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FLOURINE COUPLING CONSTANTS

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CONTENTS

1. INTRODUCTION

In an earlier volume of this series[1] we have discussed fluorine chemical shifts, and the present review is intended to complement that article. Our aim is to provide a short, critical survey of the attempts to calculate coupling to fluorine, and to present most of the data published up to 1972 in cross-referenced tables in the appendix.

Coupling constants are potential sources of information on electronic structure, but there are difficulties in finding a reliable, and practical, method of calculation, and we will attempt to assess the usefulness of the existing procedures. In addition, coupling constants may be related in a direct way to molecular shape and we will attempt to judge how useful coupling to fluorine can be in this respect.

2. THEORY OF SPIN-SPIN COUPLING

2.1 *The hamiltonian*

The discovery of spin-spin coupling was quickly followed by a description of how such effects arise in the classic paper by N. F. Ramsey,[2] and almost all subsequent work has used the formalism put forward for the hamiltonian. Ramsey suggested three mechanisms by which the nuclear coupling could be transmitted, and the contribution of each mechanism to the hamiltonian were stated. Thus the total hamiltonian $\mathscr{H}$ is written as,

$$\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_1 + \mathscr{H}_2 + \mathscr{H}_3 \tag{1}$$

where $\mathscr{H}_1$, $\mathscr{H}_2$ and $\mathscr{H}_3$ are perturbations to $\mathscr{H}_0$ arising from spin-spin coupling. The three mechanisms and their corresponding hamiltonians are as follows.

Spin-orbital. The orbital motion of an electron, described by the angular momentum operator $\underset{\sim}{L}$, produces a magnetic field at the nucleus, and the energy of the nucleus in this field depends upon its magnetic moment $\underset{\sim}{\mu}_N$, by the relationship,

$$E_{\text{spin-orbital}} = \underset{\sim}{\mu}_N \cdot \frac{2\beta \underset{\sim}{L}}{r^3} \tag{2}$$

where $\beta = e\hbar/2mc$ is the Bohr magneton. Since $\underset{\sim}{\mu}_N$ is related to the nuclear spin angular momentum $\underset{\sim}{I}$, by

$$\underset{\sim}{\mu}_N = \gamma_N \hbar \underset{\sim}{I}$$

then equation (2) can be written as,

$$E_{\text{spin-orbital}} = 2\beta\gamma_N\hbar \underset{\sim}{I} \cdot \underset{\sim}{L}\, r^{-3} \tag{3}$$

The hamiltonian representing the electron-orbital, nuclear-spin interaction is, summed over all electrons and nuclei,

$$\mathscr{H}_{1b} = 2\beta\hbar \sum_N \sum_K \gamma_N \underset{\sim}{I}_N \cdot \underset{\sim}{L}_{NK}\, r_{NK}^{-3} \tag{4}$$

A second contribution to the hamiltonian arises from the spin-orbital interaction, which can be thought of as representing the energy of interaction of two nuclei N and N' with the electron k. The hamiltonian has the form,

$$\mathscr{H}_{1a} = \frac{e^2\hbar^2}{2mc^2} \sum_{KN\neq N'} \sum \gamma_N\gamma_{N'} (\underset{\sim}{I}_N \times \underset{\sim}{r}_{KN}) \cdot (\underset{\sim}{I}_{N'} \times \underset{\sim}{r}_{KN'}) r_{KN}^{-3}\, r_{KN'}^{-3} \tag{5}$$

Spin dipolar. The magnetic moments of an electron, K, and a nucleus, N, have a mutual potential energy, represented by the dipolar hamiltonian,

$$\mathscr{H}_2 = 2\beta\hbar \sum_K \sum_N \gamma_N \{(\underset{\sim}{I}_N \cdot \underset{\sim}{r}_{KN})(\underset{\sim}{S}_K \cdot \underset{\sim}{r}_{KN}) r_{KN}^{-5} - (\underset{\sim}{I}_N \cdot \underset{\sim}{S}_K) r_{KN}^{-3}\} \quad (6)$$

where $\underset{\sim}{S}_K$ is the electron spin angular momentum operator.

Fermi-contact term. The hamiltonian given by equation (6) is not applicable when r_{KN} is zero, that is, when the electron and nucleus are in contact. The value of r_{KN} can be zero for electrons in *s* atomic orbitals, and the Fermi-contact term in the hamiltonian is an attempt to allow for this situation. The same problem arises for the electron-nucleus coupling, and in this case it has been shown that the operator with the form,[2,3]

$$\mathscr{H}_3 = \frac{16\pi\beta\hbar}{3} \sum_K \sum_N \gamma_N \delta(\underset{\sim}{r}_{KN}) \cdot \underset{\sim}{S}_K \cdot \underset{\sim}{I}_N, \quad (7)$$

does give an accurate description of the hyperfine interaction in the hydrogen atom. The application of $\mathscr{H}_3$ to the calculation of spin-spin coupling was first proposed by Ramsey and Purcell,[4] and it has been used in all subsequent calculations. The use of a delta function in $\mathscr{H}_3$ is incorrect, and leads to a second-order energy of $-\infty$. The energy is finite provided the nucleus is given a finite size,[5] but the implications of this imperfection in $\mathscr{H}_3$ for spin-spin coupling is probably unimportant.

2.2 *Calculational Procedures*

In order to explain the form of an NMR spectrum it is necessary to include a term

$$\mathscr{H}_J = \underset{\sim}{J}_{ij}\, \underset{\sim}{I}_i\, \underset{\sim}{I}_j \quad (8)$$

in the nuclear spin hamiltonian, and it is this equation which defines the spin coupling tensor $\underset{\sim}{J}_{ij}$. Note that $\mathscr{H}_J$ operates only on nuclear spin variables, and in order to obtain the magnitude of $\underset{\sim}{J}_{ij}$ we need to operate with the hamiltonian of equation (1) on the total wavefunction, Ψ. Writing Ψ as a product of a function $\Psi_{electronic}$ which describes the spatial and spin properties of the electrons, and $\Psi_{nuclear}$, which describes the spin properties of the nuclei, then the time-independent Schrodinger equation is,

$$\mathscr{H}\Psi = (\mathscr{H}_o + \mathscr{H}_{1a} + \mathscr{H}_{1b} + \mathscr{H}_2 + \mathscr{H}_3)\, \Psi_{electronic}\, \Psi_{nuclear}$$

$$= E\Psi \quad (9)$$

The magnitude of $\underset{\sim}{J}_{NN'}$ is obtained by operating on $\Psi_{electronic}$ with $\mathscr{H}$, and selecting those terms multiplying $\underset{\sim}{I}_N \cdot \underset{\sim}{I}_{N'}\, \Psi_{nuclear}$. But, the function $\Psi_{electronic}$ is not known and hence the problem posed by equation (9) is how to determine the electronic wavefunction belonging to the hamiltonian of equation (1). The function $\Psi_{electronic}$ is derived by approximate methods, such as the variation or perturbation techniques.

Detailed descriptions of the calculational procedures are given in the reviews by Barfield and Grant[6], Murrell[7], and Ditchfield and Ellis[8], and only a general discussion will be given here, with attention focussed on their application to coupling to fluorine.

The variational method is described by O'Reilly[9], who included hydrogen fluoride amongst the molecules studied, but there have been few other attempts to apply this technique, and we will not discuss it further.

Perturbation methods are appropriate for calculating $\Psi_{electronic}$ since the terms $\mathscr{H}_1$ to $\mathscr{H}_3$ are each very small perturbations compared with $\mathscr{H}_o$. The basic principle is to expand the energy, E, as a Taylor series,

$$E = E_o + \sum_r \lambda_r \left(\frac{\partial E}{\partial \lambda_r}\right)_{\lambda_r = 0} + \tfrac{1}{2} \sum_r \sum_s \lambda_r \lambda_s \left(\frac{\partial^2 E}{\partial \lambda_r \partial \lambda_s}\right)_{\lambda_r = \lambda_s = 0} + \ldots \quad (10)$$

The λ_r are small perturbations, such that the hamiltonian can be written as,

$$\mathscr{H} = \mathscr{H}_o + \sum_r \lambda_r \mathscr{H}_r, \quad (11)$$

with $\mathscr{H}_r$ independent of λ_r. Equation (10) can be written as,

$$E = E_o + \sum_r \lambda_r E_r^{(1)} + \tfrac{1}{2} \sum_r \sum_s \lambda_r \lambda_s E_{rs}^{(2)} + \ldots\ldots \quad (12)$$

and, since the λ_r are small then the successive terms in equation (12) diminish rapidly in magnitude. The wavefunction $\Psi_{electronic}$ is also written as an expansion in the λ_r, usually only as far as the first term,

$$\Psi_{electronic} = \Psi_o + \sum_r \lambda_r \left(\frac{\partial \Psi_o}{\partial \lambda_r}\right) = \Psi_o + \sum_r \lambda_r \Psi_r^{(1)} \quad (13)$$

The correction terms $E_r^{(1)}$ and $E_{rs}^{(2)}$ are given by,

$$E_r^{(1)} = \int \Psi_o^* \mathscr{H}_r \Psi_o \, d\tau \quad (14)$$

$$E_{rs}^{(2)} = 2 \int \Psi_o^* \mathscr{H}_r \Psi_s^{(1)} \, d\tau \quad (15)$$

The value of $E_r^{(1)}$ is easily evaluated as it depends only on the function Ψ_o, the solution of the Schrodinger equation in the absence of spin-spin coupling. The second-order correction, $E_{rs}^{(2)}$, is more difficult to evaluate, and there are two main methods used. The older of the two techniques expands $\Psi_s^{(1)}$ as a linear combination of the complete set of solutions, Ψ_n, of the unperturbed hamiltonian, $\mathscr{H}_o$, excluding the ground state, i.e. n = 0. The value of $E_{rs}^{(2)}$ is then given by,

$$E_{rs}^{(2)} = 2 \sum_{n \neq 0}^{\infty} (E_o - E_n^{-1}) \int \psi_o^* \mathscr{H}_r \psi_n \, d\tau \int \psi_n^* \mathscr{H}_s \psi_o \, d\tau \quad (16)$$

The evaluation of $E_{rs}^{(2)}$, and hence of $J_{NN'}$, by equation (16) will be referred to as the sum-over-states method, abbreviated to SOS.

Later methods of evaluating $E_{rs}^{(2)}$ attempt the calculation of $\psi_s^{(1)}$ directly. Pople, McIver and Ostlund[10] first introduced the method for calculating $J_{NN'}$, and they evaluated the derivative of Ψ_o with respect to the perturbation represented by $\mathscr{H}_3$, the Fermi-contact term only, by a numerical method. The method is known as the finite perturbation method, and will be referred to by the abbreviation FP. Blizzard and Santry[11,12] extended the method to include the terms $\mathscr{H}_{1b}$ and $\mathscr{H}_2$, and they also developed analytical expressions for the evaluation of the partial derivatives of Ψ_o.

The two perturbation methods have been applied extensively and there are many examples involving fluorine. A detailed comparison of the SOS and FP methods has been made by Ditchfield *et al.*[13] Each method has its difficulties in practice. The SOS method depends on the convergence of equation (16) for $E_{rs}^{(2)}$, which can be very slow, and furthermore, successive terms do not always diminish in magnitude. This latter point is particularly unfortunate for it means that extending the number of terms in the summation, for example, by using configuration interaction, can lead to worse

results than can be obtained by a minimal basis set. The FP method relies entirely on the choice of the unperturbed wavefunction Ψ_o. Almost all calculations have used LCAO molecular orbital wavefunctions, particularly those of the INDO type proposed by Pople, Beveridge and Dobosh.[14]

2.3 *Coupling Constant Contributions*

The three terms in the hamiltonian, $\mathscr{H}_1$, $\mathscr{H}_2$ and $\mathscr{H}_3$, give rise to four contributions to the magnitude of the elements of the coupling constant tensor. Thus an element $J_{ij\alpha\beta}$ is in general given by,

$$J_{ij\alpha\beta} = J^{(1)}_{ij\alpha\beta} + J^{(2)}_{ij\alpha\beta} + J^{(3)}_{ij\alpha\beta} + J^{(4)}_{ij\alpha\beta} \qquad (17)$$

Expressions for calculating these terms have been given by Buckingham and Love,[15] for the SOS method, and by Ditchfield and Ellis[8] for the FP method. We give here a discussion of the properties of each term in equation (17), particularly as they affect coupling to fluorine.

$J^{(1)}_{ij\alpha\beta}$, *the spin-orbital term.* There are two terms arising from this mechanism of spin-spin coupling, corresponding to the two contributions $\mathscr{H}_{1a}$ and $\mathscr{H}_{1b}$ (see equations (4) and (5)) to the total hamiltonian. The term $\mathscr{H}_{1a}$ is bilinear in the nuclear spins, and hence gives a contribution to coupling, $J^{(1a)}_{ij\alpha\beta}$, arising from the substitution of $\mathscr{H}_{1a}$ in the equation (14).

The calculation of this term depends only on a knowledge of the unperturbed wavefunction, Ψ_o. The magnitude of the term $J^{(1a)}_{ij\alpha\beta}$ is always small, and in calculations using LCAO molecular orbital functions it is usually assumed zero.

The second spin-orbital term, $J^{(1b)}_{ij\alpha\beta}$, arises from second-order terms obtained with the hamiltonian $\mathscr{H}_{1b}$. The dependence of $\mathscr{H}_{1b}$ on the electron orbital angular momentum operator, L_{ik}, means that $J^{(1b)}_{ij\alpha\beta}$ is significantly different from zero only if one of the coupled nuclei belongs to an atom having electrons in atomic orbitals with non-zero azimuthal quantum numbers. Thus, the term is always non-zero in theory for coupling to fluorine. The tensor $J^{(1b)}_{ij}$ is unsymmetric and has non-zero diagonal and off-diagonal terms.

$J^{(2)}_{ij\alpha\beta}$, *the spin-dipolar term,* arises from the substitution of $\mathscr{H}_2$ (equation (6)) into equation (14), that is, it is a second-order term. In order to be significantly different from zero both nuclei must belong to atoms bearing 2p atomic orbitals, hence the term is non-zero in theory for C-F, F-F, P-F etc, but zero for F-H coupling. The tensor $J^{(2)}_{ij}$ is unsymmetric, and has non-zero diagonal and off-diagonal elements.

$J^{(3)}_{ij\alpha\beta}$, *the Fermi-contact term,* arises from substitution of $\mathscr{H}_3$ (equation (7)) into equation (14). In contrast with the other contributions to coupling the tensor $J^{(3)}_{ij}$ is symmetric and isotropic, that is, there are only non-zero diagonal elements, and these comprise three equal values. The magnitude of $J^{(3)}_{ij\alpha\alpha}$ are such that they are always the dominant contribution to the magnitude of $J_{ij\alpha\alpha}$, the diagonal elements of the total coupling tensor for F-H coupling; in most other cases of coupling to fluorine the magnitude of $J^{(3)}_{ij\alpha\alpha}$ are large, but may not be dominant.

$J^{(4)}_{ij\alpha\beta}$, *the spin-dipolar, Fermi-contact term,* is the only non-zero term arising from the substitution into equation (14) of two different terms in the hamiltonian. The tensor $J^{(4)}_{ij\alpha\beta}$ is symmetric, and has zero sum for the diagonal elements, which means (see below) that it does not contribute to the coupling constant measured from isotropic solutions. For this reason the magnitude of $J^{(4)}_{ij\alpha\beta}$ has been calculated only when the total tensor J_{ij} is of interest.

2.4 *Evaluation of integrals when using LCAO molecular orbital wavefunctions*

Most calculations approximate the wavefunctions with linear combinations of atomic orbitals,

$$\psi_n = \sum_j C_{nj}\,\phi_j$$

If the ϕ_j are not allowed to vary in form (i.e. have fixed exponential forms) then the integrals to be evaluated in calculating the coupling constant are of the type

$$a_{AmBn} = \int \phi_{Am}\,\delta(r_{KA})\,\phi_{Am}\,d\tau \int \phi_{Bn}\,\delta(r_{KB})\,\phi_{Bn}\,d\tau$$

$$= S_{Am}(0)^2\,S_{Bn}(0)^2$$

$$b_{AqBs} = \int \phi_{Aq} r_{KA}^{-3}\,\phi_{As}\,d\tau \int \phi_{Bq}\,r_{KB}^{-3}\,\phi_{Bs}\,d\tau$$

$$= \langle r^{-3}\rangle_{Aq}\,\langle r^{-3}\rangle_{Bs}$$

The term $S_{Am}(0)^2$ is the probability of an electron in the m^{th} orbital centred on nucleus A being of the nucleus, and is non-zero for s orbitals only. The term $\langle r^{-3}\rangle_{Aq}$ is the average value of r^{-3} for an electron in the q^{th} orbital on atom A which has azimuthal quantum number greater than zero, and is non-zero therefore for 2p, 3p, 3d etc orbitals.

The values of a_{AmBn} and b_{AqBs} are usually evaluated for SCF wavefunctions,[125] but this has been found to give the magnitude of J_{AB} as too small, and in many calculations the integrals are arbitrarily scaled so as to give the correct coupling constant.[10,12]

2.5 *Isotropic and Anistropic Coupling Tensors*

The coupling constant tensor $\underset{\sim}{J}_{ij}$ may be written as the sum of symmetric, $\underset{\sim}{J}_{ij}^{(5)}$, and anti-symmetric, $\underset{\sim}{J}_{ij}^{(a)}$, tensors,[15]

$$\underset{\sim}{J}_{ij} = \underset{\sim}{J}_{ij}^{(s)} + \underset{\sim}{J}_{ij}^{(a)}$$

In NMR experiments using large magnetic fields the anti-symmetric term does not have a significant effect on the spectrum, hence only $\underset{\sim}{J}_{ij}^{(s)}$ is measurable. The symmetric term may be expressed as the sum of isotropic and anisotropic parts,

$$\underset{\sim}{J}_{ij}^{(s)} = J_{ij}^{iso} + J_{ij}^{aniso} \qquad (18)$$

The isotropic term is given by,

$$J_{ij}^{iso} = \frac{1}{3}\sum_{\alpha} J_{ij\alpha\alpha}^{(s)}, \qquad (19)$$

and is the magnitude of the coupling constant obtained from the spectra of isotropic solutions. The anistropic term, J_{ij}^{aniso}, has a zero diagonal sum and hence does not influence spectra of isotropic solutions. It does however, affect the spectra obtained in anisotropic media, and in favourable cases its magnitude can be derived. It should be noted, however, that the magnitude of J_{ij}^{aniso} cannot be derived directly from the spectra of oriented molecules, but only as part of a total, anisotropic spin-spin coupling, T_{ij}, which is a sum of J_{ij}^{aniso} and the dipolar coupling constant, D_{ij}.[16] Thus,

$$T_{ij} = 2D_{ij} + J_{ij}^{aniso} \qquad (20)$$

There are contributions to J_{ij}^{aniso} only from the terms $J_{ij}^{(1)}$, $J_{ij}^{(2)}$ and $J_{ij}^{(4)}$, with the latter being usually the largest term. Also, the magnitude of J_{ij}^{aniso} is small when one of the coupled nuclei is a proton, thus it is usually unimportant in comparison with D_{HF} for HF coupling.

Values of J_{ij}^{aniso} have been derived only from the spectra of molecules dissolved in liquid crystalline solvent, and in this case the derived parameter is $\langle J_{ijzz}^{aniso} \rangle$, the component of the tensor in the applied field direction, averaged over the motion in the liquid crystal medium. The relationship between $\langle J_{ijzz}^{aniso} \rangle$ and components of J_{ij} in a molecule-fixed axis system, $\alpha\beta\gamma$, is,

$$\langle J_{ijzz}^{aniso} \rangle = J_{ij}^{iso} + \frac{2}{3} \sum_{\alpha,\beta} J_{ij\alpha\beta} S_{\alpha\beta} \qquad (21)$$

The term $S_{\alpha\beta}$ refers to the Saupe ordering matrix,[16] whose components are given by,

$$S_{\alpha\beta} = \langle \tfrac{3}{2} \cos\Theta_{\alpha z} \cos\Theta_{\beta z} - \tfrac{1}{2} \rangle,$$

where $\Theta_{\alpha z}$ is the angle between the α and z axes, and $\langle\rangle$ denotes an ensemble average. The magnitude of the $S_{\alpha\beta}$ may be derived from the magnitude of dipolar couplings, D_{ij}.

There are only a small number of measured J_{ij}^{aniso} values, almost all for F-F coupling, compared with many thousand values of J_{ij}^{iso}, hence it is not surprising that only recently have attempts been made to calculate J_{ij}^{aniso} values as well as J_{ij}^{iso}. However, J_{ij}^{aniso} values often pose a more severe test of a calculational procedure than J_{ij}^{iso}, and in future it is to be hoped that calculations of all the components of $J_{ij}^{(5)}$ will be made, rather than just J_{ij}^{iso}.

In the rest of the text we will refer to J_{ij}^{iso} simply as J_{ij}, and no distinction will be made between $J_{ij}^{(s)}$ and J_{ij}.

3. MEDIUM EFFECTS

The state of a sample can affect the coupling constants measured from the nmr spectrum. The dependence of the magnitudes of coupling constants on solvent, temperature or pressure have been noted for many examples where changes in molecular conformation, or exchange between different molecular species, are absent. Two recent reviews deal with the solvent dependence of all coupling constants. Smith[17] has collected together the experimental data up to early 1970, whilst Barfield and Johnston[18] review the theories of medium effects and critically assess their application to the available data. We will concentrate attention on F-X coupling, and those seeking a wider view are recommended to consult the review by Barfield and Johnston.

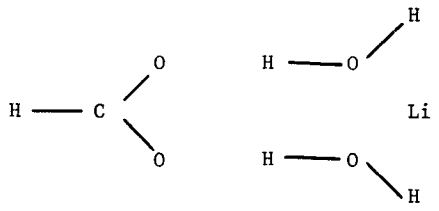
3.1 *Molecular Models of Medium Effects*

Medium effects arise because the coupling constant between two nuclei in an isolated molecule is altered by the presence of other molecules in the sample. An obvious approach to attempting to calculate such an effect is to carry out SOS or FP calculations on groups rather than single molecules. In a complete theory calculations must be performed on all possible configurations of molecules with a Boltzmann weighting of each configuration. Clearly this is impossibly time consuming and to be practicable the number of molecules in each configuration must be small, and only a limited number of configurations can be considered. In spite of these restrictions, however, this approach is the only one which has the capability of revealing information on the dependence of coupling constants on molecular ordering, and hence of giving information about liquid structure. Most attempts to explain medium effects on coupling constants (or chemical shifts) drastically simplify the problem by treating intermolecular effects as arising from the effect on one molecule of

a surrounding continuum. Thus macroscopic properties of a continuum are used to approximate the statistical average of intermolecular interactions.

Most attempts to explain solvent dependent coupling constants have used continuum models, but there have been some attempts to retain a molecular approach, although with large approximations about liquid structure.

Thus Maciel et al[19] compared the value of $^1J_{CH}$ calculated for the formate ion $HCOO^-$ and for a cluster of the ion with two water molecules and a lithium ion,



They used the FP method with an INDO wavefunction extending over the whole group. The calculated values of $^1J_{CH}$ are 106.5 Hz for the isolated ion, and 178.8 Hz for the cluster. No allowance was made for other configurations, but the magnitude of the change in $^1J_{CH}$ suggests that this kind of calculation could be profitably pursued for associated species.

A more detailed study of the effect of liquid structure on coupling has been attempted by Barfield and Johnston[20]. Their basic idea was to consider a group of molecules in a particular configuration. They consider the solute molecule surrounded by six solvent molecules in a cubic, close-packed orientation as shown in figure 1. The calculation used the FP method, hence the wavefunction modified by the presence of spin-spin coupling was calculated directly by the inclusion in the molecular hamiltonian of a coupling term. Unlike Maciel et al[19] they did not treat all seven molecules as one entity, but made the approximation that overlap of atomic orbitals on different molecules can be set to zero. This means that the only intermolecular terms in the hamiltonian arise from coulomb forces between electrons localized in solute atomic orbitals, and electrons and nuclei located in the solvent molecules

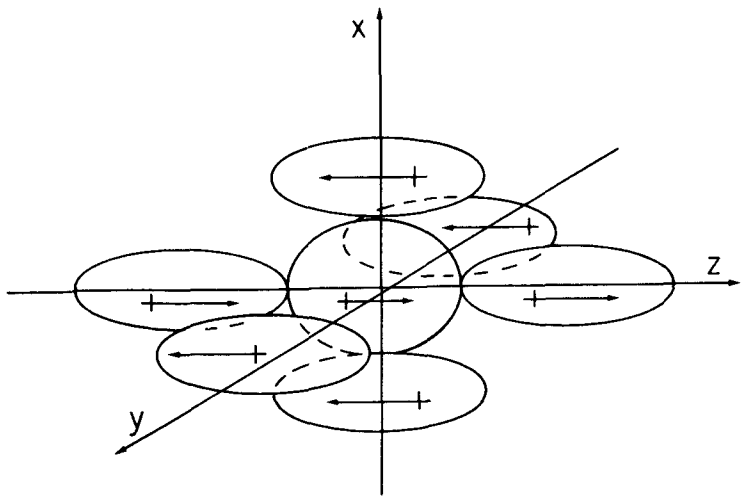


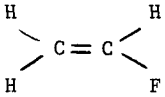
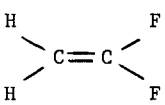
Figure 1. Arrangement of six, dipolar, solvent molecules around a dipolar solute. (Barfield and Johnston[20]).

Barfield and Johnston[20] calculated the molecular orbitals by the INDO method, and only the Fermi-contact term, $\mathscr{H}_3$, was included in the calculation. The calculation of $J^{(3)}_{NN'}$ requires the evaluation of $S^2_N(0)$ and $S^2_{N'}(0)$, the electron densities at nuclei N and N', and it is found (see section 4) that when these quantities are obtained from SCF wavefunctions, then the coupling constants are too small by about a factor of two. It is usual to adjust the values of $S^2_N(0)$ in order to give the correct magnitude for $J_{NN'}$ (equal to $J^{(3)}_{NN'}$), however, Barfield and Johnston did not adopt this scaling procedure, hence it is to be expected that their calculated changes in $J^{(3)}_{NN'}$ brought about by intermolecular effects will err on the low side. Also, since only $J^{(3)}_{NN'}$ was calculated the values obtained for the solvent effect on F-F and ^{13}C-F coupling are likely to be in poor agreement with experiment, since for these pairs of nuclei the terms $J^{(1)}_{NN'}$ and $J^{(2)}_{NN'}$ can be large. Barfield and Johnston[20] calculated $\Delta J^{(3)}_{NN'}$, the difference produced by changing from cyclohexane to another solvent, and their results are given in column A of table 1. The ΔJ_{HH} and ΔJ_{HF} are in reasonably good agreement with experiment, but ΔJ_{FF} and ΔJ_{CF}, as expected, are not.

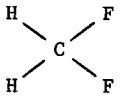
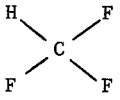
The fixed orientation of the molecules shown in figure 1 is probably the lowest energy state, but a more realistic treatment would repeat the calculation for a number of relative molecular orientations, and average the results according to the Boltzmann distribution of states at equilibrium. Such a calculation is hardly practicable, and hence before any allowance can be made for solvent motion the calculational procedure must be simplified. Barfield and Johnston[21] examined the consequences of molecular rotation by treating the solvent molecules as point dipoles, and their results are shown as column B in table 1. In some cases the rotating dipole model gives considerably different results to those obtained with the fixed cluster of solvent molecules, and this can be regarded as indicating the importance of including more than one configuration in a calculation of solvent effects.

Table 1. Changes in $J^{(3)}_{NN'}$ (in Hz) produced by solvents calculated using (A) an oriented cluster, (B) rotating dipole and (C) reaction field models (Barfield and Johnston[18,20,21,23]).

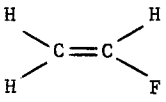
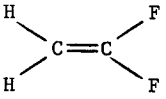
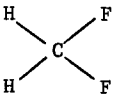
1. H-H Coupling

Molecule	Solvent		$\Delta J^{(3)}_{NN'}$ A	B	C	obs.
	CH_3CN		-2.39	-2.58	0.11	-2.20
	acetone	gem	-0.32	-0.09	-0.09	-0.26
		cis	0.01	-0.03	0.04	-0.04
		trans	-0.03	-0.02	0.00	-0.19
	DMF	gem	-0.09	-0.10	-0.09	-0.33
		cis	0.01	-0.03	0.05	-0.07
		trans	0.00	-0.03	0.00	-0.21
	neat	gem	-0.96	-	-	-0.07
	CH_3CN	gem	-0.85	-0.53	-0.22	-0.62
	DMF	gem	-1.18	-0.14	-0.22	-0.76
	CH_3NO_2	gem	-1.56	-0.66	-0.22	-0.64

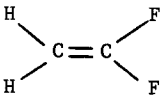
2. C-H Coupling

Molecule	Solvent		$\Delta J_{NN'}^{(3)}$			
			A	B	C	obs.
	neat		2.95	1.44	0.89	2.9
	acetone		0.86	1.52	2.28	2.70
	acetone		-	-	4.05	7.25
	DMSO		-	-	4.38	9.20

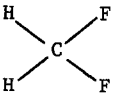
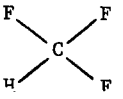
3. H-F Coupling

	acetone	gem	1.71	1.50	0.14	1.47
		cis	0.87	1.69	1.14	1.42
		trans	3.77	4.68	3.90	2.85
	DMF	gem	1.76	1.66	0.15	1.80
		cis	1.39	1.89	1.22	1.93
		trans	3.64	5.25	4.19	3.64
	neat	cis	0.86	-	-	0.15
		trans	3.07	-	-	-0.02
	CH_3CN	cis	0.58	1.36	0.62	0.50
		trans	1.70	5.69	3.12	1.71
	DMF	cis	0.85	1.00	0.62	0.69
		trans	3.36	3.81	3.12	2.39
	CH_3NO_2	cis	1.08	1.19	0.62	0.53
		trans	4.80	5.21	3.12	1.80
	neat		0.87	0.38	0.14	0.00
	acetone		0.46	0.39	0.35	0.35

4. F-F Coupling

	neat	-2.62	-	-	5.77
	CH_3CN	-5.90	5.90	-	6.76
	DMF	-5.34	-1.98	-0.37	6.10
	CH_3NO_2	-13.40	1.83	-	6.97

5. C-F Coupling

	neat	-1.39	10.28	-	1.78
	acetone	-1.05	12.19	3.13	3.80
	acetone	-	-	3.02	0.10
	DMSO			3.28	-1.00

3.2 *Continuum Models of Medium Effects*

In continuum models of intermolecular effects the solute molecule is imagined to occupy a cavity in a continuous medium whose molecular structure is not considered. In such a model the solvent-induced change, $\Delta J_{NN'}$, in a coupling constant is related to bulk properties of the medium, thus Raynes[22] suggested writing $\Delta J_{NN'}$ as,

$$\Delta J_{NN'} = \Delta J^{M}_{NN'} + \Delta J^{E}_{NN'} + \Delta J^{W}_{NN'} + \Delta J^{C}_{NN'} \qquad (22)$$

The term $J^{M}_{NN'}$ describes the dependence of $J_{NN'}$ on the magnetic susceptibility, χ_V, of the solvent through the equation,

$$J^{M}_{NN'} = \frac{-28\,\chi_V h\gamma_N\gamma_{N'}}{3\pi a^3}, \qquad (23)$$

where a is the effective radius of the solute molecule. The magnitude of $\Delta J^{M}_{NN'}$, is typically 0.1 Hz, and is usually neglected. The remaining terms in equation (22) cannot be given explicit forms. The term $J^{E}_{NN'}$, arises from intermolecular electrostatic interactions, $J^{W}_{NN'}$, results from dispersion effects, and $J^{C}_{NN'}$, describes "specific" effects. The last term really is a measure of the errors in the model arising because the medium cannot be regarded as a continuum, but some account must be taken of local molecular ordering.

There have been many attempts to demonstrate the importance of $J^{E}_{NN'}$, and to a lesser extent of $J^{W}_{NN'}$, and it is important to understand what such experiments can hope to achieve. No direct information can be obtained about molecular ordering from continuum models of $\Delta J_{NN'}$. But if models for calculating $J^{E}_{NN'}$, and $J^{W}_{NN'}$, were available which gave good agreement with experimental values of $\Delta J_{NN'}$, for most solvents, but failed for some specific solvents, then this could be taken as indicating the importance of liquid structure at the molecular level for these solvents. This would reveal appreciable values of $J^{C}_{NN'}$, according to equation (22), and such a case is often referred to as showing "complex" formation between solvent and solute molecules. However, the experimental evidence so far obtained suggests that continuum models for $J^{E}_{NN'}$, and $J^{W}_{NN'}$, are inadequate for most solute-solvent systems and hence in our view values of $J^{C}_{NN'}$, have little significance, unless they are unusually large.

Electrostatic effects, $J^{E}_{NN'}$,

Barfield and Johnston[23] have attempted a direct calculation of the effect of an electric field on the Fermi-contact term, $J^{(3)}_{NN'}$. To do so they considered a molecule of dipole moment $\underset{\sim}{\mu}$ in a uniform electric field $\underset{\sim}{E}$, so that the molecular hamiltonian is modified to include a term $-\underset{\sim}{E}.\underset{\sim}{\mu}$. The FP method with INDO molecular orbitals was used, and the dependence of $J^{(3)}_{NN'}$ on $\underset{\sim}{E}$ investigated. It was also assumed that $\underset{\sim}{\mu}$ and $\underset{\sim}{E}$ were co-linear. Figure 2 shows their results for $^1J_{CH}$ in fluoroform and $^2J_{CH}$ in 1,1-difluoroethylene. The calculated linear dependence of $J^{(3)}_{NN'}$ for these two examples support the idea of a linear dependence of $J^{E}_{NN'}$, on E for those couplings where $J^{(3)}_{NN'}$, is the dominant term, i.e. HH, CH, HF, but not CF, FF etc, for which $J^{(1)}_{NN'}$, and $J^{(2)}_{NN'}$, can be larger than $J^{(3)}_{NN'}$.

The field $\underset{\sim}{E}$ experienced by a molecule of dipole moment $\underset{\sim}{\mu}$ immersed in a solvent whose molecules have zero dipole moment may be described by Onsager's[24] reaction field model, such that

$$\underset{\sim}{E} = \left[2(\varepsilon - 1)(n^2 - 1)\underset{\sim}{\mu}\right]\left[3\alpha(2\varepsilon + n^2)\right]^{-1}. \qquad (24)$$

The terms $\underset{\sim}{n}$ and α refer to the solute and are the refractive index and polarisability, whilst ε is the dielectric coefficient of the solvent. Higher-order terms also contribute to $\underset{\sim}{E}$, but are usually neglected. Barfield and Johnston[23] have used equation (24) for $\underset{\sim}{E}$ in their direct calculation of the of the electric field effect on the coupling constants by the FP method, and their results are compared with the molecular models in table 1 column C. It is seen from table 1 that the reaction field model

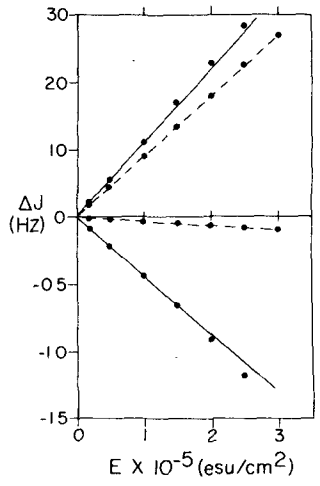


Figure 2. Calculated dependence of electric field induced changes, ΔJ, in coupling constants as a function of the electric field, E. The upper plot shows ΔJ_{CH} for fluoroform based on calculations by the SOS (dashed line) and FP (solid line) methods. The lower plot gives analogous data for $\Delta^2 J_{HH}$ in 1,1-difluoroethylene. Barfield and Johnston[23].

gives the correct solvent behaviour for many HH and HF coupling constants, but there are enough deviations between observed and calculated $\Delta J_{NN'}$ values to conclude that some structuring of the solute-solvent interaction is necessary for most systems, and in some cases, e.g. formaldehyde, the correct sign of $\Delta J_{NN'}$ is calculated only by including local order.

The extent to which there are linear correlations between observed values of $\Delta J_{NN'}$ and calculated reaction fields has been investigated for HF and FF couplings. Good correlations have been found for HH and HF in fluoroethylenes,[25] but not for HF in fluorobenzenes.[26] For FF coupling the reaction field does not correlate with the solvent effects, thus $^3J_{FF}$ in trans-1,2-difluoroethylene shows an appreciable solvent dependence even though the molecule has a zero dipole moment (see table 5).[27-32] Also, studies on fluoroaromatics revealed no consistent trend of ΔJ_{FF} with dielectric coefficients.

We conclude that from the available evidence the reaction field model is inadequate for the purpose of revealing meaningful values of $J^C_{NN'}$, that is, evidence of unusual liquid structure. For HF coupling the model provides a guide as to what to expect for ΔJ_{HF}, but caution should be exercised in reading any significance into deviations from predicted behaviour.

Dispersion effects, $J^W_{NN'}$.

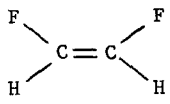
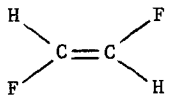
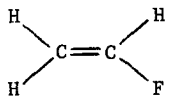
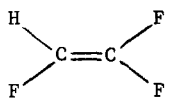
There have not been any calculations reported on the magnitude of $J^W_{NN'}$, but Barfield and Johnston[18] argue that it should be important only when the spin-dipolar contribution, $J^{1(a)}_{NN'}$, is large (see section 2.3). The experimental evidence for the magnitude of $J^W_{NN'}$ does support the view that it is significant only for coupling between atoms with p or d atomic orbitals. For polar molecules it is not possible to separate an experimental $\Delta J_{NN'}$ value into contributions from $\Delta J^E_{NN'}$ and $\Delta J^W_{NN'}$, hence in order to investigate the magnitude of $J^W_{NN'}$ it is necessary to look at the solvent, or pressure dependence of coupling between nuclei in a non-polar molecule. The best evidence for the effect of dispersive forces on a coupling constant is provided by the observed pressure dependence[33] of $^1J_{SiF}$ in the molecule SiF_4.

3.3 *Experimental Data for Solvent Dependence of Coupling Constants*

There have been several studies of the solvent variation of coupling to fluorine, which show the magnitude of the phenomenon, but which did not attempt to relate the results to liquid structure. In most cases the results were correlated with reaction fields. We will not attempt a detailed

criticism of each study since this has been done by Smith[17] and by Barfield and Johnston.[18] In tables 2-9 we collect together the published data on solvent dependent FH, FF, CF, SiF, PF, and SnF coupling constants so that the order of magnitude of these effects can be seen. In these tables we give under the heading "range" the maximum change observed in $J_{NN'}$ from a standard solvent, usually cyclohexane.

Table 2. Solvent variation of geminal hydrogen-fluorine coupling, $^2J_{HF}$.

Compound	$^2J_{HF}$ (cyclohexane soln)	range*	Reference
	71.70	+1.10	25
	75.10	-0.07 to 0.36	25
CH_2F_2	50.22	-0.1 to +0.1	32
CHF_3	79.25	0	32
	84.56	+2.0	34
	70.51	0.58 to 0.41	35
BrClCFH	52.1	-1.5	36

*The change in $^2J_{HF}$ relative to cylohexane solution.

Table 3. Solvent variation of vicinal hydrogen-fluorine coupling constants, $^3J_{HF}$

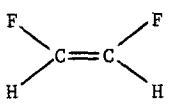
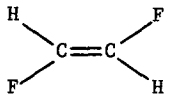
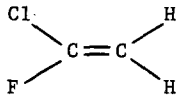
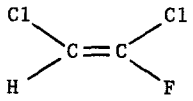
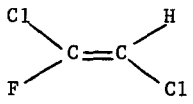
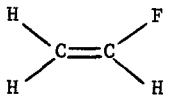
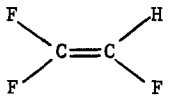
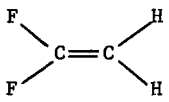
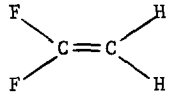
Compound	$^3J_{HF}$ (in cyclohexane)	range*	Reference
	19.63	+1.31	25

Table 3. (contd.)

Compound		$^3J_{HF}$ (in cyclohexane)	range*	Reference
		2.80	+1.77	25
	cis	7.7	-0.2 to 4.6	37
	trans	37.7	-0.8 to 1.1	37
		3.80	+0.6	38
		17.45	+2.95	38
$(CF_3)_2PH$		9.7 (TMS)	+0.6	39
	cis	19.63	+2.14	34,35
	trans	51.81	+4.57	
	cis	-4.19	0.1 to -0.15	35
	trans	12.52	+1.80	
	cis	0.60	0.69	
	trans	33.85	-0.06 to 2.81	40

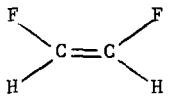
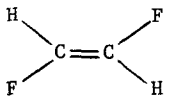
*Change in $^3J_{HF}$ in changing solvent from cyclohexane.

Table 4. Solvent variation of geminal fluorine-fluorine coupling constants, $^2J_{FF}$.

Compound	$^2J_{FF}$ (cyclohexane soln)	Range*	Reference
	31.65	-1.64 to 5.27	32
	30.72	-1.99 to 6.79	40
ClF_3	441 ± 8 (gas		
	442 ± 0.5 (liq.)		42

*Change in $^2J_{FF}$ relative to value in cyclohexane solution.

Table 5. Solvent Variation of vicinal fluorine-fluorine coupling constants, $^3J_{FF}$.

Compound	$^3J_{FF}$	Range*	Reference
	-18.74†	+0.22 to -1.85	25,32
	-133.46	-0.33 to 3.26	25.32

*Change in $^3J_{FF}$ relative to cyclohexane solution.

†Quoted as positive in references 19 and 12, but since shown to be negative (see section 6.3)

Table 6. Solvent variation of one bond carbon-fluorine coupling constants, $^1J_{CF}$.

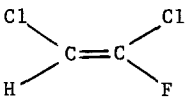
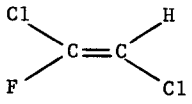
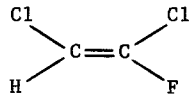
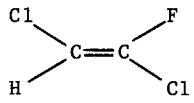
Compound	$J_{^{13}CF}$ (cyclohexane soln)	Range*	Reference
CH_2F_2	-236.58	+4.46	32
CHF_3	-274.22	-1.0	32
	-300	+1.7	38

Table 6. (contd.)

Compound	J_{13} CF (cyclohexane soln)	Range*	Reference
	-307.0	+3.6	38

*Change in $^1J_{CF}$ in going from cyclohexane solution.

Table 7. Solvent dependence of two bond carbon-fluorine coupling constants, $^2J_{CF}$.

Compound	$^2J_{CF}$	Range*	Reference
	53.6	-0.6 to 0.1	38
	20.0	-2.0	38

*Change in $^2J_{CF}$ in going from cyclohexane solution

Table 8. Solvent dependence of fluorine coupling constants in aromatic compounds.

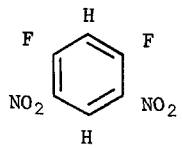
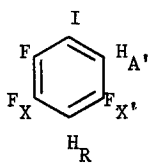
Compound	Coupling Constant	Range	Reference
	$^3J_{HF}$ = 9.71 ($CHCl_3$ soln) $^4J_{HF}$ = 7.54 ($CHCl_3$ soln)	0.91 -0.54 to 0.25	28
	$^3J_{F_AH_X}$ = 7.58 (CCl_4 soln) $^3J_{F_XH_R}$ = 8.83 (CCl_4 soln)	0.42 0.47	 43

Table 8. (contd.)

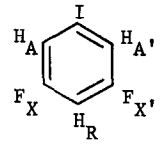
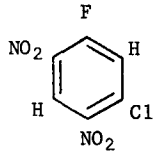
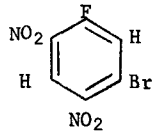
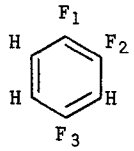
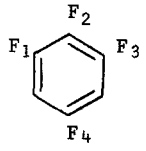
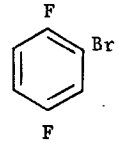
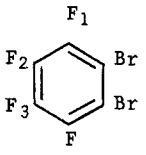
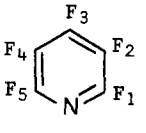
Compound	Coupling Constant	Range	Reference
	$^5J_{F_XH_{A'}}$ = 1.28 (CCl_4 soln)	0.00	
	$^4J_{F_XF_{X'}}$ = 6.23 (CCl_4 soln)	0.12	
	$^3J_{FH}$ = 9.57 (CCl_4 soln)	0.71	43
	$^4J_{FH}$ = 7.07 (CCl_4 soln)	0.00	
	$^3J_{FH}$ = 9.39 (CCl_4 soln)	0.83	43
	$^4J_{FH}$ = 6.96 (CCl_4 soln)	0.14	
	$^3J_{F_1F_2}$ = -20.22 (pentane soln)	0.80 to -1.25	30
	$^4J_{F_2F_3}$ = 3.08 (pentane soln)	0.21	
	$^5J_{F_1F_3}$ = 15.10 (pentane soln)	-0.08 to 0.23	
	$^3J_{F_1F_2}$ = -20.00 (pentane soln)	1.03 to -1.10	30
	$^4J_{F_3F_4}$ = 1.52 (pentane soln)	0.43	
	$^5J_{F_2F_4}$ = 11.15 (pentane soln)	-0.34	
	$^5J_{FF}$ = 15.31 (pentane soln)	-0.06 to 0.31	30
	$^3J_{F_1F_2}$ = -21.05 (pentane soln)	0.05 to -1.29	30
	$^4J_{F_1F_3}$ = 2.80 (pentane soln)	-0.07 to 0.23	
	$^5J_{F_1F_4}$ = 8.30 (pentane soln)	-0.43 to 0.03	
	$^3J_{F_1F_2}$ = -20.2 (cyclohexane)	1.9 to -1.2	31
	$^3J_{F_2F_3}$ = -17.6 (cyclohexane)	0.8 to -1.4	
	$^4J_{F_1F_3}$ = 13.4 (cyclohexane)	1.4	
	$^4J_{F_2F_4}$ = 0.0 (cyclohexane)	0.9	
	$^4J_{F_1F_5}$ = -14.7 (cyclohexane)	-1.1	
	$^5J_{F_1F_4}$ = 25.9 (cyclohexane)	-1.5 to 0.4	

Table 9. Solvent dependence of coupling constants between fluorine and silicon, phosphorus and tin.

Compound	Coupling Constant	Range	Reference
SiF_4	$^1J_{SiF}$ = 169.00 (gas, 30 atm)	9.61	33
	$^1J_{SiF}$ = 170.2 (gas, 200 atm)		18
PF_3	$^1J_{PF}$ = 1404 (gas)	19	44
$(CF_3)_2PH$	$^2J_{PF}$ = 69.4 (TMS soln)	0.6 to -5.5	39
$(C_2H_5N)_2SnF_6$	$^1J_{SnF}$ = 1557 (H_2O soln)		45
	1571 (MeOH soln)		
	1593 (DMSO soln)		

3.4 *Temperature Dependent Coupling Constants*

There are several examples of temperature dependent coupling constants involving fluorine, and the experimental data is summarised in table 10. We exclude the familiar temperature dependence which arises because of exchange processes. Internal rotation in molecules can also give rise to temperature dependent coupling constants, and table 10 excludes those molecules in which there are two or three different minima in the variation of energy with rotational angle ϕ. There are, however, subtleties in the treatment of the variation of $J_{NN'}$ with ϕ which are particularly important for fluorine, and we will return to these later in this section.

The hamiltonian of equation (1) does not contain temperature explicitly, hence the temperature dependence of $J_{NN'}$ must arise because of the existence of more than one energy state for the molecule, or aggregate of molecules. The distribution of molecules amongst these energy states must vary with temperature, and the coupling constants, $J^i_{NN'}$, must also change with the energy state. Thus if p_i is the normalised probability of the state with energy E_i then the observed coupling will be,

$$J_{NN'} = \sum_i p_i J^i_{NN'} \tag{25}$$

For a system at equilibrium p_i is

$$p_i = g_i \exp(-E_i/KT) \left[\sum_i \exp(-E_i/KT)\right]^{-1}, \tag{26}$$

where g_i is the state degeneracy. In order to understand a temperature dependent $J_{NN'}$ we must identify these energy states which are close enough to the ground state to be substantially populated at temperatures accessible to NMR spectroscopists, i.e. normally -150 to 200°C.

Table 10. Temperature dependence of coupling to fluorine.

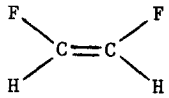
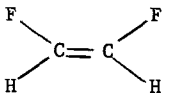
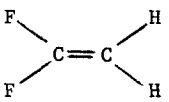
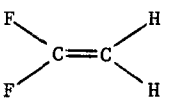
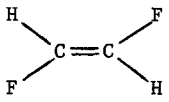
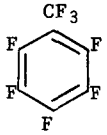
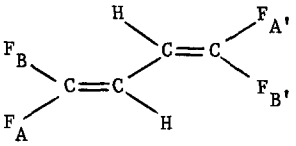
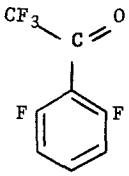
Compound	Coupling Constant	Solvent	Temperature Coefficient	Reference
	$^2J_{FH}$ = 71.70 (23°C)	n-hexane	-0.08	25
	71.76	CS_2	0.24	
	72.01	$CHCl_3$	-0.09	
	72.12	Et_2O_2	-0.16	
	72.36	methyl acetate	-0.26	
	72.37	CH_2Cl_2	0.18	
	72.73	acetone	0.09	
	72.77	DMF	0.12	
	$^3J_{FH}$ trans 19.63	n-hexane	-0.45	
	20.04	CS_2	-0.16	
	20.31	$CHCl_3$	-0.48	
	20.43	Et_2O	-1.09	
	20.36	methyl acetate	-1.32	
	20.37	CH_2Cl_2	-0.74	
	21.49	DMF	-0.71	
	$^3J_{FF}$ = -18.74 (23°C)	n-hexane	+1.37	25
	-19.66	CS_2	1.68	
	-19.10	$CHCl_3$	1.07	
	-18.98	Et_2O	1.92	
	-18.70	methyl acetate	1.45	
	-18.94	CH_2Cl_2	1.29	
	-18.89	acetone	1.52	
	-19.45	DMF	1.47	
	$^3J_{FH}$ cis = 0.61 (23°C)	n-hexane	0.08	25
	0.67	CS_2	0.12	
	0.79	$CHCl_3$	0.09	
	1.04	methyl acetate	-0.07	
	0.88	CH_2Cl_2	-0.06	
	1.07	acetone	-0.08	
	1.19	DMF	-0.09	
	$^3J_{HF}$ trans = 33.76 (23°C)	n-hexane	-0.29	25
	34.01	CS_2	-0.29	
	34.40	$CHCl_3$	-0.56	
	35.23	methyl acetate	-0.96	
	34.85	CH_2Cl_2	-0.51	
	35.42	acetone	-0.78	
	36.15	DMF	-0.52	

Table 10. (contd.)

Compound	Coupling Constant		Solvent	Temperature Coefficient	Reference
	$^2J_{FF}$ =	31.65	n-hexane	1.39	
		30.01	CS_2	1.27	
		32.58	$CHCl_3$	0.93	
		36.73	methyl acetate	0.37	
		33.86	CH_2Cl_2	0.59	
		36.51	acetone	0.30	
		36.92	DMF	0.16	
	$^2J_{HF}$ =	75.06 (23°C)	CS_2	0.34	25
		75.23	Et_2O	0.11	
		75.10	acetone	0.06	
	$^3J_{HF}$ cis =	2.84 (23°C)	CS_2	0.02	25
		3.17	Et_2O	-0.40	
		3.36	acetone	-0.19	
	$^J_{CF_3-F_{ortho}}$ =	22.48 (-27°C)	CCl_4	0.45	27
	$^5J_{F_AF_{A'}}$ =	35.7 (30°C)	neat	2.4	57
	$^5J_{F_AF_{B'}}$ =	8.0	neat	-0.5	
	$^5J_{F_BF_{B'}}$ =	4.8	neat	0.5	
	$^2J_{F_AF_B}$ =	36.6	neat	2.3	
	$^5J_{CF_3-F}$ =	-	-	0.5	46
CF_3CFCl_2	$^3J_{FF}$ =	5.6 (90°C)	neat	-0.3	58
CF_3CF_2COOH	$^3J_{FF}$ =	1.3 (85°C)	neat	-0.4	58

*Change in J for 100° change in temperature.

For liquid samples we have discussed already (section 3.1) the effect of molecular ordering on $J_{NN'}$ and in figure (1) we show one possible arrangement of solute and solvent molecules. Other molecular configurations will exist, and it is possible that $J_{NN'}$ will depend on the molecular ordering sufficiently to show a temperature dependence as the p_i values change with temperature. There have not been any attempts to calculate the magnitude of such temperature effects, but they have been invoked to explain the temperature dependent J_{FF} values in benzotrifluorides[46] and fluoroethylenes.[25]

Isolated molecules also may have thermally accessible energy states in which $J_{NN'}$ differs from the ground state, and population of these states may produce a temperature variation of $J_{NN'}$. The most general phenomenon is the existence of low frequency vibrational modes, but as yet there are no published calculations of how coupling to fluorine depends on vibrational motion. Restricted internal rotation in molecules has been much studied by NMR spectroscopy, and in most cases a simplified view is taken of the problem. Thus for substituted ethanes it is usual to assume that the averaged coupling constant is given by,

$$J_{NN'} = p_I J^I_{NN'} + p_{II} J^{II}_{NN'} + p_{III} J^{III}_{NN'}, \tag{26}$$

where p_I, $J^I_{NN'}$, etc, refer to the three possible positions of energy minima as the rotational angle ϕ changes between 0 and 360^o. The justification of equation (26) lies in the assumption that the barriers to internal rotation are large enough to make the probability of intermediate values of ϕ negligible. However, there is evidence that this assumption is not always valid and the averaging process should extend over all ϕ. An approximate method of doing this averaging is to assume a classical model for the rotation, such that each value of ϕ describes an energy state, giving

$$J_{NN'} = \int_0^{2\pi} J_{NN'}(\phi) \exp(-V(\phi)/KT)\, d\phi \Big[\int_0^{\pi} \exp(-V(\phi)/KT) d\phi\Big]^{-1} \tag{27}$$

In order to apply equation (27) it is necessary to know the form of $V(\phi)$, and $J_{NN'}(\phi)$, the variation of $J_{NN'}$ with ϕ. Equation (27) is a considerable improvement on (26), particularly for F-F coupling, but it is possible to go a step further and to treat the rotation quantum mechanically. To do so it is necessary to start by assuming a functional form for $V(\phi)$, and a Fourier series expansion has been found convenient in that it appears to be reasonable to truncate the series at the minimum number of terms dictated by symmetry.[47] Thus for no symmetry $V(\phi)$ can be written as,

$$V(\phi) = \tfrac{1}{2}V_1(1 - \cos\phi) + \tfrac{1}{2}V_2(1 - \cos 2\phi) + \tfrac{1}{2}V_3(1 - \cos 3\phi) + V_4 \sin\phi + V_5 \sin 2\phi \tag{28}$$

Substitution of $V(\phi)$ into the Schrödinger equation gives a differential equation which may be solved by numerical methods[48] to yield a set of rotation energy states E_i and eigenfunctions $\psi_i(\phi)$. The values of $p_i(\phi)$ are given by,

$$p_i(\phi) = \psi_i(\phi)^* \psi_i(\phi)$$

and may be used to calculate a total probability distribution $p(\phi)$, such that,

$$p(\phi) = \sum_i p_i(\phi) \exp(-E_i/KT) \Big[\sum_i \exp -E_i/KT\Big]^{-1}$$

The rotational average of $J_{NN'}$ is then obtained as,

$$J_{NN'} = \int_0^{2\pi} p(\phi)\, J_{NN'}(\phi)\, d\phi \tag{29}$$

Equation (26) predicts temperature independent values of $^3J_{NN'}$, between CH_3 or CF_3 groups and a vicinal neighbour, whereas equations (27) and (29) allow for a possible temperature variation of $^3J_{NN'}$, depending on the nature of $J_{NN'}(\phi)$. The rotational potential for a fragment CH_3-CH-, or fragments with the same 3-fold symmetry but with H replaced by F, is

$$V(\phi) = \tfrac{1}{2}V_3(1 - \cos 3\phi), \qquad (30)$$

higher terms in the Fourier series being neglected. Substitution of equation (30) into the Schrödinger equations yields a 3-fold Mathieu equation,

$$\frac{\partial^2}{\partial\phi^2}\psi(\phi) + (a - q\cos 3\phi)\psi(\phi) = 0 \qquad (31)$$

The constants a and q are,

$$a = 8\pi^2 I_r h^{-2}(E_i - \tfrac{1}{2}V_3)$$

$$q = 4\pi^2 I_r V_3 h^{-2},$$

in which I_r is the reduced moment of inertia. The solution of equation (31) is possible by standard numerical methods,[49] to yield $\psi_i(\phi)$, E_i and hence $p(\phi)$. If $^3J_{NN'}$ has a Karplus-type dependence on ϕ, then it is found that $^3J_{NN'}$ is independent of temperature for 3-fold symmetry i.e. $^3J_{HH}$ and $^3J_{FH}$ when CH_3- or CF_3 groups are involved.[46,50] In the case of $^3J_{FF}$ coupling both theory and experiment (see section 6.3) suggest that the ϕ dependence is not of the Karplus type, and there may be appreciable dependence on temperature for coupling involving CF_3 groups.[50] As an example consider the molecule CF_3CFH_2, for which Hirao *et al*[51] have calculated the variation of $^3J_{FF}$ with ϕ. Using their $J(\phi)$, and a barrier to rotation of V_3 = 12 KJ mol^{-1} gives the averaged value of $^3J_{FF}$ to be 4.51 Hz for T = 173°K and 5.06 Hz for T = 373°K. It should also be noted that the average value is predicted to be 3.19 Hz if only three positions (ϕ = 0, 120 and 240°) are appreciably populated, and 7.52 Hz for free rotation.[50] The observed value is 15.5 Hz, thus the calculated $^3J_{FF}$ values are considerably in error, however, the trends suggested by these calculations are that equation (26) is not appropriate for coupling between fluorine nuclei, and that if reliable $J(\phi)$ values were available it would be possible to obtain V_3 by comparison of the observed and calculated average values.

4. FLUORINE-HYDROGEN COUPLING

In Tables A1- A8 we collect together most of the data on F-H coupling published prior to 1973, and in this section we will discuss attempts either to calculate F-H coupling, or to relate their values to structure and substituents.

4.1 $^1J_{FH}$ *in Hydrogen Fluoride*

Hydrogen fluoride is the ideal molecule for testing the various methods of calculating coupling constants, and table 11 summarises the results of several attempts to calculate $^1J_{FH}$. It is very obvious from table 11 that the calculated value of $^1J_{FH}$ is sensitive to the wavefunction used, and there is no clear indication of which method is the best. All methods agree, however, that the Fermi-contact term is the dominant one, contributing about 80% of the total magnitude of $^1J_{FH}$. With the Nesbet, extended basis-set, MO wavefunction and the SOS method it is possible to get very close to the experimental value, and similarly for the variation method with Duncan's MO function. All other calculations are hopelessly incorrect, giving the wrong sign to the coupling constant, and emphasising the importance of the choice of wavefunction in these calculations. It would be interesting to see if the FP method can get the correct result with the Nesbet or Duncan MO wavefunctions.

Table 11. Calculated spin-spin coupling in the hydrogen fluoride molecule (experimental value[54] = 530 Hz)

Method		$J^{1(a)}_{HF}$	J^{1b}_{HF}	J^{2}_{HF}	J^{3}_{HF}	Total J_{HF}	Reference
SOS	Slater MO	2.1	-215.9	97.9	-1160.6	-1276.5	55
SOS	Ransil MO	2.1	-143.0	57.1	-1399.0	-1482.9	55
SOS	Karo and Allen MO	5.1	-266.5	110.3	-459.5	-610.6	55
SOS	Mukherji and Karplus MO	1.67	-180.9	64.8	-696.1	-810.5	55
SOS	Nesbet MO	*	*	36.6	+584.7	621.3	55
SOS	Nesbet MO	*	*	*	528.1	528.1	52
SOS	Nesbet MO with configuration interaction	*	*	*	835.6	835.6	52
SOS	McLean and Yoshimine MO		-46.4†	-21.5	-1489	-1560	53
FP	INDO-MO		*	*	-150.2	-150.2	10
FP	Ransil-MO		*	*	-1399	-1399	56
Variation	Duncan MO					531.2	9
Variation	Ballinger MO					54.8	9

† $J^{1(a)}_{HF} + J^{1(b)}_{HF}$

* value not calculated

Murrell, Turpin and Ditchfield[52] have investigated the dependence of the calculated value of $^1J_{FH}$ on the inter-nuclear distance. They used the SOS method with the Nesbet MO wavefunction, and found that replacing hydrogen by deuterium changes the coupling constant by -13.3 Hz, when allowance is made for the change in gyromagnetic ratios.

The calculation by Buckingham and Love[53] also evaluated the anisotropies, $\Delta J = J_{||} - J_{\perp}$, for each term; however, the result they obtain for the isotropic average of $^1J_{FH}$ of -1560 Hz is so far from the observed[54] value of 530 Hz as to cast doubt on the significance of their result.

4.2 *Geminal Fluorine-Hydrogen Coupling*

4.2.1 *Calculations of* $^2J_{FH}$

There have been several attempts to calculate $^2J_{FH}$ values, but in most cases the results are in poor agreement with experiment.[10,59,60,61] Ditchfield and Snyder[62] have made a theoretical study of all the measurable couplings in methyl fluoride, i.e. $^1J_{CH}$, $^1J_{CF}$, and $^2J_{HF}$, by the FP method, and using a molecular orbital wavefunction calculated from a basis set of gaussian functions (known as STO-4-31 G[63]). For $^2J_{FH}$ they obtain the results:

$$^2J^{(1)}_{FH} = 12.3, \quad ^2J^{(2)}_{FH} = -4.2, \quad ^2J^{(3)}_{FH} = 58.5, \text{ and } ^2J_{FH} = 66.6 \text{ Hz}.$$

The total coupling of 66.6 Hz compares well with the experimental value of 46.5 Hz.[64] This calculation was made in order to determine the magnitude to be expected for Δ^2J_{HF}, the total anisotropy in the coupling (see section 2.5), because the results of an analysis of the spectrum of $^{13}CH_3F$ dissolved in a liquid crystalline solvent were interpreted by Bernheim and Krugh[65] as showing a large anisotropy in some, at least, of the coupling constants. Later experiments have shown this interpretation to be incorrect,[66] but the original experimental work stimulated a lot of useful work, including the calculation by Ditchfield and Snyder. The anisotropy was calculated to be:

$$\Delta^2J_{FH}^{(1)} = -18.9, \quad \Delta^2J_{FH}^{(2)} = -4.8, \quad \Delta^2J_{FH}^{(4)} = -83.8, \text{ and } \Delta^2J_{FH} = -107.5 \text{ Hz.}$$

At first sight this appears to be a large quantity, but it must be compared to $2D_{HF}$ for a completely aligned molecule, which has a value of -24,300 Hz, hence $^2J_{HF}^{aniso}$ (see equation (20)) contributes only about 0.5% to the observed total, anisotropic, H-F coupling.

4.2.2 *Dependence of $^2J_{FH}$ on HF distance and HCF angle*

The calculation by Ditchfield and Snyder on methyl fluoride predicts the spin-orbital term, $^2J_{HF}^{(1)}$, to be appreciable in magnitude, and this is in agreement with an earlier calculation of this term by Pople,[66] who proposed that $^2J_{HF}^{(1)}$ depends on r_{FH}, the F-H separation, and θ, the HCF angle, such that,

$$^2J_{FH}^{(1)} = 75.2\ r_{FH}^{-3}\ (3\cos^2\theta - 1) \times 10^{-24} \text{ Hz}$$

The other contributions to the total value of $^2J_{FH}$ will also be distance and angular dependent, and it is therefore probable that there will be an angular and distance dependence of $^2J_{FH}$, however, it is unlikely to be of a simple functional form. Examination of the tabulated $^2J_{FH}$ values in tables A clearly show that any dependence on r_{FH} and θ is much less important than a dependence on substitution of other groups on both α and β carbon atoms. Aranda, Jullien and Martin[67] have assumed that small variations in $^2J_{FH}$ in some cyclopentyl and cyclohexyl derivatives do arise from changes in the HCF angle. It is more probable, however, that the observed changes arise from the substituent effects described in the following sections.

4.2.3 *Effect on $^2J_{FH}$ of substitution*

There are large changes in $^2J_{FH}$ in compounds of the type CFHXY and SiFHXY as the electronegativity of X and Y are changed. When X or Y is itself a complex molecular fragment then there may be added, but smaller, substituent effects. However, if X or Y for complex fragments is taken to be the first atom then the following relationships predict $^2J_{FH}$ to an accuracy of about ±2Hz[68]

CHFXY:

$$^2J_{FH} = 78.76 + 8.45\ E_XE_Y - 16.73\ (E_X + E_Y) \tag{32}$$

SiHFXY

$$^2J_{FH} = 49.08 + 7.85\ E_XE_Y - 9.03\ (E_X + E_Y) \tag{33}$$

When X or Y is not a single atom then there may be small added substituent effects on $^2J_{FH}$, which are conformationally dependent. A careful examination of the values of $^2J_{FH}$ in conformationally rigid molecules enabled Phillips and Wray[69] to propose the following rules for the change in $^2J_{FH}$ on substitution at an adjacent carbon atom in fluorocarbohydrate molecules

1. Value of $^2J_{FH}$ for

is 50 Hz

2. Replacement of α carbon by oxygen changes $^2J_{FH}$ by +1 Hz
3. Replacement of α carbon by sulphur changes $^2J_{FH}$ by -4 Hz
4. Substitution effects for X (= O, OR, F) groups vicinal to H,F

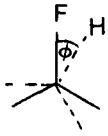
Orientation of F	Orientation of X	
F axial	X equatorial	+ 1Hz
F equatorial	X equatorial	
F axial	S or O in ring	
F equatorial	X axial	- 2Hz
F axial	X axial	
F equatorial	O or S in ring	

Application of these rules to a wide range of fluorocarbohydrates, polyfluoro-1,4-dioxans, and polyfluoro-1,4-oxathians gave good agreement between observed and calculated $^2J_{HF}$ values. In particular, the rules were used to re-assign the structures of some of the dioxans and oxathians.

4.3 *Vicinal Fluorine-Hydrogen Coupling*

4.3.1. *Saturated compounds*

The most interesting aspect of $^3J_{FH}$ coupling is undoubtably the dependence in saturated compounds on the dihedral angle, ϕ, between CH and CF bonds,



The relationship between $^3J_{HH}$ and ϕ is well-established, both from experiment and theory, and a similar, Karplus-type, ϕ-dependence appears to hold for F-H coupling, but with a larger substituent effect.[70-73] All theoretical calculations agree in predicting an angular dependence of the form,

$$^3J_{HF}(\phi) = A + B\cos\phi + C\cos^2\phi \qquad (34)$$

Figure 3 shows the results of calculations by Gopinathan and Narasimhan,[74] who compared calculated values of $^3J_{FH}$ for ethyl fluoride using the FP method with CNDO-2 and INDO wavefunctions, and the Pople-Santry method[75] with an extended-Hückel (EHT) function. With the INDO method the three coefficients in equation (34) are calculated to be A = 0.212, B = -5.042 and C = 31.379 Hz, and these values predict observed values with a standard deviation of 0.2 Hz.

Govil[76] has also calculated $^3J_{FH}(\phi)$ for ethyl fluoride using the Pople-Santry method with EHT wavefunctions, and obtained similar results to Gopinathan and Narasimhan. One interesting point about Govil's calculations is that he compares the result of using two different basis sets of Slater atomic orbitals to construct the EHT molecular orbitals. In one set the orbital exponents are calculated with

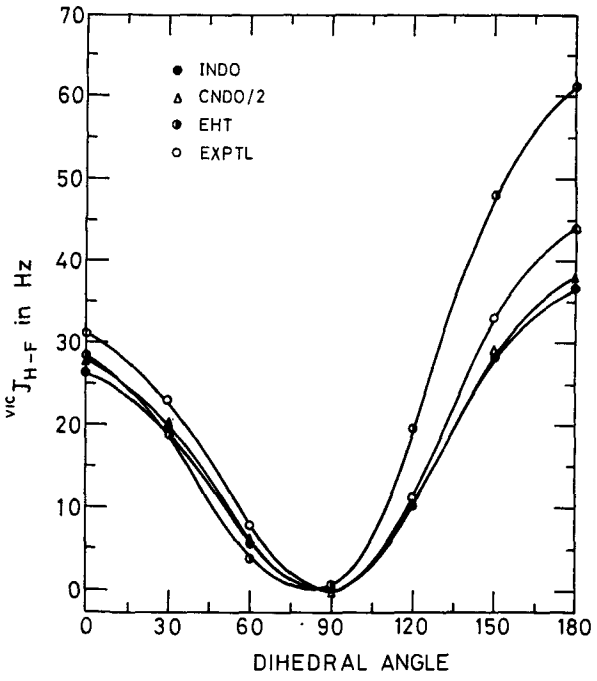


Figure 3. Calculated variation of $^3J_{FH}$ with dihedral angle in substituted ethanes. Gopinathan and Narisimhan[74]

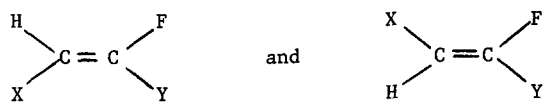
Slater's rules,[77] which is the usual set adopted in almost all approximate wavefunction calculations. The other basis set also uses Slater orbitals, but with orbital exponents calculated by the modifications to Slater's rules suggested by Burns.[78] As one might expect there is a considerable difference in the magnitude of $^3J_{FH}$ calculated by the two sets, but each gives the same kind of angular dependence, with the Burns set closer to experiment.

Govil[76] also has calculated $^3J_{FH}(\phi)$ in substituted ethanes CH_2XCH_2F and CH_3CHXF, in which X is C, N, O and F, and the results are shown in Figure 4. It is seen that the substituent effects on $^3J_{FH}$ differ for the two kinds of molecule, in that increasing the electronegativity of X decreases $^3J_{FH}$ for CH_2XCH_2F, but increases for CH_3CH_2X. Note too that the curves are not symmetrical about $\phi = 180^o$, hence in substituted ethanes the two gauche $^3J_{FH}$ values are likely to be different, and this has been observed experimentally.[70]

Jensen and Schaumburg[60] have made a very thorough experimental and theoretical study of all the coupling constants in ethyl fluoride. Their calculations used the SOS method with CNDO-2 and INDO wavefunctions, and for $^3J_{FH}$ they reproduce the observed, averaged value quite well.

4.3.2. *Unsaturated compounds*

There are very large substituent effects on the $^3J_{FH}$ couplings in substituted olefines, but for the pair of compounds,



$^3J_{FH}$(cis) is always smaller than $^3J_{FH}$ (trans) for the same X and Y, and this also holds within single molecules having Y = F. The measured values of $^3J_{FH}$ (cis) cover range -4 to 20 Hz, whilst $^3J_{FH}$ (trans) lie between 10 and 100 Hz. Thus a $^3J_{FH}$ > 25 Hz or <5 is clearly a <u>trans</u> or <u>cis</u> coupling respectively.

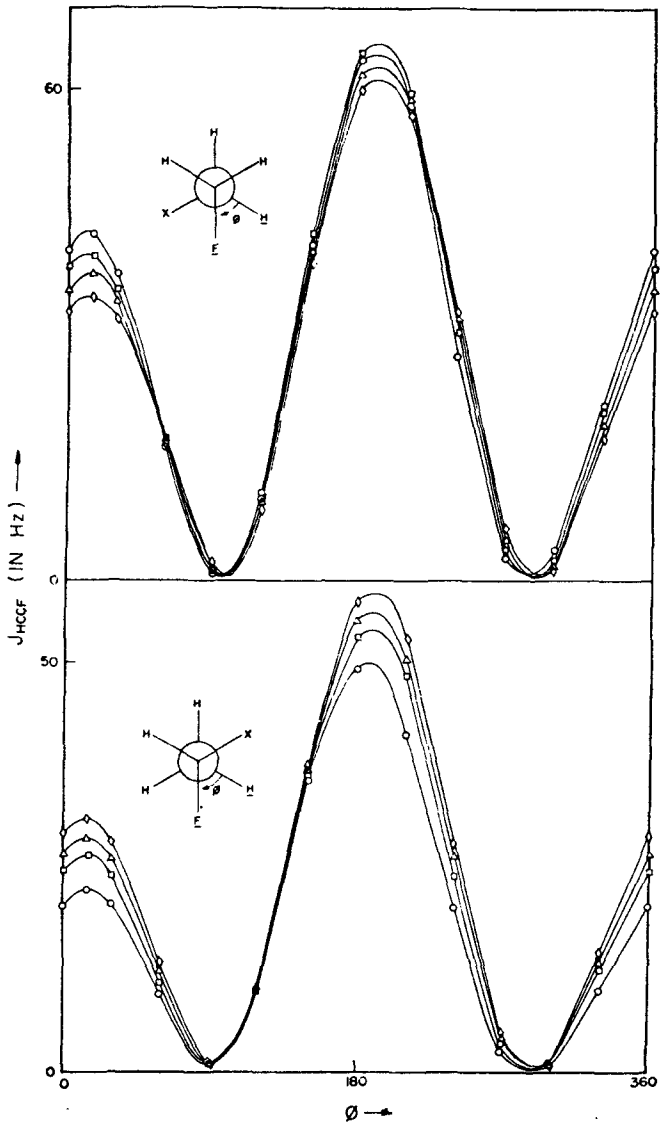
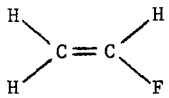


Figure 4. Substituent effects on the variation of $^3J_{FH}$ with ϕ, the dihedral angle in ethanes. X refers to: O, carbon; □ nitrogen; Δ, oxygen; and ◇, fluorine. Govil.[76]

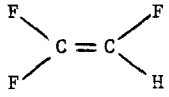
Calculations of $^3J_{FH}$ in vinyl fluoride have given good agreement with experiment:[10,79]



$^3J_{FH}$ (cis) 26.7 (calculated), 20.1 (experimental)[80]

$^3J_{FH}$ (trans) 66.20 (calculated), 52.4 (experimental)[80]

However, a calculation on trifluoroethylene by Gopinathan and Narasimhan,[79] using the same procedure, the FP method with an INDO wavefunction, as the work on vinyl fluoride, gave good agreement with the cis but poor for trans coupling:



$^3J_{FH}$ (cis) 2.78 (calculated), 3.0 (observed)[81]

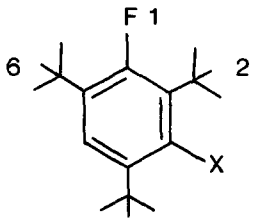
$^3J_{FH}$ (trans) 58.69 (calculated), 12.0 (observed)[81]

The poor agreement between calculated and observed $^3J_{FH}$ (trans) underlines a lack of knowledge as to why the FP method gives such varied results.

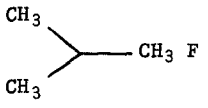
Haigh and Sykes[82] have calculated the anisotropies ΔJ of $^3J_{FH}$ values in olefines and substituted benzenes, and predict that ΔJ is largest for $^3J_{FH}$ (trans), when it may be 1% of the corresponding dipolar coupling constant. The other anisotropies are predicted to be less than 0.5% of their dipolar coupling, and these results are in accord with upper limits to ΔJ values determined from the analysis of spectra of molecules dissolved in liquid crystalline solvents.[16]

4.4 *Long-range fluorine-hydrogen coupling*

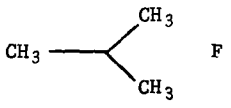
Values of $^nJ_{FH}$ with $n > 3$ tend to be larger than corresponding $^nJ_{HH}$ values, a factor leading to more complex spectra for fluorocarbons, but which may also have some useful diagnostic features. In many molecules a long-range F-H coupling is observed only when the two nuclei are close through space. For example, Mhyre et al[83] have argued convincingly that the larger coupling between methyl protons and fluorine in compounds,



when X is increased in bulk, arise because conformation (I) is more favoured than II,



(I)



(II)

Thus, when X=H the values of $^5J_{FH}$ are,

$$^5J_{FH}^{1,2} = {}^5J_{FH}^{1,6} = 1.2 \text{ Hz}$$

Myhre et al[83] took their results to show that there must be strong dependence of $^5J_{FH}$ on distance, and this has been supported by calculations by the FP method by Barfield and Wasylishen.[124] The calculations examined many different molecular systems and it was concluded that long-range F-H coupling should be both distance and orientation (of C-F and C-H bonds) dependent. There has been a great deal of discussion of the "mechanism" of long-range F-X coupling, and the subject has been reviewed recently by Hilton and Sutcliffe.[84]

A great deal of information exists for the long-range $^nJ_{FH}$ in aromatic systems, and the data in the tables A of the appendix has been used to show the additivity of substitutent effects, and a correlation with substituent electronegativity.[126]

5. CARBON-FLUORINE COUPLING

As soon as we consider coupling between fluorine and a nucleus other than hydrogen then we can expect the spin-dipolar and spin-orbital terms to be important, as well as the Fermi-contact term. Thus the total value of J_{CF} may have three contributions, possibly varying in sign as well as magnitude, and it is to be expected that substituent and structural effects may be large and complex. This is certainly true for $^1J_{CF}$ in fluoro-methanes, which vary between -150 and -380 Hz depending on the substituents. The $^1J_{CF}$ values for other compounds also fall within this range, thus, unlike $^1J_{CH}$,

the one-bond coupling is not a good indication of the hybridisation of the carbon atom.

5.1 *One bond C-F coupling*

There have been several attempts to calculate $^1J_{CF}$ for the fluoromethanes, CF_nH_{4-n}, and the results are shown in table 12. The molecule CH_3F has been the subject of special attention, because of the suggestion by Bernheim and Krugh[65] that $^1J_{CF}$ in this molecule might have a particularly large value of the anisotropic part, $^1J_{CF}^{aniso}$ (see section 2.5). Recent experiments by Burnelle, Council and Ulrich[85] show that $^1J_{CF}^{aniso}$ for methyl fluoride is small, and this is supported by the calculations, even though they differ considerably on the magnitude and signs of the different contributions to the coupling constant and its anisotropy. Indeed, the calculations on CH_3F illustrate once more how difficult it is to calculate coupling constants, and the sensitivity to the choice of calculational method and wavefunction. It should also be noted that the calculations in table 12 differ in their methods of calculating $S_N(0)^2$ and $\langle r^{-3}\rangle_N$ values (see section 2.4). The Blizzard and Santry[12] calculations do obtain the correct trends in going from CF_4 to CF_3H, but this has been achieved by treating $S_N(0)$ and $\langle r^{-3}\rangle_N$ as adjustable parameters whose values are optimised to give the best fit to experiment.

Table 12. Calculated values of $^1J_{CF}$ in fluoromethanes.

Molecule	Method	$^1J_{CF}^{(1)}$	$\Delta J^{(1)}$	$^1J_{CF}^{(2)}$	$\Delta J^{(2)}$	$^1J_{CF}^{(3)}$	$\Delta J^{(4)}$	J	ΔJ	Ref.
CH_3F	Pople-Santry	-13.8	-	5.3	-	-124.6	-	-133.1	-	10
(expt	CNDO-2									
-157.5)										
	FP-INDO	-	-	-	-	-237.1	-	-237.1	-	86
	FP-INDO	-15	27	15	26	-97	208	-97	261	87
	FP-INDO	-65	-	31	-	-169		-203	-	12
	FP-(4-31G)	32.4	-75.2	19.6	35.0	-149.5	303.8	-97.5	263.6	62
	SOS-INDO	-6.3	4.6	9.4	-16.2	-99.2	93.5	-96	114.2	88
	SOS-INDO-C1*	-4.1	-	6.9	-	-126.3	-	-123.5	-	59
	SOS-INDO-C1*	-	-	-	-	-150.9	-	-150.9	-	59
CH_2H_2	FP-INDO	-118.2	-	23.0	-	-164.5	-	-259.6	-	12
(expt	SOS-INDO-C1*	-12.5	-	4.5	-	-132.6	-	-140.7	-	59
-234.8)	SOS-INDO-C1*	-	-	-	-	-241.7	-	-241.7	-	59
CF_3H	FP-INDO	-149.7	-	17.1	-	-152.6	-	-285.2	-	12
(expt	SOS-INDO-C1*	-17.5	-	3.3	-	-125.5	-	-139.7	-	59
-274.3)	SOS-INDO-C1*	-	-	-	-	-279.0	-	-279.0	-	59
CF_4	FP-INDO	-164.6	-	4.3	-	-106.8	-	-267.0	-	12
(expt	SOS-INDO-C1*	-20.2	-	2.4	-	-85.3	-	-103.1	-	59
-259.2)	SOS-INDO-C1*	-	-	-	-	-251.3	-	-251.3	-	59

*These calculations differ only in the choice of values for $S_C(0)^2S_F(0)^2$ and $\langle r^{-3}\rangle_C\langle r^{-3}\rangle_F$.

The calculations reported in table 12 agree that the Fermi-contact term is not the only important term contributing to $^1J_{CF}$, and the spin-orbital term $J^{(1)}$ is of comparable magnitude. There is a striking disagreement on the sign of $J^{(1)}$ for methyl fluoride, the calculation by Ditchfield and Snyder[62] obtaining 32.4 Hz, whereas all others obtain a negative value. The distinguishing feature of the Ditchfield and Snyder calculation lies in the use of a STO 4-31G gaussian basis set for their wavefunction calculation, whereas the others all use an INDO wavefunction.

5.2 *Two-bond C-F coupling*

Although there are now many experimental determinations of $^2J_{CF}$ values, the lack of success in calculating $^1J_{CF}$ values appears to have deterred theoreticians from investigating the ability of calculational procedures to predict these coupling constants. The only extensive investigation is by Jensen and Schaumburg[60] on the molecule ethyl fluoride. They determine $^2J_{CF}$ in this compound to be 11.51 ± 0.30 Hz, and using the SOS method with an INDO wavefunction they found that the calculated value is -11.30 Hz. Including configuration interaction (CI) into the calculation of the INDO wavefunction leads to a change in the calculated value to -1.71 Hz. The use of configuration interaction with the SOS method at first sight ought to improve calculated coupling constants since more states are used in the summation of equation (16); however the result obtained for ethyl fluoride shows that the convergence of the summation is not monotonic, that is increasing the number of virtual states by using CI may not lead to better calculated $J_{NN'}$ values unless very large numbers of states are included. The calculations found the terms $^2J_{CF}^{(1)}$ and $^2J_{CF}^{(3)}$ to be almost equal in magnitude but opposite in sign, and it is this cancelling effect which makes calculation of $^2J_{CF}$ so difficult.

Jensen and Schaumburg also stress the sensitivity of the calculated value of $^2J_{CF}$ to the structure for the molecule used in the calculation, and suggest that good agreement with experiment should be expected only if an accurate structure is known.

5.3 *Long-range C-F coupling*

The proton noise-decoupled spectra of fluorocarbons reveal the magnitudes of long range C-F coupling, but the signs are not obtained, and consequently it is impossible to be sure of the effects of structure or substitution. Sign determinations have been made for some aromatic compounds by double resonance techniques, and it has been found that $^2J_{CF}$ is probably always negative.[89,90] Similarly, $^3J_{CF}$ and $^4J_{CF}$ are always positive and substituent effects are additive in the series $C_6F_mH_{6-m}$. The magnitudes of $^nJ_{CF}$ in aromatic compounds always decrease as n increases for a given compound. For saturated compounds there is some evidence that $^3J_{CF}$ and $^4J_{CF}$ may be conformationally dependent.[91]

6. FLUORINE-FLUORINE COUPLING

There is a wealth of data on F-F coupling, and many interesting features have been revealed, however, attempts to relate the couplings to electronic and geometrical structure have had mixed success. We will attempt to highlight some of the interesting problems, most of which still require much theoretical work before they are understood.

6.1 *One-bond F-F coupling*

It is not possible to measure $^1J_{CF}$ for the fluorine molecule, but values of the various contributions to its magnitude have been made by Buckingham and Love[53] using the SOS method and Ransil's ab inito molecular orbital wavefunction.[92] The results are,

$J^{(1)}$	$\Delta J^{(1)}$	$J^{(2)}$	$\Delta J^{(2)}$	$J^{(3)}$	$\Delta J^{(4)}$	J(total)	ΔJ(total)
-272.1	408.1	50.0	116.6	-791.9	-370.9	-1014.0	147.7 Hz

Thus, contributions from $J^{(1)}$ and $J^{(2)}$ are appreciable, and this is a feature of other F-F coupling constants, and is one reason for the difficulty in calculating their values.

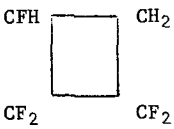
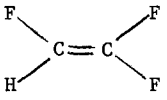
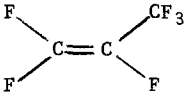
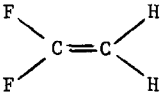
6.2 *Two-bond F-F coupling*

There are two striking features of $^2J_{FF}$ values in fluorocarbons. Firstly, they vary widely, and their values are obviously very sensitive to structure and substituents. Secondly, they can

have a large anisotropy. Both features have been extensively investigated, but not with much success, and it is interesting to speculate on this failure.

It would be of considerable importance to understand the sensitivity of $^2J_{FF}$ to structure and substituents, but there has not yet been a sufficiently systematic study of these effects by theoreticians, largely because of uncertainty in the reliability of the calculational methods. This is illustrated by the calculations on a number of compounds shown in table 13. The striking feature of these calculations is that $^2J_{FF}^{(1)}$, $^2J_{FF}^{(2)}$ and $^2J_{FF}^{(3)}$ are of comparable magnitude, and this is probably the reason why the calculated values are in some cases so far from those observed.

Table 13. Calculated $^2J_{FF}$ in fluorocarbons.

	Method[a,b]		$J^{(1)}$	$J^{(2)}$	$J^{(3)}$	J	J(obs)
CF_2H_2	SOS-INDO		76.9	36.4	-103.9	9.2	∿ 150-250*
CF_3H	FPT-INDO		47.3	20.1	36.3	103.7	
	SOS-INDO		57.7	31.5	-17.2	72.1	150[c]
 A B	SOS-INDO	A	63.3	28.5	-11.3	80.5	202-230[d]
		B	61.5	27.9	-5.0	84.4	
	FPT-INDO		56.4	19.9	5.4	81.7	87[e]
	SOS-INDO		44.4	29.9	-15.0	59.3	
	FPT-INDO		41.6	19.2	3.4	64.2	60.0[f]
	SOS-INDO		12.2	24.5	-2.1	34.6	
	FPT-INDO		48.6	19.2	-0.9	66.9	27[g]
	SOS-INDO		19.9	22.2	-20.4	21.6	

* not observable, but estimated from observed coupling constants in CF_2 groups

[a] SOS-INDO calculation reference 93
Uses $S_F^2(0)\ S_F^2(0) = 143.185$ au
$\langle r^{-3}\rangle\ \langle r^{-3}\rangle_F = 56.942$ au

[b] FPT-INDO reference 12.
Uses $S_F^2(0)\ S_F^2(0) = 548.418$ au
$\langle r^{-3}\rangle\ \langle r^{-3}\rangle_F = 35.410$ au

[c] Reference 94.

[d] Reference 95.

[e] Reference 96.

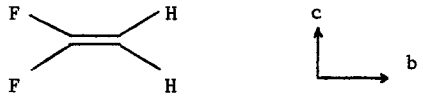
[f] Reference 97.

[g] Reference 81.

Nakatsuji, Hirao and Kato[98] have calculated the angular variation of the various contributions to $^2J_{FF}$ for the molecules difluoromethane and 1,1-difluoroethylene. They used the SOS method with an INDO wavefunction, and for both molecules find that only $J^{(3)}$ is appreciably angular dependent. In the case of difluoromethane the calculations predict large changes in $^2J_{FF}$ over the range of angles 110-120°, and this could be one reason why the values of $^2J_{FF}$ vary so widely in saturated fluorocarbons.

The anisotropy of $^2J_{FF}$ in 1,1-difluoroethylene has been determined experimentally by MacLean et al.[99,100] and also calculated by Nakatsuji et al[88] by the SOS method. The calculated values have the correct sign, but are too small, as shown in table 14. Haigh and Sykes[82] have also attempted to calculate the anisotropy of $^2J_{FF}$ in this molecule using the FP method but their results are in poor agreement with experiment, which they attribute to the sensitivity of the calculated values to the geometry of the molecule.

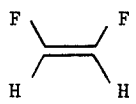
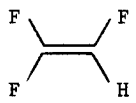
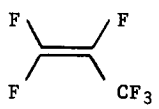
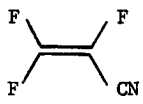
Table 14. Components of $^2J_{FF}$ in 1,1-difluoroethylene derived from experimental data[100] and calculated by the SOS method.[88]



	observed	calculated (Hz)
J_{aa}	342 ± 264	87
J_{bb}	-1215 ± 132	-93
J_{cc}	970 ± 132	69

6.3 *Three-bond fluorine-fluorine coupling*

The data in tables B of the appendix reveal on the one hand useful regularities, like the constancy of $^3J_{FF}$ in substituted benzenes, and on the other, large variations in value in saturated systems. Even in olefins, where $^3J_{FF}$ (trans) is always larger in magnitude than $^3J_{FF}$ (cis), there are some striking variations in value. Particularly interesting is the case of $^3J_{FF}$ (cis) in fluoroethylenes, whose values are,

	$^3J_{FF}$ (cis) Hz
	-18.7
	+33
	+40.3
	+35

A strong urge to believe that $^3J_{FF}$ (cis) must have a simple variation with substitution led to the sign of $^3J_{FF}$ (cis) in 1,2-difluoroethylene to be assigned a positive value when studying the effects of solvent.[25] A calculation on this molecule by Nakatsuji et al[93] by the SOS method with an INDO wavefunction gave the results,

$$J^{(1)} \quad -2.6, \quad J^{(2)} = 1.2, \quad J^{(3)} = 49.0, \text{ and } {}^2J_{FF} = 47.6 \text{ Hz},$$

and thus casting doubt on the negative sign, particularly as positive signs were calculated for the other compounds, in agreement with experiment. However, including configuration interaction into the SOS calculation gave[101]

$$J^{(1)} = -8.1, \quad J^{(2)} = -1.1, \quad J^{(3)} = -8.8, \text{ and } {}^3J_{FF} = -16.6 \text{ Hz}.$$

A FP calculation also gave a negative result not only for the 1,2-difluoroethylene, but also for other fluoroethylenes and hence is of doubtful significance. This example illustrates the difficulty of understanding F-F coupling and the widely varying results that can be obtained by calculation. The coupling in cis 1,2-difluoroethylene has been firmly established as negative.[96,102-5]

Calculations of $^3J_{FF}$ (trans) have been uniformly successful in predicting a large, negative value, in agreement with experiment.[93,12] MacLean and den Otter[106] have found evidence for a large anisotropy in the value of $^3J_{FF}$ in trans-1,2-difluoroethylene, and calculations by Haigh and Sykes[82] by the FP method with an INDO wavefunction have been very successful at reproducing the experimental values. Large anisotropies in $^3J_{FF}$ values are the exception not the rule,[16] thus $^3J_{FF}$ (cis) in olefins and $^3J_{FF}$ in fluorinated benzenes appear to be almost entirely isotropic. A large anisotropy has been found for $^3J_{FF}$ (cis) in perfluorocyclopropane.[107]

The available values of $^3J_{FF}$ for saturated fluorocarbons suggest that substituent effects dominate any possible dependence on dihedral angle, and hence these couplings have been found to be of no use as indications of structure. The changes with substitution of the angular dependence of $^3J_{FF}$ in saturated fluorocarbons has been the subject of calculations by Nakatsuji et al,[93] who confirmed the large changes produced by substitution. The calculations are by the SOS method with an INDO wavefunction, and do not predict the correct average values of $^3J_{FF}$, however, they are of considerable interest in indicating the probability of non-Karplus type angular dependence of $^3J_{FF}$ values.

6.4 *Four-bond fluorine-fluorine coupling*

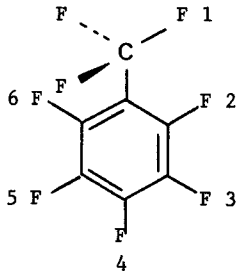
It is a striking feature of the spectra of fluorocarbons that $^4J_{FF}$ is often larger in magnitude than $^3J_{FF}$. For saturated compounds there is some evidence of a stereochemical dependence of $^4J_{FF}$, which could be a useful indication of structure. Thus for six-membered ring compounds it has been found[108-111] that the $^4J_{FF}$ values follow a consistent pattern, for example, in perfluoromethyl cyclohexane[108-110] the values are,

$$J_{ax\text{-}ax} = 26 \text{ Hz}$$

$$J_{eq\text{-}eq} = -6 \text{ to } -9 \text{ Hz}$$

$$J_{ax\text{-}eq} \approx 0$$

The axial-axial orientation has the two C-F bonds eclipsed, and in other kinds of molecule in which the CF bonds are also eclipsed there is a large, positive $^4J_{FF}$ value. For example, perfluoro toluene (I),[112] fluorinated bicyclo (II),[113] and 1,8-difluoronaphthalenes (III)[114] have the $^4J_{FF}$ values shown below.



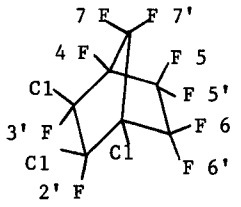
(I)

$^4J_{FF}^{1,2}$ = 22.68 Hz

$^4J_{FF}^{2,4}$ = 5.54

$^4J_{FF}^{3,5}$ = -0.43

$^4J_{FF}^{2,6}$ = -7.52



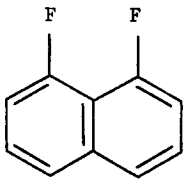
(II)

$^4J_{FF}^{2'6'}$ = 81 Hz

$^4J_{FF}^{3'5'}$ = 78

$^4J_{FF}^{57'}$ = 28

$^4J_{FF}^{67'}$ = 26



(III)

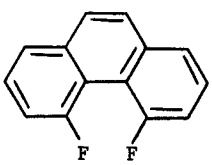
$^4J_{FF}$ = 58.8 Hz

The large magnitudes of $^4J_{FF}$ in (I) and (III), and similar compounds, have been cited as evidence of a "thru space" mechanism for large $^4J_{FF}$ couplings, however, the couplings in (II) clearly demonstrate that close approach through space is not the only situation giving rise to large $^4J_{FF}$ values. The eclipsing of the two CF bonds does, however, appear to be essential for the largest couplings.

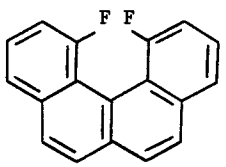
Calculations of $^4J_{FF}$ suggest that the Fermi contact term is the major contribution to the total coupling,[93] but, although predicting the largest magnitude for the eclipsed conformation, the sign was negative, contrary to experiment. The calculation, by the SOS method with an INDO wavefunction, also found that $^4J_{FF}$ can change sign within one molecule, in agreement with observed values.

6.5. *Long-range coupling*

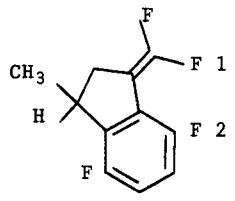
Very large values of $^nJ_{FF}$ with n > 4 observed when the two nuclei are close through space, for example



$^5J_{FF}$ = 174 Hz [115]



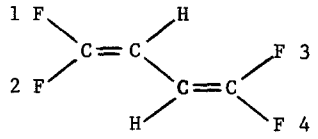
$^6J_{FF}$ = 43.2 Hz [116]



$^5J_{FF}^{1,2}$ = 68.39 Hz [117]

Again, as with $^4J_{FF}$ the planar arrangement of CF bonds, together with a close proximity through space appear to be essential for large $^5J_{FF}$ values.

Calculation of $^5J_{FF}$ by the SOS method[93] suggests the Fermi contact term to be dominant, and that the large couplings are positive. The angular dependence of $^5J_{FF}$ has been calculated by Hirao et al[98] who predict that $^5J_{FF}$ should have the largest value in compounds like the difluorophenanthrene above when in a planar form, and should decrease rapidly for non-planar forms. Both theory[98] and experiment[118] agree that the $^5J_{FF}$ values in butadienes follow a different pattern, with $^5J_{FF}^{1,4}$ being greater than $^5J_{FF}^{2,3}$

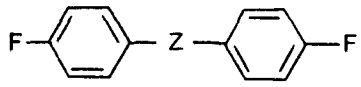


$^5J_{FF}^{1,4}$ = 35.7 Hz

$^5J_{FF}^{2,3}$ = 4.8 Hz

In the case of hexafluorobutadiene the same couplings are[119] $^5J_{FF}^{1,4}$ = 4.8 Hz and $^5J_{FF}^{2,3}$ = 11.3 Hz, whereas theory[98] still predicts the same relative magnitude as in tetrafluorobutadiene. Hirao et al[98] suggest therefore that hexafluorobutadiene is not planar, and a cisoid rather than transoid form.

Very long range couplings have been observed in molecules of the type[120]



where Z is a group, such as C=C, N=N, > C=O, which aids the transmission of electronic effects throughout the molecules. Thus, when Z = -C=C-C(=O)-C=C- there is a 0.2 Hz coupling between the two fluorines which are 14 bonds appart. When Z is a non-transmissive group, such as -N=N(=O)-, -S-, >C(OH)H, then the F-F coupling is unobserved.

6.6 *Fluorine-fluorine coupling in aromatic compounds*

$^3J_{FF}$ values in aromatic compounds are remarkably insensitive to substitution, and are found to be within a few hertz of -20 Hz. In contrast, the $^4J_{FF}$ and $^5J_{FF}$ are very sensitive to substitution, but Abraham et al[121,122] pointed out that such couplings can be predicted by additive substituent parameters. For para coupling only one parameter for each substituent is necessary to calculate the value of $^5J_{FF}$, and those derived by Abraham et al[122] are given in table 14, together with a substituent parameter for -N- in pyridines, determined by Emsley and Phillips.[123] The $^4J_{FF}$ couplings require three parameters per substituent, to allow for the three different substitution sites in 1,3-difluorobenzene. The coupling constants are calculated from the equations,

$$^4J_{FF}^{X,Y,\cdots} = 5.8 + {}^4J^{X(i)} + {}^4J^{Y(i)} + \cdots . \text{ Hz} \qquad (34)$$

$$^5J_{FF}^{X,Y,\cdots} = 18.1 + {}^5J^{X} + {}^5J^{Y} + \cdots . \text{ Hz} \qquad (35)$$

Table 14. Substituent parameters for $^4J_{FF}$ and $^5J_{FF}$ in benzenes and pyridines.

Substituent (X)	$^4J^{X(i)}$			$^5J^X$
	ortho-ortho (i = 1)	ortho-meta (i = 2)	meta-para (i = 3)	
NH_2	7.2	-8.7	0.5	-2.9
OH	4.7	-7.7	-0.8	-3.0
CH_3	0.7	-2.0	0.1	-0.3

Table 14. (contd.)

Substituent (X)	$^4J^{X(i)}$			$^5J^X$
	ortho-ortho (i = 1)	ortho-meta (i = 2)	meta-para (i = 3)	
Ph	0.6	-1.6	0.4	-0.3
H	0.0	0.0	0.0	0.0
F	-0.1	-3.8	-0.3	-3.2
Cl	-3.2	-0.4	0.7	-2.0
Br	-3.4	-0.5	0.1	-2.1
I	-3.1	0.5	0.7	-1.4
CF_3	-5.5	4.2	2.0	0.0
CN	-5.7	4.3	1.9	-0.3
NO_2	-5.7	4.3	1.9	-0.3
N	-	12.8	2.3	15.7

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APPENDIX

The appendix consists of lists of spin-spin coupling constants involving fluorine, in a wide variety of compounds both organic and inorganic. The data have been compiled from the literature by using the authors' own records and the literature abstracting services provided by Preston Technical Abstracts Co., Illinois. Most of the available published data, up to January 1972, is reported here.

The appendix comprises three main sections, devoted respectively to fluorine-hydrogen, fluorine-fluorine and fluorine-"other nuclei" coupling. Each of these main sections is, for convenience, divided into a large number of subsections according to the detailed environment of each of the coupled nuclei. Full details of the classification precedes the tables, and the reader is urged to study this prior to attempting to use the appendix. Compounds containing a variety of coupling situations may appear in more than one table, and in order to facilitate searching, each entry is given its own serial number together with those of other entries in which the same compound appears.

Each table consists of (1) a literature reference number corresponding to the list at the end of the appendix, (2) the entry serial number(s), (3) a code letter to indicate the solvent in which the compound was dissolved (referring to the list immediately prior to the data tables, (4) the molecular formula of the compound, (5) the structure of the compound, (6) a listing of the relevant coupling constants classified as ^{1}J (directly bonded) ^{2}J (geminal) ^{3}J (vicinal) and ^{n}J (longer range).

Each table is arranged according to an index of molecular formulae, and the convention adopted for priority of elements is C,F,H and then the other elements in alphabetical order.

List of Tables

A. FLUORINE-HYDROGEN COUPLING

1. *Fluorine bonded to carbon in acyclic system, hydrogen bonded to carbon in either an acyclic or cyclic system.*
   a) fluorine bonded to sp^3 carbon, **hydrogen** bonded to sp^3 carbon
   b) fluorine bonded to sp^3 carbon, hydrogen bonded to sp^2 carbon other than carbonyl
   c) fluorine bonded to sp^3 carbon, hydrogen bonded to sp^2 carbon of carbonyl group
   d) fluorine bonded to sp^3 carbon, hydrogen bonded to sp carbon
   e) fluorine bonded to sp^2 carbon other than of carbonyl group, hydrogen bonded to sp^3 carbon
   f) fluorine bonded to sp^2 carbon of carbonyl group, hydrogen bonded to sp^3 carbon
   g) fluorine bonded to sp^2 carbon other than of carbonyl group, hydrogen bonded to sp^2 carbon other than of carbonyl group
   h) fluorine bonded to sp^2 carbon of carbonyl group, hydrogen bonded to sp^2 carbon other than of carbonyl group
   i) fluorine bonded to sp^2 carbon other than of carbonyl group, hydrogen bonded to sp^2 carbon of carbonyl group

j) fluorine bonded to sp carbon, hydrogen bonded to sp carbon

2. *Fluorine bonded to carbon in alicyclic non-aromatic system, hydrogen bonded to carbon in either acyclic or cyclic systems*

a) fluorine bonded to carbon in three membered ring, hydrogen bonded to carbon in the same ring
b) fluorine bonded to carbon in three membered ring, hydrogen bonded to carbon outside this ring
c) fluorine bonded to carbon in four membered ring, hydrogen bonded to carbon in the same ring
d) fluorine bonded to carbon in four membered ring, hydrogen bonded to carbon outside this ring
e) fluorine bonded to carbon in five membered ring excluding steroids, hydrogen bonded to carbon in the same ring
f) fluorine bonded to carbon in five membered ring excluding steroids, hydrogen bonded to carbon outside this ring
g) fluorine bonded to carbon in six membered ring excluding steroids, hydrogen bonded to carbon in the same ring
h) fluorine bonded to carbon in six membered ring excluding steroids, hydrogen bonded to carbon outside this ring
i) fluorine bonded to carbon in steroid nucleus, hydrogen bonded to carbon in the same system
j) fluorine bonded to carbon in seven membered ring, hydrogen bonded to carbon in the same ring
k) fluorine bonded to carbon in larger rings, hydrogen bonded to carbon in the same ring

3. *Fluorine bonded to carbon in non-aromatic heterocyclic systems, hydrogen bonded to carbon in either acyclic or cyclic systems*

a) fluorine bonded to carbon in non-aromatic nitrogen heterocycle, hydrogen bonded to carbon in the same ring
b) fluorine bonded to carbon in non-aromatic nitrogen heterocycle, hydrogen bonded to carbon outside this ring
c) fluorine bonded to carbon in non-aromatic oxygen heterocycle other than carbohydrate, hydrogen bonded to carbon in the same ring
d) fluorine bonded to carbon in non-aromatic oxygen heterocycle other than carbohydrate, hydrogen bonded to carbon outside this ring
e) fluorine bonded to carbon in carbohydrates
f) fluorine bonded to carbon in non-aromatic di-oxygen heterocycle, hydrogen bonded to carbon in the same ring
g) fluorine bonded to carbon in non-aromatic heterocyclic systems with more than one heteratom, hydrogen bonded to carbon in the same ring

4. *Fluorine bonded to carbon in alicyclic aromatic systems, hydrogen bonded to carbon in either aromatic or non-aromatic systems*

a) fluorine bonded to carbon in substituted monofluorobenzenes, hydrogen bonded to carbon in the same ring
b) fluorine bonded to carbon in substituted difluorobenzenes, hydrogen bonded to carbon in the same ring
c) fluorine bonded to carbon in substituted trifluorobenzenes, hydrogen bonded to carbon in the same ring
d) fluorine bonded to carbon in substituted tetrafluorobenzenes, hydrogen bonded to carbon in the same ring
e) fluorine bonded to carbon in pentafluorobenzene, hydrogen bonded to carbon in the same ring

f) fluorine bonded to carbon in substituted monofluorobenzenes, hydrogen bonded to carbon outside this ring
g) fluorine bonded to carbon in substituted difluorobenzenes, hydrogen bonded to carbon outside this ring
h) fluorine bonded to carbon in substituted trifluorobenzenes, hydrogen bonded to carbon outside this ring
i) fluorine bonded to carbon in substituted tetrafluorobenzenes, hydrogen bonded to carbon outside this ring
j) fluorine bonded to carbon in substituted pentafluorobenzenes, hydrogen bonded to carbon outside this ring

5. *Fluorine bonded to carbon in heterocyclic aromatic systems, hydrogen bonded to carbon in either heterocyclic aromatic or non-aromatic systems*

a) fluorine bonded to carbon in aromatic heterocycle containing nitrogen, hydrogen boned to carbon in the same ring
b) fluorine bonded to carbon in aromatic heterocycle containing sulphur, hydrogen bonded to carbon in the same ring
c) fluorine bonded to carbon in aromatic heterocycle containing nitrogen, hydrogen bonded to carbon outside this ring
d) fluorine bonded to carbon in aromatic heterocycle containing sulphur, hydrogen bonded to carbon outside this ring

6. *Fluorine bonded to element, M, other than carbon, hydrogen bonded to carbon*

a) M = arsenic (As)
b) M = boron (B)
c) M = germanium (Ge)
d) M = nitrogen (N)
e) M = phosphorus (P)
f) M = sulphur (S)
g) M = selenium (Se)
h) M = silicon (Si)
i) M = tin (Sn)
j) M = tellurium (Te)
k) M = tunsten (W)

7. *Fluorine bonded to carbon, hydrogen bonded to element, M, other than carbon*

a) M = nitrogen (N)
b) M = oxygen (O)
c) M = phosphorus (P)
d) M = sulphur (S)
e) M = silicon (Si)

8. *Fluorine bonded to element, M, other than carbon, hydrogen bonded to element other than carbon*

a) M = boron (B)
b) coupling in hydrogen fluoride
c) M = nitrogen (N)
d) M = phosphorus (P)
e) M = sulphur (S)
f) M = silicon (Si)

B. FLUORINE-FLUORINE COUPLING

1. *One fluorine bonded to carbon in acyclic system, the other fluorine bonded to carbon in either acyclic or cyclic system*
   a) both fluorines bonded to sp^3 carbon
   b) one fluorine bonded to sp^3 carbon, the other to sp^2 carbon
   c) one fluorined bonded to sp^3 carbon, the other to an aromatic ring
   d) one fluorine bonded to sp^3 carbon, the other to a heteroaromatic ring
   e) one fluorine bonded to sp^3 carbon, the other to sp carbon
   f) both fluorines bonded to sp^2 carbon (both non carbonyl)
   g) one fluorine bonded to sp^2 carbon of a carbonyl group, the other to sp^3 or sp^2 carbon

2. *Fluorine bonded to carbon in alicyclic, non-aromatic ring systems*
   a) three membered rings
   b) four membered rings
   c) five membered rings
   d) six membered rings
   e) seven membered rings

3. *Fluorine bonded to carbon in heterocyclic, non-aromatic ring systems*
   a) heterocycles containing one nitrogen atom
   b) heterocycles containing one oxygen atom (excluding carbohydrates)
   c) carbohydrates
   d) heterocycles containing one metal atom
   e) heterocycles containing two nitrogen atoms
   f) heterocycles containing two oxygen atoms
   g) heterocycles containing two sulphur atoms
   h) heterocycles containing two phosphorus atoms
   i) heterocycles containing both oxygen and nitrogen
   j) heterocycles containing both oxygen and sulphur

4. *Fluorine bonded to carbon in alicyclic aromatic systems*
   a) substitued difluorobenzenes
   b) substituted trifluorobenzenes
   c) substituted tetrafluorobenzenes
   d) substituted pentafluorobenzenes
   e) condensed-ring systems

5. *Fluorine bonded to carbon in heterocyclic aromatic systems*
   a) heterocycles containing nitrogen
   b) heterocycles containing sulphur

6. *Fluorine bonded to elements other than carbon*
   a) one fluorine bonded to carbon, the other bonded to nitrogen
   b) one fluorine bonded to carbon, the other bonded to oxygen
   c) one fluorine bonded to carbon, the other bonded to phosphorus
   d) one fluorine bonded to carbon, the other bonded to sulphur
   e) one fluorine bonded to carbon, the other bonded to silicon

f) both fluorines bonded to the same element, M (other than carbon)

i) M = arsenic (As)
ii) M = boron (B)
iii) M = chlorine (Cl)
iv) M = germanium (Ge)
v) M = iodine (I)
vi) M = nitrogen (N)
vii) M = phosphorus (P)
viii) M = rhenium (Re)
ix) M = sulphur (S)
x) M = antimony (Sb)
xi) M = silicon (S)
xii) M = tin (Sn)
xiii) M = tantalum (Ta)
xiv) M = tellurium (Ta)
xv) M = titanium (Ti)
xvi) M = tungsten (W)

f) each fluorine bonded to an element (other than carbon)

C. FLUORINE COUPLING TO AN ELEMENT, M, OTHER THAN HYDROGEN OR FLUORINE

(In alphabetical order)

1. M = silver (Ag)
2. M = arsenic (As)
3. M = boron (B)
4. M = beryllium (Be)
5. M = bismuth (Bi)
6. M = carbon (C)
7. M = deuterium (D)
8. M = germanium (Ge)
9. M = mercury (Hg)
10. M = nitrogen (N)
11. M = biobium (Nb)
12. M = phosphorus (P)
13. M = platinum (Pt)
14. M = rhodium (Rh)
15. M = antimony (Sb)
16. M = selenium (Se)
17. M = silicon (Si)
18. M = tin (Sn)
19. M = tellurium (Te)
20. M = titanium (Ti)
21. M = vanadium (V)
22. M = tungsten (W)
23. m = xenon (Xe)

Solvent abbreviations used in the tables

A	Chloroform (deuterochloroform)
B	Neat
C	The nematic phase of a liquid crystal
D	Cyclohexane
E	Acetone
F	Dimethyl sulphoxide
G	Carbon tetrachloride
H	Benzene
I	Anisole
J	Dichloromethane
K	Nitrobenzene
L	Dimethylformamide
M	Acetonitrile
N	Nitromethane
O	Hydrogen fluoride-antimony pentafluoride (low temperature)
P	Trichlorofluoromethane
Q	Carbon disulphide
R	Diethyl ether
S	Sulphuric acid - water
T	n-Hexane
U	1,2-Dichloroethane
V	Ethylemthylketone
W	n-Pentane
X	1,1,2-Trichloroethylene
Y	Diisopropyl ether
Z	1,1-Dichloroethane
A^2	Water (deuterium oxide)
B^2	Sulphur dioxide
C^2	Antimony pentafluoride-sulphur dioxide
D^2	Dioxane
E^2	Methanol (deuteromethanol)
F^2	Fluorosulphonic acid-antimony pentafluoride-sulphur dioxide
G^2	1,1,2,2-Tetrachloroethane
H^2	Pyridine
I^2	Tetrachloroethylene
J^2	Ethanol
K^2	Trifluoroacetic acid
L^2	Propionic acid
M^2	Diethylamine
N^2	Cyclopentanone
O^2	2-Nitropropane
P^2	Propene carbonate
Q^2	Xylene
R^2	Diethylene glycol diethyl ether
S^2	Tetramethyl silane
T^2	Toluene

U^2 Tetrahydrofuran
V^2 Dimethylacetamide
W^2 Freon 112
X^2 Decalin
Y^2 Dichlorofluoromethane
Z^2 Fluorosulphonic acid-sulphur dioxide
A^3 Hexafluorobenzene
B^3 Methylcyclohexane
C^3 Chlorocyanomethane
D^3 Liquid hydrogen fluoride
E^3 Thiophene
F^3 Formamide
G^3 Tetramethyltin
H^3 Tetraethoxysilane
I^3 Chlorobenzene
J^3 Tetrafluorosilane
K^3 Hexafluorodisiloxane ($F_3Si.O.SiF_3$)
L^3 Cyanotrifluoromethane
M^3 Chlorotrifluoromethane
N^3 Trifluorosilylmethane (CH_3SiF_3)
O^3 Bromotrifluorosilane
P^3 Ethyltrifluorosilane
Q^3 Trifluorosilylethylene ($CH_2=CHSiF_3$)
R^3 Difluorodimethylsilane $(CH_3)_2SiF_2$)
S^3 Fluorotrimethylsilane ($(CH_3)_3SiF$)
T^3 Dichlorodifluoromethane
U^3 Dibromodifluorosilane
V^3 Tetramethylsilane
W^3 Tribromofluorosilane
X^3 Tribromoborane
Y^3 Tetrabromosilane
Z^3 Acetic acid
A^4 Acetic anhydride
B^4 n-Butane
C^4 Chloroethane
D^4 cis-But-2-ene
E^4 1,1,2-Trichloro-1,2,2-trifluoroethane
F^4 Acetaldehyde
G^4 Dimethyl ether
H^4 25% Aqueous ortho phosphoric acid
I^4 Propan-1-ol
J^4 Formic acid
K^4 Ethane-thiolic acid
L^4 Dithioacetic acid
M^4 Mesitylene
N^4 1,4-Bis(trifluoromethyl)benzene
O^4 40% Trichlorofluoromethane, 25% 1,2-dichlorodifluoroethylene, 10% Hexafluorobenzene, 25% compound
P^4 Bromoethane

Q^4 2-Methylbutan-2-ol

R^4 Fluorosulphuryl chloride

S^4 Chlorocyanomethane

T^4 Sulphuryl fluoride

U^4 Butan-1-ol

V^4 1,2-Dibromotetrafluoroethane

W^4 Thioacetone

X^4 Thionyl chloride

Y^4 3-Chloroprop-1-ene

Z^4 Propylene

A. Fluorine-hydrogen coupling. 1. Fluorine bonded to carbon in acyclic system, hydrogen bonded to carbon in either an acyclic or cyclic system. Table A.1.a. Fluorine bonded to sp^3 carbon, hydrogen bonded to sp^3 carbon.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1	1	A	$CFHCl_2$	$CFHCl_2$	53.5		
2	2		$CFHCl_2$	$CFHCl_2$	53.6		
3	3	B	$CFHCl_2$	$CFHCl_2$	54		
4	4	B	$CFHCl_2$	$CFHCl_2$	53.6		
5	5	C*	CFH_3	CFH_3	+46.3		
	(5386)						
6	6		CFH_3	CFH_3	46.4		
	(5385)						
7	7	C*	CFH_3	CFH_3	+45		
182	8	F	CFH_3	CFH_3	45		
1	9	A	CF_2HCl	CF_2HCl_2	63		
4	10	C*	CF_2H_2	CF_2H_2	50.4		
6	11		CF_2H_2	CF_2H_2	50.2		
	(5392)						
8	12	D	CF_2H_2	CF_2H_2	50.1		
	(5395)	E			50.3		
		F			50.2		
1	13	A	CF_3H	CF_3H	79		
6	14	D	CF_3H	CF_3H	79.7		
	(5399)						
9	15	A	CF_3H	CF_3H	79.25		
		D			79.31		
		G			79.23		
		H			79.27		
		I			79.26		
		J			79.35		
		E			79.40		
		K			79.32		
		L			79.37		
		M			79.38		
		N			79.38		
8	16	E	CF_3H	CF_3H	79.25		
	(5401)	F			79.30		
		G			79.25		
10	17	A	CF_3H_2N	FCH_2NF_2	48		
11	(2205)						
12	18		CF_6H_2S	FCH_2SF_5	45.9		
	(4801, 5041a)						
13	20	O	CF_7H_4OSb	$FCH_2OH_2^+SbF_6^-$	47.9		

Table A.1.a. (contd.)

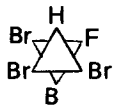
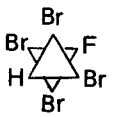
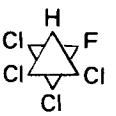
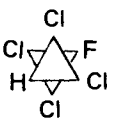
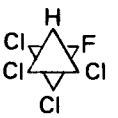
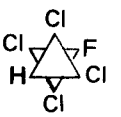
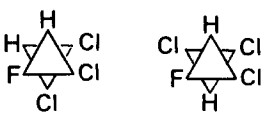
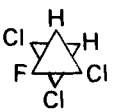
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
15-17	21	P	C_2FHBr_4			1.15	
		Q				1.5	
		R				1.7	
		E		**178**		1.8	
		P				22.2	
		Q				23.6	
		R				24.0	
		E		**178**		24.5	
		P		$CFBr_2CHBr_2$ (278^oK)		6.85	
18	22	B	C_2FHCl_4			1.00	
						18.2	
19	23	Q	C_2FHCl_4			<2	
						17.9	
20	24	B	$C_2FH_2Cl_3$	$FCHClCHCl_2$	49.0	9.4	
18	25	B	$C_2FH_2Cl_3$		±49.1	±13.2 ∓ 2.8	
					±49.1	±37.3	
2	26		$C_2FH_2NaO_2$	FCH_2CO_2Na	48		
21	27		$C_2FH_3N_2O_5$	$FC(NO_2)_2CH_2OH$		15.0	
22	28	G	C_2FH_4Br	$FCHBrCH_3$	50.5	21	
23	29	G	C_2FH_4Br	FCH_2CH_2Br	46	18.5	
23	30	G	C_2FH_4Cl	FCH_2CH_2Cl	46	23	
14	31	B	$C_2FH_4Cl_3Si$	$FCH_2CH_2SiCl_3$	48	20.5	
14	32	B	$C_2FH_4Cl_3Si$	$CH_3CFHSiCl_3$	46	26.4	
21	33		$C_2FH_4NO_2$	$FCH(NO_2)CH_3$	51	21	

Table A.1.a. (contd.)

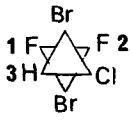
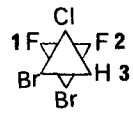
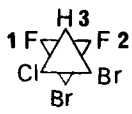
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
23	34	G	C_2FH_4I	FCH_2CH_2I	47		19	
24	35		C_2FH_5	FCH_2CH_3			25.2	
25	36		C_2FH_5	FCH_2CH_3	47.5		25.7	
26	37	B	C_2FH_5	FCH_2CH_3	46.7		25.2	
27	38	B	C_2FH_5	FCH_2CH_3	47.3		25.8	
28	39		C_2FH_5O	FCH_2CH_2OH			29.3	
29	40	S	$C_2FH_6N_3O_8S$	$FC(NO_2)_2CH_2^+NH_3HSO_4^-$			11.0	
30	41		$C_2F_2HBr_2Cl$	$CF_2BrCHClBr$			7	
	(2586)							
183	42		$C_2F_2HBr_2Cl$			1,3	<2	
						2,3	18.9	
						1,3	18.5	
						2,3	<2	
				 -150		1,3	1.8	
						2,3	3.4	
31	43		$C_2F_2HCl_3$	$FCHClCFCl_2$			3.5	
	(2588)							
14	44	B	$C_2F_2HCl_5Si$	$CHCl_2CF_2SiCl_3$			10.1	
184	45	B	$C_2F_2H_2BrCl$	CF_2BrCH_2Cl			12.0	
20	46	B	$C_2F_2H_2Br_2$	FCHBrCFHBr (dl)	49.2		6.5	
	(2859)							
20	47	B	$C_2F_2H_2Br_2$	FCHBrCFHBr (meso)	48.4		11.8	
	(2859)							
32	48		$C_2F_2H_2Br_2$	CF_2BrCH_2Br			22	
							4	
33	49		$C_2F_2H_2BrCl$	CF_2BrCH_2Cl			21	
							3	
34	50		$C_2F_2H_2Cl_2$	FCH_2CFCl_2	46.5		13.6	
	(2591)							
34	51		$C_2F_2H_2Cl_2$	FCHClCFHCl (dl)	48.8		7.0	
	(2592)							
34	52		$C_2F_2H_2Cl_2$	FCHClCFHCl (meso)	49.1		7.2	
	(2592)							
2	53		$C_2F_2H_2Cl_2$	CF_2HCHCl_2	55		8	
32	54		$C_2F_2H_2Cl_2$	CF_2ClCH_2Cl			16	
	(2590)						6	
14	55		$C_2F_2H_2Cl_4Si$	$CH_2ClCF_2SiCl_3$			14.3	

Table A.1.a. (contd.)

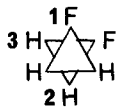
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
34	56		$C_2F_2H_3Br$	FCH_2CHFBr	1,3	46.5	1,4	11.9	
	(2593)			(1)(3)(4)(2)	2,4	51.6	2,3	20.4	
							2,3	22.5	
25	57		$C_2F_2H_3Br$	CF_2BrCH_3				15.9	
25	58		$C_2F_2H_3Cl$	CF_2ClCH_3				15.0	
35	59		$C_2F_2H_3Cl$	CF_2ClCH_3				14.8	
36	60		$C_2F_2H_3Cl_2P$	$CF_2HCH_2PCl_2$		56.0		16.8	
	(5823)								
14	61		$C_2F_2H_3Cl_3Si$	$CF_2HCH_2SiCl_3$		57			
14	62		$C_2F_2H_3Cl_3Si$	$CH_3CF_2SiCl_3$				22.7	
37	63		$C_2F_2H_3I$	CF_2HCH_2I		57.0		15.5	
38	64	A*	$C_2F_2H_4$	FCH_2CFH_2		48.00		29.69	
	(2594)	B*				48.00		30.27	
		D*				47.52		28.57	
		E*				47.94		30.58	
		G*				48.60		29.10	
		J*				47.79		30.17	
		M*	(10% v/v)			47.96		30.82	
		R*				48.02		29.62	
		T*				47.71		28.69	
		W*				47.73		28.63	
		X*				47.86		29.57	
		Y*				48.13		29.28	
		Z*				47.82		30.16	
				 				30.6	
								0	
							1,2	45	
							1,3	15	
25	65		$C_2F_2H_4$	CF_2HCH_3		57.2		20.8	
39	66		$C_2F_2H_4$	CF_2HCH_3				20.9	
40	67	P	$C_2F_2H_4O$	CF_2HOCH_3		74.4			
41	68		$C_2F_2H_4O_3S$	CH_3CHFSO_3F		56.5		22	
36	69	B	$C_2F_2H_5P$	$CF_2HCH_2PH_2$		57.6		17.5	

Table A.1.a (contd)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
33	70		C_2F_3HBrCl	$FCHBrCF_2Cl$		48		3.9	
847	(2614)							7.1	
32	71		C_2F_3HBrCl	$FCHClCF_2Br$		48		3.5	
42	(2613)							6.3	
845									
846									
33	72		$C_2F_3HBr_2$	$FCHBrCF_2Br$		48		3.2	
847	(2615)							9.1	
185	73		$C_2F_3HCl_2$	$FCHClCF_2Cl$		48.1		3.7	
	(2617)							5.0	
20	74	B	$C_2F_3HCl_2$	$FCHClCF_2Cl$		48.1		3.6	
	(2616)							5.2	
44	75		$C_2F_3HCl_4Si$	$FCHClCF_2SiCl_3$		48.1		6.6	
	(2619)							10.1	
185	76		$C_2F_3HCl_4Si$	$FCHClCF_2SiCl_3$		46.6		5.0	
	(2618)							11.3	
14	77	B	$C_2F_3HCl_4Si$	$CF_2HCFClSiCl_3$		54		5.1	
	(2620)					55			
20	78	B	$C_2F_3H_2Br$	FCH_2CF_2Br		46.0			
	(2621)								
25	79		$C_2F_3H_2Br$	CF_3CH_2Br				8.9	
35	80		$C_2F_3H_2Br$	CF_3CH_2Br				9.0	
20	81	B	$C_2F_3H_2Cl$	FCH_2CF_2Cl		46.5			
	(2622)								
25	82		$C_2F_3H_2Cl$	CF_3CH_2Cl				8.4	
35	83		$C_2F_3H_2Cl$	CF_3CH_2Cl				8.5	
43	84	G	$C_2F_3H_2ClO_2S$	$CF_3CH_2SO_2Cl$				8.3	
36	85	B	$C_2F_3H_2Cl_2P$	$FCH_2CF_2PCl_2$		49.1		13.1	
	(2623, 5849)								
36	86		$C_2F_3H_2Cl_2P$	$CHF_2CHFPCl_2$	1,4	46.7	2,4	12.0	
	(2624, 5850)			(5)(2,3)(4)(1)	2,5	53.3	3,4	7.5	
					3,5	52.9	1,5	8.1	
14	87	B	$C_2F_3H_2Cl_3Si$	$FCH_2CF_2SiCl_3$		46			
	(2626)								
14	88	B	$C_2F_3H_2Cl_3Si$	$CF_2HCFHSiCl_3$	1,4	46	2,4	12.0	
	(2625)			(2,3)(5)(1)(4)	2,5	54	3,4	16.4	
					3,5	56	1,5	8.2	
20	89	B	$C_2F_3H_2I$	FCH_2CF_2I		46.4			
	(2627)								
20	90	B	$C_2F_3H_3$	FCH_2CF_2H	1,2	46.0			
	(2629)			(1)(2)					

Table A.1.a (contd.)

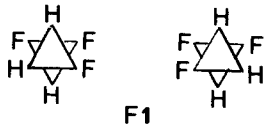
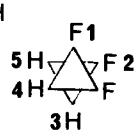
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ	
					$J_{(CHF_2)}$	$J_{(CH_2F)}$	$J_{(CH_2CF_2)}$	$J_{(CHCF)}$	
38	91		$C_2F_3H_3$	FCH_2CF_2H					
	(2628)	A*			54.44	46.10	13.27	6.86	
		B*			54.22	45.91	13.48	7.23	
		E*			54.11	46.09	14.09	8.39	
		F*			53.65	45.89	15.10	10.54	
		G*			54.61	46.20	12.84	5.88	
		J*			54.32	46.07	13.39	7.14	
		M*	(10% v/v)		53.80	45.99	14.38	9.20	
		Q*			54.62	46.22	12.97	6.16	
		R*			54.39	46.12	13.18	6.65	
		T*			54.72	46.19	12.68	5.57	
		W*			54.67	46.26	12.75	5.67	
		X*			54.44	46.17	13.25	6.55	
		Y*			54.33	46.14	13.22	6.52	
		Z*			54.37	46.01	13.48	7.48	
							15.5	12.7	
							12.4	4.8	
					1,3	(20)	^3J 2,4 12.7	1,5	(10)
							4.8		
25	92		$C_2F_3H_3$	CF_3CH_3			12.8		
35	93		$C_2F_3H_3$	CF_3CH_3			12.8		
185	94		$C_2F_3H_3ClP$	$FCHClCF_2PH_2$		49.0	7.1		
	(2630)						5.6		
45	95	A	$C_2F_3H_3O$	CF_3CH_2OH			8		
35	96		$C_2F_3H_3O$	CF_3CH_2OH			8.9		
46	97		$C_2F_3H_3O_2S$	$CF_3S(O)OCH_3$					1.2
41	98		$C_2F_3H_3O_3S$	$CH_3CF_2SO_3F$			15		
	(4806)								
11	99	A	$C_2F_3H_4N$	$FCH_2CH_2NF_2$ (1)(2)(3)	1,2	48	1,3 23		

Table A.1.a. (contd.)

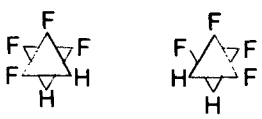
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
36	100 (5851)	B	$C_2F_3H_4P$	$FCH_2CF_2PH_2$		54.6		3.5	
20	101	B	$C_2F_4HBrO_2S$	$CF_2BrCHFSO_2F$	1,4	43.0	2,4	3.6	
186	[2426 2635 4810]			(2,3)(4)(1)			3,4	11.7	
36	102 [2636 5857]	B	$C_2F_4HCl_2P$	$CF_2HCF_2PCl_2$		53.3		5.0	
14	103 (2637)	B	$C_2F_4HCl_3Si$	$CF_2HCF_2SiCl_3$		54		5.0	
25	104		$C_2F_4H_2$	CF_2HCF_2H		52.1		4.8	
47	105		$C_2F_4H_2$	CF_2HCF_2H					
38	(2640)	A*				53.378		2.990	
		B*				53.420		3.269	
		D*				53.658		2.581	
		E*				52.789		4.566	
		G*	(10% v/v)			53.520		2.610	
		H*				53.260		3.353	
		L*				52.264		5.138	
		Q*				53.516		2.762	
		T*				53.701		2.495	
		U*				53.125		3.557	
		V*				52.811		4.445	
									5.1
									1.8
							1,2	(8.4)	
25	106		$C_2F_4H_2$	CF_3CH_2F		45.5		8.0	
38	107 (2638)	A*	$C_2F_4H_2$	CF_3CH_2F		45.66		8.03	

Table A.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
		B*				45.68		8.04		
		D*				45.93		7.94		
		E*				45.31		8.34		
		G*				45.87		8.02		
		M*	(10% v/v)			45.30		8.34		
		Q*				45.61		8.00		
		R*				45.52		8.17		
		W*				46.00		7.92		
		X*				45.88		8.01		
		Y*				45.54		8.11		
		Z*				45.64		8.07		
540	108	A	$C_2F_4H_2N_2O_3S$	$CF_3CH_2N_2^+SO_3F^-$				6.1		
540	109	A	$C_2F_4H_2O_3S$	$CF_3CH_2OSO_2F$				7.5		
	(4811)									
49	110		$C_2F_4H_3NO_4S_2$	$CF_3SO_2N(CH_3)SO_2F$					1,2	0.7
	(4812)			(1) (2)						
36	111	B	$C_2F_4H_3P$	$CF_2HCH_2PF_2$		55.6		18.6†		
50	112		$C_2F_4H_4Si$	$CF_2HCF_2SiH_3$	1,3	55.8	2,3	4.9		
	[2515 2642]			(1) (3)(2)						
51	113	A^2	$C_2F_4H_{15}N_4O_5SRh$	$[Rh(CF_2HCF_2)(NH_3)_4(H_2O)]^{2+}$ SO_4^{2-}		55		4		
	[2643 6632]									
51	114	A^2	$C_2F_4H_{16}N_5O_4SRh$	$[Rh(CF_2HCF_2)(NH_3)_5]^{2+}SO_4^{2-}$		56		4.9		
	[2644 6653]									
25	115		C_2F_5H	CF_3CF_2H		52.6		2.6		
	(2649)									
52	116		C_2F_5HO	CF_2HCF_2OF		56				
20	117	B	$C_2F_5HO_2S$	CF_3CFHSO_2F		44.2		5.2		
186	[2650 4813 2427]									
40	118	P	$C_2F_5HO_3S$	$CF_3SO_3CF_2H$		68.5				
	(2651)									
53	119		$C_2F_6H_2Br_2OS$	$FCHBrCHBrOSF_5$	I	49.9		10.5		
	(5052)				II	49.9		~ 4.2		
53	120		$C_2F_6H_2Cl_2OS$	$FCCl_2CH_2OSF_5$				12.6		
	(5054)									
53	121		$C_2F_6H_2Cl_2OS$	$FCHClCHClOSF_5$	I	49.6		5.0		
	(5053)				II	49.6		6.5		

Table A.1.a. (contd.)

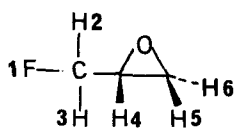
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
14	122 [2460 4853 2669]	B	$C_2F_6H_2Si$	$FCH_2CF_2SiF_3$	46	15.2†	
14	122a [2461 4854 6696 2672]	B	C_2F_7HSi	$CF_2HCF_2SiF_3$	54	5.0	
54	123 [2678 4825 5064]	B	C_2F_8HBrS	$CF_2BrCHFSF_5$	43.0	1.8 12.6	
187	124 [2679 4826 5065]		C_2F_8HClOS	$CF_2ClCFHOSF_5$	54.0	3.0	
54	125 [2681 4828 5067]	B	C_2F_8HClS	$FCHClCF_2SF_5$	46.8	1.2 13.0	
54	126 [2680 4827 5066]	B	C_2F_8HClS	$CF_2ClCHFSF_5$	43.0	3.4 10.1	
55	127	B	$C_3FH_3Cl_2O$	$FCH_2COCHCl_2$	46.7		1.8
55	128	B	C_3FH_4ClO	$FCHClCOCH_3$	51		3.5
55	129	B	C_3FH_4ClO	FCH_2COCH_2Cl	47		2.5
11	130	A	C_3FH_4N	FCH_2CH_2CN	45	22	
56	131	B^2	C_3FH_5	$FCH_2CH{=}CH_2$	47.5		
57	132 (775)	*	C_3FH_5	$FCH_2CH{=}CH_2$	46.75		
21	133		$C_3FH_5N_2O_4$	$FC(NO_2)_2CH_2CH_3$		19.7	
58	134	A	$C_3FH_5N_2O_5$	$CF(NO_2)_2CHOHCH_3$ (1 2 3)		1,2 17	1,3 1.2
59	135		C_3FH_5O				
		A*			1,2	47.17 1,3	12.25 1,5 3.67
		B*				47.35	12.00 3.87
		G*				47.18	11.74 3.60
		M*				47.15	11.85 3.96
		A*			1,3	47.61	1,6 -1.22
		B*				47.77	-1.57

Table A.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
		G*				47.84			-1.32
		M*				47.99			-1.63
55	136		C_3FH_5O	FCH_2COCH_3		47			4
60	137	B	C_3FH_2O	$FCH_2CO_2CH_3$		46.83			
		F				46.48			
		G				47.45			
		J				47.01			
		M				46.83			
61	138	C[2]	$C_3FH_6^+$	$(CH_3)_2{}^+CF$				25.4	
23	139	G	C_3FH_6Br	CH_3CHFCH_2Br	1,2	47	1,3	1.7	
				(4)(2)(1)(3)			1,4	23	
23	140	G	C_3FH_6I	CH_3CHFCH_2I	1,2	48	1,3	8	
				(4)(2)(1)(3)			1,4	22.5	
21	141		$C_3FH_6NO_2$	$FCH(NO_2)CH_2CH_3$		54		23	
29	142	G	$C_3FH_6N_3O_4$	$FC(NO_2)_2CH_2NHCH_3$				18.7	
62	143		C_3FH_7	$FCH_2CH_2CH_3$		47.35		23.55	
28	144		C_3FH_7O	CH_3CHFCH_2OH			1,2	23.6	
				(2) (1)(3)			1,3	23.6	
63	145		$C_3F_2HCl_5$	$CHCl_2CF_2CCl_3$				9.23	
63	146		$C_3F_2H_2Cl_4$	$CHCl_2CF_2CHCl_2$				8.74	
63	147		$C_3F_2H_2Cl_4$	$CH_2ClCF_2CCl_3$				14.20	
64	148		$C_3F_2H_2N_2$	$CH_2FC(=N)F$		46			
	(2213)								
	(4700)								
64	149		$C_3F_2H_2N_2$	$CH_2FC(=N)F$		46			
	(2214, 4701)								
63	150		$C_3F_2H_3Cl_3$	$CH_3CF_2CCl_3$				17.42	
57	151	*	$C_3F_2H_4$	$CF_2HCH=CH_2$		55.90			
	(776)								
63	152		$C_3F_2H_4Cl_2$	$CH_3CF_2CHCl_2$			1,2	5.85	
				(3)(1)(2)			1,3	17.84	
60	153	B	$C_3F_2H_4O$	CF_2HCOCH_3		53.85			1.56
		G				54.30			1.39
		M				53.60			1.61
60	154	B	$C_3F_2H_4O_2$	$CF_2HCO_2CH_3$		53.21			0.47
		F				52.57			0.49
		G				53.22			0.43
		J				53.41			0.45
		M				52.96			0.47
63	155		$C_3F_2H_5Cl$	$CH_3CF_2CH_2Cl$			1,2	11.41	
				(3) (1)(2)			1,3	17.92	
63	156		$C_3F_2H_6$	$CH_3CF_2CH_3$				17.76	
41	157		$C_3F_2H_6$	$CH_3CF_2CH_3$				19	
61	158		$C_3F_2H_6$	$CH_3CF_2CH_3$				17.6	

Table A.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
20	159	B	$C_3F_3HBr_2O$	$CF_2BrCHBrC(O)F$			4.8		
	[983 2685 3645]						13.6		
65	160		$C_3F_3HCl_6Si$	$CF_3CHClCCl_2SiCl_3$			5.3		
66	161		$C_3F_3HCl_6Si$	$CF_3CHClCCl_2SiCl_3$			5.4		
65	162		$C_3F_3H_2Cl_5Ge$	$CF_3CH_2CCl_2GeCl_3$			8.8		
65	163		$C_3F_3H_2Cl_5Si$	$CF_3CHClCHClSiCl_3$			5.9		
							5.5		
66	164		$C_3F_3H_2Cl_5Si$	$CF_3CH_2CCl_2SiCl_3$			8.8		
43	165	G	$C_3F_3H_2NS$	CF_3CH_2SCN			9.7		
65	166		$C_3F_3H_3Cl_4Ge$	$CF_3CH_2CHClGeCl_3$			8.8		
66	167		$C_3F_3H_3Cl_4Si$	$CF_3CHClCH_2SiCl_3$			6.1		
66	168		$C_3F_3H_3Cl_4Si$	$CF_3CH_2CHClSiCl_3$			9.3		
65	169		$C_3F_3H_3Cl_4Si$	$CF_3CH_2CHClSiCl_3$			9.6		
67	170		$C_3F_3H_3N_2O_4$	$CF_3C(NO_2)_2CH_3$					1.2
60	171	A	$C_3F_3H_3O$	CF_3COCH_3					0.99
		B							0.97
		F							1.00
		G							0.96
		M							0.99
68	172		$C_3F_3H_3O$	CF_3COCH_3					1.1
69	173		$C_3F_3H_4Br$	$CF_3CH_2CH_2Br$			10.06		
70	174	Q	$C_3F_3H_4Br$	$CF_3CH_2CH_2Br$			+9.8		−0.2
69	175		$C_3F_3H_4Cl$	$CF_3CH_2CH_2Cl$			10.1		
70	176	Q	$C_3F_3H_4Cl$	$CF_3CH_2CH_2Cl$			+9.95		−0.15
185	177		$C_3F_3H_4ClO$	$FCHClCF_2OCH_3$		48.8	3.3		
	(2686)						4.6		
185	178		$C_3F_3H_4ClS$	$FCHClCF_2SCH_3$		49.0	6.6		
	(2687)						5.1		
65	179		$C_3F_3H_4Cl_3Ge$	$CF_3CH_2CH_2GeCl_3$			8.3		
65	180		$C_3F_3H_4Cl_3Si$	$CF_3CH_2CH_2SiCl_3$			9.8		
71	181	H	$C_3F_3H_4Cl_3Sn$	$CF_3CH_2CH_2SnCl_3$			9.7		
	(6781)								
69	182		$C_3F_3H_4I$	$CF_3CH_2CH_2I$			10.1		
70	183	Q	$C_3F_3H_4I$	$CF_3CH_2CH_2I$			+9.85		−0.3
72	184	D[2]	$C_3F_3H_4NO$	$CF_3CONHCH_3$				1,2	
	(2493)			(1) (2)					
67	185		$C_3F_3H_4NO_2$	$CF_3CH(NO_2)CH_3$			6.2		0.6
68	186		$C_3F_3H_4O^+$	$CF_3{}^+C(OH)CH_3$				1,2	1.3
				(1) (2)					
188	187		$C_3F_3H_5$	$CF_2HCH_2CFH_2$	1,3	56.5	1,5 16.0		
	(2688)			(1)(3)(5)(2)(4)	2,4	48.7	2,5 25.4		
73	188		$C_3F_3H_5$	$CF_3CH_2CH_3$			10.6		0.4

Table A.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
20	189 (2689)	B	$C_3F_3H_5O$	$FCH_2CF_2OCH_3$		46.3			
68	190		$C_3F_3H_5O$	$CF_3CHOHCH_3$				7.5	
43	191	B	$C_3F_3H_5O_3S$	$CF_3CH_2OSO_2CH_3$				8.0	
20	192 (2690)	B	$C_3F_3H_5S$	$FCH_2CF_2SCH_3$		46.2			
11	193 (2221)	A	$C_3F_3H_6N$	$FCH_2CH_2CH_2NF_2$ (1)(2)(3)	1,2	48	1,3	25	
46	194		$C_3F_3H_6NOS$	$CF_3S(O)N(CH_3)_2$					1.4
68	195		$C_3F_3H_6O^+$	$CF_3CH(O^+H_2)CH_3$				5.7	
189	196 (5925)	B	$C_3F_3H_6PS_2$	$CF_3P(SCH_3)_2$					0.74
74	197 (2692)	B	C_3F_4HClO	CF_2HCOCF_2Cl		51			
68	198		$C_3F_4H_2O$	$CF_2HC(O)CF_2H$		54.5			5
188	200 (2694)		$C_3F_4H_4$	$FCH_2CH_2CF_3$ (1)(3)(4)(2)	1,3	47.7	1,4 2,4	22.8 10.7	
188	201		$C_3F_4H_4$	FCH_2CFHCF_2H (1)(4)(2)(5)(3)(6)	1,4 2,5 3,6	47.7 47.1 55.0			
64	202 (2223, 4704)		$C_3F_4H_4N_2$	$FCH_2C(=N-F)CH_2NF_2$		47			2.4
64	203 (2222, 4703)		$C_3F_4H_4N_2$	$FCH_2C(=N-F)CH_2NF_2$		46			2.8
20	204	B	$C_3F_4H_4O_3S$	$CF_2(OCH_3)CHFSO_2F$ (2,3) (4)(1)	1,4	44.4	2,4 3,4	3.6 5.9	
186	[2695, 4833, 2431]								
75	205		$C_3F_4H_6NP$	$CF_3PFN(CH_3)_2$					0.7
76	206 (4770)	P	$C_3F_4H_6NPS$	$CF_3PF(S)N(CH_3)_2$					0.8
77	207 (2699)		$C_3F_5HBr_2$	$CF_3CHBrCF_2Br$ (1) (3) (2)			1,3 2,3	6.0 8.7	
184	208 (2700)	B	C_3F_5HClI	$CF_3CHClCF_2I$ (1) (3)(2)			1,3 2,3	11.3 8.2	
184	209 (2703)	B	$C_3F_5HCl_2$	$CF_3CF_2CHCl_2$				8.8	0.4
40	210	P	$C_3F_5HO_2$	$CF_3CO_2CF_2H$		68.8			
73	211 (2707)		$C_3F_5H_2Br$	$FCHBrCF_2CF_2H$ (1)(4)(3)(2)(5)	1,4 2,5	48.7 52.9	3,4 3,5	7.4 4.6	

Table A.1.a. (contd.)

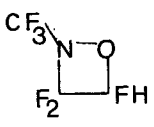
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
73	212		$C_3F_5H_2Br$	$FCH_2CF_2CF_2Br$	1,4	46.0	2,4	11.7	3,4	0.9
	(2706)			(1)(4)(2)(3)						
77	213		$C_3F_5H_2Br$	$CF_3CHBrCF_2H$		55.0				
77	214		$C_3F_5H_2Br$	$CF_2BrCH_2CF_3$			1,3	13.0		
				(1) (3)(2)			2,3	8.6		
73	215		$C_3F_5H_2Cl$	$FCHClCF_2CF_2H$	1,4	47.5	3,4	7.2		
				(1)(4)(3)(2)(5)	2,5	52.3	3,5	4.6		
73	216		$C_3F_5H_2Cl$	$FCH_2CF_2CF_2Cl$	1,4	45.9	2,4	11.8	3,4	1.0
	(2708)			(1)(4)(2)(3)						
73	217		$C_3F_5H_3$	$FCH_2CF_2CF_2H$	1,4	45.9	3,4	12.0	1,5	1.5
	(2710)			(1)(4)(3)(2)(5)	2,5	52.6	3,5	4.2	2,4	1.4
188	218		$C_3F_5H_3$	$CF_2HCFHCF_2H$	1,3	54.7	2,3	8.0		
	(2711)			(1)(3)(2)(4)	2,4	46.2				
188	219		$C_3F_5H_3$	$CF_2HCH_2CF_3$	1,3	54.4	1,4	13.4		
	(2712)			(1)(3)(4)(2)			2,4	10.0		
78	220		$C_3F_5H_3O$	$CF_2HCFHOCF_2H$	1,4	54	1,5	4.5		
	(2713)			(1)(4)(2)(5)(3)(6)	2,5	57	2,4	3.0		
					3,6	72				
40	221		$C_3F_5H_3O$	$CF_2HOCH_2CF_3$	1,3	72	2,4	8.0		
	(2714)			(1)(3)(4)(2)						
45	222	G	$C_3F_5H_3S$	$CF_3CF_2CH_2SH$				15		
190	223		$C_3F_5H_3Se$	$CF_3CF_2SeCH_3$					1,2	1.0
560	(2715)			(1) (2)						
79	224		$C_3F_5H_4OP$	$CF_2HP(OCH_3)CF_3$		50.4				
80										
81	225	J	C_3F_6HAg	$(CF_3)_2CHAg$				13.5		
	(5289)									
73	226		C_3F_6HCl	$CF_3CHClCF_3$				5.9		
20	227	B	C_3F_6HI	$FCHICF_2CF_3$	1,5	47.9	2,5	1.2	4,5	∿1.0
	(2730)			(1)(5)(2,3)(4)			3,5	19.2		
20	228	B	C_3F_6HI	$CF_2ICFHCF_3$	1,5	43.4	2,5	4.7	4,5	5.5
	(2729)			(2,3)(1)(5)(4)			3,5	13.3		
988	229		C F HNO							
	[2732 1780 4096]									
				(-79°) Isomer I						<1
				Isomer II						<1
73	230		$C_3F_6H_2$	$FCH_2CF_2CF_3$		46.0		11.7		
	(2733)									
188	231		C_3F_6H	$CF_2HCFHCF_3$	1,4	53.9	1,5	7.2		
	(2734)			(1)(4)(2)(5)(3)	2,5	45.1	2,4	6.8		

Table A.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
							3,5	5.9	
73	232		$C_3F_6H_2$	$CF_2HCF_2CF_2H$		52.7		8.5	
82	233		$C_3F_6H_2$	$CF_2HCF_2CF_2H$		53			
73	234		C_3F_6H	$CF_3CH_2CF_3$				9.2	
74	235	B	$C_3F_6H_2O$	$CF_3CHOHCF_3$				6.0	
45	236	A	$C_3F_6H_2O$	$CF_3CHOHCF_3$				6	
68	237		$C_3F_6H_2O$	$CF_3CHOHCF_3$				6	
78	238		$C_3F_6H_2S$	$CF_2HCFHSCF_3$	1,3	54	1,4	12	
	(2735)			(1)(3)(2)(4)	2,4	49			
83	239		$C_3F_6H_2S$	$CF_3CHSHCF_3$				7	
84	240		$C_3F_6H_3DNOP$	$(CF_3)_2P(O)NDCH_3$					0.5
	(5941)								
84	241		$C_3F_6H_3DNP$	$(CF_3)_2PNDCH_3$					0.6
	(5942)								
84	242		$C_3F_6H_3DNPS$	$(CF_3)_2P(S)NDCH_3$					0.6
	(5943)								
85	243		$C_3F_6H_3N$	$(CF_3)_2CHNH_2$				7	
46	244		$C_3F_6H_3NO_2S_2$	$(CF_3S(O))_2NCH_3$					1.5
12	245		$C_3F_6H_3NS$	$(CF_3)_2NSCH_3$					0.47
68	246		$C_3F_6H_3O^+$	$CF_3CH(^+OH_2)CF_3$				6	
86	247		$C_3F_6H_3OP$	$(CF_3)_2POCH_3$					0.46
	(5944)								
86	248		$C_3F_6H_3OP$	$(CF_3)_2P(O)CH_3$					0.78
	(5945)								
86	249		$C_3F_6H_3O_2P$	$(CF_3)_2P(O)OCH_3$					0.37
36	250	B	$C_3F_6H_3P$	$(CF_3)_2PCH_3$					~0
	(5947)								
85	251		$C_3F_6H_4ClN$	$(CF_3)_2CHNH_3Cl$				8	
84	252		$C_3F_6H_4NOP$	$(CF_3)_2P(O)NHCH_3$					0.6
73	253		C_3F_7H	$CF_2HCF_2CF_3$		52.1		4.5	
	(2753)								
87	254		C_3F_7H	CF_3CFHCF_3		45		5.5	
	(2756)								
41	255		$C_3F_7H_6Sb$	$(CH_3)_2{}^+CFSbF_6^-$				26	
64	256		C_3F_7	$CF_3C(=NF)CHFNF_2$		50			
	(2751, 4708a)								
54	257	B	$C_3F_8H_4OS$	$CH_3OCF_2CHFSF_5$		43.6		7.7	
	[2433, 2769, 4837, 5074]							2.9	

Table A.1.a. (contd).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
354	258		$C_4FH_6BrO_2$	$CH_2BrCHFOC(O)CH_3$		∿50		∿15		
29	259	A-E	$C_4FH_6N_3O_6$	$FC(NO_2)_2CH_2NHCH_2CO_2H$				18.0		
56	260	B[2]	C_4FH_7	$FCH_2C(CH_3)=CH_2$		46				
88	261	E[2]	$C_4FH_7N_4O_5$	$FC(NO_2)_2CH_2NHNHCOCH_3$				19		
89	262		C_4FH_7O	$(CH_3)_2CFCHO$			1,2	22		
90	(901)			(2) (1)						
90	263		C_4FH_7O	$CH_3CH_2CHFCHO$	1,2	51				
	(903)									
91	264	G	$C_4FH_7O_2$	$CFH_2CO_2CH_2CH_3$		47.0				
92	265	F[2]	$C_4FH_8^+$	$CH_3CH_2\overset{+}{C}FCH_3$				22		
								26		
23	266	G	C_4FH_8Br	$CH_3CHFCHBrCH_3$	1,2	46.5	1,3	23.4	1,5	1.6
				(3) (2)(1)(4)(5)						
				(Erythro-dl-)			1,4	9.9		
23	267	G	C_4FH_8Br	$CH_3CHFCHBrCH_3$	1,2	46.4	1,3	23.2		
				(3) (2)(1)(4)						
				(Threo-dl-)			1,4	16.6		
92	268	G	C_4FH_8Br	$FC(CH_3)_2CH_2Br$			1,2	21		
				(1) (2) (3)			1,3	15		
23	269	G	C_4FH_8Cl	$CH_3CHFCHClCH_3$	1,2	46.5	1,3	23.5	1,5	1.2
				(3) (2)(1)(4)(5)			1,4	9.7		
				(Erythro-dl-)						
23	270	G	C_4FH_8Cl	$CH_3CHFCHClCH_3$	1,2	46.4	1,3	23.2	1,5	0.7
				(3) (2)(1)(4)(5)			1,4	16.0		
				(Threo-dl-)						
92	271	G	C_4FH_8Cl	$FC(CH_3)_2CH_2Cl$			1,2	21		
				(1) (2) (3)			1,3	16		
23	272	G	C_4FH_8I	$CH_3CHFCHICH_3$	1,2	47.0	1,3	23.6	1,5	1.0
				(3) (2)(1)(4)(5)			1,4	10.6		
				(Erythro-dl-)						
23	273	G	C_4FH_8I	$CH_3CHFCHICH_3$	1,2	47.0	1,3	23.5		
				(3) (2)(1)(4)			1,4	19.0		
				(Threo-dl-)						
92	274	G	C_4FH_8I	$FC(CH_3)_2CH_2I$			1,2	21		
				(1) (2) (3)			1,3	16		
62	275		C_4FH_9	$FCH_2(CH_2)_2CH$		47.5				
35	276		C_4FH_9	$FC(CH_3)_3$				20.4		
28	277		C_4FH_9O	$FC(CH_3)_2CH_2OH$			1,2	21.0		
				(1) (2) (3)			1,3	19.5		
28	278	P	C_4FH_9O	$CH_3CHFCHOHCH_3$	1,2	47.5	1,3	24.1	1,5	1.35
93				(3)(2)(1)(4)(5)						
				(Erythro)			1,4	15.0		

Table A.1.a. (contd.)

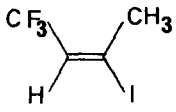
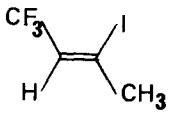
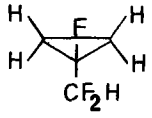
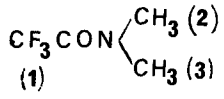
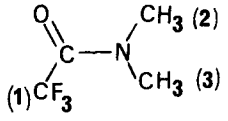
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
28	279	P	C_4FH_9O	$CH_3CHFCHOHCH_3$	1,2	48.3	1,3	24.1	1,5	0.81
93				(3)(2)(1)(4)(5)						
				(Threo)			1,4	15.5		
92	280	P	C_2FH_9O	$FCH_2C(CH_3)_2OH$		49		2		
92	281	F^2	$C_4FH_{10}O^+$	$FCH_2C(CH_3)_2{}^+OH_2$		49		1		
94	282	B	$C_4FH_{11}Si$	$FCH_2Si(CH_3)_3$		46.8				0.7
29	283	E	$C_4F_2H_6N_4O_8$	$(FC(NO_2)_2CHNH)_2$				17.5		
95	284	B	$C_4F_2H_7Cl_3NP$	$CHCl_2CF_2PClN(CH_3)_3$			1,3	9.0		
	(2781, 5994)			(3) (1,2)			2,3	10.5		
40	285	P	$C_4F_2H_8O$	$CF_2HOCH(CH_3)_2$		75.4				
440	286 (787)	P	$C_4F_3H_4I$							2.1
440	287 (788)	B	$C_4F_3H_4I$							2.0
262	288 1185 2783	B	$C_4F_3H_5$			54				
								^5J		
96	289	G	$C_4F_3H_6NO$				1,2	0.7	1,3	1.5
97	290	A	$C_4F_3H_6NO$				1,2	0.80	1,3	1.60
		B						0.80		1.63
		D						0.60		1.50
		E						0.80		1.63
		G	(4% w/w)					0.60		1.50
		H						0.70		1.60
		M						0.80		1.68
		G^2						0.80		1.65
		H^2						0.80		1.65
185	291 (2784)		$C_4F_3H_7ClP$	$FCHClCF_2P(CH_3)_2$		47.6		4.8, 10.7		
95	292 (6010)	B	$C_4F_3H_7Cl_2NP$	$CHCl_2CF_2PF(NCH_3)_2$			1,3	9		
				(3) (1,2)			2,3	10		
20	293 (2785)	B	$C_4F_3H_7O$	$FCH_2CF_2OCH_2CH_3$		46.1				

Table A.1.a. (contd.)

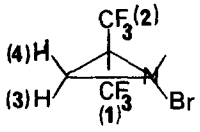
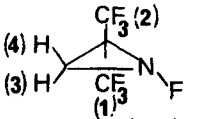
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		
20	294 (2786)	B	$C_4F_3H_7S$	$FCH_2CF_2SCH_2CH_3$		47.5				
36	295 (6012)	B	$C_4F_3H_9NP$	$CF_2HCH_2PFN(CH_3)_2$		56.5		18.3		
98	296 (2791)	F* P* H^{2*}	$C_3F_5H_5$	$CF_3CH_2CF_2CH_3$ (1)(2) (3)			1,2	10.80 10.23 10.48	1,3	0.56 0.77 0.64
114	297 (2799)	G	$C_4F_6H_2BrN$						1,3 2,4	2.2 0.6
85	298 (2800)		$C_4F_6H_3N$	$(CF_3)_2C{=}NCH_3$						2.5 { 1.8
68	299		$C_4F_6H_3O$	$(CF_3)_2C(OH)CH_3$						1
94	300	B	$C_4F_6H_4Cl_3NSi$	$(CF_3)_2NCH_2CH_2SiCl_3$ (1) (2)					1,2	1.4
36	301	B	$C_4F_6H_5P$	$(CF_3)_2PCH_2CH_3$ (1) (2)					1,2	∿0
99	302 (6042)	P	$C_4F_6H_6AsP$	$(CF_3)_2AsP(CH_3)_2$						0.7
99	303 (6041)	P	$C_4F_6H_6AsP$	$(CF_3)_2PAs(CH_3)_2$						0.7
99	304	P	$C_4F_6H_6As_2$	$(CF_3)_2AsAs(CH_3)_2$						0.6
100	305 (6044)		$C_4F_6H_6NP$	$(CF_3)_2PN(CH_3)_2$						0.5
76	306 (6046)	P	$C_3F_6H_6NPS$	$(CF_3)_2P(S)N(CH_3)_2$						0.7
99	307 (6048)	P	$C_4F_6H_6P_2$	$(CF_3)_2PP(CH_3)_2$						0.7
101	308		$C_4F_7H_2Br_2N$	$(CF_3)_2NCHBrCFHBr$ (1) (3)(2)(4) (Erythro)	2,4	48.0	1,3 2,3	1.1 8.0		
101	309		$C_4F_7H_2Br_2N$	$(CF_3)_2NCHBrCFHBr$ (1) (3) (2)(4) (Threo)	2,4	49.6	1,3 2,3	3.0 3.0		
32	310		$C_4F_7H_2I$	$CF_3CF_2CF_2CH_2I$				{ 29 6		
114	311 (2807 4717)	K	$C_4F_7H_2N$						1,3 2,4	2.4 0.8
101	312		$C_4F_7H_3BrN$	$FCHBrCH_2N(CF_3)_2$		52.0				
37	313 (2808)		$C_4F_7H_3ClN$	$FCHClCH_2N(CF_3)_2$ (2) (3,4) (1)			2,3 2,4	10.1 25.7	1,3 1,4	1.2 1.6
37	314		$C_4F_7H_3ClN$	$CH_2ClCHFN(CF_3)_2$		46.3				

Table A.1.a. (contd.)

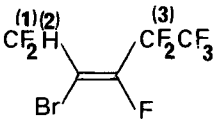
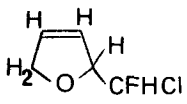
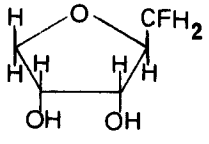
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
37	315		$C_4F_7H_3IN$	$CH_2ICHFN(CF_3)_2$		46.8				
190	316 (918)		C_4F_8HBr		1,2	53.6			2,3	5.6
77	317		C_4F_8HI	$CF_2ICH(CF_3)_2$			1,3	10.0		
	(2817)			(1) (3)(2)			2,3	7.3		
77	318		C_4F_8HI	$CF_3CF_2CHICF_3$			1,2	6.9		
	(2818)			(2)(1)						
87	319		C_4F_9H	$(CF_3)_3CH$				7		
102	320 (2823)		C_4F_9HBrN	$FCHBrCF_2N(CF_3)_2$		47.7				
102	321 (2824)		C_4F_9HClN	$FCHClCF_2N(CF_3)_2$		47.8				
102	322 (2825)		C_4F_9HClN	$CF_2ClCFHN(CF_3)_2$		42.4				
102	323 (2827)		C_4F_9HIN	$FCHICF_2N(CF_3)_2$		47.5				
102	324 (2826)		C_4F_9HIN	$CF_2ICFHN(CF_3)_2$		42.1				
83	325		$C_4F_9HS_3$	$CF_3CH(SCF_3)S_2CF_3$				7		
191	326	G	C_5FH_6ClO			50				
103	327	A	$C_5FH_8BrO_2$	$CH_2BrCF(CH_3)CO_2CH_3$			1,2	21		
				(1)(2)						
29	328	A	$C_5FH_8N_3O_4$	$FC(NO_2)_2CH_2NHCH_2CH{=}CH_2$				19.7		
29	329	G	$C_5FH_8N_3O_6$	$FC(NO_2)_2CH_2NHCO_2CH_2CH_3$				14.9		
90	330		C_5FH_9O	$FC(CH_3)_2COCH_3$				21		5
90	331		C_5FH_9O	$CH_3CH_2CHFCOCH_3$		50		24		5
91	332	G	$C_5FH_9O_2$	$CH_3CHFCO_2CH_2CH_3$		48.3		22.8		
104	333	G-P	$C_5FH_9O_3$	$CH_3CHFCHOHCO_2CH_3$	1,2	47.6	1,3	24.0		
				(3)(2)(1)(4)						
				(Erythro)			1,4	16.0		
104	334	G-P	$C_5FH_9O_3$	$CH_3CHOHCHFCO_2CH_3$		47.9		21.1		2.1
				(Erythro)						
104	335	G-P	$C_5FH_9O_3$	$FCH_2C(CH_3)OHCO_2CH_3$		47.5				2.0
105 355	336		$C_5FH_9O_3$			54		12		

Table A.1.a. (contd.)

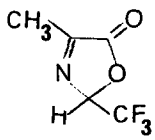
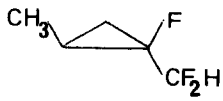
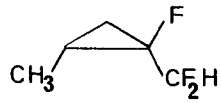
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
92	337	G	$C_5FH_{10}Br$	$FC(CH_3)_2CHBrCH_3$			1,2	21	1,4	
				(1) (2) (3) (4)			1,3	9		
92	338	G	$C_5FH_{10}Cl$	$FC(CH_3)_2CHClCH_3$			1,2	21	1,4	1
				(1)(2) (3)(4)			1,3	9		
92	339	G	$C_5FH_{10}I$	$FC(CH_3)_2CHICH_3$			1,2	21		
				(1) (2) (3)			1,3	9		
106	340		C_5FH_{11}	$FC(CH_3)_2CH_2CH_3$			1,2	21		
				(1) (2)						
106	341		C_5FH_{11}	$CH_3CHFCH_2CH_2CH_3$	1,2	46	1,3	23		
				(3)(2)(1)						
62	342		C_5FH_{11}	$FCH_2(CH_2)_3CH_3$		47.5		24.8		
28	343		$C_5FH_{11}O$	$FC(CH_3)_2CHOHCH_3$			1,2	21.6		
				(1) (2) (3)			1,3	11.5		
107	344		$C_5F_2H_8O$	$CH_3CF_2C(O)CH_2CH_3$				20.0		
107	345		$C_5F_2H_8O$	$CH_3CH_2CF_2C(O)CH_3$				16		
108	346	G	$C_5F_2H_8O$	$CH_3CH_2CF_2C(O)CH_3$				17		
109	347	G*	$C_5F_2H_8O$	$FCH_2CHFCO_2CH_2CH_3$	1,3	+46.59	2,3	+30.25		
	(2448)			(1)(3,4)(5)(2)	1,4	+47.94	2,4	+21.30		
					2,5	+47.31	1,5	+28.42		
110	348	B	$C_5F_3H_4NO_2$					4.6		
111	349		$C_5F_3H_6N$	$CF_3CH_2CH(CN)CH_3$				10.6		
111	350		$C_5F_3H_6N$	$CF_3CH(CH_3)CH_2CN$				7.5		
262	351	B	$C_5F_3H_7$			+56†				
	(1187 2849)									
262	352	B	$C_5F_3H_7$			{ 51 53				
	1188 2850									
67	353		$C_5F_3H_8NO_2$	$CF_3C(CH_3)_2CH_2NO_2$					1,2	0.77
				(1) (2)						
20	354		$C_5F_3H_9S$	$FCH_2CF_2SCH(CH_3)_2$		46.9				
	(2851)									
185	355		$C_5F_3H_{10}ClSi$	$FCHClCF_2Si(CH_3)_3$		49.0		6.2		
	(2852)							11.9		
189	356	T	$C_5F_3H_{12}As_2P$	$CF_3P[As(CH_3)_2]_2$						0.34
	(6090)									

Table A.1.a. (contd.)

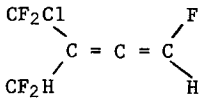
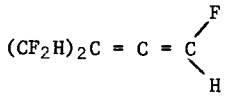
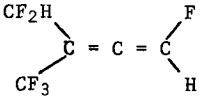
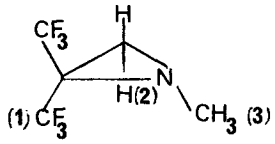
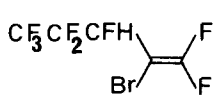
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
75	357 (6094)		$C_5F_3H_{12}N_2P$	$CF_2P[N(CH_3)_2]_2$			0.7
112	358 (6801)		$C_5F_4H_{10}Sn$	$CF_2HCF_2Sn(CH_3)_3$	57.5	5.5	
50	359 (2517)		$C_5F_4H_{13}NSi$	$CF_2HCF_2SiH_3N(CH_3)_3$	55.7	6.5	
192	360 (804, 1040)		$C_5F_5H_2Cl$		55		
192	361		$C_5F_5H_2Cl$	$(CF_2H)_2CFC{\equiv}CCl$	55	5.6	
192	362 (805, 1041)		$C_5F_5H_3$		55		
192	363 (1044, 807)		$C_5F_6H_2$		55		
113	364		$C_5F_6H_4O$	$(CF_3)_2CHCOCH_3$		8	
114	365 (2860)	J	$C_5F_6H_5N$				1,3 2.0 1,2 2.7
115	366		$C_5F_6H_7As$	$(CF_3)_2CHAs(CH_3)_2$		10	0.95
94	367	B	$C_5F_6H_7Cl_2NSi$	$(CF_3)_2NCH_2CH_2SiCl_2CH_3$ (1) (2)			1.3
83	368 (6102)		$C_5F_6H_7O_3P$	$(CF_3)_2CHP(O)(OCH_3)_2$		7	
36	369 (6103)	B	$C_5F_6H_7P$	$(CF_3)_2P(CH_2)_2CH_3$			≈0
67	370		$C_5F_7H_4NO_2$	$CF_3CF(NO_2)CH_2CH_2CF_3$		8.8	
190	371 [2869, 3272, 3518]	P	C_5F_8HBr		42.7	5.9 13.8	

Table A.1.a. (contd.)

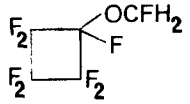
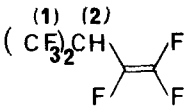
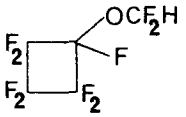
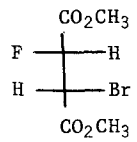
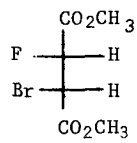
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
116	372		$C_5F_8H_2O$		50			
117	373	B	$C_5F_8H_2O$	$CF_2HCOCH(CF_3)_2$	53.5		7.3	
118	374 (3273, 3520)	G	C_5F_9H			1,2	7.1	
116	376 (1230)		C_5F_9HO		71			
40	377 (2884)	P	$C_5F_9HO_2$	$CF_3(CF_2)_2CO_2CF_2H$	68.6			
119	378		$C_5F_9H_2Br_2N$	$CF_3CHBrCHBrN(CF_3)_2$ (1)(2)		1,2	5.7	
120	379		$C_5F_9H_2NO$	$CF_3CH_2CON(CF_3)_2$ (1)(2)		1,2	0.9	
119	380		$C_5F_9H_3BrN$	$CF_3CHBrCH_2N(CF_3)_2$			6.5	
119	381		$C_5F_9H_3IN$	$CF_3CH_2CHIN(CF_3)_2$			9.3	
83	382		$C_5F_9H_3S_2$	$CF_3CH_2S_2CH(CF_3)_2$ (1)(3) (4)(2)		1,3 2,4	9 7	
119	383		$C_5F_9H_4N$	$CF_3CH_2CH_2N(CF_3)_2$			10.2	
121	384		$C_6FH_8BrO_4$		46.0		23.7	
121	385		$C_6FH_8BrO_4$		46.0		18.4	
29	386	E	$C_6FH_8N_3O_6$ (1)	$CF(NO_2)_2CH_2NHCH(CO_2H)CH_2CO_2H$ (1) (2,3)		1,2 1,3	15.0 15.0	
104	387	G	$C_6FH_9O_5$	$CH_3O_2CCHFCHOHCO_2CH_3$	47		23.3	
29	388	G	$C_6FH_{10}N_3O_6$	$CF(NO_2)_2CH_2NHCH_2CO_2CH_2CH_3$			18.0	
193	389	G	$C_6FH_{11}O$	$CH_3(CH_2)_2CFHCOCH_3$	51.1			
104	390	G	$C_6FH_{11}O_3$	$(CH_3)_2CFCHOHCO_2CH_3$ (2) (1)(3)		1,2 1,3	21.1 14.1	
105	391		$C_6FH_{11}O_3$	$CH_3CHFCHOHCO_2CH_2CH_3$ (3)(2)(1)(4)	1,2 47.0	1,3 1,4	23.5 16.3	

Table A.1.a. (contd.)

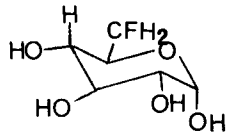
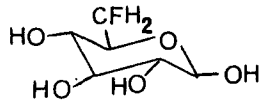
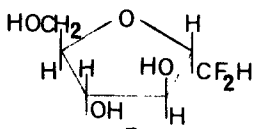
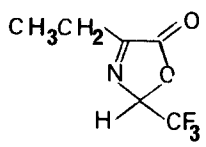
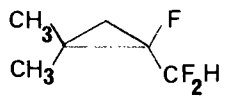
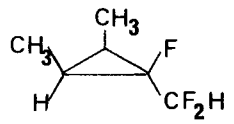
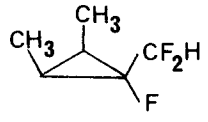
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
357	392	A^2	$C_6FH_{11}O_5$			47.3		28.0		
357	393	A^2	$C_6FH_{11}O_5$			47.5		27.0		
122	394	G	$C_6FH_{12}Br$	$CH_2BrCHF(CH_2)_3CH_3$ (3) (2) (1)	1,2	46.8	1,3	17.4		
62	395		C_6FH_{13}	$FCH_2(CH_2)_4CH_3$		47.5		24.5		
107	396		$C_6CH_{13}O$	$FC(CH_3)_2COH(CH_3)_2$				23		
88	397	M	$C_6F_2H_7N_5O_{10}$	$[FC(NO_2)_2CH_2]_2NCH_2CO_2H$				18.5		
108	398 (2900)	G	$C_6F_2H_9NO$	$CH_3CH_2CF_2COH(CN)CH_3$				17		
40	399	P	$C_6F_2H_{10}O_2$	$CF_2HO_2C(CH_2)_3CH_3$		70.8				
361	400	A^2	$C_6F_2H_{10}O_4$			55		12		
36	401 (6135)	B	$C_6F_2H_{15}N_2P$	$CF_2HCH_2P[N(CH_3)_2]_2$		57.2		$17.9^{\dagger}$		
123	402		$C_6F_3H_5$	$CF_3C{\equiv}CCH_2CH{=}CH_2$ (1) (2)					1,2	3.78
110	403	B	$C_6F_3H_6NO_2$					4.5		
262	404 (1189, 2901)	B	$C_6F_3H_9$			{ 55, 55				
262	405 (1190, 2903)	B	$C_6F_3H_9$			56				
262	406 (1191, 2904)	B	$C_6F_3H_9$			52				

Table A.1.a. (contd.)

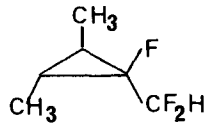
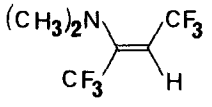
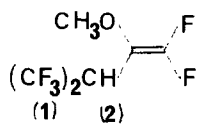
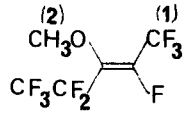
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
263	407 (1192 2902)	B	$C_6F_3H_9$		53 54		
20	408 (2905)	B	$C_6F_3H_{11}S$	$FCH_2CF_2SC(CH_3)_3$	47.3		
66	409		$C_6F_3H_{12}ClSi$	$CF_3CH_2CHClSi(CH_3)_3$		9.7	
66	410		$C_6F_3H_{12}ClSi$	$CF_3CHClCH_2Si(CH_3)_3$		6.3	
71	411 (6805)	H	$C_6F_3H_{13}Sn$	$CF_3CH_2CH_2Sn(CH_3)_3$		10.4	
124	412 (2906)		$C_6F_4HCoO_4$	$CF_2HCF_2Co(CO)_4$	57.1	3.7	
125	413	A	$C_6F_6H_4O_3$	$(CF_3)_2CHC(O)CH_2CO_2H$		7.7	
126	414		$C_6F_6H_6S$	$(CF_3)_2CHSCH_2CH{=}CH_2$		8	
127	415 (830)		$C_6F_6H_7N$				1,2 1.7
67	416		$C_6F_6H_7NO_2$	$CF_3CH_2CH_2C(CF_3)(NO_2)CH_3$		9.5	
71	417 (6811)	H	$C_6F_6H_8Cl_2Sn$	$(CF_3CH_2CH_2)_2SnCl_2$		9.9	
74	418 (2917)	B	$C_6F_6H_8O$	$CF_3CH(CH_3)C(OH)(CH_3)CF_3$		8	
128	419		$C_6F_6H_{10}OGe$	$(CF_3)_2CHOGe(CH_3)_3$		6.1	
128	420		$C_6F_6H_{10}OSi$	$(CF_3)_2CHOSi(CH_3)_3$		6.0	
129	421		$C_6F_6H_{10}OSi$	$(CF_3)_2CHOSi(CH_3)_3$		5.7	
128	422		$C_6F_6H_{10}OSn$	$(CF_3)_2CHOSn(CH_3)_3$		6.1	
112	423 [2918 6812 5519]		$C_6F_6H_{10}Sn$	$CF_3CFHCF_2Sn(CH_3)_3$ (1)(2)(5)(3,4)	2,5 45.9	1,5 6.5 3,5 13.9 4,5 11.3	
115	424		$C_6F_6H_{10}Sn$	$(CF_3)_2CHSn(CH_3)_3$		11.5	0.5
118	425 (951 3543)	B	$C_6F_8H_4O$			1,2 8.0	
194	426 (3291 2929)		$C_6F_9H_3O$				1,2 0.6

Table A.1.a. (contd.)

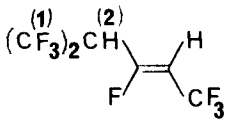
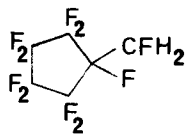
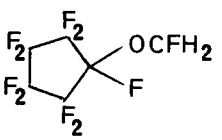
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J
113	427 [835 953 1083 3294]		$C_6F_{10}H_2$			1,2	7.5
113	428		$C_6F_{10}H_2$	$CF_3CH_2CF{=}C(CF_3)_2$			9
116	429		$C_6F_{10}H_2$		50		
116	431		$C_6F_{11}HO$		11.3		
634	430 [3295 3547 5569]		$C_6F_{11}HHg$	$(CF_3)_2CHHgC(CF_3){=}CF_2$			68
83	432		$C_6F_{12}HClS_2$	$(CF_3)_2CHS_2CCl(CF_3)_2$			7
634	433 (5570)		$C_6F_{12}H_2Hg$	$[(CF_3)_2CH]_2Hg$			11.3
83	434		$C_6F_{12}H_2OS_2$	$(CF_3)_2CHS_2COH(CF_3)_2$			8.0
83	435		$C_6F_{12}H_2S_2$	$(CF_3)_2CHS_2CH(CF_3)_2$			7
130	436	G	$C_7FH_2MnO_6$	$CFH_2C(O)Mn(CO)_5$	50		
131	437	P	C_7FH_6Br	para-$BrC_6H_4CFH_2$	47.9		
131	438	P	C_7FH_6Cl	meta-$ClC_6H_4CFH_2$	47.2		
131	439	P	C_7FH_6Cl	para-$ClC_6H_4CFH_2$	48.1		
131	440	P	$C_7FH_6NO_2$	meta-$NO_2C_6H_4CFH_2$	47.2		
131	441	P	$C_7FH_6NO_2$	para-$NO_2C_6H_4CFH_2$	46.9		
131	442	P	C_7FH_7	$CFH_2C_6H_5$	48		
132							
133	4443 (6197)	A^2	$C_7FH_{11}NO_3P$	$FCH_3P(O)(OH)O^-$ $N^+H_3C_6H_5$	46.3		
134	444		$C_7FH_{11}O$	$(CF_3)_2CFC(O)C(CH_3){=}CH_2$			20
91	445	G	$C_7FH_{11}O_2$	$CH_2{=}CHCH_2CHFCO_2CH_2CH_3$	48.5		23.8
90	446 (904)		$C_7FH_{13}O$	$CH_3(CH_2)_4CHFCHO$	52		
135	447	G	$C_7FH_{13}O_2$	$(CH_3CH_2)_2CFCO_2CH_3$			16.5

Table A.1.a. (contd.)

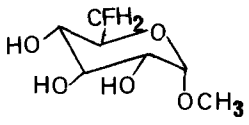
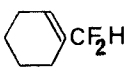
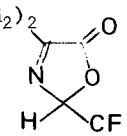
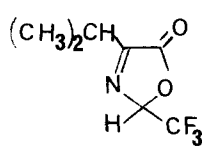
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
358	448		$C_7FH_{13}O_5$			54		19		
62	449	B	C_7FH_{15}	$FCH_2(CH_2)_5CH_3$		47.5		24.3		
136										
122	450	G	$C_7FH_{15}O$	$CH_3(CH_2)_4CHFCH_2OH$ (2)(1)(3)	1,2	51.6	1,3	24.1		
191	451		$C_7FH_{16}ClSi$	$FCHClSi(CH_2CH_3)_3$		45.5				
124	452		$C_7F_2HCl_2MnO_5$	$CF_2HCCl_2Mn(CO)_5$		61.0				
124	453		$C_7F_2HCl_2MnO_5$	$CHCl_2CF_2Mn(CO)_5$				11.0		
137	454		$C_7F_2HCl_2O_5Re$	$CHCl_2CF_2Re(CO)_5$				11.0		
130	455		$C_7F_2HMnO_6$	$CF_2HC(O)Mn(CO)_5$		59				
138	456		$C_7F_2H_5BrO$	para-$BrC_6H_4OCF_2H$		+73.2				
138	457		$C_7F_2H_5NO_3$	para-$NO_2C_6H_4OCF_2H$		+72.2				
131	458		$C_7F_2H_6$	m-$FC_6H_4CFH_2$		48.0				
131	459		$C_7F_2H_6$	p-$FC_6H_4CFH_2$		48.2				
138	460		$C_7F_2H_6O$	$C_6H_5OCF_2H$		+73.9				
29	461	A	$C_7F_2H_9N_5O_8$	$[FC(NO_2)_2CH_2]_2NCH_2CH=CH_2$				18.0		
139	462 (840)		$C_7F_2H_{10}$			56.1				
58	463	N	$C_7F_2H_{10}N_4O_{10}$	$[FC(NO_2)_2CH(OH)CH_2]_2CH_2$				19		
88	464	G	$C_7F_2H_{11}N_5O_9$	$[FC(NO_2)_2CH_2]_2NCH_2OCH_2CH_3$				17		
134	465		$C_7F_2H_{12}O$	$(CH_3)_2CFC(O)CF(CH_3)_2$				20		
140	466		$C_7F_3HClMnO_5$	$FCHClCF_2Mn(CO)_5$	1,4	52.0	2,4	5.5		
	(2952)			(1)(4)(2,3)			3,4	12.5		
140	467		$C_7F_3HClMnO_5$	$CF_2HCFClMn(CO)_5$	1,4	61.3	3,4	5.3		
	(2953)			(1,2)(4)(3)	2,4	63.7				
137	468		$C_7F_3HClO_5Re$	$FCHClCF_2Re(CO)_5$	1,4	52.5	2,4	5.3		
				(1)(4)(2,3)			3,4	11.8		
123	469		$C_7F_3H_7$	$CF_3C\equiv CCH_2C(CH_3)=CH_2$ (1) (2)					1,2	3.78
110	470		$C_7F_3H_8NO_2$	$CH_3(CH_2)_2$ 				4.0		
110	471		$C_7F_3H_8NO_2$					4.2		

Table A.1.a. (contd.)

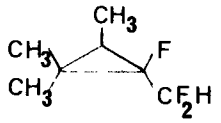
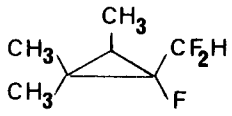
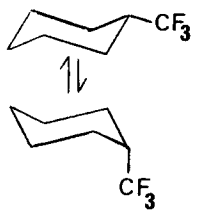
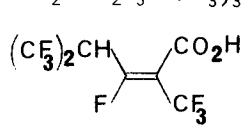
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
67	472		$C_7F_3H_{10}NO_4$	$CF_3C(NO_2)(CH_3)CH_2CH_2CO_2CH_3$ (1) (2) (3)		1,2 1,3	1.1 0.5
262	473 1197 2954	B	$C_7F_3H_{11}$		55 56		
262	474 1198 2955	B	$C_7F_3H_{11}$		54†		
300	475	A D E P E^2	$C_7F_3H_{11}$			8.0 7.7 8.3 7.8 8.0	
141	476 (2956)		$C_7F_4HCoN_5^{3-}$	$[CF_2HCF_2Co(CN)_5]^{3-}$	55.9	7.5	
141	477 (2957)		$C_7F_4HMnO_5$	$CF_2HCF_2Mn(CO)_5$	58.0	5.3	
142	478 (2958)		$C_7F_4HN_5Rh^{3-}$	$[CF_2HCF_2Rh(CN)_5]^{3-}$	52.8	7.4	
137	479 (2959)		$C_7F_4HO_5Re$	$CF_2HCF_2Re(CO)_5$	59.0	5.7	
61	480	B^2	$C_7F_6H_2$	$C_6F_5CFH_2$	47.8		
125	481	E	$C_7F_6H_6O_3$	$(CF_3)_2CHC(O)CH(CH_3)CO_2H$		8.4	
125	482	A	$C_7F_6H_6O_3$	$(CF_3)_2CHC(O)CH_2CO_2CH_3$		7.9	
67	483		$C_7F_6H_8N_2O_4$	$(CF_3CH_2CH_2)_2C(NO_2)_2$		9.4	
126	484		$C_7F_6H_8S$	$(CF_3)_2CHSCH_2C(CH_3)=CH_2$		8	
143	485		$C_7F_7H_5IN$	$CF_3CF_2CF_2CH_2CHICH_2CN$		20	
143	486		$C_7F_7H_5O_2$	$CF_3CF_2CF_2CH_2CH=CHCO_2H$		18	
112	487		$C_7F_8H_{10}Sn$	$CF_2H(CF_2)_3Sn(CH_3)_3$	52.0	5.9	
113	488 (3302 955)		$C_7F_{10}H_2O_2$			7.2	

Table 1.A.a. (contd.)

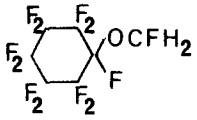
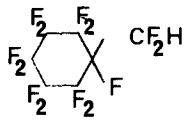
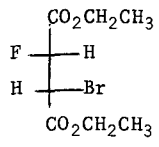
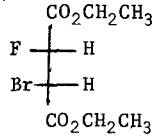
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
116	489		$C_7F_{12}H_2O$		50		
113	490		$C_7F_{12}H_2O$	$(CF_3)_2CHC(O)CH(CF_3)_2$		7	
83	491		$C_7F_{12}H_4S_3$	$(CF_3)_2CHSC(CF_3)_2S_2CH_3$		7	
85	492		$C_7F_{12}H_5NO$	$(CF_3)_2CHNHCH_2C(CF_3)_2OH$		7	
116	493		$C_7F_{13}HO$		75		
194	494 (2982)		$C_7F_{13}HO$	$CF_3CF_2CFHC(O)CF_2CF_2CF_3$	46		
74	495	B	$C_7F_{14}H_2O$	$(CF_3)_2CFCHOHCF(CF_3)_2$		10	
193	496	G	C_8FH_6BrO	$FCHBrCOC_6H_5$	49.7		
131	497		C_8FH_6N	meta-$CNC_6H_4CFH_2$	47.4		
131	498		C_8FH_6N	para-$CNC_6H_4CFH_2$	47.2		
58	499	A	$C_8FH_7N_2O_5$	$FC(NO_2)_2CHOHC_6H_5$		19	
107	500		C_8FH_7O	$FCH_2C(O)C_6H_5$	48		
61	501	C[2]	$C_8FH_8^+$	$CH_3{}^+CFC_6H_5$		22.8	
265	502	G	C_8FH_8BrO	$FCHBrCHOHC_6H_5$ (Erythro)	52.2	14.1	
265	503	G	C_8FH_8BrO	$FCHBrCHOHC_6H_5$ (Threo)	52.2	10.6	
144	504	G	C_8FH_8Cl	$CH_2ClCHFC_6H_5$ (3,4) (2)(1)	1,2 47	1,3 17 1,4 22	
131	505	P	$C_8FH_8NO_2$	para-$NO_2C_6H_4CH_2CFH_2$	46.7	25.0	
131	506	P	C_8FH_9	meta-$CH_3C_6H_4CFH_2$	48.0		
131	507	P	C_8FH_9	para-$CH_3C_6H_4CFH_2$	48.3		
131	508	P	C_8FH_9	$FCH_2CH_2C_6H_5$	47.0	23.6	
131	509	P	C_8FH_9O	meta-$CH_3OC_6H_4CFH_2$	48.2		
131	510	P	C_8FH_9O	para-$CH_3OC_6H_4CFH_2$	48.7		
145	511		C_8FH_9O	$FCH_2CHOHC_6H_5$	47.8	15.4	
121	512		$C_8FH_{12}BrO_4$		46.8	23.4	
121	513		$C_8FH_{12}BrO_4$		46.5	17.5	

Table A.1.a. (contd.)

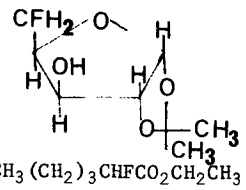
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
91	514	G	$C_8FH_{13}O_2$	$CH=CHCH_2CF(CH_3)CO_2CH_2CH_3$		1,2	20.9		
				(2)(1) (3)		1,3	20.9		
193	515	G	$C_8FH_{13}O_3$	$(CH_3)_2CHCFHCOCO_2CH_2CH_3$	48.7		25.4		
193	516	G	$C_8FH_{13}O_3$	$CH_3CH_2CH_2CFHCOCO_2CH_2CH_3$	48.0		25.4		
362	517	E	$C_8FH_{13}O_4$		47		16		
91	518	G	$C_8FH_{15}O_2$	$CH_3(CH_2)_3CHFCO_2CH_2CH_3$	49.4		24.2		
104	519	G-P	$C_8FH_{15}O_3$	$(CH_3)_2CFC(CH_3)OHCO_2CH_2CH_3$		1,2	20.9	1,4	0.89
				(2,3)(1) (4)		1,3	20.6		
29	520	B	$C_8FH_{16}N_3O_6$	$FC(NO_2)_2CH_2NHCH_2CH(OCH_2CH_3)_2$			17.8		
30	521		$C_8F_2H_6Br_2$	$CF_2BrCHBrC_6H_5$		1,3	6		
	(2987)			(1,2) (3)		2,3	15		
843	522		$C_8F_2H_6Cl$	$CF_2ClCHClC_6H_5$		1,3	6		
	(2988)					2,3	9		
40	523		$C_8F_2H_6O_2$	$CF_2HO_2CC_6H_5$	70.7				
41	524	C[2]	$C_8F_2H_8$	$CH_3CF_2C_6H_5$			17.8		
61									
138	525		$C_8F_2H_8O$	para-$CH_3C_6H_4OCF_2H$	74.2				
138	526		$C_8F_2H_8O_2$	para-$CH_3OC_6H_4OCF_2H$	74.4				
146	527	G	$C_8F_2H_{10}Cl_6O$	$[CH_3CH(CFClCCl_2H)_2]O$		1,2	16(t)		
				(3)(1) (2)			2(g)		
						1,3	18(t)		
88	528	A	$C_8F_2H_{13}N_5O_8$	$[FC(NO_2)_2CH_2]_2NC(CH_3)_3$			14		
139	529		$C_8F_2H_{15}Cl$	$CF_2HCHCl(CH_2)_5CH_3$ (1,2),3	56.2	1,4	11.9		
	(2989)			(1,2)(3)(4)		2,4	9.5		
140	530		$C_8F_3H_3ClMnO_5$	$CH_3CF_2CFClMn(CO)_5$		1,4	13.0	3,4	2.0
	(2990)			(4)(1,2)(3)		2,4	18.5		
147	531		$C_8F_3H_5Br_2$	para-$FC_6H_4CHBrCF_2Br$			17		
							5		
250			$C_8F_3H_6NO_2$	para-$NO_2C_6H_4CH_2CF_3$			10.5		
148	532	B	$C_8F_3H_7O$	$CF_3CHOHC_6H_5$			6.9		
149	(861)	G					6.7		
		H[2]					7.3		
88	533		$C_8F_3H_8N_7O_{14}$	$[FC(NO_2)_2CH_2]_2NCH_2CO_2CH_2CF(NO_2)_2$		1,3	17.5		
				(1) (3) (4)(2)		2,4	15.0		
123	534		$C_8F_3H_9$	$CF_3C\equiv CCH_2CH=C(CH_3)_2$				1,2	3.78
				(1) (2)					

Table A.1.a. (contd.)

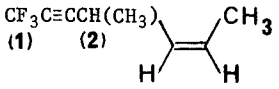
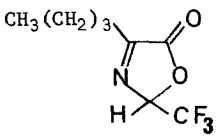
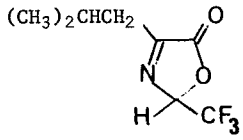
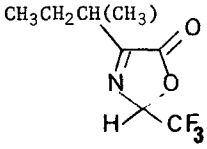
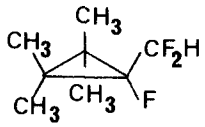
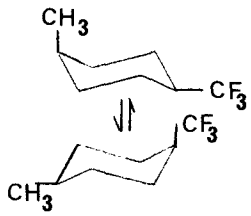
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ
123	535		$C_8F_3H_9$				1,2	3.78
110	536	G	$C_8F_3H_{10}NO_2$			4.0		
110	537	G	$C_8F_3H_{10}NO_2$			4.0		
110	538	G	$C_8F_3H_{10}NO_2$					
262	539 (1201 / 2991)	B	$C_8F_3H_{13}$		54			
300	540	A	$C_8F_3H_{13}$			8.2		
		D				7.9		
		E				8.7		
		P				8.1		
		E^2				8.2		
300	541	A	$C_8F_3H_{13}$			7.4		
		D				7.5		
		E				8.0		
		P				7.4		
		E^2				7.6		
150	542	G	$C_8F_3H_{16}BrSi$	$CF_3CHBrSi(CH_2CH_3)_3$				10
187	543		$C_8F_3H_{19}GeSn$	$CF_2HCF[Sn(CH_3)_3]Ge(CH_3)_3$ (1,2)(4)(3)	1,4 58 2,4 62.4	3,4		9.7
	(2993)							
187	544		$C_8F_3H_{19}GeSn$	$(CH_3)_3SnCF_2CFHGe(CH_3)_3$ (1,2)(3)(4)	3,4 46.3	1,4 2,4		39.4 8
	(2992)							

Table A.1.a. (contd.)

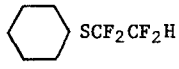
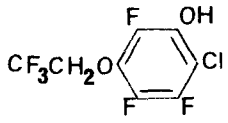
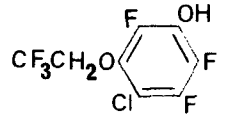
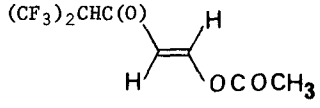
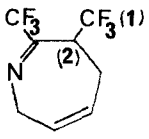
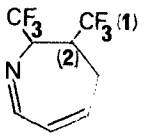
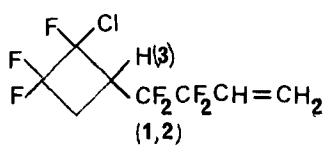
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		
195	545		$C_8F_3H_{19}SiSn$	$CF_2HCF[Sn(CH_3)_3]Si(CH_3)_3$	1,4	57.6	3,4	10.9		
	(2995)			(1,2)(4)(3)	2,4	58.5				
195	546		$C_8F_3H_{19}SiSn$	$(CH_3)_3SnCF_2CFHSi(CH_3)_3$	3,4	43.1	1,4	36		
	(2994)			(1,2)(3)(4)			2,4	9.6		
140	547		$C_8F_4H_3MnO_5$	$CH_3CF_2CF_2Mn(CO)_5$			2,3	18.9	1,3	2.5
	(2996)			(3)(2)(1)						
137	548		$C_8F_4H_3O_5Re$	$CH_3CF_2CF_2Re(CO)_5$			2,3	20.0	1,3	2.5
	(2997)			(3)(2)(1)						
147	549		$C_8F_4H_5Br$	para-$CF_2BrC_6H_4CF_2H$		57				
147	550		$C_8F_4H_6$	para-$CF_2HC_6H_4CF_2H$		57				
151	551	B	$C_8F_4H_6$	$CF_2HCF_2C_6H_5$		56		3		
146	552	G	$C_8F_4H_{10}Cl_4O$	$[CH_3CH(CFClCHFCl)]_2O$		48				
152	553		$C_8F_4H_{12}S$			55		3.5		
	(2998)									
147	554		$C_8F_5H_5$	$CF_2HC_6H_4CF_3$		57				
892	555	B	$C_8F_6H_3ClO_2$					8.7		
	(4189)									
892	556	B	$C_8F_6H_3ClO_2$					8.7		
	(4190)									
117	557	E	$C_8F_6H_6O_3$					8.0		
215	558		$C_8F_6H_7N$				1,2	9.6		
	(3009)									
215	559		$C_8F_6H_7N$				1,2	9.5		
	(3010)									
125	560	E	$C_8F_6H_8O_3$	$(CF_3)_2CHC(O)C(CH_3)_2CO_2H$				7.5		
71	561	H	$C_8F_6H_{14}Sn$	$(CF_3CH_2CH_2)_2Sn(CH_3)_2$				10.3		
	(6817)									
196	562		$C_8F_7H_4Cl$				1,2	9		
							2,3	16		

Table A.1.a. (contd.)

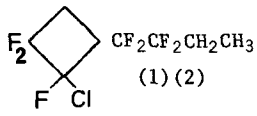
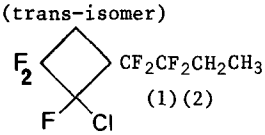
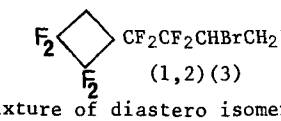
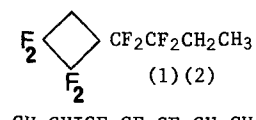
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J
196	563 (3771, 3014)		$C_8F_7H_8Cl$	 $CF_2CF_2CH_2CH_3$ (1)(2) (trans-isomer)		1,2	18.5
196	564		$C_8F_7H_8Cl$	 $CF_2CF_2CH_2CH_3$ (1)(2) (cis-isomer)		1,2	∿18
41	565		$C_8F_7H_8Sb$	$C_6H_5{}^+CFCH_3SbF_6{}^-$			23
197	566 (4419)		$C_8F_8H_2O$	$CF_3CH_2OC_6F_5$			8.8
196	567 (3018, 3774)		$C_8F_8H_6Br_2$	 $CF_2CF_2CHBrCH_2Br$ (1,2)(3) (Mixture of diastero isomers)		1,3 2,3	13.8 9.0 9.0
196	568 (3775)		$C_8F_8H_8$	 $CF_2CF_2CH_2CH_3$ (1)(2)		1,2	18.5
198	569 (3024)		$C_8F_9H_6I$	$CF_3CF_2CH_2CHICF_2CF_2CF_2CH{=}CH_2$ (3) (1,2)		1,3 2,3	21.7 6.7
143	570		$C_8F_9H_6IO_2$	$CF_3(CF_2)_3CH_2CHICH_2CO_2H$			19
198	571		$C_8F_9H_9$	$CF_3CF_2CH_2CH_2CF_2CF_2CH_2CH_3$ (2)(1)		1,2	∿15
113	572 (3035)		$C_8F_{12}H_4O$	$(CF_3)_2CHC(OCH_3){=}C(CF_3)_2$			7
128	573		$C_8F_{12}H_8O_2Sn$	$[(CF_3)_2CHO]_2Sn(CH_3)_2$			6.2
83	574		$C_8F_{12}H_8S_3$	$(CF_3)_2CHSC(CF_3)_2S_2CH_2CH_3$			7
116	575		$C_8F_{13}H_3O$	 $OCFHCFH_2$ (1)(3)(2)(4)	1,3 2,4	55 45	1,4 2,3	5 10
116	576		$C_8F_{14}H_2O$	 $OCFHCF_2H$ (1)(3)(2)(4)	1,3 2,4	55 55		
116	577		$C_8F_{14}H_2O$	 OCH_2CF_3				15
116	578		$C_8F_{15}HO$	 OCF_2CF_2H		55		3
116	579		$C_8F_{15}HO$	 $OCFHCF_3$		55		

Table A.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
193	580	G	C_9FH_9O	$C_6H_5CFHCOCH_3$		48.3				
91	581	G	$C_9FH_9O_2$	$C_6H_5CFHCO_2CH_3$		47.5				
193	582		$C_9FH_{10}BrO$	$CH_3CFBrCHOHC_6H_5$			1,2	19.8		
				(2)(1) (3)			1,3	12.3		
				(Erythro)						
193	583		$C_9FH_{10}BrO$	$CH_3CFBrCHOHC_6H_5$			1,2	19.8		
				(2)(1) (3)			1,3	8.5		
				(Threo)						
153	584	P	$C_9FH_{10}Cl$	$C_6H_5CFHCHClCH_3$		46.7		14.6		
				(Threo)						
93	585	P	$C_9FH_{11}O$	$CH_3CHFCHOHC_6H_5$	1,2	47.4	1,3	24.0		
				(3)(2)(1)(4)			1,4	12.0		
				(Erythro)						
145	586		$C_9FH_{11}O$	$CH_3CHFCHOHC_6H_5$	1,2	47.4	1,4	13.0		
				(3)(2)(1)(4)						
				(Erythro)						
93	581	P	$C_9FH_{11}O$	$CH_3CHFCHOHC_6H_5$	1,2	49.0	1,3	23.8		
				(3) (2)(1)(4)			1,4	12.5		
				(Threo)						
145	588		$C_9FH_{11}O$	$CH_3CHFCHOHC_6H_5$	1,2	50.1	1,4	11.6		
				(3) (2)(1)(4)						
				(Threo)						
93	589	P	$C_9FH_{11}O$	$C_6H_5CHFCHOHCH_3$		47.1		15.5		1.50
				(Erythro)						
145	590		$C_9FH_{11}O$	$C_6H_5CHFCHOHCH_3$		47.0		15.5		
				(Erythro)						
93	591	P	$C_9FH_{11}O$	$C_6H_5CHFCHOHCH_3$		47.9		14.0		1.00
				(Threo)						
145	592		$C_9FH_{11}O$	$C_6H_5CHFCHOHCH_3$		47.6		14.4		
				(Threo)						
131	593	P	$C_9FH_{11}O$	para-$CH_3OC_6H_4CH_2CFH_2$		47.0		23.4		
91	594	G	$C_9FH_{17}O_2$	$CH_3(CH_2)_3CF(CH_3)CO_2CH_2CH_3$				20.6		
107	595		$C_9F_2H_8O$	$CH_3CF_2C(O)C_6H_5$				20		
154	596		$C_9F_2H_{10}$	$C_6H_5CHFCHFCH_3$	1,3	48	1,4	~14	1,5	1.6
	(3042)			(3)(1)(4)(2)(5)			2,3	~15		
				(Erythro)			2,5	23		
154	597		$C_9F_2H_{10}$	$C_6H_5CHFCHFCH_3$	1,3	48	1,4	14	1,5	<0.5
	(3042)			(3)(1)(4)(2)(5)			2,3	15		
				(Threo)			2,5	23		
108	598	G	$C_9F_2H_{10}O$	$C_6H_5CF_2CHOHCH_3$				10		
	(3043)									
88	599	E^2	$C_9F_2H_{14}N_6O_{10}$	$[FC(NO_2)_2CH_2NH(COCH_3)_2]CH_2$				17		
155	600	A	$C_9F_3H_6N$	$C_6H_5CH(CN)CF_3$				7		

Table A.1.a. (contd.)

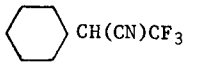
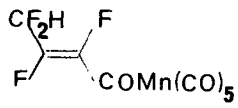
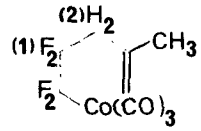
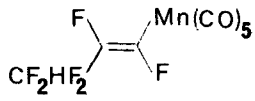
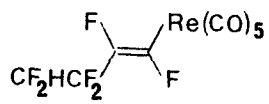
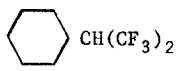
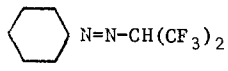
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
151	601 (3044)	B	$C_9F_3H_9O$	$CF_2HCF(OCH_3)C_6H_5$	56		3		
125	602		$C_9F_3H_{11}O_5$	$CH_3O_2CCH(CH_3)COCH(CF_3)CO_2CH_3$ (3) (2) (1)		1,2	8.3	1,3	6.4
155	603		$C_9F_3H_{12}N$				8		
199	604 [964 3314 3580]		$C_9F_4HMnO_6$		51.8				
156	605		$C_9F_4H_6FeO_2$	$CF_2HCF_2Fe(CO)_2\pi C_5H_5$	57.9		4.6		
200	606		$C_9F_4H_7CoO_3$			1,2	21.0 21.0		
151	607		$C_9F_4H_8$	$CH_3CF_2CF_2C_6H_5$			18		
199	608 [3589 3322 3588]		$C_9F_6HMnO_5$		53.5				
199	609		$C_9F_6HMnO_5$		60.0				
199	610 (3590)		$C_9F_6HO_5Re$		53.4				
201	611		$C_9F_6H_6N_2$	$(CF_3)_2CHC(CN)_2CH_2CH{=}CH_2$			8		
125	612		$C_9F_6H_{10}O_3$	$(CF_3)_2CHC(O)C(CH_3)_2CO_2CH_3$			7.4		
157	613		$C_9F_6H_{12}$				9		
157	614		$C_9F_6H_{12}N_2$				7		
126	615		$C_9F_6H_{12}S$	$(CF_3)_2CHSCH_2C(CH_3){=}C(CH_3)_2$			8		
113	616 (3068)		$C_9F_9H_7O_3$	$(CF_3)_2CHC(OCH_3){=}C(CF_3)CO_2CH_3$ (1) (3) (4) (2)		1,3	7	2,4	0.7
71	617 (6818)	H	$C_9F_9H_{12}ClSn$	$(CF_3CH_2CH_2)_3SnCl$			10.1		

Table A.1.a. (contd.)

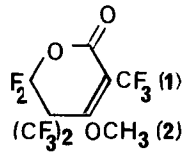
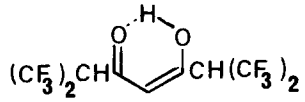
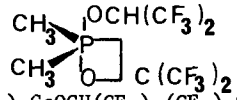
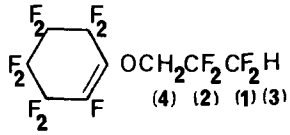
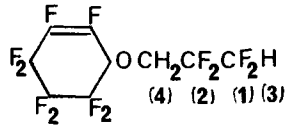
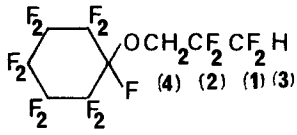
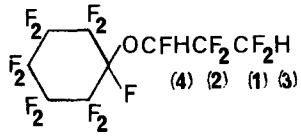
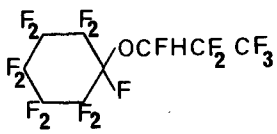
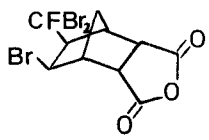
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
113	618 (3073)		$C_9F_{11}H_3O_3$					1,2	2
125	619	A	$C_9F_{12}H_4O_2$				7.7		
158	620	A	$C_9F_{12}H_9O_2P$				5.5		
128	621		$C_9F_{12}H_{10}O_2Ge$	$(CH_3)_3GeOCH(CF_3)_2(CF_3)_2CO$			6.1		
128	622		$C_9F_{12}H_{10}O_2Si$	$(CH_3)_3SiOCH(CF_3)_2(CF_3)_2CO$			5.8		
128	623		$C_9F_{12}H_{10}O_2Sn$	$(CH_3)_3SnOCH(CF_3)_2(CF_3)_2CO$			6.1		
159	624		$C_9F_{13}H_2O$		1,3	63	2,4 2,3	13.5 4	
159	625		$C_9F_{12}H_2O$		1,3	50	2,4 2,3	15 4	
116	626		$C_9F_{15}H_3O$		1,3	53	2,4 2,3	12 4	
116	627		$C_9F_{16}H_2O$		1,3	53	2,4 2,3	5 5	
116	628		$C_9F_{17}HO$			53		5	
296	629	E	$C_{10}FH_8Br_3O_3$	 (-50°C)					

Table A.1.a. (contd.)

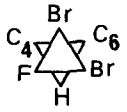
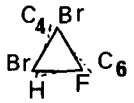
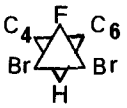
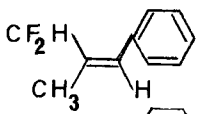
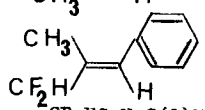
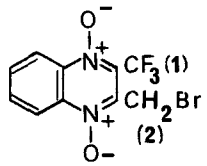
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
								13.5 Angle HF = 60		
								∿ 0 Angle HF = 90		
								33.5 Angle HF = 180		
153	630	P	$C_{10}FH_{10}ClO_2$	$C_6H_5CFHCHClCO_2CH_3$ (Threo)		46.9		14.9		
104	631	G-P	$C_{10}FH_{11}O_3$	$C_6H_5CFHCHOHCO_2CH_3$ (Erythro)		45		15		
145	632		$C_{10}FH_{13}O$	$(CH_3)_2CFCHOHC_6H_5$ (1)(2)			1,2	11.5		
145	633		$C_{10}FH_{13}O$	$C_6H_5CHFCOH(CH_3)_2$		45.8				
154	634		$C_{10}FH_{13}O$	$CH_3CFHCH(OCH_3)C_6H_5$ (3)(1)(2)(4)(5)	1,2	47	1,3 1,4	24 8	1,5	<0.5
160	635		$C_{10}FH_{21}N_2$	$CH_3CFHN{=}NC(CH_3)_2CH_2C(CH_3)_3$		56		22		
161	636	G	$C_{10}F_2H_{10}$			56				
161	637	G	$C_{10}F_2H_{10}$			56				
147	638		$C_{10}F_2H_{11}NO$	para-$CF_2HC_6H_4C(O)N(CH_3)_2$		57				
151	639		$C_{10}F_2H_{12}O_2$	$C_6H_5C(OCH_3)_2CF_2H$		56				
88	640	G	$C_{10}F_2H_{17}N_5O_{10}$	$[FC(NO_2)_2CH_2]_2NCH_2CH(OCH_2CH_3)_2$				17		
162	641		$C_{10}F_2H_{20}$	$(CH_3(CH_2)_3CHF)_2$		50		20		
163	642	I^2	$C_{10}F_3H_6BrN_2O_2$						1,2	1.3

Table A.1.a. (contd.)

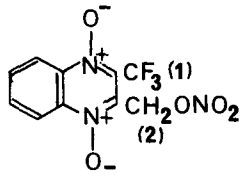
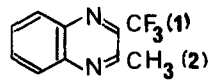
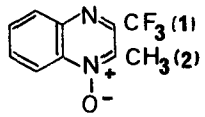
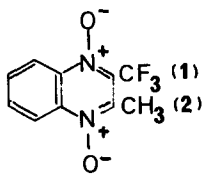
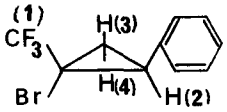
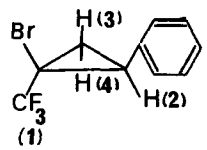
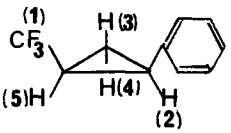
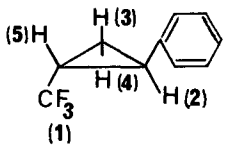
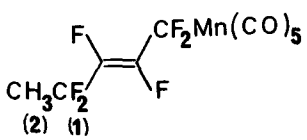
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ
163	643	A	$C_{10}F_3H_6N_3O_5$				1,2	2.0
163	644	A	$C_{10}F_3H_7N_2$				1,2	1.6
163	645	A	$C_{10}F_3H_7N_2O$				1,2	1.2
163	646	A	$C_{10}F_3H_7N_2O_2$				1,2	3.0
275	647	A*	$C_{10}F_3H_8Br$				1,2 1,3 1,4	0.93 -0.03 1.62
275	648	A*	$C_{10}F_3H_8Br$				1,3 1,4	1.35 -0.03
275	649	A*	$C_{10}F_3H_9$		1,5	7.49	1,2 1,3 1,4	0.99 0.27 1.36
275	650	A*	$C_{10}F_3H_9$		1,5	6.59	1,2 1,3 1,4	0.51 1.09 0.43
151	651	B	$C_{10}F_3H_{11}O$	$C_6H_5CF(OCH_3)CF_2CH_3$ (2) (1) (3)	1,3	19	2,3	1.5
164	652 [971 3082 3331 3595]		$C_{10}F_6H_3MnO_5$		1,2	18.8		

Table A.1.a. (contd.)

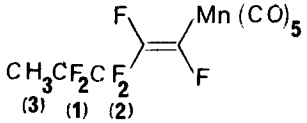
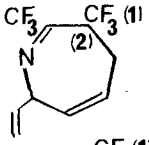
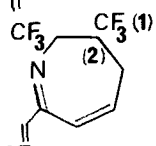
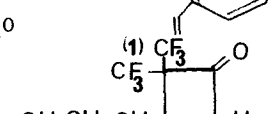
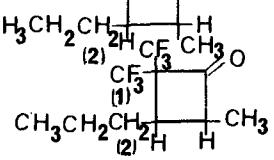
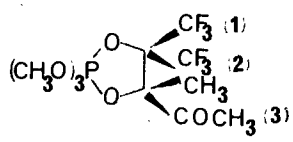
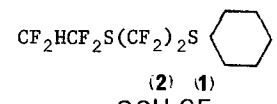
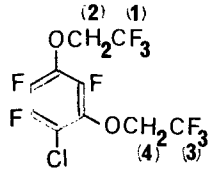
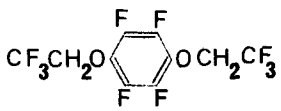
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
164	653 [972 3332 3596]		$C_{10}F_6H_3MnO_5$		1,3 18.2	2,3 2.4	
215	654 (3089)		$C_{10}F_6H_9N$		1,2 10		
215	655 (3090)		$C_{10}F_6H_9N$		1,2 9.5		
117	656 (3092)	B	$C_{10}F_6H_{12}O$			1,2	<1
117	657 (3091)	B	$C_{10}F_6H_{12}O$			1,2	1.0
117	658	E	$C_{10}F_6H_{12}O_2$	$(CF_3)_2CHC(O)C(CH_3)=CHO(CH_2)_2CH_3$		7.5	
165	659	A	$C_{10}F_6H_{15}O_6P$			1,2 2.0 1,3 0.8	
166	660		$C_{10}F_8HMnO_6$	$CF_2H(CF_2)_3C(O)Mn(CO)_5$	50		
152	661 (3098)		$C_{10}F_8H_{12}S_2$		54	3.5	
197	662 (4199)		$C_{10}F_9H_4ClO_2$			1,2 8.7 3,4 8.7	
113	663		$C_{10}F_9H_9O_3$	$(CF_3)_2C{=}C(OCH_3)CH(CF_3)CO_2CH_2CH_3$ (3) (2)(1)		1,2 7	1,3 2
71	664 (6821)	H	$C_{10}F_9H_{15}OSn$	$(CF_3CH_2CH_2)_3SnOCH_3$		10.5	
71	665 (6822)	H	$C_{10}F_9H_{15}Sn$	$(CF_3CH_2CH_2)_3SnCH_3$		10.3	
197	666		$C_{10}F_{10}H_4O_2$			9.0	

Table A.1.a. (contd.)

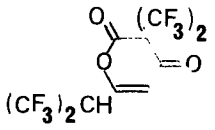
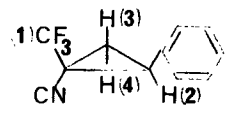
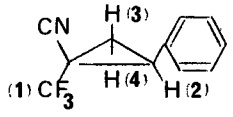
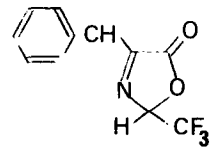
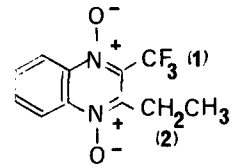
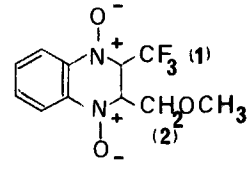
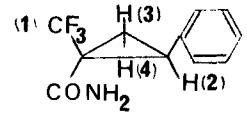
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
125	667	A	$C_{10}F_{12}H_2O_3$			7.2	
198	668		$C_{10}F_{14}H_6$	$CF_3CF_2CH_2CH_2CF_2CF_2CH{=}CHCF_2CF_3$ (1)(3)(4)(2)		1,3 15.5 2,4 ∿15	
198	669		$C_{10}F_{14}H_8$	$(CF_3CF_2CH_2CH_2CF_2)_2$ (1) (2)		1,2 ∿17	
83	670		$C_{10}F_{18}H_4S_4$	$(CF_3)_2CHSC(CF_3)_2SC(CF_3)_2S_2CH_3$		7	
121	671		$C_{11}FH_{12}BrO_2$	$C_6H_5CFHCHBrCO_2CH_2CH_3$	45.6	17.5	
91	672	G	$C_{11}FH_{13}O_2$	$C_6H_5CH_2CFHCO_2CH_2CH_3$	48.9	20.7 29.2	
104	673	G-P	$C_{11}FH_{13}O_3$	$C_6H_5C(CH_3)FCHOHCO_2CH_3$ (Threo)		22.9 20.4	
88	674	A	$C_{11}F_2H_{11}N_5O_8$	$[FC(NO_2)_2CH_2]_2NCH_2C_6H_5$		17	
151	675	B	$C_{11}F_2H_{14}O_2$	$C_6H_5C(OCH_3)_2CF_2CH_3$		16	
275	676	A*	$C_{11}F_3H_8N$				1,2 1.33 1,3 -0.15 1,4 1.6
275	677	A-H	$C_{11}F_3H_8N$				1,2 0.50 1,3 1.30 1,4 -0.34
110	678	G	$C_{11}F_3H_3NO_2$			∿ 4.5	
163	679	A	$C_{11}F_3H_9N_2O_2$				1,2 2.1
163	680	A	$C_{11}F_3H_9N_2O_3$				1,2 2.0
275	681	A*	$C_{11}F_3H_{10}NO$				1,2 1.24 1,3 -0.06 1,4 1.94

Table A.1.a. (contd.)

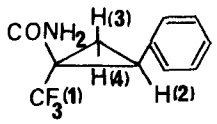
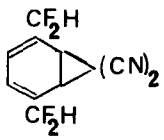
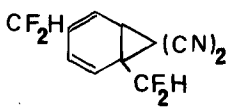
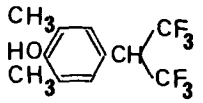
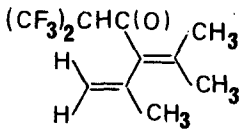
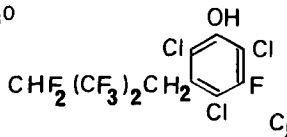
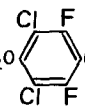
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
275	682	A*	$C_{11}F_3H_{10}NO$				1,3 1.96 1,4 -0.01
300	683	A	$C_{11}F_3H_{19}$			7.4	
		D				7.2	
		E				8.0	
		P				7.4	
		E^2				7.8	
300	684	A	$C_{11}F_3H_{19}$			11.1	
		D				10.9	
		E				11.3	
		P				11.1	
		E^2				11.5	
167	685 (3108)	E	$C_{11}F_3H_6N_2$		54.1		
167	686	E	$C_{11}F_4H_6N_2$		55		
1083	687 (884, 3111)	P	$C_{11}F_6H_{10}O$			8.4	
125	688	B	$C_{11}F_6H_{12}O$			8.0	
83	689		$C_{11}F_6H_{21}NO_3S_2$	$(CF_3)_2CHSSO_3^-\overset{+}{N}(CH_2CH_3)_4$		8	
892	690	B	$C_{11}F_9H_4Cl_3O$		54.0	12.2	
197	691		$C_{11}F_{10}H_3Cl_3O$	$CF_2HCF_2CF_2CF_2CH_2O$  (1)(3) (2)(4)	1,3 54.0	2,4	12.2
197	692 (4444)		$C_{11}F_{13}H_3O$	$CF_2HCF_2CF_2CF_2CH_2OC_6F_5$ (1)(3) (2)(4)	1,3 54.0	2,4	14.0
83	693		$C_{11}F_{18}H_6S_4$	$(CF_3)_2CHSC(CF_3)_2SC(CF_3)_2S_2CH_2CH_3$			7
91	694	G	$C_{12}FH_{15}O_2$	$C_6H_5CH_2CF(CH_3)CO_2CH_2CH_3$ (3,4)(1)(2)		1,2 1,3 1,4	20.3 25.5 20.9

Table A.1.a. (contd.)

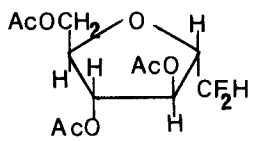
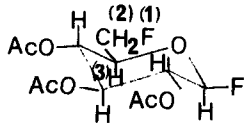
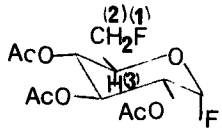
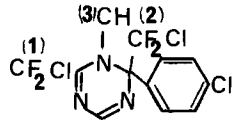
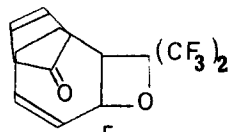
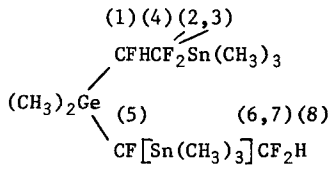
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
144	695	G	$C_{12}FH_{16}N$	$C_6H_5CFHCH_2N$		48	∿29 ∿20			
160	696		$C_{12}FH_{25}N_2$	$(CH_3)_2CHCFHN{=}N{-}C(CH_3)_2CH_2C(CH_3)_2$		56		20		
361	697	A	$C_{12}F_2H_{16}O_7$			55		12		
378	698 (1716 3119)	A	$C_{12}F_2H_{16}O_7$		1,2	46.6†	1,3	20.6		
378	699 (1715 3118)	A	$C_{12}F_2H_{16}O_7$		1,2	47.0†	1,3	23.9		
168	700	H	$C_{12}F_3H_2Co_3O_9$	$CF_2CH_2C(Co)_3(CO)_9$				9.5		
169	701		$C_{12}F_4H_3Cl_3N_3$						1,3 2,3	1.9 1.9
202	702		$C_{12}F_6H_8O_2$							2 0.8
187	703		$C_{12}F_6H_{26}GeSn_2$	$(CH_3)_2Ge\left[\underset{(3)}{CF}\left[Sn(CH_3)_3\right]\underset{(1,2)(4)}{CF_2H}\right]_2$	1,4 2,4	65 58	3,4	10		
187	704		$C_{12}F_6H_{26}GeSn_2$	$(CH_3)_2Ge\left[\underset{(1)(4)(2,3)}{CFHCF_2Sn(CH_3)_3}\right]_2$	1,4	45	2,4 3,4	42 5		
187	705		$C_{12}F_6H_{26}GeSn_2$		1,4 6,8 7,8	45 60 56	2,4 3,4 5,8	42 5 10		

Table A.1.a.

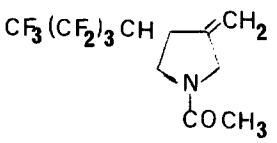
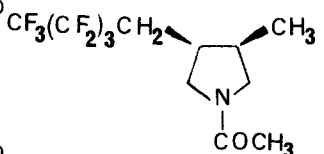
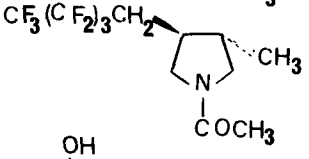
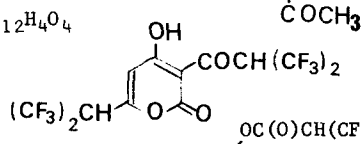
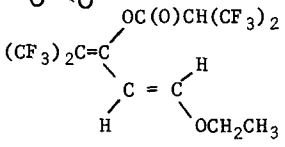
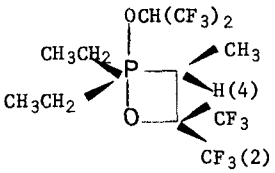
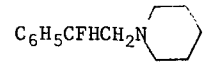
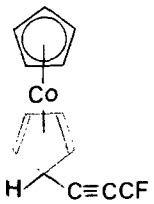
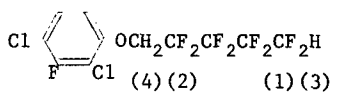
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
170	705	G	$C_{12}F_9H_{12}NO$				20		
170	707	G	$C_{12}F_9H_{14}NO$				20		
170	708	G	$C_{12}F_9H_{14}NO$				20		
25	709	A	$C_{12}F_{12}H_4O_4$			1,3 2,4	7.5 7.5		
117	710 (3131)	B	$C_{12}F_{12}H_8O_3$	 (3) (1)			8.0		
158	711 (3133)	A	$C_{12}F_{12}H_{15}O_2P$			1,3	7.2	2,4	2.3
71	712 (6826)	H	$C_{12}F_{12}H_{16}Sn$	$(CF_3CH_2CH_2)_4Sn$			10.6		
104	713	G-P	$C_{13}FH_{17}O_3$	$C_6H_5C(CH_3)FC(CH_3)OHCO_2CH_2CH_3$ (Erythro)			22.2		2.0
144	714	G	$C_{13}FH_{18}N$		48		28.5 19.5		
29 88	715	A	$C_{13}F_2H_{20}N_6O_{12}$	$[FC(NO_2)_2CH_2NHCHCO_2CH_2CH_3]_2CH_2$			19.0		
168	716		$C_{13}F_3H_{10}Co$						2.8
197	717		$C_{13}F_{11}H_6Cl_3O_2$	$H(CF_2)CH_2O$  (4)(2) (1)(3)	1,3	54.1	2,4	12.0	

Table A.1.a. (contd.)

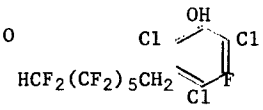
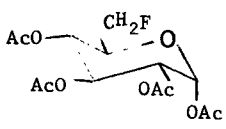
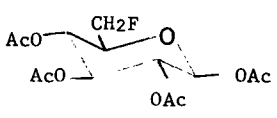
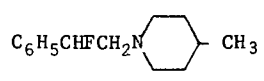
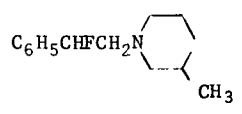
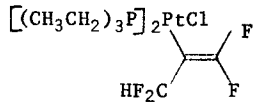
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
892	718		$C_{13}F_{13}H_4Cl_3O$		54.1	12.1	
107	719		$C_{14}FH_{11}O$	$C_6H_5CFHC(O)C_6H_5$	51		
145	720		$C_{14}FH_{13}O$	$C_6H_5CFHCHOHC_6H_5$ (Erythro)	45.7	13.0	
93	721	P	$C_{14}FH_{13}O$	$C_6H_5CFHCHOHC_6H_5$ (Erythro)	45.9	12.8	
145	722		$C_{14}FH_{13}O$	$C_6H_5CFHCHOHC_6H_5$ (Threo)	47.2	13.6	
93	723	P	$C_{14}FH_{13}O$	$C_6H_5CFHCHOHC_6H_5$ (Threo)	48.0	13.1	
378	724	A	$C_{14}FH_{19}O_9$		46.9†	23.1	
378	725	A	$C_{14}FH_{19}O_9$		47.0 46.8	21.9	
144	726	G	$C_{14}FH_{20}N$		47.5	28.5 19	
144	727	G	$C_{14}FH_{20}N$	 I II	48 48	29 ∿19 29 19.0	
171	728 (3145)		$C_{14}F_2H_{12}$	$(C_6H_5)_2CFCFH_2$	48	∿20	
172	729		$C_{14}F_2H_{26}O_4P_2Pt_2$	$[CH_2{=}CH(CH_2)_3PH_2Pt(O_2CCH_2F)]_2$	48		
171	730 (3147)		$C_{14}F_3H_{11}$	$(C_6H_5)_2CFCF_2H$	52		
128	731		$C_{14}F_{24}H_8O_4Sn$	$(CH_3)_2Sn[OCH(CF_3)_2]_2.2(CF_3)_2CO$		6.0	
173	732 (3614, 6574)		$C_{15}F_4H_{31}ClP_2Pt$		55		
83	733		$C_{15}F_6H_{29}NO_3S_2$	$(CF_3)_2CHSSO_3^{-+}N(CH_2CH_2CH_3)_4$		8	
71	734 (6838)	H	$C_{15}F_9H_{17}Sn$	$(CF_3CH_2CH_2)_3SnC_6H_5$		10.1	

Table A.1.a. (contd.)

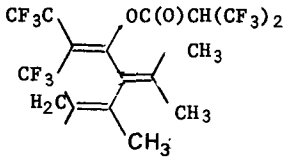
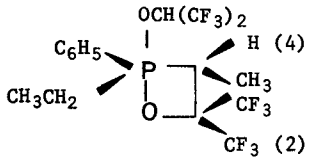
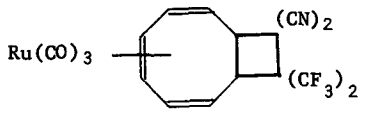
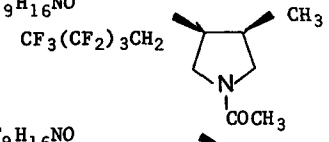
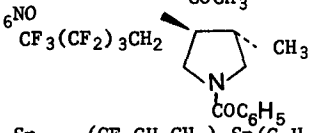
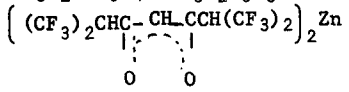
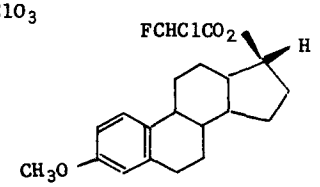
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
125	735 (3158)		$C_{15}F_{12}H_{12}O_2$			7.3	
174	736	B	$C_{15}F_{24}H_6O_3$	$[HCF_2CF_2(CF_2)_3CF_2CH_2O]_2C(O)$			
				(4)(1)(2) (3) (5) 1,4	51.2	2,4 6.0	
						3,5 13.2	
91	737	G	$C_{16}FH_{15}O_2$	$C_6H_5CH_2CF(C_6H_5)CO_2CH_3$		1,2 28.8	
				(2,3)(1)		1,3 20.2	
				(3)(1)			
158	738 (3164)	A	$C_{16}F_{12}H_{15}O_2P$			1,3 5	2,4 2
202	739 (3167)		$C_{17}F_6H_8N_2O_3Ru$				5.0 0.0
170	740	G	$C_{17}F_9H_{16}NO$			19	
170	741	G	$C_{17}F_9H_{16}NO$			19	
71	742 (6841)	H	$C_{18}F_6H_{18}Sn$	$(CF_3CH_2CH_2)_2Sn(C_6H_5)_2$		10.3	
175	743	H	$C_{18}F_{12}H_{10}$	$(CF_3)_2CHC_6H_4C(CF_3)_2C_6H_5$		9	
125	744	E	$C_{18}F_{24}H_6O_4Zn$			8.5	
176	745	A	$C_{19}FH_{37}O_2$	$CH_3(CH_2)_5CHF(CH_2)_{10}CO_2CH_3$	49.1		
177	746 (6438 6588)	A	$C_{19}F_5H_{25}I_2P_2Pt$	$[(P(CH_3)_2C_6H_5]_2PtI_2(CH_3)CF_2CF_3$ (2) (1)			1,2 1.1
315	747	A	$C_{20}FH_{24}ClO_3$		51		

Table A.1.a. (contd.)

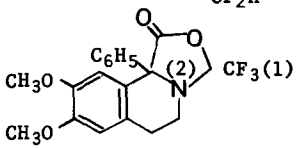
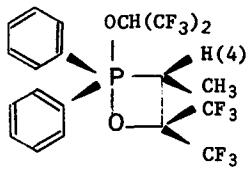
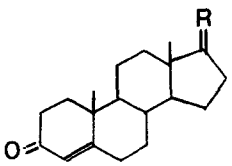
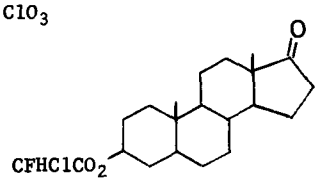
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
178	748 (3177)	M	$C_{20}F_2H_{16}Cl_5OSb$	$(C_6H_5)_2{}^+C$–(C$_6$H$_3$)–CF_2H $SbCl_5OH^-$	56		
350	749		$C_{20}F_3H_{18}NO_4$			1,2 6.5	
177	750 (6590)	A	$C_{20}F_3H_{30}As_2IPt$	$CF_3CH_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$ (1)(2) (3)		1,2 15	1,3 1.1
177	751 (6591)	A	$C_{20}F_3H_{30}IP_2Pt$	$CF_3CH_2PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$		1,2 15	
158	752 (3179)	A	$C_{20}F_{12}H_{15}O_2P$	(3) (1) 		1,3 6	2,4 3.0
315	753	A	$C_{21}FH_{28}O_3$				
				R = αH, β $O_2CCFHCl$	50.8		
				R = α$O_2CCFHCl$, β H	51.1		
315	754	A	$C_{21}FH_{30}ClO_3$		50.7		
71	755 (6843)	H	$C_{21}F_3H_{19}Sn$	$CF_3CH_2CH_2Sn(C_6H_5)_3$		10.2	
177	756 (6594)	A	$C_{21}F_5H_{30}As_2IPt$	$CF_3CF_2CH_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$ (1)(2) (3)			1,3 1.4
177	757 (6595)	A	$C_{21}F_5H_{30}IP_2Pt$	$CF_3CF_2CH_2PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$ (1)(2) (3)		1,2 25	
177	758 (3180 / 6596)	A	$C_{21}F_7H_{28}As_2IPt$	$CF_3CF_2CF_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$			1.4
177	759	A	$C_{22}F_7H_{30}As_2IPt$	$CF_3CF_2CF_2CH_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$			1.2

Table A.1.a.

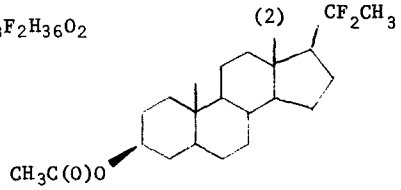
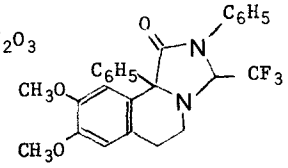
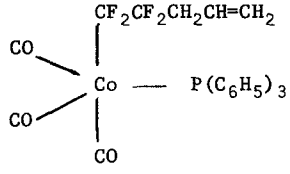
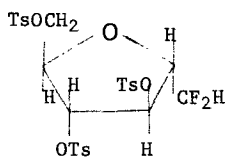
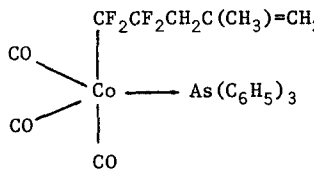
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
174	760	B	$C_{22}F_{36}H_{10}O_3$	$(HCF_2CF_2(CF_2)_2CF_2CH_2O)_3H$					
				(4)(1)(2) (3)(5)	1,4	47.8	2,4	4.9	
							3,5	12.2	
313 346	761		$C_{23}F_2H_{36}O_2$						1,2 2
124	762 (3187 6464)		$C_{23}F_4H_{16}CoO_3$	$HCF_2CF_2Co(CO)_3P(C_6H_5)_3$		57.0		5.5	
177	763 (3191 6602)	A	$C_{25}F_{15}H_{28}As_2IPt$	$CF_3(CF_2)_5CF_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$					1,2 1.6
350	764		$C_{26}F_3H_{23}N_2O_3$					6.5	
200	765 (6490)	A	$C_{26}F_4H_{20}CoO_3P$					19.0	
179	766	A	$C_{27}FH_{25}O_2PRh$	$FCH_2CO_2Rh[P(C_6H_5)_3]$ 		48			
361	767	A	$C_{27}F_2H_{28}O_{10}S_3$			54		12	12 (?)
				(Ts = para-$CH_3C_6H_4SO_2$)					
200	768	A	$C_{27}F_4H_{22}AsCoO_3$					19.0	

Table A.1.a. (contd.)

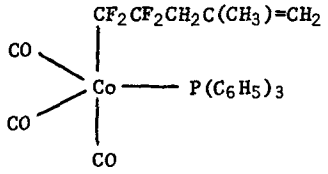
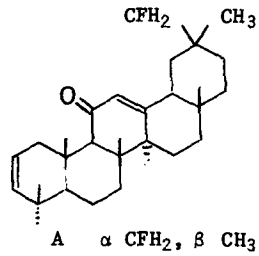
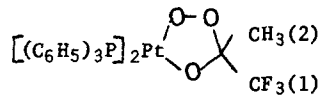
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
200	769 (6505)	A	$C_{27}F_4H_{22}CoO_3P$			19.0	
174	770	B	$C_{28}F_{36}H_{14}O_3$	$(CF_2HCF_2(CF_2)_3CF_2CH_2O)_3CC_6H_5$			
				(1)(4)(2) (3)(5) 1,4	48.5	2,4 4.5	
						3,5 12.0	
174	771	B	$C_{29}F_{48}H_{12}O_4$	$(CF_2HCF_2(CF_2)_3CF_2CH_2O)_4C$ 1,4	48.2	2,4 5.1	
				(1)(4)(2) (3)(5)		3,5 12.0	
345	772	A	$C_{30}FH_{44}O$				
				A α CFH_2, β CH_3	~49		
				B α CH_3, β CFH_2	~49		
180	773		$C_{38}F_4H_{31}Cl_2P_2Rh$	$CF_2HCF_2RhCl_2[P(C_6H_5)_3]_2$	52	7	
181	774	J	$C_{39}F_3H_{33}O_3P_2Pt$				1,2 1.7

Table A.1.b. Fluorine bonded to sp^3 carbon, hydrogen bonded to sp^2 carbon other than carbonyl.

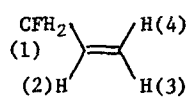
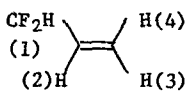
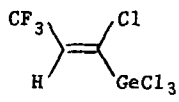
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
57	775 (132)	*	C_3FH_5		1,2 14.53	1,3 -0.89	
						1,4 -4.32	
57	776 (151)	*	$C_3F_2H_4$		1,2 8.63	1,3 -0.14	
						1,4 -3.66	
65	777		$C_3F_3HCl_4Ge$		6.5		

Table A.1.b. (contd.)

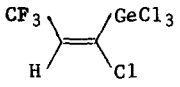
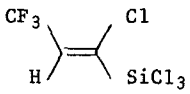
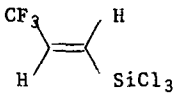
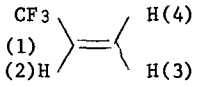
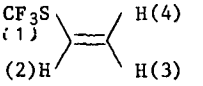
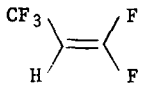
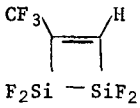
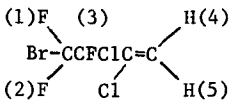
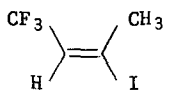
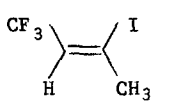
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J	^5J
65	778		$C_3F_3HCl_4Ge$			8.3			
65	779		$C_3F_3HCl_4Si$			6.6			
65	780		$C_3F_3H_2Cl_3Ge$	$CF_3CH{=}CHGeCl_3$ (trans and cis)		4.4			
65	781		$C_3F_3H_2Cl_3Si$			5.5			
57	782	*	$C_3F_3H_3$		1,2	6.28	1,3 1,4	+0.03 -2.22	
225	783	B	$C_3F_3H_3S$				1,2	~0	1,3 1.4 1,4 0.6
77	784 1017 3460 3229		C_3F_5H			6.7			
203	785 (2469 4855)		$C_3F_7HSi_2$					1.6	
						^4J		^5J	^5J
204	786 (2782)	B* E* G* H* M*	$C_4F_3H_2BrCl_2$		3,4	+2.41 +2.41 +2.41 +2.47 +2.40	1,4	<0.05 <0.04 <0.05 <0.05 <0.05	1,5 0.51 0.54 0.50 0.48 0.52
		B* E* G* H* M*			3,5	+5.24 +5.31 +5.30 +5.27 +5.30	2,4	0 0 0 0 0	2,5 0.0 0.0 0.0 0.0 0.0
440	787 (286)	B	$C_4F_3H_4I$			7.1			
440	788 (287)	B	$C_4F_3H_4I$			7.7			
67	789		$C_4F_3H_4NO_2$	$CF_3C(CH_3){=}CHNO_2$				1.45	

Table A.1.b. (contd.)

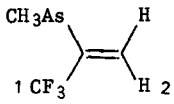
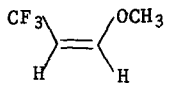
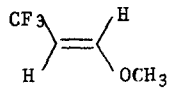
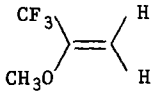
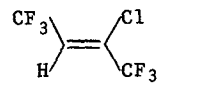
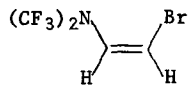
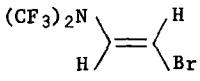
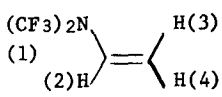
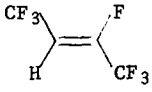
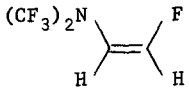
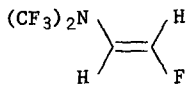
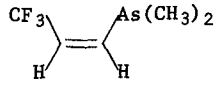
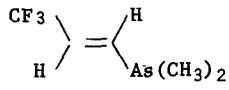
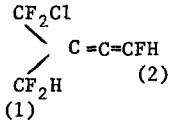
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ
127	790		$C_4F_3H_5As$			1,2	2		
205	791		$C_4F_3H_5O$		8.2				
205	792		$C_4F_3H_5O$		6.3		2.0		
205	793		$C_4F_3H_5O$				1.8		
206	794 (2798)	B	C_4F_6HCl		6.6		~1		
119	795	B	$C_4F_6H_2BrN$				5.5		
119	796	B	$C_4F_6H_2BrN$				1.5		0.7
207	797		$C_4F_6H_3N$			1,2	1.85	1,3 1,4	0.8 0.5
206	798 (1022 / 3250)		C_4F_7H		6.8				
101	799 (1025 / 3254)		$C_4F_7H_2N$				1.7		
101	800 (1026)		$C_4F_7H_2N$				1.4		
127	801		$C_5F_3H_8As$		8				
127	802		$C_5F_3H_8As$		6		2		
192	803 (1039 / 3256)		$C_5F_5HCl_2$	$(CF_2Cl)_2C{=}C{=}CFH$ (1) (2)				1,2	1.1
92	804 (360 / 1040)		$C_5F_5H_2Cl$					1,2	3

Table A.1.b. (contd.)

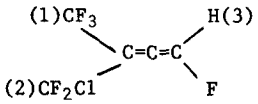
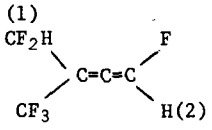
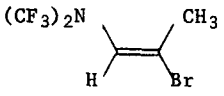
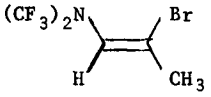
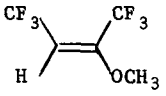
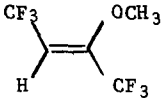
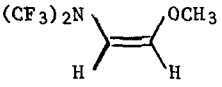
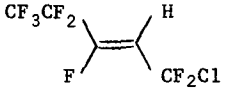
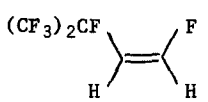
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
192	805 (362, 1041)		$C_5F_5H_3$	$(CF_2H)_2C{=}C{=}CFH$ (1) (2)					1,2	3
192	806 (1042, 3266)		C_5F_6HCl						1,3 2,3	1.1 1.2
192	807 (363, 1044)		$C_5F_6H_2$						1,2	3
101	808		$C_5F_6H_4BrN$					1.9		
101	809		$C_5F_6H_4BrN$					1.8		
205	810 (2859)		$C_5F_6H_4O$			8				
205	811		$C_5F_6H_4O$			8				
207	812		$C_5F_6H_5NO$					1.9		
192	813 (1045, 3269)		C_5F_7H	$(CF_3)_2C{=}C{=}CFH$						1.2
208	814 [1046, 2871, 3273]	P	C_5F_8HCl			10.2				
209	815 [1047, 2872, 3274]		$C_5F_8H_2$	(1) (2)  (3) (4)	2,3	22.8	2,4 1,3	2.1 0.8	1,4	0

Table A.1.b. (contd.)

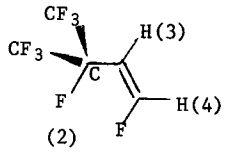
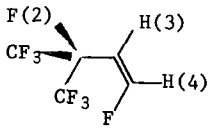
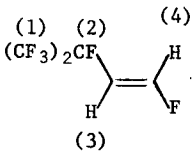
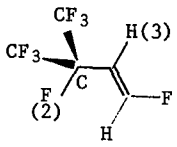
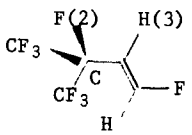
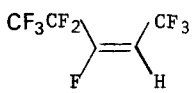
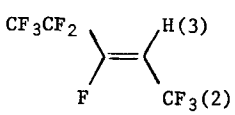
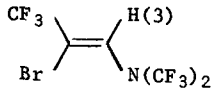
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
				 (2)	2,3	23.9	2,4	±2.2		
					2,3	4.1 (±2)	2,4	±0.1 (±0.3)		
209	816 [1048 2873 3275]		$C_5F_8H_2$	 (3)	2,3	21.1	2,4 1,3	∿0 ∿0	1,4	∿0
					2,3	25.0 (±0.7)				
					2,3	3.9 (±1)				
190	817 [1049 2880 3279]		C_5F_9H			7.8		0.5		
190	818 [1050 2881 3280]		C_5F_9H	(1) 			1,3 2,3	1.9 7.0		
120	819		C_5F_9HBrN	(1) 			1,3 2,3	1.1 2.0		

Table A.1.b. (contd.)

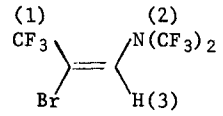
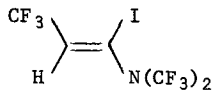
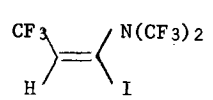
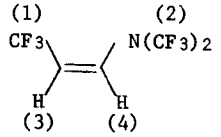
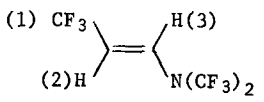
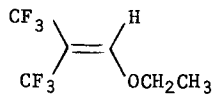
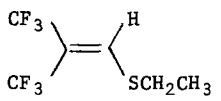
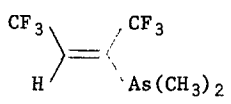
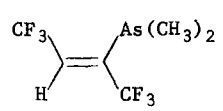
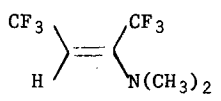
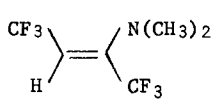
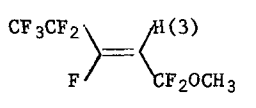
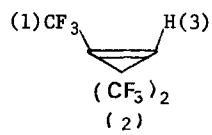
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ
120	820		C_5F_9HBrN				1,3	1.0	
	(2882)						2,3	0.8	
119	821		C_5F_9HIN			6.6			
119	822		C_5F_9HIN			6.4			
	(2883)								
120	823		$C_5F_9H_2N$		1,3	6.6	1,4	2.5	
	(2885)						2,4	2.0	
119	824		$C_5F_9H_2N$		1,2	6.3	1,3	2.3	
210	825	J^2	$C_6F_6H_6O$					0.9	
	(2915)	H						1.6	
210	826		$C_6F_6H_6S$					1.3	
	(2915)								
211	827		$C_6F_6H_7As$			8.3		≤1	
127									
211	828		$C_6F_6H_7As$			8.3		2.0	
127	(2916)								
211	829		$C_6F_6H_7N$			9.1		≤1	
127									
211	830		$C_6F_6H_7N$			9.1		≤1	
127	(415)								
190	831		$C_6F_8H_4O$		1,3	7.1			
	1082				2,3	7.2			
	2925								
	3290			(1,2)					
115	832		C_6F_9H				1,3	1.3	
	(2927)						2,3	1.0	

Table A.1.b. (contd.)

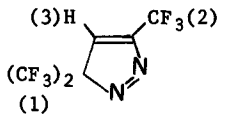
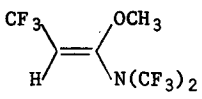
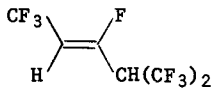
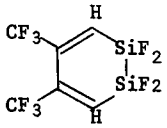
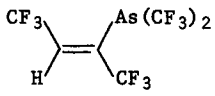
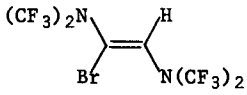
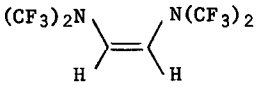
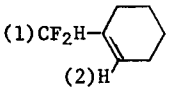
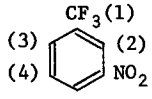
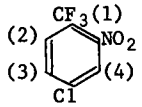
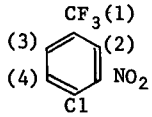
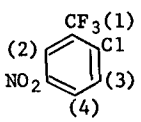
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
115	833		$C_6F_9HN_2$			1,3 2.4 2,3 5.7	
120	834		$C_6F_9H_4NO$		7.2		
113	835 [953 427 1083 3294]		$C_6F_{10}H_2$		7		
203	836 (4857)		$C_6F_{10}H_2Si_2$			0.6	
211	837		$C_6F_{12}HAs$		7.5	1.5	
119 120	838		$C_6F_{12}HBrN_2$			2.0	
120	839		$C_6F_{12}H_2N_2$			0.8	
139	840 (462)		$C_7F_2H_{10}$				1,2 1.0
212	841	E	$C_7F_3H_3BrNO_2$			1,2 -0.58 1,3 -0.68	1,4 0.82
212	842	E	$C_7F_3H_3ClNO_2$			1,2 -0.65	1,3 0.50 1,4 0.61
212	843	E	$C_7F_3H_3ClNO_2$			1,2 -0.68 1,3 -0.67	1,4 0.90
212	844	E	$C_7F_3H_3ClNO_2$			1,2 -0.55	1,3 0.74 1,4 0.49

Table A.1.b. (contd.)

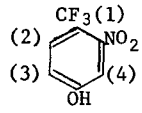
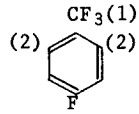
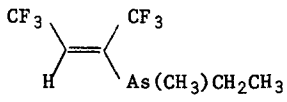
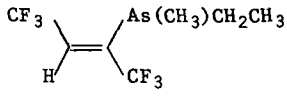
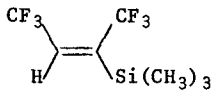
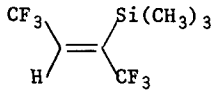
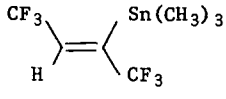
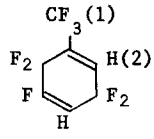
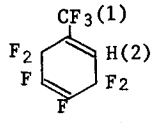
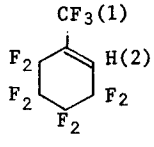
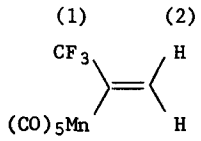
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J		^nJ	
212	845	E	$C_7F_3H_4NO_3$			1,2	-0.58	1,3 1,4	0.49 0.49
61	846 (1841 3355)		$C_7F_4H_4$			1,2	0.5		
211	847		$C_7F_6H_9As$		8.5		≤1		
211	848		$C_7F_6H_9As$		8.5		2.0		
211	849		$C_7F_6H_{10}Si$		8.6		≤0.6		
211	850		$C_7F_6H_{10}Si$		8.8		2.5		
211	851		$C_7F_6H_{10}Sn$		7.5		2.3		
213	852 [1333 2969 3940 3299]		$C_7F_8H_2$			1,2	1		
213	853 (2971)		C_7F_9H			1,2	1.2		
213	854 (2976)		$C_7F_{11}H$			1,2	1.1		
168	855		$C_8F_3H_2O_5Mn$			1,2	2		

Table A.1.b. (contd.)

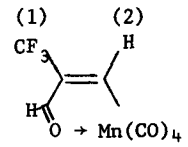
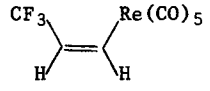
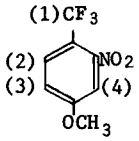
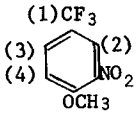
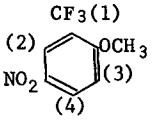
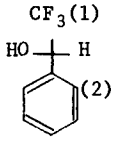
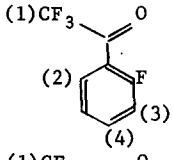
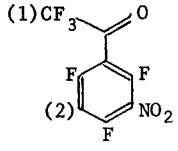
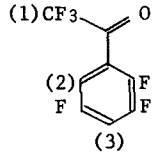
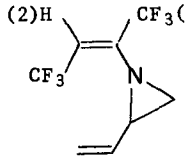
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
168	856		$C_8F_3H_2O_5Mn$			1,2 1.5	
214	857		$C_8F_3H_2O_5Re$		8.5		
212	858	E	$C_8F_3H_6NO_3$			1,2 -0.61	1,3 0.51 1,4 0.58
212	859	E	$C_8F_3H_6NO_3$			1,2 -0.71 1,3 -0.72	1,4 0.77
212	860	E	$C_8F_3H_6NO_3$			1,2 -0.65	1,3 0.76 1,4 -0.54
148	861 (532)	G	$C_8F_3H_7O$				1,2 0.7
401	862 (3362)		$C_8F_4H_4O$				1,2 0.6 1,3 0.6 1,4 0.6
401	863 (3363)		$C_8F_6HNO_3$				1,2 0.6
401	864 (3364)		$C_8F_6H_2O$				1,2 0.6 1,3 0.6
117	865	B	$C_8F_6H_6O_2$	$(CF_3)_2C{=}C{=}CHCO_2CH_2CH_3$ (1) (2)			1,2 2.5
215	866 (3011)		$C_8F_6H_7N$			1,2 9.2	

Table A.1.b. (contd.)

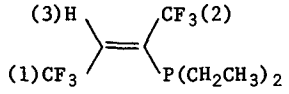
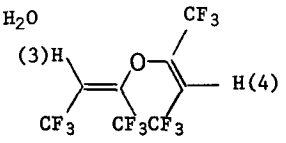
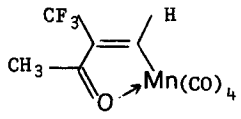
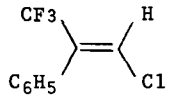
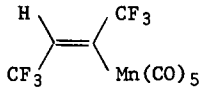
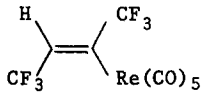
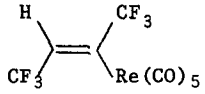
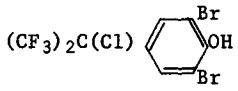
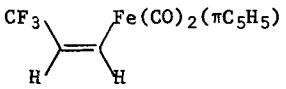
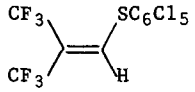
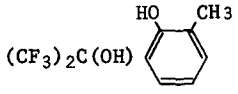
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J	^nJ
206	867 (6257)	B	$C_8F_6H_{11}P$		1,3	7.5	2,3	1.7	
206	868 (3034)	B	$C_8F_{12}H_2O$	 (1) (2)	1,3 2,4	7.8 7.1			
168	869		$C_9F_3H_4MnO_5$					1.8	
150	870	B	$C_9F_3H_6Cl$					1.1	
216	871	B	$C_9F_3H_{11}BrCl_3$	$CCl_3CF_2CFBrCH{=}CH(CH_2)_3CH_3$		13.5			
211	872		$C_9F_6HMnO_5$			9.6		2.3	
211	873		$C_9F_6HO_5Re$			9.1		2.5	
137	874		$C_9F_6HO_5Re$			9.1		2.5	
1083	875		$C_9F_6H_3Br_2ClO$						0.7
214	876	B	$C_{10}F_3H_7FeO_2$			8.5			
210	877 (3081)	A	$C_{10}F_6HCl_5S$					1.4	
1083	878		$C_{10}F_6H_8O_2$						1.1

Table A.1.b. (contd.)

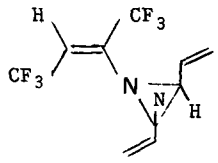
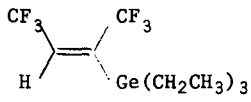
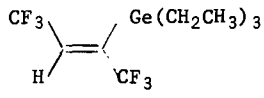
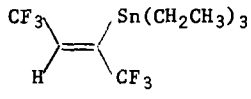
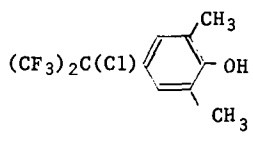
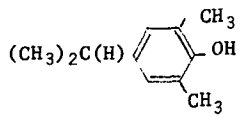
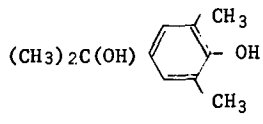
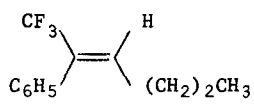
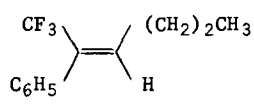
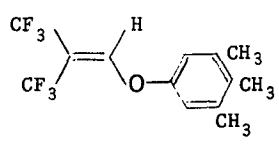
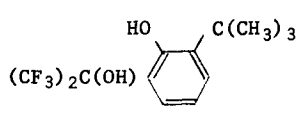
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
215	879 (3088)		$C_{10}F_6H_9N$		9.2		
211	880		$C_{10}F_6H_{10}Ge$		8.0	≤1	
211	881		$C_{10}F_6H_{16}Ge$		8.0	2.5	
211	882		$C_{10}F_6H_{16}Sn$		7.5	2.5	
1083	883		$C_{11}F_6H_9ClO$				0.8
1083	884 (687, 3111)		$C_{11}F_6H_{10}O$				0.6
1083	885		$C_{11}F_6H_{10}O_2$				1.1
217	886		$C_{12}F_3H_{13}$			1.4	
217	887		$C_{12}F_3H_{13}$			0.7	
210	888 (3140)	A	$C_{13}F_6H_{12}O$			0.9 1.5	
1083	889		$C_{13}F_6H_{14}O_2$				1.0

Table A.1.b. (contd.)

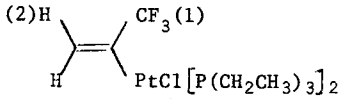
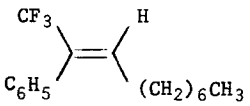
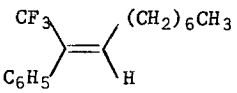
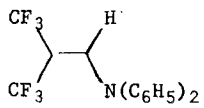
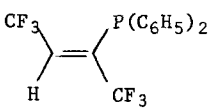
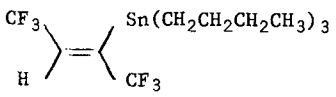
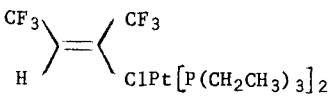
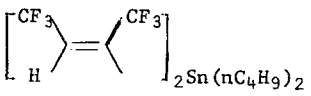
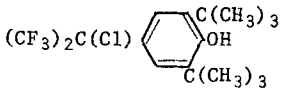
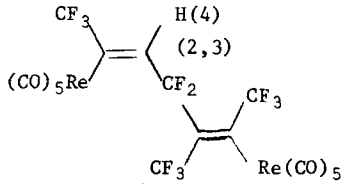
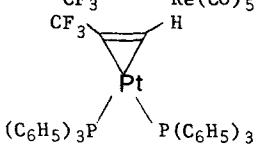
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J	^nJ
168	890 (6572)		$C_{15}F_3H_{32}ClPPt$			1,2	2	
217	891		$C_{16}F_3H_{21}$				1.5	
217	892		$C_{16}F_3H_{21}$				<0.7	
210	893 (3162)	A	$C_{16}F_6H_{11}N$				0.8 1.1	
127	894		$C_{16}F_6H_{11}P$		9.0			
211	895		$C_{16}F_6H_{28}Sn$		7.0		1.5	
173	896 (3163 6580)		$C_{16}F_6H_{31}ClP_2Pt$		9.6			
218	897		$C_{16}F_{12}H_{20}Sn$		8			
1083	898		$C_{17}F_6H_{21}ClO$					0.8
219	899 (3172)		$C_{18}F_{11}HO_{10}Re_2$	(1) 	2,4 3,4	2.9 7.3	1,4 2.0	
168	900 (6542 6619)		$C_{39}F_3H_{31}P_2Pt$				2.8	

Table A.1.c. Fluorine bonded to sp^3 carbon, hydrogen bonded to sp^2 carbon of carbonyl group.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
89	901 (262)		C_4FH_7O	$(CH_3)_2CFCHO$	5		
90	902		C_4FH_7O	$(CH_3)_2CFCHO$	5		
90	903 (263)		C_4FH_7O	$CH_3CH_2CFHCHO$	5		
90	904 (446)		$C_7FH_{13}O$	$CH_3(CH_2)_4CFHCHO$	5		

Table A.1.d. Fluorine bonded to sp^3 carbon, hydrogen bonded to sp carbon.

220	905	C	C_3F_3H	$CF_3C{\equiv}CH$		3.3 (±0.1)	
119	906		C_4F_6HN	$(CF_3)_2NC{\equiv}CH$			0.6

Table A.1.e. Fluorine bonded to sp^2 carbon other than of carbonyl group, hydrogen bonded to sp^3 carbon.

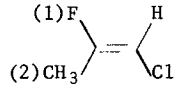
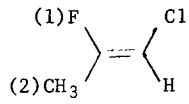
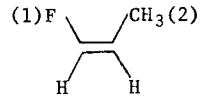
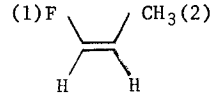
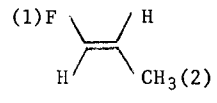
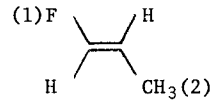
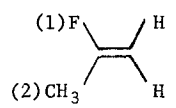
222	907 (1010)		C_3FH_4Cl		1,2	16.85		
222	908 (1011)		C_3FH_4Cl		1,2	16.3		
223	909 (1014)		C_3FH_5				1,2	2.6
224	910 (1015)		C_3FH_5				1,2	2.4
223	911 (1012)		C_3FH_5				1,2	3.3
224	912 (1013)		C_3FH_5				1,2	3.3
224	913 (1016)		C_3FH_5		1,2	16.0		

Table A.1.e. (contd.)

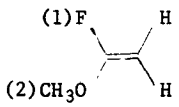
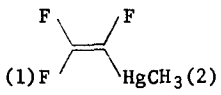
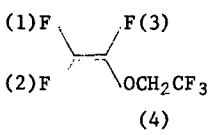
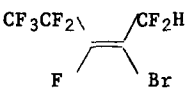
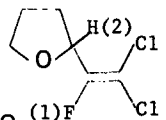
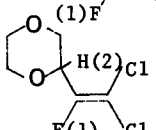
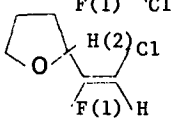
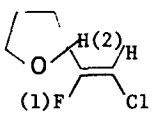
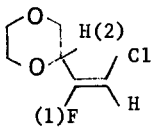
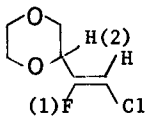
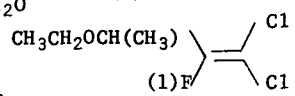
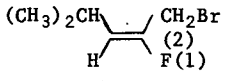
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
226	914 (1019)		C_3FH_5O		1,2	2.8				
243	915 (5563)		$C_3F_3H_3Hg$						1,2	+0.28
227	916 (6021)		$C_4F_4H_6N_2P$	$[(CH_3)_2N]_2PFCF=CF_2$ (2) (1)					1,2	0.9
1046	917 (3245 / 3492)		$C_4F_6H_2O$		3,4	1.5			1,4 2,4	<0.5 <0.5
849	918 (316)		C_4F_8HBr							
230	919	G	$C_6FH_7Cl_2O$		1,2	26				
230	920	G	$C_6FH_7Cl_2O_2$		1,2	23				
230	921 (1051)	G	C_6FH_8ClO		1,2	27				
230	922 (1052)	G	$C_6FH_8ClO_2$		1,2	13				
230	923 (1053)	G	$C_6FH_8ClO_2$		1,2	23				
230	924 (1054)	G	$C_6FH_8ClO_2$		1,2	13				
230	925	G	$C_6FH_9Cl_2O$		1,2	25				
193	926 (1055)	G	$C_6FH_{10}Br$		1,2	20.9				

Table A.1.e.

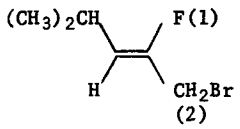
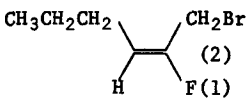
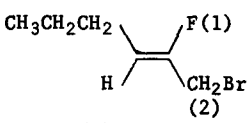
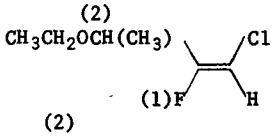
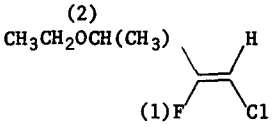
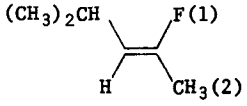
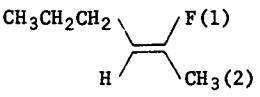
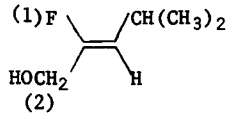
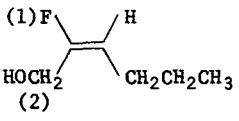
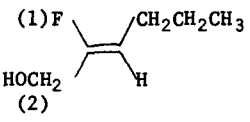
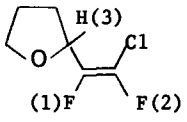
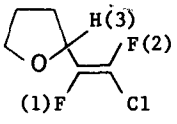
Ref. No.	Serial No.	Sovlent	Molecular formula	Structure	^3J		^4J	^nJ
193	927 (1056)	G	$C_6FH_{10}Br$		1,2	19.1		
193	928 (1057)	G	$C_6FH_{10}Br$		1,2	20.7		
193	929 (1058)	G	$C_6FH_{10}Br$		1,2	19.8		
230	930 (1059)	G	$C_6FH_{10}ClO$		1,2	27		
230	931 (1060)	G	$C_6FH_{10}ClO$		1,2	15		
193	932 (1061)	G	C_6FH_{11}		1,2	16.2		
193	933 (1062)	G	C_6FH_{11}		1,2	16.2		
193	934 (1063)	G	$C_6FH_{11}O$		1,2	14.5		
193	935 (1064)	G	$C_6FH_{11}O$		1,2	20.5		
193	936 (1065)	G	$C_6FH_{11}O$		1,2	14.3		
230	937 (3524)	G	$C_6F_2H_7ClO$		1,3	28	2,3	3
230	938 (3525)	G	$C_6F_2H_7ClO$		1,3	29	2,3	5

Table A.1.e. (contd.)

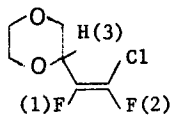
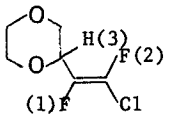
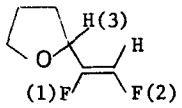
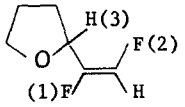
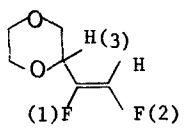
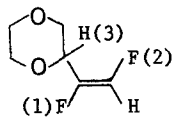
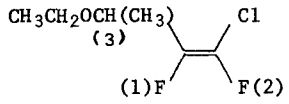
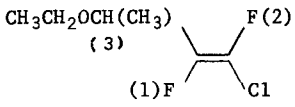
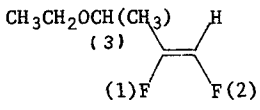
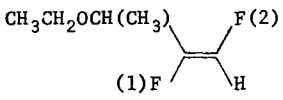
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
230	939 (3526)	G	$C_6F_2H_7ClO_2$		1,3	25	2,3	2		
230	940 (3527)	G	$C_6F_2H_7ClO_2$		1,3	25	2,3	4		
230	941 (1067 / 3528)	G	$C_6F_2H_8O$		1,3	20				
230	942 (1068 / 3529)	G	$C_6F_2H_8O$		1,3	28	2,3	5		
230	943 (1070 / 3530)	G	$C_6F_2H_8O_2$		1,3	13	2,3	4		
230	944 (1069 / 3531)	G	$C_6F_2H_8O_2$		1,3	25	2,3	6		
230	945 (3532)	G	$C_6F_2H_9ClO$		1,3	28	2,3	3		
230	946 (3533)	G	$C_6F_2H_9ClO$		1,3	29	2,3	5		
230	947 (1074 / 3534)	G	$C_6F_2H_{10}O$		1,3	20	2,3	20		
230	948 (1073 / 3535)	G	$C_6F_2H_{10}O$		1,3	28	2,3	6		
227	949		$C_6F_3H_{12}NP$	$[(CH_3)_2\overset{(2)}{N}]_2\overset{(1)}{P}CF=CF_2$					1,2	0.8
227	950 (3540 / 6172)		$C_6F_6H_6NP$	$(CH_3)_2\overset{(2)}{N}P(\overset{(1)}{C}F=CF_2)_2$					1,2	0.6

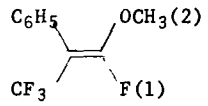
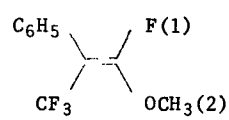
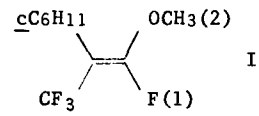
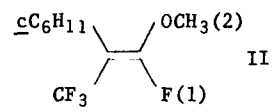
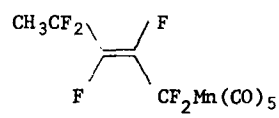
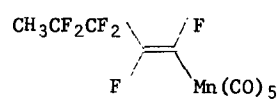
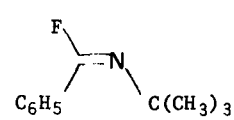
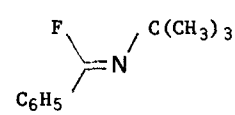
Table A.1.e.(contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ
118	951 (425, 3543)	B	$C_6F_8H_4O$	(3) $(CF_3)_2CH$ F(1); CH_3O F(2); (4)			1,3 ∿1.2	2,4	∿2.0
194	952 (2928, 3289)		$C_6F_9H_3O$	(1)F OCH_3(2); CF_3 CF_2CF_3				1,2	3.2
113	953 [427, 835, 1083, 3294]		$C_6F_{10}H_2$	$(CF_3)_2CH$(2) H; (1)F CF_3	1,2	22			
231	954 (6204)		$C_7F_2H_{18}N_3P$	$[(CH_3)_2N]_3P{=}CF_2$ (2) (1)				1,2	2.86
113	955 (488, 3302)		$C_7F_{10}H_2O_2$	(2) $(CF_3)_2CH$ CO_2H; (1)F CF_3	1,2	29			
198	956 (1101, 3309)		$C_8F_8H_4$	CF_3 H; (1)F CH_3(2); F_2 F_2				1,2	1.8
193	957 (1103)	G	C_9FH_8Br	C_6H_5 F(1); H CH_2Br (2)	1,2	20.1			
154	958 (1104)		C_9FH_9	C_6H_5 CH_3(2); (1)F H			1,2	2.2	
154	959 (1106)		C_9FH_9	C_6H_5 H; (1)F CH_3(2)			1,2	2.5	
193	960 (1105)	G	C_9FH_9	C_6H_5 F(1); H CH_3(2)	1,2	16.2			
193	961		C_9FH_9O	C_6H_5 F(1); H CH_2OH (2)	1,2	13.8			

Table A.1.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J	^nJ
232	962 (1108)	G	$C_9FH_{16}ClO_2$	$CH_2{=}CFCH(OCH_2CH_2Cl)(O(CH_2)_3CH_3)$ (1)(2)	1,2	3.5		
139	963		$C_9F_2H_8$	$CF_2{=}C(CH_3)(C_6H_5)$			3.0	
199	964 [604 3314 3580]	A	$C_9F_4HMnO_6$	CF_2H(4), F, (1)F, $COMn(CO)_5$	1,2	14.6		
193	965 (1113)	G	$C_{10}FH_{10}BrO$	para-$CH_3OC_6H_4$, F(1), H, CH_2Br(2)	1,2	19.9		
193	966 (1114)	G	$C_{10}FH_{11}O$	para-$CH_3OC_6H_4$, F(1), H, CH_3(2)	1,2	16.8		
193	967 (1115)	E	$C_{10}FH_{11}O_2$	para-$CH_3OC_6H_4$, F(1), H, CH_2OH(2)	1,2	13.4		
233	968 (3324 3325)	B	$C_{10}F_4H_7ClO$	para-ClC_6H_4, OCH_3(2), CF_3, F(1) I				
				and para-ClC_6H_4, F(1), CF_3, OCH_3(2) II				
				Mixture A: 94% I 6% II	1,2	1.1		
				Mixture B: 8% I 92% II	1,2	1.0		

Table A.1.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
233	969 (3326, 3327)	B	$C_{10}F_4H_8O$	 I and  II			
				Mixture A: 96% I 4% II	1,2	1.0	
				Mixture B: 4% I 96% II	1,2	0.9	
233	970 (3328, 3329)		$C_{10}F_4H_{14}O$	 I and  II			
				Mixture A: 96% I 4% II	1,2	1.0	
				Mixture B: 4% I 96% II	1,2	1.0	
164	971 (652, 3082, 3331, 3595)		$C_{10}F_6H_3MnO_5$			2.6	2.6
164	972 (653, 3332, 3596)		$C_{10}F_6H_3MnO_5$				2.6
234	973		$C_{11}FH_{14}N$				1
234	974		$C_{11}FH_{14}N$				~0

TableA.1.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
233	975 (3339 / 3340)	B	$C_{11}F_4H_{10}O_2$	para-$CH_3OC_6H_4$, OCH_3(2), CF_3, F(1) I and para-$CH_3OC_6H_4$, F(1), CF_3, OCH_3(2)			
				Mixture A: 92% I 8% II	1,2	1.0	
				Mixture B: 6% I 94% II	1,2	0.9	
233	976 (3344 / 3345)	B	$C_{11}F_6H_8O$	C_6H_5, OCH_3(2), CF_3CF_2, F(1) I and C_6H_5, F(1), CF_3CF_2, OCH_3(2) II			
				Mixture A: 90% I 10% II	1,2	1.0	
				Mixture B: 9% I 91% II	1,2	1.0	
231	977 (6355)		$C_{13}F_2H_{30}N_3P$	CF_2(1)=P(2)$[N(CH_2CH_3)_2]_3$			1,2 1.9

Table A.1.f. Fluorine bonded to sp^2 carbon of carbonyl group, hydrogen bonded to sp^3 carbon.

251	978	B	C_2FHCl_2O	Cl, O, F, Cl, H	-4.23		
				H, O, Cl, Cl, F	25.0		

Table A.1.f. (contd.)

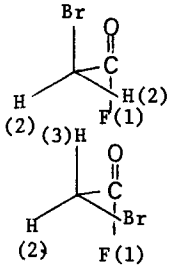
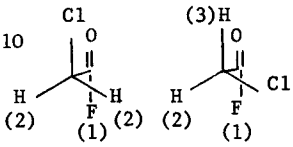
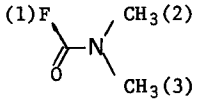
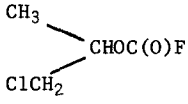
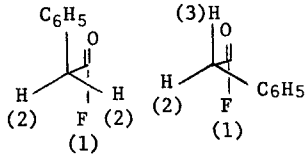
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
251	979		C_2FH_2BrO				
					^3J		
		B			1,2 -8.34	1,3 42.3	
		E			1,2 -7.55	1,3 38.2	
251	980	B	C_2FH_2ClO		1,2 -6.54 1,3 31.6		
35	981		C_2FH_3O	$CH_3C(O)F$	6.9		
252	982	G	C_3FH_6NO			1,2 0.8	
		B				1,3 0.3 1,2 1.1 1,3 0.4	
20	983 [159 2685 3645]	B	$C_3F_3HBr_2O$	$CF_2BrCHBrC(O)F$	3.1		
253	984		$C_4FH_6ClO_2$	$Cl(CH_2)_3OC(O)F$		2	
253	985		$C_4FH_6ClO_2$			2	
125	986		$C_5F_2H_6O_2$	$(CH_3)_2C[C(O)F]_2$			0.8
251	987	E	C_8FH_7O		1,2 -8.75 1,3 48.3		

Table A.1.g. Fluorine bonded to sp^2 carbon other than of carbonyl group, hydrogen bonded to sp^2 carbon other than of carbonyl group.

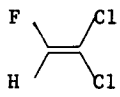
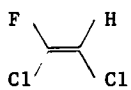
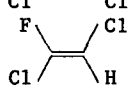
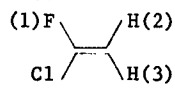
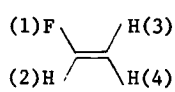
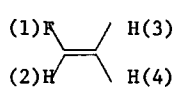
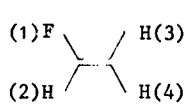
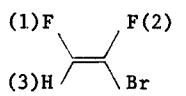
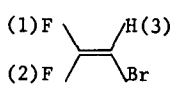
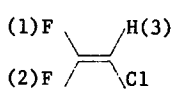
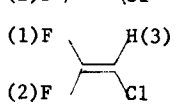
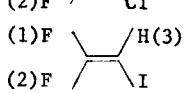
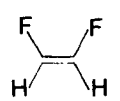
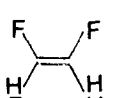
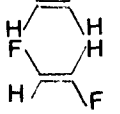
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
235	988		C_2FHCl_2		81		
236	989 (5408)	A	C_2FHCl_2			4.05	
236	990 (5409)	A	C_2FHCl_2			18.10	
235	991		C_2FH_2Cl			1,2 8 1,3 40	
239	992		C_2FH_3		1,2 +84.7	1,3 +20.1 1,4 +52.4	
237	993	B	C_2FH_3		1,2 84.6	1,3 19.8 1,4 52.7	
						^3J	
238	994	A*	C_2FH_3		1,2 85.49	1,3 20.53	1,4 53.61
		D*			84.67	19.63	51.81
		E*			86.14	21.05	54.66
		F*			86.54	21.77	56.38
		L*			86.47	21.56	55.45
		K^{2*}			86.54	21.77	56.38
240	995 (3415)		C_2F_2HBr		1,3 72.9	2,3 13.5	
240	996 (3414)		C_2F_2HBr			1,3 0.3 2,3 19.0	
235	997 (3417)		C_2F_2HCl			1,3 <3 2,3 13	
184	998 (3418)		C_2F_2HCl			1,3 1.0 2,3 16.6	
184	999 (3421)		C_2F_2HI			1,3 2.1 2,3 23.1	
241	1000 (3426)		$C_2F_2H_2$		+72.7	+20.4	
242	1001 (3424)		$C_2F_2H_2$		71.9	20.1	
241	1002 (3427)		$C_2F_2H_2$		+74.3	+4.4	

Table A.1.g. (contd.)

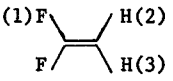
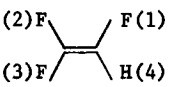
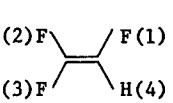
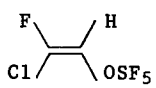
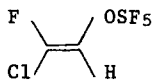
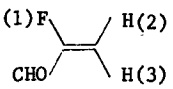
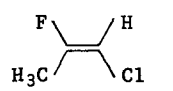
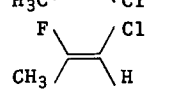
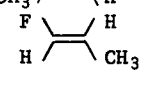
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
235	1003		$C_2F_2H_2$			1,2 ∿1	
	(3422)					1,3 34	
235	1004		C_2F_3H		1,4 72	2,4 12	
	(3430)					3,4 <3	
238	1005	A*	C_2F_3H		1,4 70.61	2,4 12.79	3,4 -4.24
	(3430)	D*			70.51	12.52	-4.19
		E*			70.39	13.53	-4.31
		F*			69.93	14.32	-4.30
		G*			70.59	12.57	-4.18
		J*			70.73	13.00	-4.27
		L*			70.08	14.01	-4.31
		N*			70.55	13.30	-4.34
		Q*			70.58	12.76	-4.24
		R*			70.28	13.09	-4.27
		K^{2*}			70.92	12.63	-4.26
		L^{2*}			70.52	13.09	-4.24
		M^{2*}			70.20	13.37	-4.24
		N^{2*}			70.21	13.70	-4.27
		O^{2*}			70.43	13.26	-4.30
		P^{2*}			70.43	13.65	-4.20
53	1006		C_2F_6HClOS	$CFH{=}CCl(OSF_5)$	75		
	(5049)			Stereochemistry not known			
187	1007		C_2F_6HClOS			13.2	
	[2430 5051 4817]						
53	1008		C_2F_6HClOS			47.0	
	(5050 4816)						
232	1009	G	C_3FH_3O			1,2 3.5	
	(1134)					1,3 27	
222	1010		C_3FH_4Cl			10.8	
	(907)						
222	1011		C_3FH_4Cl			24.2	
	(908)						
223	1012		C_3FH_5		+84.8	+19.9	
	(911)						

Table A.1.g. (contd.)

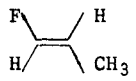
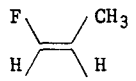
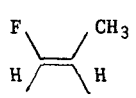
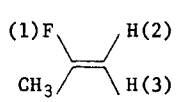
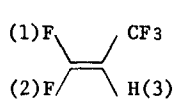
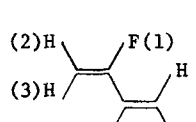
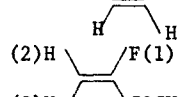
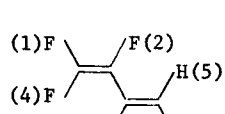
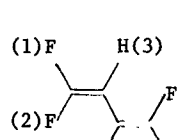
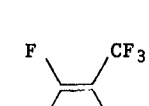
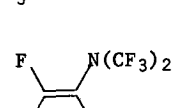
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
224	1013 (912)		C_3FH_5		+84.8	+19.9	
223	1014 (909)		C_3FH_5		+89.9	+41.8	
224	1015 (910)		C_3FH_5		+85.2	+41.5	
224	1016 (913)		C_3FH_5			1,2 +16.6 1,3 +48.6	
77	1017 [784 3460 3229]		C_3F_5H			1,3 21.7 2,3 1.6	
244	1018	Q[2]*	C_4FH_5			1,2 15.76 1,3 47.93	
226	1019 (914)		C_4FH_5O			1,2 14.1 1,3 47.9	
245	1020 (3471)		$C_4F_3H_3$		1,4 71.5	2,4 16.0 3,5 48.4 3,6 18.1	2,5 3.9 2,6 3.9 3,4 3.3
1064	1021 (3478)		$C_4F_4H_2$			1,3 or 2,3 +36.6	1,4 or 2,4 +30
206	1022 (798 3250)	B	C_4F_7H			29	
101	1023 (3251)		C_4F_7HBrN		76.5		

Table A.1.g. (contd.)

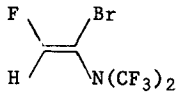
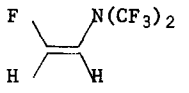
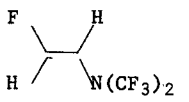
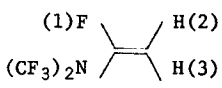
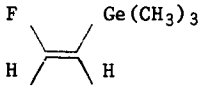
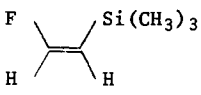
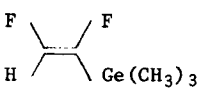
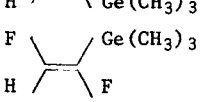
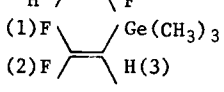
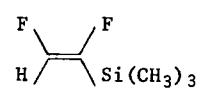
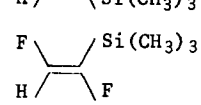
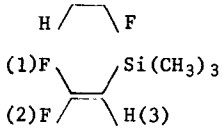
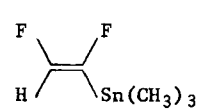
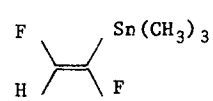
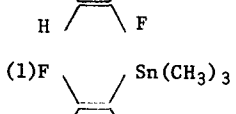
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
101	1024 (3252)		C_4F_7HBrN		75.5		
101	1025 (799, 3254)		$C_4F_7H_2N$		73.2	26.2	
101	1026 (800)		$C_4F_7H_2N$		76.0	6.2	
37	1027 (3253)		$C_4F_7H_2N$			1,2 4.9 1,3 30.5	
187	1028		$C_5FH_{11}Ge$		78.	96	
195	1029	B	$C_5FH_{11}Si$		82	96	
187	1030		$C_5F_2H_{10}Ge$		76	23	
187	1031		$C_5F_2H_{10}Ge$		74	15	
187	1032		$C_5F_2H_{10}Ge$			1,3 42 2,3 9	
195	1033		$C_5F_2H_{10}Si$		75	22	
195	1034		$C_5F_2H_{10}Si$		78	12	
195	1035		$C_5F_2H_{10}Si$			1,3 40 2,3 7	
246	1036		$C_5F_2H_{10}Sn$		77	25.5	
246	1037		$C_5F_2H_{10}Sn$		78	15	
246	1038		$C_5F_2H_{10}Sn$			1,3 46 2,3 9	

Table A.1.g. (contd.)

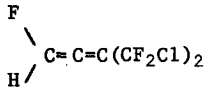
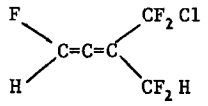
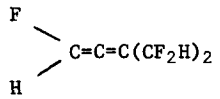
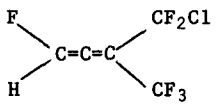
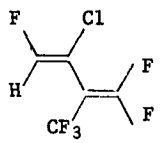
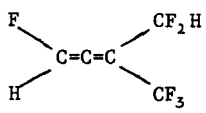
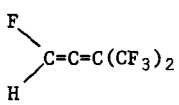
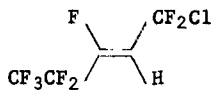
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
192	1039 (803, 3265)		$C_5F_5HCl_2$		77		
192	1040 (360, 804)		$C_5F_5H_2Cl$		78		
192	1041 (362, 805)		$C_5F_5H_3$		77		
192	1042 (806, 3266)		C_5F_6HCl		76.6		
192	1043 (3267)		C_5F_6HCl		77		
192	1044 (363, 807)		$C_5F_6H_2$		80		
192	1045 (813, 3269)		C_5F_7H		77		
208	1046 [814, 2871, 3273]	P	C_5F_8HCl			28.0	

Table A.1.g. (contd.)

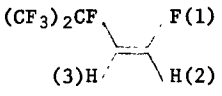
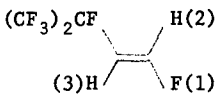
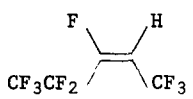
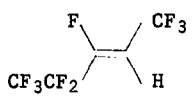
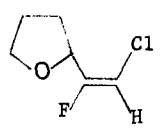
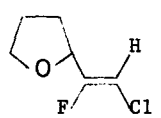
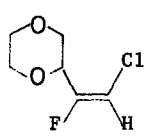
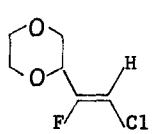
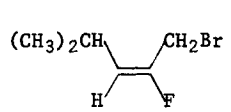
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
209	1047 [815 2872 3274]		$C_5F_8H_2$		1,2	77.3	1,3	36.7	
209	1048 [816 2873 3275]		$C_5F_8H_2$		1,2	78.0	1,3	16.5	
190	1049 [817 280 3279]		C_5F_9H					19.2	
190	1050 [818 2881 3280]		C_5F_9H					28.8	
230	1051 (921)		C_6FH_8ClO					11	
230	1052 (922)		C_6FH_8ClO					25	
230	1053 (923)		$C_6FH_8ClO_2$					11	
230	1054 (924)		$C_6FH_8ClO_2$					25	
193	1055 (926)		$C_6FH_{10}Br$					20.9	

Table A.1.g. (contd.)

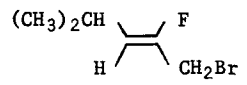
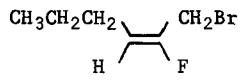
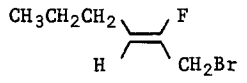
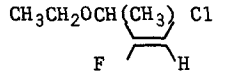
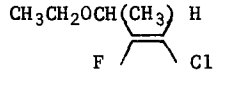
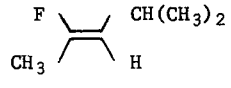
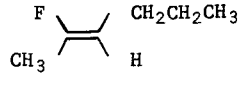
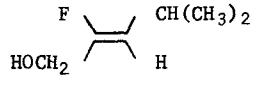
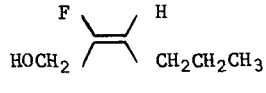
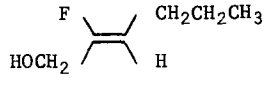
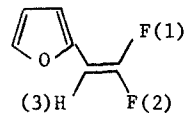
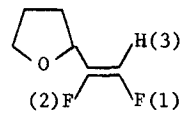
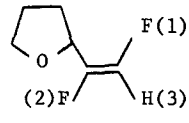
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
193	1056 (927)		$C_6FH_{10}Br$				33.8	
193	1057 (928)		$C_6FH_{10}Br$				20.7	
1193	1058 (929)		$C_6FH_{10}Br$				33.9	
230	1059 (930)		$C_6FH_{10}ClO$				11	
230	1060 (931)		$C_6FH_{10}ClO$				25	
193	1061 (932)	G	C_6FH_{11}				36.7	
193	1062 (933)	G	C_6FH_{11}				37	
193	1063 (934)	G	$C_6FH_{11}O$				36	
193	1064 (935)	G	$C_6FH_{11}O$				20.5	
193	1065 (936)	G	$C_6FH_{11}O$					
250	1066	G	$C_6F_2H_4O$				1,3 25.7 2,3 3.3	
230	1067 (941 / 3528)	G	$C_6F_2H_8O$		1,3	76	2,3 15	
230	1068	G	$C_6F_2H\ O$		1,3	73	2,3 7	

Table A.1.g. (contd.)

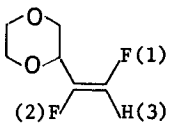
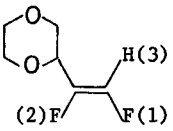
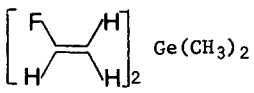
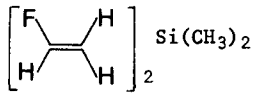
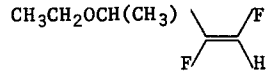
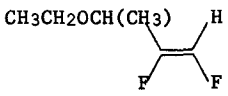
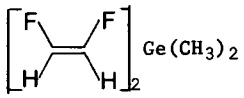
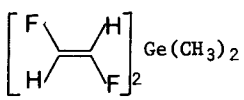
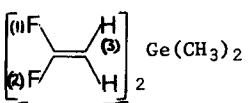
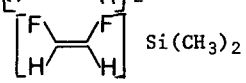
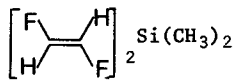
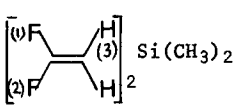
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
230	1069 (944 / 3531)		$C_6F_2H_8O_2$		1,3	71	2,3	8	
230	1070 (943 / 3530)		$C_6F_2H_8O_2$		1,3	74	2,3	18	
187	1071		$C_6F_2H_{10}Ge$			78		95	
195	1072		$C_6F_2H_{10}Si$			76		95	
230	1073 (948 / 3535)		$C_6F_2H_{10}O$			74		8	
230	1074 (947 / 3534)		$C_6F_2H_{10}O$			73		17	
187	1075		$C_6F_4H_8Ge$			75		22	
187	1076		$C_6F_4H_8Ge$			73		15	
187	1077		$C_6F_4H_8Ge$				1,3	7	
							2,3	42	
195	1078		$C_6F_4H_8Si$			74		21	
195	1079		$C_6F_4H_8Si$			74		15	
195	1080		$C_6F_6H_6Si$				1,3	7	
							2,3	30	

Table A.1.g. (contd.)

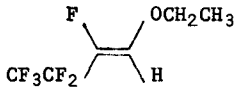
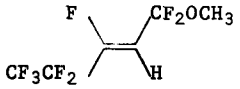
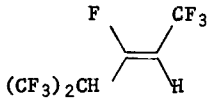
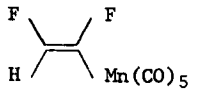
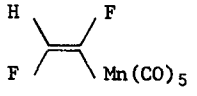
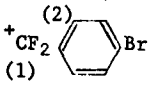
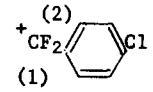
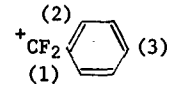
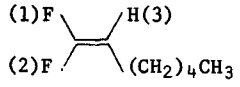
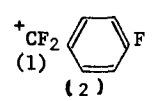
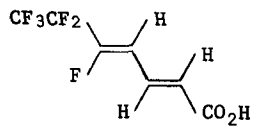
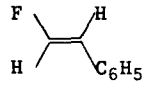
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
194	1081		$C_6F_6H_6O$			21	
190	1082 [831, 2925, 3290]	P	$C_6F_8H_4O$			30.0	
113	1083 [427, 835, 953, 3294]		$C_6F_{10}H_2$			31	
173 247	1084		$C_7F_2HMnO_5$		80.0	25.0	
173 247	1085		$C_7F_2HMnO_5$		86.5	10.2	
61	1086	C^2	$C_7F_2H_4Br^+$				1,2 1.0
61	1087	C^2	$C_7F_2H_4Cl^+$				1,2 1.0
61	1088	C^2	$C_7F_2H_5^+$				1,2 1.0
248	1089 (3550)		$C_7F_2H_{12}$			1,3 3.5 2,3 25	
61	1090 (1837, 3354)	C^2	$C_7F_3H_4^+$			1,2 1.1	
143	1091	G	$C_7F_6H_4O_2$			16	
249	1092	P	C_8FH_7		82.1	19.9	

Table A.1.g. (contd.)

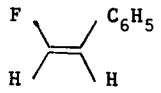
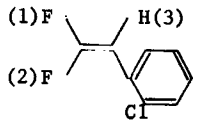
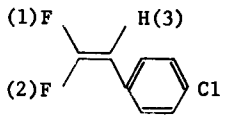
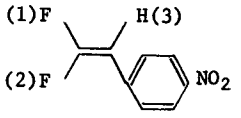
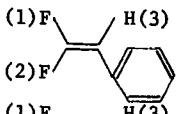
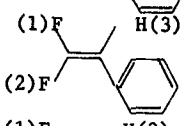
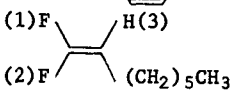
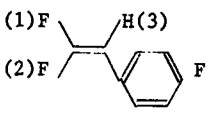
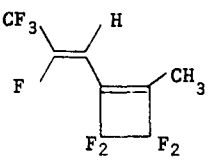
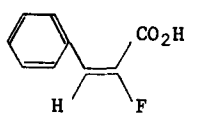
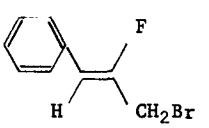
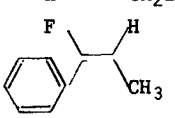
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
249	1093	P	C_8FH_7		82.6	44.6	
248	1094 (3554)	G	$C_8F_2H_5Cl$			1,3 4.5 2,3 25	
248	1095 (3555)	G	$C_8F_2H_5Cl$			1,3 4.5 2,3 26	
250	1096	G	$C_8F_2H_5NO_2$			1,3 3.8 2,3 25	
250	1097	G	$C_8F_2H_6$			1,3 4.3 2,3 25	
248	1098 (3556)	G	$C_8F_2H_6$			1,3 4.5 2,3 26	
248	1099 (3557)	G	$C_8F_2H_{14}$			1,3 3.5 2,3 25	
147 250	1100	G	$C_8F_3H_5$			1,3 5 2,3 25	
198	1101 (956, 3309)		$C_8F_8H_4$			33.6	
249	1102	P	$C_9FH_7O_2$			21.9	
193	1103 (957)	G	C_9FH_8Br			35.3	
154	1104 (958)		C_9FH_9			22	

Table A.1.g. (contd.)

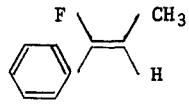
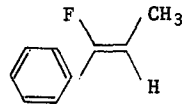
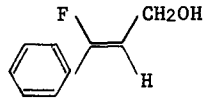
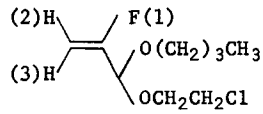
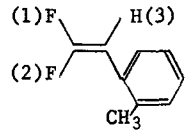
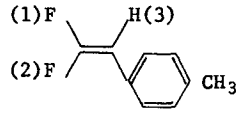
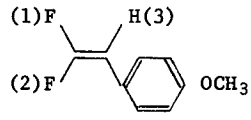
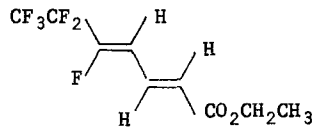
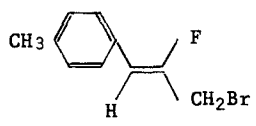
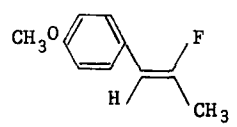
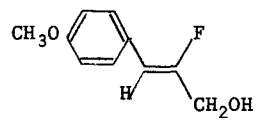
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
193	1105 (960)		C_9FH_9			38.1	
154	1106 (959)		C_9FH_9			36	
193	1107		C_9FH_9O			38.8	
232	1108 (232)	G	$C_9FH_{16}ClO_2$		1,2 1,3	17.5 48.5	
248	1109 (3575)	G	$C_9F_2H_8$		1,3 2,3	5.5 24	
248	1110 (3576)	G	$C_9F_2H_8$		1,3 2,3	4.5 26	
248	1111 (3577)	G	$C_9F_2H_8O$		1,3 2,3	4.5 25	
143	1112	B	$C_9F_6H_8O_2$			16	
193	1113 (965)	G	$C_{10}FH_{10}BrO$			35.7	
193	1114	G	$C_{10}FH_{11}O$			39.1	
193	1115 (967)	E	$C_{10}FH_{11}O_2$			39.7	

Table A.1.g. (contd.)

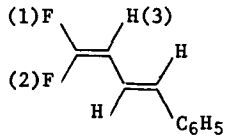
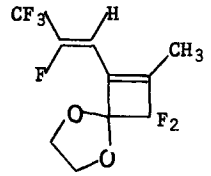
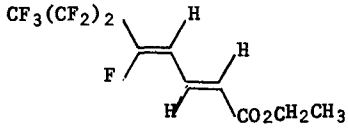
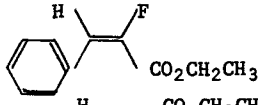
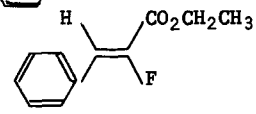
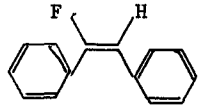
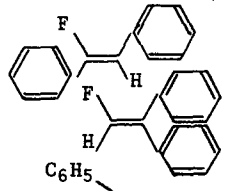
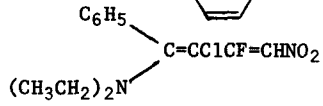
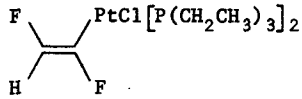
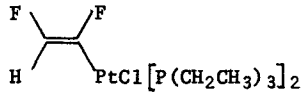
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
248	1116 (3591)	G	$C_{10}F_2H_8$			1,3 2.0 2,3 24	
198	1117 (3333)		$C_{10}F_6H_8O_2$			36.5	
143	1118		$C_{10}F_8H_8O_2$			11	
249	1119	P	$C_{11}FH_{11}O_2$			22.6	
249	1120	P	$C_{11}FH_{11}O_2$			34.3	
160	1121		$C_{12}FH_{23}N_2$	$CH_3CH{=}CH{-}CF{=}NNHC(CH_3)_2CH_2C(CH_3)_3$		23	
107	1122		$C_{14}FH_{11}$			21	
107	1123		$C_{14}FH_{11}$			67	
171	1124		$C_{14}FH_{11}$		83		
288	1125		$C_{14}FH_{16}ClN_2O_2$			23	
173	1126		$C_{14}F_2H_{31}ClP_2Pt$		84	7.8	
173	1127		$C_{14}F_2H_{31}ClP_2Pt$		82.3	24	

Table A.1.h. Fluorine bonded to sp^2 carbon of carbonyl group, hydrogen bonded to sp^2 carbon other than of carbonyl group.

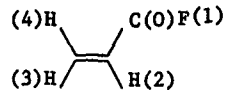
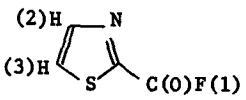
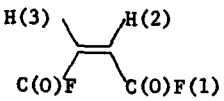
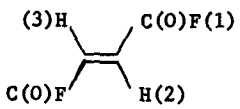
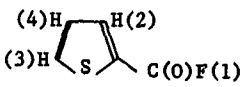
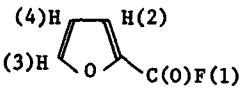
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J			
254	1128	M	C_3FH_3O		1,2	9.02	1,3	2.95	1,4	-0.28
		P				7.95		2.92		-0.31
		Q				8.22		2.79		-0.33
255	1129	R^{2*}	C_4FH_2NOS						1,2	0.80
									1,3	2.15
256	1130		$C_4F_2H_2O_2$		1,2	4.17	1,3	1.83		
257	(3647 5454)	M*				4.44		1.54		
256	1131		$C_4F_2H_2O_2$		1,2	7.51	1,3	0.21		
257	(3648 5455)									
255	1132	R^{2*}	C_5FH_3OS				1,2	<0.2	1,3	2.44
258									1,4	1.99
258	1133	R^{2*}	$C_5FH_3O_2$				1,2	+0.55	1,3	+2.43
									1,4	+0.78

Table A.1.i. Fluorine bonded to sp^2 carbon other than of carbonyl group, hydrogen bonded to sp^2 carbon of carbonyl group.

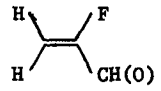
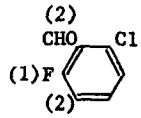
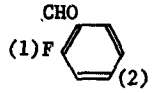
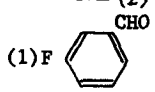
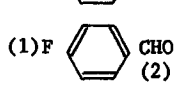
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J		^nJ	
232	1134 (1009)	G	C_3FH_3O		16				
395	1135 (1827)	E*	C_7FH_4ClO			1,2	-1.08		
395	1136	E*	C_7FH_5O			1,2	-0.38		
395	1137	E*	C_7FH_5O					1,2	1.85
395	1138	E*	C_7FH_5O					1,2	-0.44

Table A.1.j. Fluorine bonded to sp carbon, hydrogen bonded to sp carbon.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J
259	1139		C_2FH	F-C≡C-H	21

A.2. Fluorine bonded to carbon in alicyclic non-aromatic system, hydrogen bonded to carbon in either acyclic or cyclic system.

Table A.2.a. Fluorine bonded to carbon in three membered ring, hydrogen bonded to carbon in the same ring.

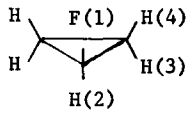
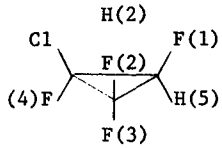
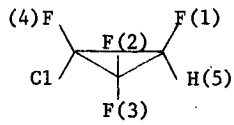
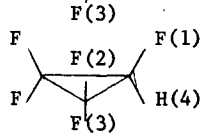
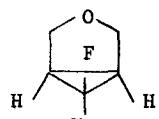
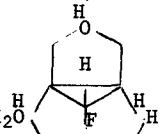
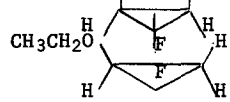
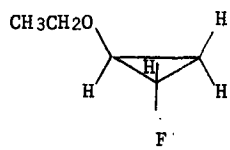
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
260	1140	H-P	C_3FH_5		1,2	64.90	1,3	9.87	
							1,4	21.02	
261	1141 (3671)	B	C_3F_4HCl		1,5	57	2,5	2.1	
							3,5	9.1	
							4,5	16.8	
261	1142 (3670)	B	C_3F_4HCl		1,5	57	2,5	1.3	
							3,5	10	
							4,5	1.3	
261	1143 (3675)	B	C_3F_5H		1,4	56	2,4	1.3	
							3,4	13.2	
263	1144	G	C_5FH_7O			66.0		8.0	
263	1145	G	C_5FH_7O			69.0		18.5	
263	1146	G	C_5FH_9O			63.0			
263	1147	G	C_5FH_9O			63.0			

Table A.2.a. (contd.)

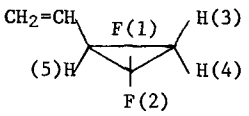
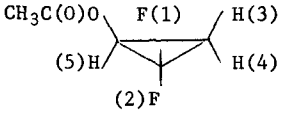
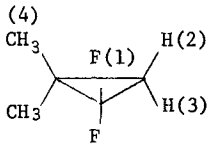
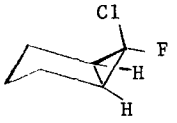
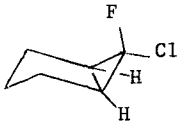
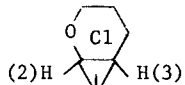
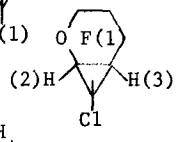
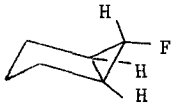
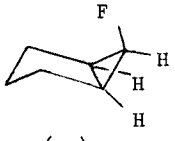
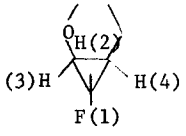
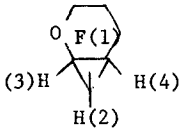
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
265	1148 (3680)		$C_5F_2H_6$			2,5 ∿12.4 2,4 ∿12.4 2,3 5.0 1,3 12.0	
266	1149 (3681)	A*	$C_5F_2H_6O_2$			— ^3J — 1,3 15.5 2,3 4.8 1,4 6.7 2,4 14.2 1,9 -2.3 2,5 9.9	
265	1150 (1186 3682)		$C_5F_2H_8$			1,2 ∿8.5 1,3 ∿8.5	
267	1151	G	C_6FH_8Cl			19	
267	1152	G	C_6FH_8Cl			8	
268	1153		C_6FH_8ClO			1,2 12 1,3 22	
268	1154		C_6FH_8ClO			1,2 2 1,3 6	
263 267	1155	G	C_6FH_9		64.3	21	
263 267	1156	G	C_6FH_9		66.3	10	
263 268	1157	G	C_6FH_9O		1,2 61.5	1,3 12.0 1,4 26.6	
263 268	1158	G	C_6FH_9O		1,2 64.5	1,3 0 1,4 13.2	

Table A.2.a. (contd.)

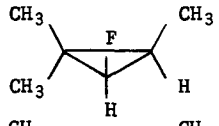
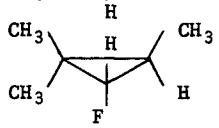
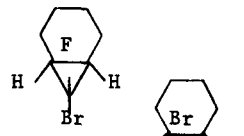
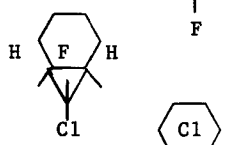
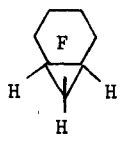
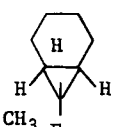
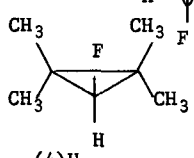
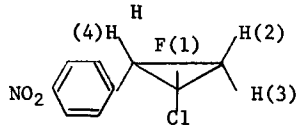
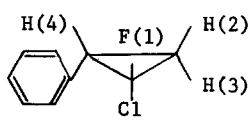
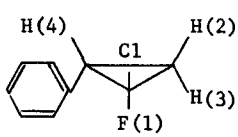
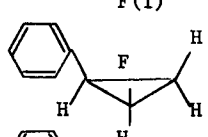
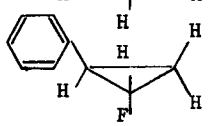
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
263	1159	G	C_6FH_{11}		66.5	12.0	
263	1160	G	C_6FH_{11}		65.0	22.5	
267	1161	G	$C_7FH_{10}Br$			13	
267	1162	G	$C_7FH_{10}Br$			40	
270	1163		$C_7FH_{10}Cl$			5	
270	1164		$C_7FH_{10}Cl$			19	
263 270	1165	G	C_7FH_{11}		68.0	9.0	
263 270	1166	G	C_7FH_{11}		65.0	18.0	
263	1167	G	C_7FH_{13}		65.7		
266	1168	A*	$C_9FH_7ClNO_2$			1,2 15.4 1,3 6.2 1,4 16.2	
266	1169	A*	C_9FH_8Cl			1,2 15.7 1,3 6.2 1,4 17.1	
266	1170	A*	C_9FH_8Cl			1,2 7.5 1,3 16.0 1,4 1.8	
263	1171	G	C_9FH_9		65.9		
263	1172	G	C_9FH_9		64.1		

Table A.2.a. (contd.)

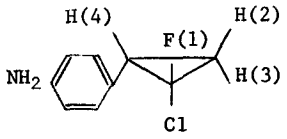
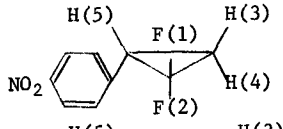
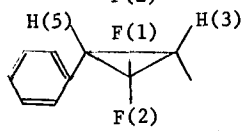
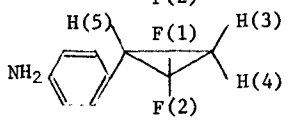
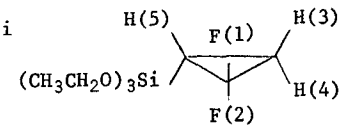
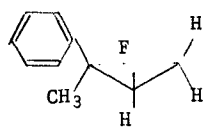
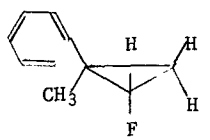
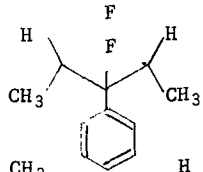
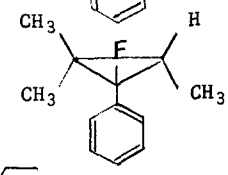
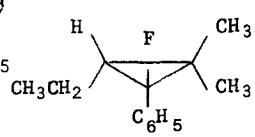
Ref. No.	Serial No.	Solvent	Molecular formulae	Structure	^2J	^3J	^nJ
266	1173	A*	C_9FH_9ClN			1,2 15.7 1,3 6.2 1,4 17.0	
						— ^3J —	
266	1174 (3692)	A*	$C_9F_2H_7NO_2$			1,3 12.0 1,4 4.0 1,5 12.5	2,3 5.2 2,4 12.5 2,5 0.24
266	1175 (3693)	A*	$C_9F_2H_8$			1,3 12.5 1,4 3.8 1,5 13.4	2,3 5.0 2,4 12.6 2,5 0.40
266	1176 (3694)	A*	$C_9F_2H_9N$			1,3 12.7 1,4 4.0 1,5 13.5	2,3 4.6 2,4 12.2 2,5 -0.01
266	1177 (3695)	A*	$C_9F_2H_{18}O_3Si$			1,3 10.3 1,4 3.3 1,5 15.7	2,3 1.8 2,4 9.1 2,5 6.9
263	1178	G	$C_{10}FH_{11}$		65.9		
263	1179	G	$C_{10}FH_{11}$		65.5		
264	1180	G	$C_{11}FH_{13}$			21.5	
264	1181	G	$C_{12}FH_{15}$			12	
264	1182	G	$C_{13}FH_{15}$			23	
264	1183	G	$C_{13}FH_{17}$			15.5	

Table A.2.a. (contd.)

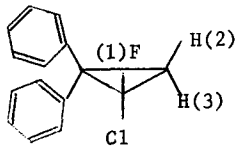
Ref. No.	Serial No.	Solvent	Molecular formulae	Structure	^2J	^3J	^nJ
277	1184	A	$C_{15}FH_{12}Cl$		1,2	+17.7	
					1,3	+6.3	

Table A.2.b. Fluorine bonded to carbon in three membered ring, hydrogen bonded to carbon outside this ring.

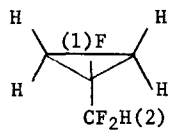
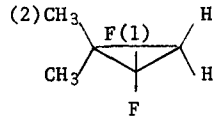
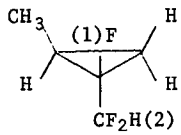
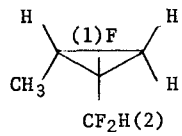
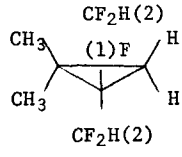
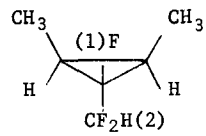
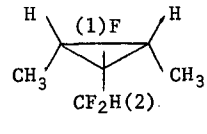
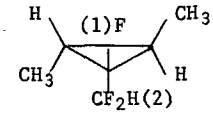
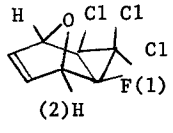
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^nJ
262	1185 (288 2783)	B	$C_4F_3H_5$		1,2 7	
265	1186 (1150 3682)		$C_5F_2H_8$		1,2	∿2
262	1187 (351 2849)	B	$C_5F_3H_7$		1,2 8	
262	1188 (352 2850)	B	$C_5F_3H_7$		1,2 13	
262	1189 (404 2901)	B	$C_6F_3H_9$		1,2 13	
262	1190 (405 2903)	B	$C_6F_3H_9$		1,2 7	
262	1191 (406 2904)	B	$C_6F_3H_9$		1,2 17	
263	1192 (407 2902)	B	$C_6F_3H_9$		1,2 13	
269	1193		$C_7FH_4Cl_3O$		1,2	2.5

Table A.2.b. (contd.)

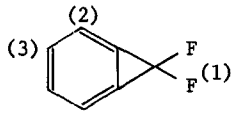
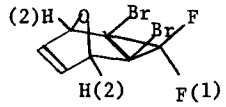
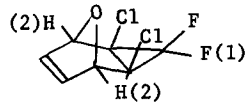
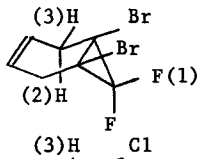
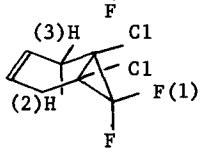
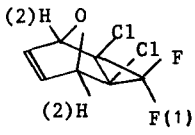
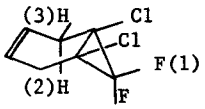
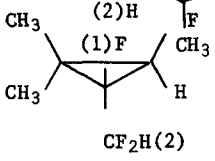
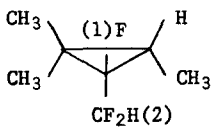
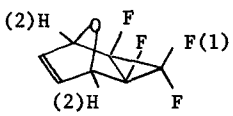
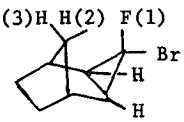
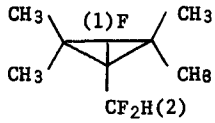
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^nJ
271 272	1193a	G*	$C_7F_2H_4$			1,2 3.61 1,3 −0.33
269	1193b (3684)		$C_7F_2H_4Br_2O$			1,2 2.0
269	1193c (3685)		$C_7F_2H_4Cl_2O$			1,2 2.5
269	1193d (3686)		$C_7F_2H_6Br_2$			1,2 3 1,3 3
269	1194 (3687)		$C_7F_2H_6Cl_2$			1,2 4 1,3 4
269	1195		$C_7F_3H_4ClO$			1,2 2
269	1196		$C_7F_3H_6Cl$			1,2 <3 1,3 <3
262	1197 (473 2954)	B	$C_7F_3H_{11}$		1,2 14	
262	1198 (474 2955)	B	$C_7F_3H_{11}$		1,2 17	
274	1199 (3690)	B	$C_7F_4H_4O$			1,2 3.2
273	1200		$C_8FH_{10}Br$			1,2 3.6 1,3 3.0
262	1201 (539 2991)	B	$C_8F_3H_{13}$		1,2 18	

Table A.2.b. (contd.)

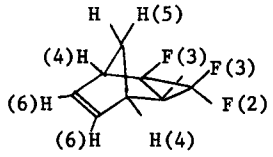
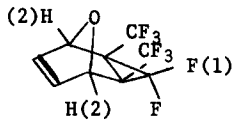
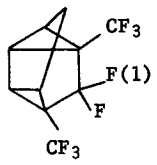
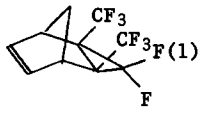
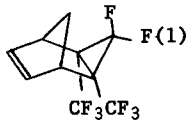
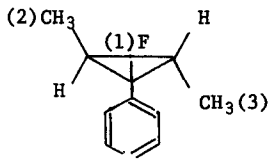
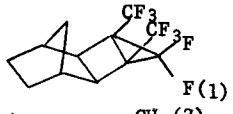
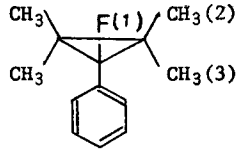
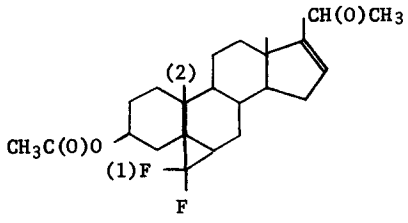
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^nJ	
274	1202 [1344 1275 3691]	B	$C_8F_4H_6$		3,4	2.3	1,6 1,4 3,5	1.8 4.3 6.3
274	1203 (3067 3696)	B	$C_9F_8H_4O$				1,2	1.2
274	1204 (3097 4002)	B	$C_{10}F_8H_6$				1,?	3.0
274	1205 (3095 3699)	B	$C_{10}F_8H_6$				1,?	2.8
274	1206 (3096 3700)	B	$C_{10}F_8H_6$				1,?	8.5
276	1207	G	$C_{11}FH_{13}$				1,2 1,3	≈2
274	1208	B	$C_{12}F_8H_{10}$				1,?	1.8
276	1209	G	$C_{13}FH_{17}$				1,2 1,3	≈2
313 347	1211	A	$C_{24}F_2H_{32}O_3$				1,2	2.3

Table A.2.c. Fluorine bonded to carbon in four membered ring, hydrogen bonded to carbon in the same ring.

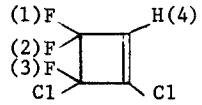
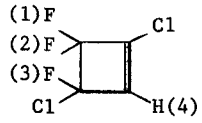
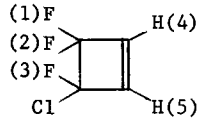
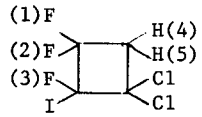
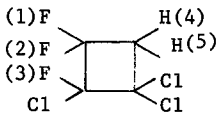
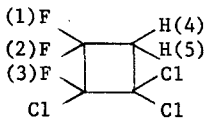
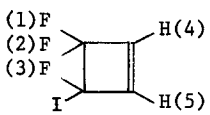
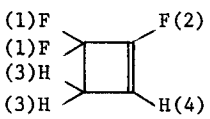
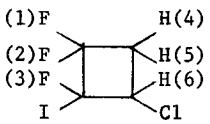
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
278	1212 (3705)	P	$C_4F_3HCl_2$			1,4 -1.5 2,4 -1.9	3,4 +6.0
278	1213 (3706)	P	$C_4F_3HCl_2$			1,4 +10.1 2,4 +9.7	3,4 -0.6
278 279	1214 (3707)	P*	$C_4F_3H_2Cl$			1,4 -1.62 2,4 -2.04 3,5 -0.85	1,5 +10.19 2,5 +11.85 3,4 +6.85
279	1215 (3709)	P*	$C_4F_3H_2Cl_2I$			1,4 +11.78 1,5 +10.59 2,4 +9.49 2,5 +8.99	3,4 +6.87 3,5 -3.03
279	1216 (3712)	P*	$C_4F_3H_2Cl_3$			1,4 +11.86 1,5 +10.69 2,4 +9.76 2,5 +10.47	3,4 +7.5 3,5 -3.1
280	1217 (3710)	B	$C_4F_3H_2Cl$			1,4 +12.03 1,5 +10.77 2,4 +9.57 2,5 +10.46	3,4 +7.40 3,5 -2.92
278 279	1218 (3713)	P	$C_4F_3H_2I$			1,4 -1.65 2,4 -2.50 3,5 -0.86	1,5 +9.72 2,5 +12.63 3,4 +4.77
278	1219 (3714)	P	$C_4F_3H_3$			1,3 +3.1 2,4 -7.6	1,4 +11.8 2,3 +12.3
279	1220 (3715)	P	$C_4F_3H_3ClI$			1,4 +13.23 1,5 +10.23 2,4 +11.71 2,5 +8.45 3,6 +6.85	1,6 +1.13 2,6 +5.6 3,4 +5.92 3,5 -2.53

Table A.2.c. (contd.)

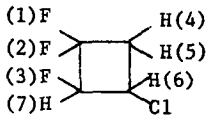
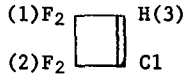
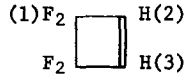
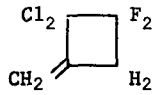
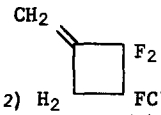
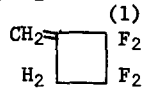
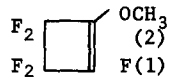
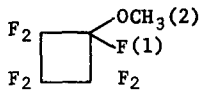
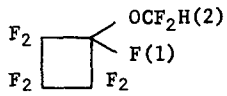
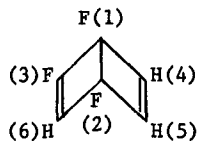
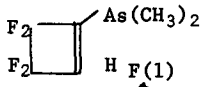
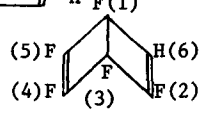
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
281	1221 (3716)		$C_4F_3H_4Cl$		3,7	50.95	1,4 1,5 1,7 2,4 2,5 2,7 3,6	15.99 20.02 8.17 2.49 9.16 7.81 14.70	1,6 2,6 3,4 3,5	3.45 2.70 11.58 -3.32
282	1222		C_4F_4HCl				1,3	2	2,3	10
280	1223 (3720)	B*	$C_4F_4H_2$				1,2	-1.65	1,3	+11.16
283	1224		$C_5F_2H_4Cl_2$					11		
283	1225 (3727)		$C_5F_3H_4Cl$				1,2	13		
283	1226		$C_5F_4H_4$					12		
159	1227		$C_5F_5H_3O$						1,2	1.2
284	1228 (3734)	P*	$C_5F_5H_3O$						1,2 3,2	1.40 0.47
116	1229		$C_5F_7H_3O$				1,2	1.8		
116	1230 (376)		C_5F_9HO				1,2	1.4		
284	1231 (3738)	P	$C_6F_3H_3$				2,6 3,6	4.4 9.9	1,6 3,5	1.4 3.5
285	1232		$C_6F_4H_7As$							∿10
284	1233 (3750)	P	C_6F_5H				2,6 1,6	10.0 3.1	3,6 4,6 5,6	1.9 3.3 ∿0

Table A.2.c. (contd.)

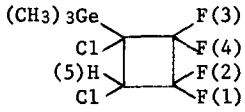
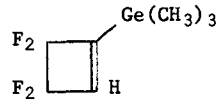
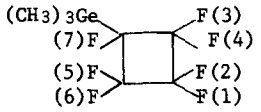
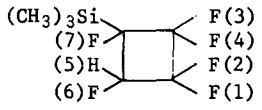
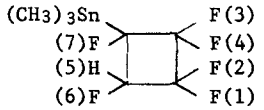
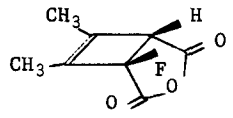
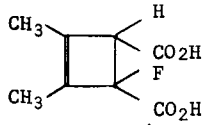
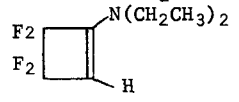
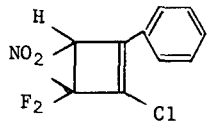
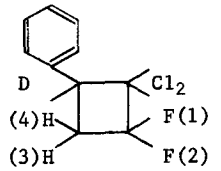
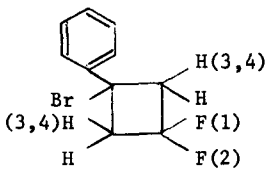
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
286	1234	B	$C_7F_4H_{10}Cl_2Ge$			1,5 2,5	12.0 4.0	3,5 4,5	8.0 ≤1
285	1235	B	$C_7F_4H_{10}Ge$					?	10.5
286	1236	B	$C_7F_6H_{10}Ge$		5,6 55	1,5 2,5 5,7	13.7 5.5 22	3,5 4,5	7.0 1.7
286	1237	B	$C_7F_6H_{10}Si$		5,6 52	1,5 2,5 5,7	∿13 ∿6 22	3,5 4,5	∿7 ∿1.5
286	1238	B	$C_7F_6H_{10}Sn$		5,6 55	1,5 2,5 5,7	12.5 5.0 22.5	3,5 4,5	7.5 2.5
287	1239	E	$C_8FH_7O_3$				0.9		
287	1240	E	$C_8FH_9O_4$				6.25		
285	1241	B	$C_8F_4H_{11}N$				3		11
288	1242		$C_{10}F_2H_6ClNO_2$				2.2 0.9		
							^3J		
289	1243		$C_{10}F_2H_7Cl_2D$			1,4 1,3 2,4 2,3	21.89 12.77 0.73 8.18 (-50°C)	20.08 12.18 2.46 8.76 (+100°C)	
289	1244		$C_{10}F_2H_9Br$			1,4 1,3 2,4 2,3	12.52 12.45 10.60 7.80 (-50°C)	11.90 11.85 10.85 9.55 (+100°C)	

Table A.2.c. (contd.)

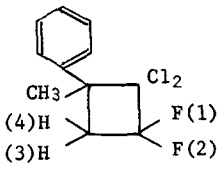
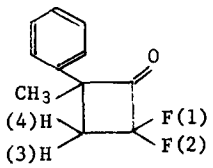
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
289	1245		$C_{11}F_2H_{10}Cl_2$		1,4	21.22	20.40
					1,3	13.65	13.63
					2,4	0.64	1.34
					2,3	8.69	8.89
						(-50°C)	(100°)
289	1246		$C_{11}F_2H_{10}O$		1,4	16.17	16.15
					1,3	10.28	10.34
					2,4	15.09	14.87
					2,3	10.97	10.79
						(30°C)	(100°C)

Table A.2.d. Fluorine bonded to carbon in four membered ring, hydrogen bonded to carbon outside this ring.

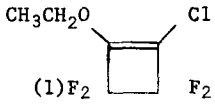
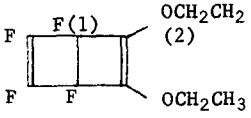
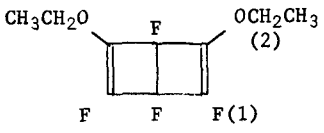
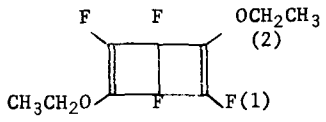
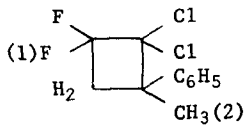
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^nJ
1095	1247 (3744)	P*	$C_6F_4H_5ClO$		1,2 0.2
290	1248 (3790)		$C_{10}F_4H_{10}O_2$		1,2 0.5
290	1249 (3791)		$C_{10}F_4H_{10}O_2$		1,2 1.3
290	1250 (3792)		$C_{10}F_4H_{10}O_2$		1,2 0.6
1099	1251		$C_{11}F_2H_{10}Cl_2$		1,2 2

Table A.2.e. Fluorine bonded to carbon in five membered ring excluding steroids, hydrogen bonded to carbon in the same ring.

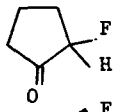
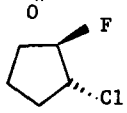
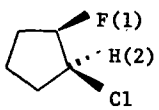
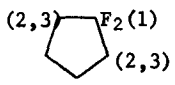
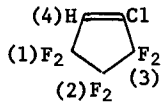
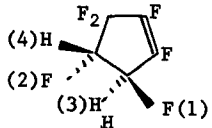
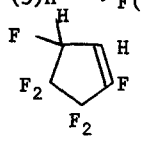
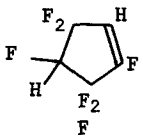
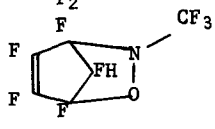
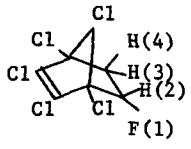
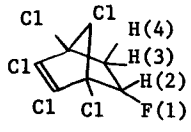
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
90	1252		C_5FH_7O		51					
153	1253	P	C_5FH_8Cl		50					
153	1254	P	C_5FH_8Cl		53.7	1,2	21			
291	1255	A	$C_5F_2H_8$			1,2 1,3	14.0 14.0			
627	1256 (3807)		C_5F_6HCl			1,4	1.6	2,4 3,4	2.7 1.5	
292	1257		$C_5F_6H_2$		1,3 2,4	57 49				
292	1258 (3809)		$C_5F_6H_2$			53				
292	1259 (3810)		$C_5F_6H_2$			49				
292	1260	B	C_6F_8HNO			59.5				
287 277	1261 (1322)	A	$C_7FH_3Cl_6$		1,2	55.1	1,3 1,4	24.7 12.2		
293	1262 (1323)	G	$C_7FH_3Cl_6$		1,2	54.31	1,3 1,4	25.10 12.01		

Table A.2.e. (contd.)

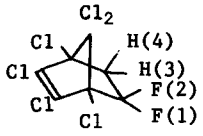
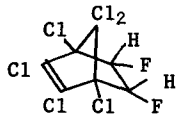
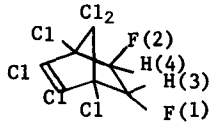
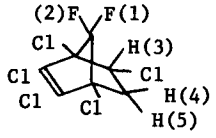
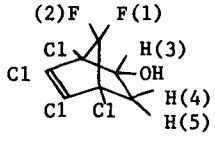
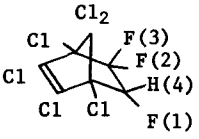
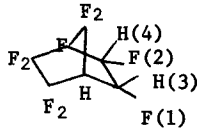
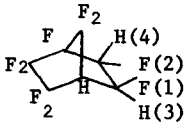
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
293	1263 (1328)	G	$C_7F_2H_2Cl_6$				1,3	15.86		
							1,4	7.36		
							2,3	4.46		
							2,4	13.07		
293	1264 (1329)	G	$C_7F_2H_2Cl_6$			52.10		1.87		
293	1265 (1330)	G	$C_7F_2H_2Cl_6$		1,3	51.73	1,4	17.71		
					2,4	52.06	2,3	13.85		
								^4J		
294	1266 (3816)	P*	$C_7F_2H_3Cl_5$				2,3	+0.81	1,3	-3.56
							2,4	-0.68	1,4	-3.21
							2,5	-5.27	1,5	-1.56
								^4J		
294	1267 (3817)	P*	$C_7F_2H_4Cl_4O$				2,3	+0.36	1,3	-3.21
							2,4	-0.45	1,4	-3.48
							2,5	-5.38	1,5	-1.95
293	1268 (1332)	G	$C_7F_3HCl_6$		1,4	51.72	2,4	0.31		
							3,4	9.13		
1151	1269 [1335 3839 3955]		$C_7F_9H_3$		1,3	52				
					2,4	54				
1151	1270 [1336 3840 3956]		$C_7F_9H_3$		1,3	48				
					2,4	48				

Table A.2.e. (contd.)

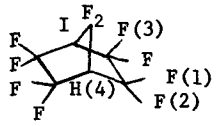
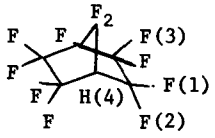
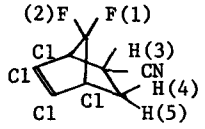
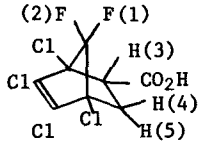
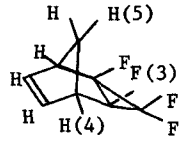
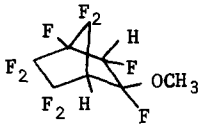
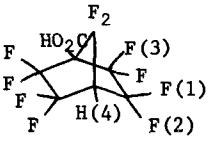
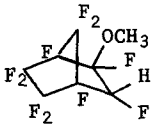
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ	
1151	1271 (1337)		$C_7F_{10}HI$			1,4 2,4	7.9 2.0	3,4	4.0
1151	1272 (1338)		$C_7F_{11}H$			1,4 2,4	9.1 2.1	3,4	5.2
							^4J		
294	1273 (3842)	P*	$C_8F_2H_3Cl_4N$			2,3 2,4 2,5	+1.12 −0.32 −4.87	1,3 1,4 1,5	−2.32 −2.74 −1.40
							^4J		
294	1274 (3843)	P*	$C_8F_2H_4Cl_4O_2$			2,3 2,4 2,5	+0.93 +0.89 −5.14	1,3 1,4 1,5	−2.81 −2.72 −1.42
274	1275 [1202 3691 1344]	B	$C_8F_4H_6$			3,4	2.3	3,5	6.3
1151	1276 [3857 3975 1345]		$C_8F_9H_5O$				50		
1151	1277 (1346)		$C_8F_{10}H_2O_2$			1,4 2,4	8.7 2.2	3,4	4.4
1151	1278 [3859 3976 1347]		$C_8F_{10}H_4O$		51				

Table A.2.e. (contd.)

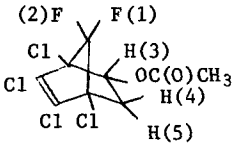
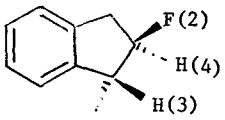
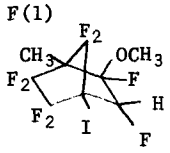
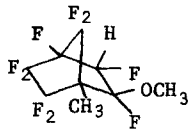
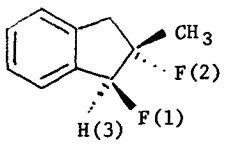
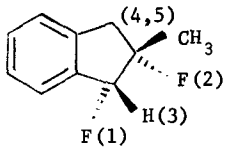
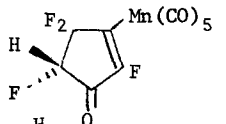
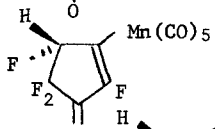
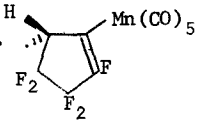
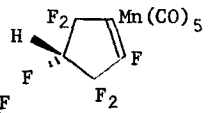
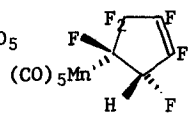
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ	
						^4J			
294	1279 (3863)	P*	$C_9F_2H_6Cl_4O_2$			2,3	+0.56	1,3	-3.24
						2,4	-0.76	1,4	-3.46
						2,5	-5.44	1,5	-1.89
295	1280 (3864, 3981)		$C_9F_2H_8$		1,3 56	1,4	16		
1151	1281 [3872, 3989, 1352]		$C_9F_8H_7IO$		45				
1151	1282		$C_9F_9H_7O$		51				
295	1283 (1305, 3875)		$C_{10}F_2H_{10}$		1,3 56	2,3	15		
295	1284 (1306, 3876)		$C_{10}F_2H_{10}$			2,3	9	1,4	2.2
						2,4	18.6		
						2,5	17.6		
292	1285 (3877)		$C_{10}F_4HMnO_6$		50.6				
292	1286 (3878)		$C_{10}F_4HMnO_6$		50				
292	1287 (3882)		$C_{10}F_6HMnO_5$		50				
292	1288 (3881)		$C_{10}F_6HMnO_5$		50				
292	1289 (3883)		$C_{10}F_6HMnO_5$		53				

Table A.2.e. (contd.)

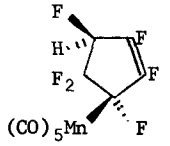
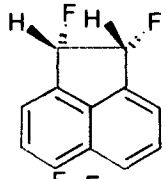
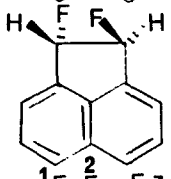
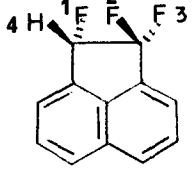
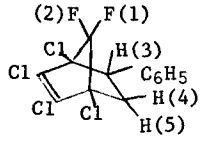
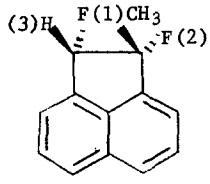
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ	
292	1290 (3884)		$C_{10}F_6HMnO_5$			≈56				
295	1291 (3891)		$C_{12}F_2H_8$			54.6	5.2			
295	1292 (3892)		$C_{12}F_2H_8$			52.2	19.4			
295	1293 (3893)		$C_{12}F_3H_7$		1,4	53.9	2,4 3,4	12.8 1.2		
								^4J		
294	1294 (3896)	P*	$C_{13}F_2H_8Cl_4$				2,3 2,4 2,5	+1.04 +0.39 -4.95	1,3 1,4 1,5	-3.04 -2.51 -0.90
295	1295 (1307, 3897)		$C_{13}F_2H_{10}$		1,3	54	2,3	5		

Table A.2.f. Fluorine bonded to carbon in five membered ring excluding steroids, hydrogen bonded to carbon outside this ring.

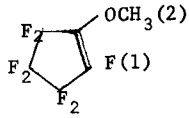
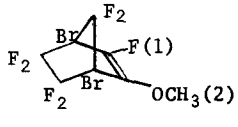
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ	
159	1296		$C_6F_7H_3O$				1,2	3.8
1151	1297 [3846, 3966, 1384]		$C_8F_7H_3Br_2O$				1,2	3.5

Table A.2.f. (contd.)

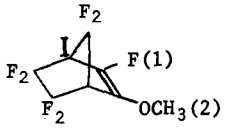
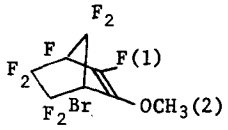
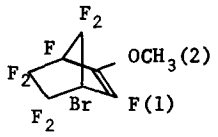
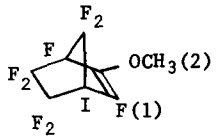
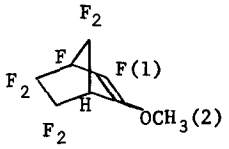
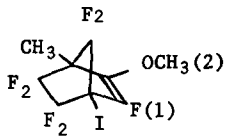
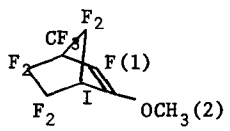
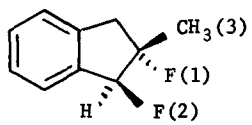
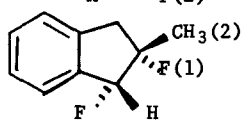
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1151	1298 [3846 3967 1385]		$C_8F_7H_3I_2O$				1,2 3.4
1151	1299 (1386)		$C_8F_8H_3BrO$				1,2 3.4
1151	1300 [3847 3968 1387]		$C_8F_8H_3BrO$				1,2 3.2
1151	1301 [3849 3970 1388]		$C_8F_8H_3IO$				1,2 3.4
1151	1302 [3852 3973 1389]		$C_8F_8H_4O$				1,2 3.2
1151	1303 [3869 3986 1393]		$C_9F_7H_6IO$				1,2 3.6
1151	1304 [3874 3991 1394]		$C_9F_{10}H_3IO$				1,2 3.6
295	1305 (1283 3875)		$C_{10}F_2H_{10}$		1,3	22	2,3 4
295	1306		$C_{10}F_2H_{10}$		1,2	22	

Table A.2.f. (contd.)

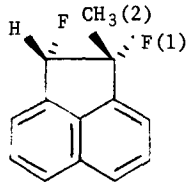
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
295	1307 (1295 3897)		$C_{13}F_2H_{10}$			1,2	22	

Table A.2.g. Fluorine bonded to carbon in six membered ring excluding steroids, hydrogen bonded to carbon in the same ring.

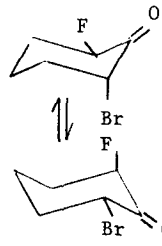
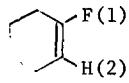
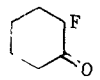
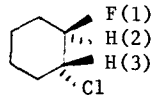
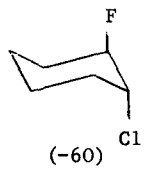
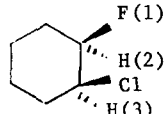
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
392	1308	F^2	$C_6FH_6^+$				1,2	8
298	1309	G	C_6FH_8BrO					
291	1310	A	C_6FH_9			1,2	17	
90	1311		C_6FH_9O		48			
153	1312	P	$C_6FH_{10}Cl$		49	1,3	7.5	
				Room temperature 	48.7			
153	1313	P	$C_6FH_{10}Cl$	 Room temperature	1,2 47.3	1,3	20	

Table A.2.g. (contd.)

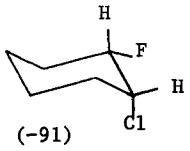
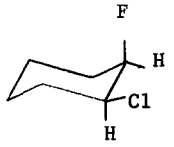
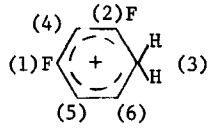
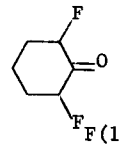
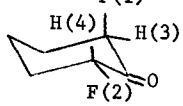
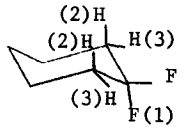
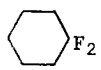
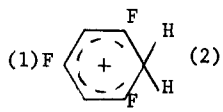
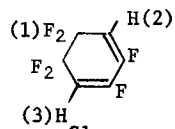
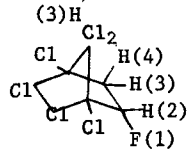
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
				 (-91)	1,2	46	1,3	6-10		
					1,2	50	1,3	30		
299	1314		C_6FH_{11}			49				
398	1315	0	$C_6F_2H_5^+$				1,4	8.5	1,6	5
392	(3910)						1,5	7	2,6	5
							2,3	8.5	1,3	8.5
							2,4	8.5		
298	1316	A	$C_6F_2H_8O$			~46				
298	1317	G	$C_6F_2H_8O$						1,4	~0
									2,3	4.6
297	1318		$C_6F_2H_{10}$				1,2	34.3		
	(3912)						1,3	11.5		
291	1319	A	$C_6F_2H_{10}$					14.0		
392	1320	F^2	$C_6F_3H_4^+$						1,2	8
	(3915)									
213	1321		$C_6F_6H_2$				1,2	15.1	1,3	3.7
	(3919)									
287	1322	A	$C_7FH_3Cl_6$		1,2	55.1	1,3	24.7		
277	(1261)						1,4	12.2		

Table A.2.g. (contd.)

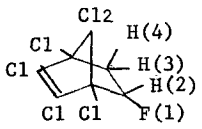
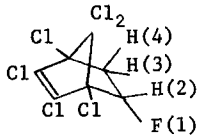
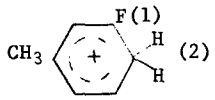
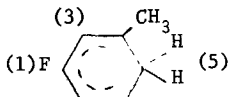
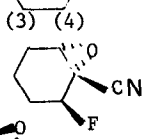
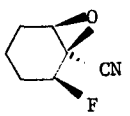
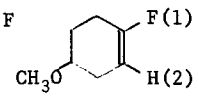
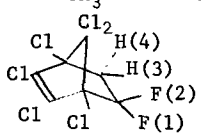
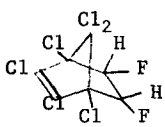
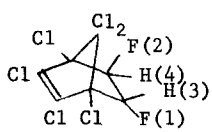
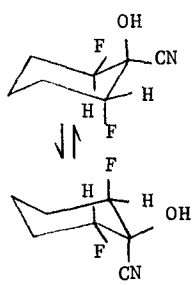
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
287 277	1322 (1261)	A	$C_7FH_3Cl_6$		1,2	55.1	1,3 1,4	24.7 12.2		
293	1323 (1262)	G	$C_7FH_3Cl_6$		1,2	54.31	1,3 1,4	25.10 12.01		
398	1324	O	$C_7FH_8^+$				1,2	9.5		
398	1324a	O	$C_7FH_8^+$				1,2 1,3	9.0 ~7	1,5 1,4	9.5 5.5
298	1325	G	C_7FH_8NO			50				
298	1326	G	C_7FH_8NO			48				
291	1327	A	$C_7FH_{11}O$				1,2	16		
293	1328 (1263)	G	$C_7F_2H_2Cl_6$				1,3 1,4 2,3 2,4	15.86 7.36 4.46 13.07		
293	1329 (1264)	G	$C_7F_2H_2Cl_6$			52.10		1.87		
293	1330 (1265)	G	$C_7F_2H_2Cl_6$		1,3 2,4	51.73 52.06	1,4 2,3	17.71 13.85		
298	1331	A	$C_7F_2H_9NO$						$^4J^{cis}$	3.75

Table A.2.g. (contd.)

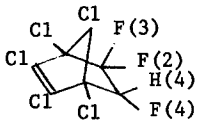
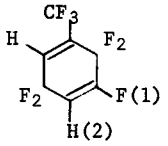
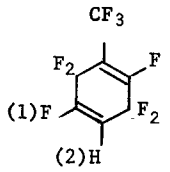
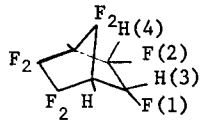
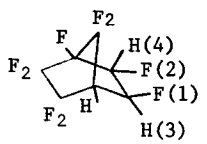
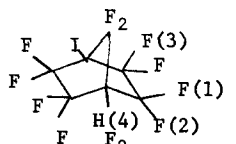
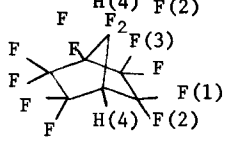
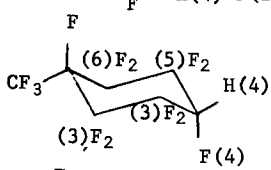
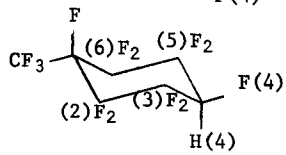
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ	
293	1332 (1268)	G	$C_7F_3HCl_6$		1,4	51.72	2,4 3,4	0.31 9.13			
213	1333 [852 2969 3940 3299]		$C_7F_8H_2$				1,2	11.3			
213	1334 [2970 3949 3300]		C_7F_9H				1,2	11.3			
1151	1335 [1269 3839 3955]		$C_7F_9H_3$		1,3 2,4	52 54					
1151	1336 [1270 3840 3956]		$C_7F_9H_3$		1,3 2,4	48 48					
1151	1337 (1271)		$C_7F_{10}HI$				1,4 2,4	7.9 2.0	3,4	4.0	
1151	1338		$C_7F_{11}H$				1,4 2,4	9.1 2.1	3,4	5.2	
301	1339 (2981 3958)	P*	$C_7F_{13}H$		4a,4e	47.6	3a:5a,4e 3e:5e,4e	5.6 5.6	2a:6a,4e 2e:6e,4e	4.0 0	
301	1340 (2980 3959)	P*	$C_7F_{13}H$		4e,4a	44.8	3a:5a,4a 3e:5e,4a	17 6	2a:6a,4a 2e:6e,4a	3.3 0	

Table A.2.g. (contd.)

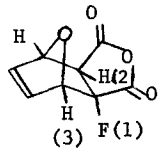
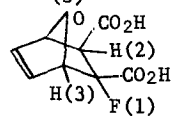
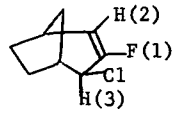
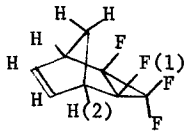
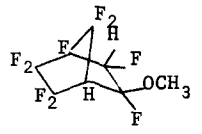
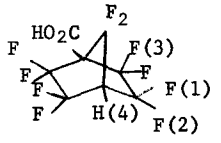
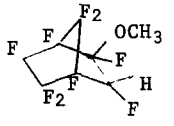
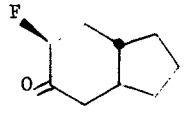
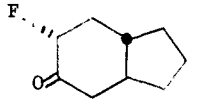
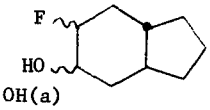
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ
277 287	1341	E-M	$C_8FH_5O_4$			1,2 1,3	10.55 2.3	
277 287	1342	E-M	$C_8FH_7O_5$			1,2 1,3	19.8 ∿2	
302	1343		$C_8FH_{10}Cl$			1,2 1,3	12.6 3.4	
274	1344 [1202 1275 3691]	B	$C_8F_4H_6$			1,2	2.3	
1151	1345 [1276 3857 3975]		$C_8F_9H_5O$		50			
1151	1346 (1277)		$C_8F_{10}H_2O_2$			1,4 2,4	8.7 2.2	3,4 4.4
1151	1347 [1278 3976 3859]		$C_8F_{10}H_4O$		51			
303	1348	G	$C_9FH_{13}O$		50			
303	1349	G	$C_9FH_{13}O$		47			
303	1350	G	$C_9FH_{14}O$					
				F(a) OH(a)	48			
				F(a) OH(e)	52			
				F(e) OH(e)	54			
				F(e) OH(a)	45			

Table A.2.g. (contd.)

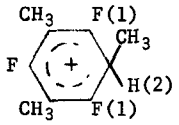
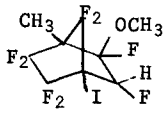
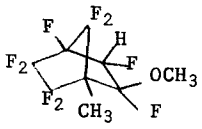
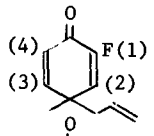
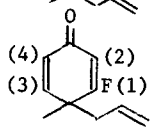
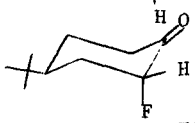
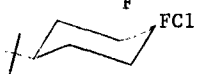
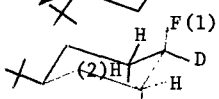
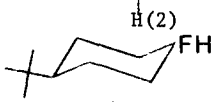
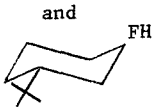
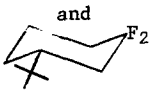
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
450	1351	F^2	$C_9F_3H_{10}^+$			1,2	6		
1151	1352 [1281 3872 3989]		$C_9F_8H_7IO$		45				
1151	1353 (3873 3990)		$C_9F_9H_7O$		51				
304	1354		$C_{10}FH_{11}O$			1,2	+13.8	1,3 1,4	+0.95 +7.25
304	1355		$C_{10}FH_{11}O$			1,2	+15.3	1,3 1,4	+12.0 +1.5
305	1356	G	$C_{10}FH_{16}O$		48				
305	1357	G	$C_{10}FH_{16}O$		~50				
306	1358	B	$C_{10}FH_{18}Cl$		~44				
				and					
					~10				
306	1359	B	$C_{10}FH_{18}D$			1,2	40		
306	1360	B	$C_{10}FH_{19}$		~46		~44 ~10		
				and					
					~10				
306	1361	B	$C_{10}F_2H_{18}$		~44				
				and					
					~10				

Table A.2.g. (contd.)

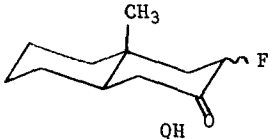
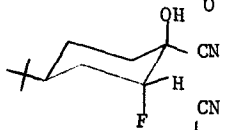
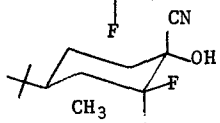
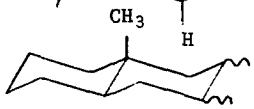
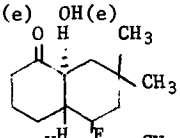
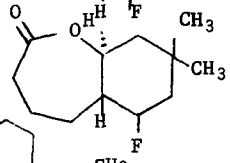
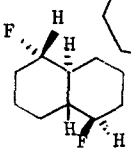
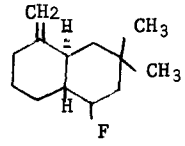
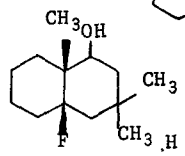
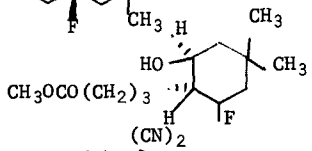
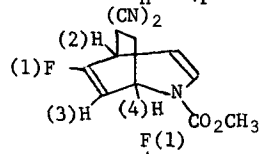
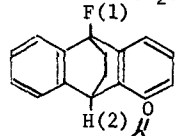
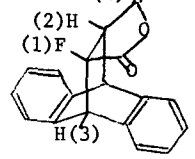
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ	
307	1362	G	$C_{11}FH_{17}O$		F(a) F(e)	50 48				
305	1363	A	$C_{11}FH_{18}NO$			48				
305	1364	A	$C_{11}FH_{18}NO$			50				
307	1365	G	$C_{11}FH_{19}O$		F(1), H(2) OH, H(3)					
					F(a) OH(a)	1,2	48	1,3	10	
					F(a) OH(e)		51		28	
					F(e) OH(a)		46			
					F(e) OH(e)		50			
308	1366		$C_{12}FH_{19}O$				50			
308	1367		$C_{12}FH_{19}O_2$				50			
308	1368		$C_{12}F_2H_{20}$				49			
308	1369		$C_{13}FH_{21}$				50			
308	1370		$C_{13}FH_{23}O$				46			
308	1371		$C_{13}FH_{23}O_3$				50			
309	1372		$C_{14}FH_8N_5O_2$					1,2 1,3	15 ~5	1,4 ~5
310	1373	G	$C_{16}FH_{13}$							1,2 <0.5
277 287	1374	L	$C_{18}FH_{11}O_3$					1,2 1,3	22.5 6.0	

Table A.2.g. (contd.)

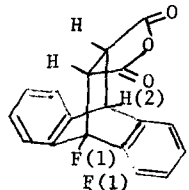
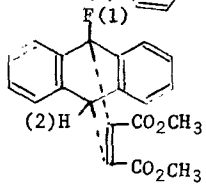
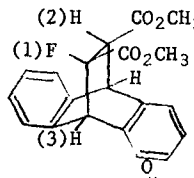
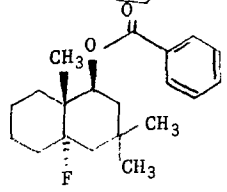
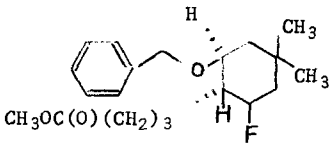
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
287	1375	F	$C_{18}FH_{11}O_3$			1,2	<0.5
310	1376	A	$C_{20}FH_{15}O_4$			1,2	0.88
277	1377	A	$C_{20}FH_{17}O_4$		1,2	30.8	
287					1,3	3.8	
308	1378		$C_{20}FH_{26}NO_4$			47 47 12 12	
308	1379		$C_{20}FH_{26}NO_6$		50		

Table A.2.h. Fluorine bonded to carbon in six membered ring excluding steroids, hydrogen bonded to carbon outside this ring.

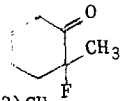
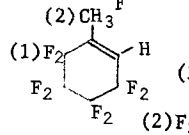
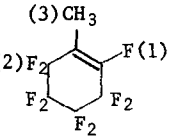
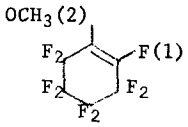
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^nJ
90	1380		$C_7FH_{11}O$		22	
213	1381		$C_7F_8H_4$			1,2 3.1
213	1382 (3954)		$C_7F_9H_3$			1,2 3.2 2,3 3.2
159	1383		$C_7F_9H_3O$			1,2 4

Table A.2.h. (contd.)

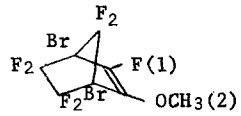
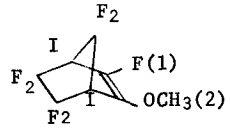
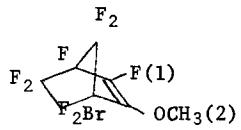
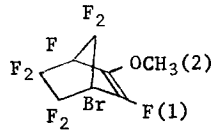
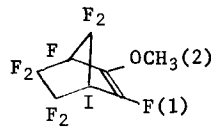
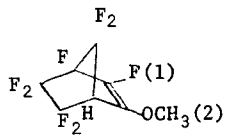
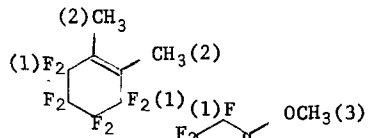
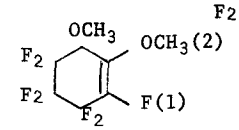
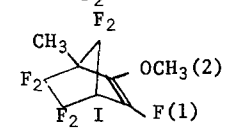
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^nJ
1151	1384 [1297 3845 3966]		$C_8F_7H_3Br_2O$		1,2	3.5
1151	1385 [1298 3864 3967]		$C_8F_7H_3I_2O$		1,2	3.4
1151	1386 (1299)		$C_8F_8H_3BrO$		1,2	3.4
1151	1387 [1300 3847 3968]		$C_8F_8H_3BrO$		1,2	3.2
1151	1388 [1301 3849 3970]		$C_8F_8H_3IO$		1,2	3.4
1151	1389 [1302 3852 3973]		$C_8F_8H_4O$		1,2	3.2
213	1390		$C_8F_8H_6$		1,2	2.7
159	1391		$C_8F_8H_6O$		1,3 2,4	0.5 1.5
159	1392		$C_8F_8H_6O_2$		1,2	4
1151	1393 [1303 3869 3986]		$C_9F_7H_6IO$		1,2	3.6

Table A.2.h. (contd.)

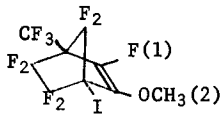
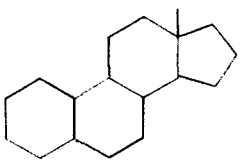
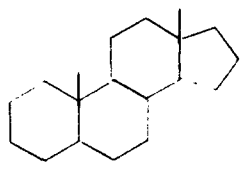
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	n_J	
1151	1394 [1304 3874 3991]		$C_9F_{10}H_3IO$		1,2	3.6

Table A.2.i. Fluorine bonded to carbon in steroid nucleus, hydrogen bonded to carbon in the same system.

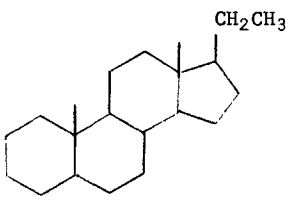
Parent steroid structures (serial No. 1395-1563)



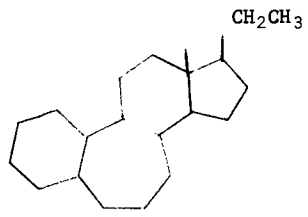
(I) Estrane



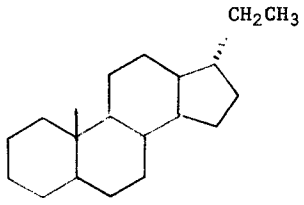
(II) Androstane



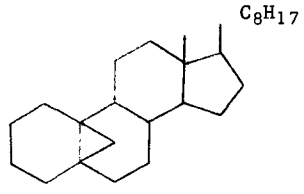
(III) Pregnane



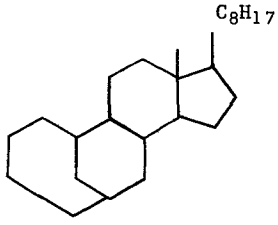
(IV) B-homo-19-norpregnane



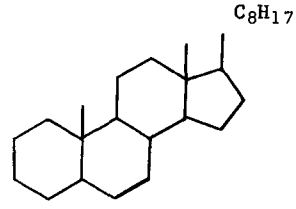
(V) 18-nor-17-isopregnane



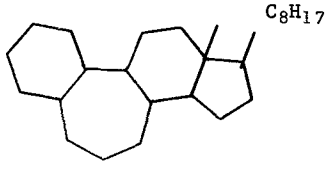
(VI) 5β,19-cyclocholestane



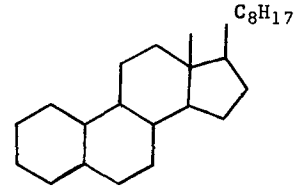
(VII) 4-Abeo(5:6)-19-nor-6β-cholestane



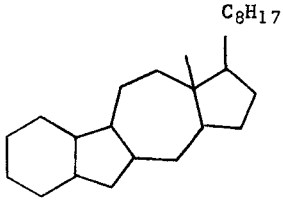
(VIII) Cholestane



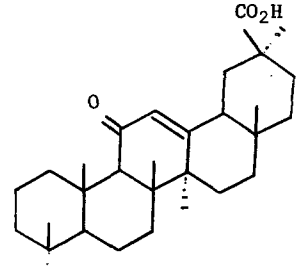
(IX) B-Homo-19-nor-cholestane



(X) 19-Norcholestane



(XI) B-Nor-C-homocholestane



(XII) Glycyrrhetic acid

Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.		J
311	1395	A	$C_{18}FH_{23}O_3$	2α-fluoro-10β-hydroxyestra-3,17-dione	(I)		49
312	1396	A	$C_{18}FH_{25}O_2$	3β-fluoro-17β-acetoxyestra-5(10)-ene	(I)		~50
313	1397	A	$C_{19}F_2H_{22}O_2$	16,16-difluoro-3-hydroxyestra-1,3,5(10)-trien-17-one-	(I)	16,18	1
314				-3-methyl ether			
313	1398	A	$C_{19}FH_{23}O_2$	16β-fluoro-3-hydroxyestra-1,3,5(10)-trien-17-one-	(I)	16,18	0.5
				-3-methyl ether			
313	1399	A	$C_{19}FH_{25}$	17α-fluoroestra-1,3,5(10)-trien-3-ol methyl ether	(I)	17,18	1.8
315							
316	1400	A	$C_{19}FH_{26}O_3$	6β-fluoro-5α-hydroxyandrostane-3,17-dione	(II)	6,19	3.7
317							
313	1401	A	$C_{19}FH_{27}O$	17α-fluoroandrost-4-en-3-one	(II)	17,18	2.1
315							
318	1402	A	$C_{19}FH_{27}O$	3β-fluoroandrost-5(6)-en-17-one	(II)		~50
315	1403	A	$C_{19}FH_{27}O$	3α-fluoroandrost-5(6)-en-17-one	(II)		51
315	1404	A	$C_{19}FH_{27}O$	17α-fluoroandrost-4-en-3-one	(II)		55.2
						17,18	2.1
313	1405	A	$C_{19}FH_{27}O_2$	2β-fluoro-5α-androstan-3,17-dione	(II)	2,19	2
319							
311	1406	A	$C_{19}FH_{27}O_2$	2β-fluoro-17β-hydroxyandrost-4-en-3-one	(II)		49
318	1407	A	$C_{19}FH_{27}O_2$	3β-fluoro-6β-hydroxy-5-methyl-19-nor-5β-androst-9-en-17-one	(II)		~ 48.5
315	1408	A	$C_{19}FH_{29}O$	3α-fluoroandrostan-17-one	(II)		48

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.		J
312	1409	A	$C_{19}FH_{29}O$	3β-fluoro-6β-methyl-17β-hydroxyestr-5(10)-ene	(I)		~50
313	1410	A	$C_{19}FH_{29}O_2$	2β-fluoro-3α-hydroxyandrostan-17-one	(II)	2,19	2
319							
311	1411	A	$C_{19}FH_{29}O_2$	5β-fluoro-4β,17β-dihydroxy-5β-androstan-3-one	(II)	5,19	10
						5,4	34
312	1412		$C_{19}FH_{29}O_2$	3β-fluoro-6β-hydroxymethyl-17β-hydroxyestr-5(10)-ene	(I)		~50
318	1413	A	$C_{19}FH_{29}O_3$	3β-fluoro-5α,6β-dihydroxyandrostan-17-one	(II)		~ 49
320	1414		$C_{19}F_2H_{24}O_2$	6,6-difluoroandrost-4-en-3,17-dione	(II)	6β,4	4.0
	(4011)					6,7	33
318	1415	A	$C_{19}F_2H_{26}O$	(R) 3β,5-difluoro-5-methyl 4(5:6)-abeo-19-nor-6β-androst-9-en-17-one	(II)	5,19	23
320	1416	A	$C_{19}F_4H_{22}O$	6,6,17,17-tetrafluoro-androst-1,4-dien-3-one	(II)	17,18	2.0
	(4012 / 3902)					6β,4	4.0
						6,7	33
						17,16	25
320	1417		$C_{19}F_4H_{24}O$	6,6,17,17-tetrafluoro-androst-1,4-dien-3-one	(II)	17,18	2.0
	(4013 / 3903)					6β,4	4.0
						6,7	33
						17,16	24
320	1418		$C_{19}F_5H_{25}O$	5α,6,6,17,17-pentafluoroandrostan-3-one	(II)	17,18	2.0
	(3904)					17,16	21
						5,4	45
320	1419		$C_{19}F_5H_{27}O$	5α,6,6,17,17-pentafluoro-3β-hydroxyandrostane	(II)	17,18	2.0
	(3905)					17,16	24
						5,4	40
313	1420	A	$C_{21}FH_{26}ClO_2$	11β-fluoro-9α-chloropregna-1,4-diene-3,20-dione	(III)	11,18	2.7
322						11,19	5.3

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.		
313	1421	A	$C_{21}FH_{27}O_3$	15β-fluoropregn.-4-ene-3,11,20-trione	III	15,18	1
323							
324	1422	A	$C_{21}FH_{28}O$	3β-fluoro-17β acetoxy-4-hydroxyandrost-5-ene	II		48.7
						3,4	6
316	1423	A	$C_{21}FH_{29}O_2$	6β-fluoropregn-4-en-3,20-dione	III	6,19	2
325							
313	1424	A	$C_{21}FH_{29}O_2$	11β-fluoropregn-4-en-3,20-dione	III	11,19	3
326						11,18	3
312	1425	A	$C_{21}FH_{29}O_3$	3β-fluoro-17β-acetoxy-19-oxoandrost-5-ene	II		∿ 50
318	1426	A	$C_{21}FH_{29}O_3$	3β-fluoro-6β-acetoxy-5-methyl 19-nor-5β-androst-9-en-17-one	II		∿ 49.5
324	1427	A	$C_{21}FH_{29}O_3$	3β-fluoro-17-acetoxyandrost-5-en-7-one	II		48
320	1428		$C_{21}FH_{29}O_4$	5α-fluoro-3α-acetoxyandrost-6,17-dione	II		50
315	1429	A	$C_{21}FH_{30}BrO_3$	6β-fluoro-3β-acetoxy-5α-bromoandrost-17-one	II		50
						6,19	4.5
312	1430	A	$C_{21}FH_{30}BrO_3$	3β-fluoro-17β-acetoxy-5α-bromo-6β,19-epoxyandrostane	II		∿50
315	1431	A	$C_{21}FH_{31}O_2$	3β-fluoro-17β-acetoxyandrost-5-ene	II		∿50
312	1432	A	$C_{21}FH_{31}O_2$	3β-fluoro-17β-acetoxyandrost-5-ene	II		∿50
327	1433	A	$C_{21}FH_{31}O_2$	7ζ-fluoro-3β-hydroxy-B-homo-19-norpreg-5(10)-en-20-one	II		50
328	1434	A	$C_{21}FH_{31}O_2$	3β-fluoro-17β-acetoxy-5-methyl-6α,10-cyclo-5β,9β,10α-estrane	I		49.5
311	1435	A	$C_{21}FH_{31}O_3$	5α-fluoro-17β-acetoxy-4α-hydroxyandrost-3-one	II	5,6	33
316	1436	A	$C_{21}FH_{31}O_3$	6β-fluoro-17β-acetoxy-5α-androstan-3-one	II	6,19	2.2
312	1437	A	$C_{21}FH_{31}O_3$	3β-fluoro-17β-acetoxy-19-hydroxyandrost-5-ene	II		∿50
312	1438	A	$C_{21}FH_{31}O_3$	3β-fluoro-17β-acetoxy-5α,6α-epoxyandrostane	II		∿50
312	1439	A	$C_{21}FH_{31}O_3$	3β-fluoro-17β-acetoxy-5β,6β-epoxyandrostane	II		∿50
312	1440	A	$C_{21}FH_{31}O_3$	3β-fluoro-17β-acetoxy-6β-hydroxymethylestrene	I		∿50
318	1441	A	$C_{21}FH_{31}O_4$	3β-fluoro-6β-acetoxy-5α-hydroxyandrost-17-one	II		∿50.5
316	1442	A	$C_{21}FH_{31}O_4$	6β-fluoro-3β-acetoxy-5α-hydroxyandrostan-17-one	II	6,19	4.5
315							

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.		J
316	1443	A	$C_{21}FH_{32}BrO_3$	6β-fluoro-3β-acetoxy-5α-bromoandrostan-17-one	II	6,19	4.5
312	1444	A	$C_{21}FH_{32}BrO_3$	3β-fluoro-17β-acetoxy-5α-bromo-6β-hydroxyandrostane	II		50
312	1445	A	$C_{21}FH_{32}BrO_3$	3β-fluoro-17β-acetoxy-6β-bromo-5α-hydroxyandrostane	II		50
312	1446	A	$C_{21}FH_{32}BrO_3$	3β-fluoro-17β-acetoxy-6α-bromo-5β-hydroxyandrostane	II		50
316	1447	A	$C_{21}FH_{33}BrO_2$	6β-fluoro-5α-bromo-3β-hydroxypregnan-20-one	III		4.8
329							
313	1448	A	$C_{21}F_2H_{28}O_3$	4,4-difluoro-17β-acetoxyandrost-5-en-3-one	II	4,19	1
330							
320	1449		$C_{21}F_3H_{29}O_3$	5α,6,6-trifluoro-3β-acetoxyandrostan-17-one	II	5,4	44
320	1450		$C_{21}F_5H_{29}O_2$	5α,6,6,17,17-pentafluoro-3β-acetoxyandrostane	II	17,18	2.0
	(3908)					17,16	24
331	1451	A	$C_{22}FH_{31}O_3$	6α-fluoro-17β-acetoxy-17β-acetoxy-17α-methyl-9β,10α-androst-4-en-3-one	II		50
						6,4	4.3
331	1452	A	$C_{22}FH_{31}O_3$	6β-fluoro-17β-acetoxy-17α-methyl-9β,10α-androst-4-en-3-one	II		50
316	1453	A	$C_{22}FH_{33}BrO_2$	6β-fluoro-5α-bromo-3β-hydroxy-16α-methylpregnan-20-one	III	6,19	4.6
332	1454	A	$C_{22}FH_{33}O_5$	6β-fluoro-3α-acetoxy-17α-hydroxypregnan-11,20-dione	III		48
331	1456	A	$C_{23}FH_{29}O_3$	6α-fluoro-17β-acetoxy-17α-ethynyl-9β,10α-androst-4-en-3-one	II		50
						6,4	4.3
331	1457	A	$C_{23}FH_{29}O_3$	6β-fluoro-17β-acetoxy-17α-ethynyl-9β,10α-androst-4-en-3-one	II		50
313	1458	A	$C_{23}FH_{29}O_4$	15β-fluoropregna-4,17(20)-diene-3,11-dione 21-carboxylic acid	III	15,18	1
323				methyl ester			
324	1459	A	$C_{23}FH_{30}O_4$	3β-fluoro-4β,17β-diacetoxyandrost-3-one	II		48
313	1460		$C_{23}FH_{31}O_5$	17α-fluoro-21-acetoxy-5β-pregnan-3,11,20-trione	III	17,18	1
321							
327	1461	A	$C_{23}FH_{31}O_5$	7-fluoro-17,20:20,21-bismethylenedioxy-B-homo-19-norpregn-4-en-3-one	II		50

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.		J
316	1462	A	$C_{23}FH_{32}O_4$	6β-fluoro-3β-acetoxy-5α-hydroxypregn-16-en-20-one	(III)	6,19	4.3
311	1463	A	$C_{23}FH_{32}O_4$	5α-fluoro-4α,17β-diacetoxyandrost-3-one	(II)	5,4	34
331	1464	A	$C_{23}FH_{33}O_3$	6α-fluoro-17β-acetoxy-17α-ethyl-9β,10α-androst-4-en-3-one	(II)		50
						6,4	4.3
331	1465	A	$C_{23}FH_{33}O_3$	6β-fluoro-17β-acetoxy-17α-ethyl-9β,10α-androst-4-en-3-one	(II)		50
312	1466	A	$C_{23}FH_{33}O_4$	3β-fluoro-17β,19-diacetoxyandrost-5-ene	(II)		50
312	1467	A	$C_{23}FH_{33}O_4$	3β-fluoro-6β-acetoxymethyl-17β-acetoxyestr-5(10)-ene	(I)		50
316	1468	A	$C_{23}FH_{33}O_5$	6β-fluoro-17α-acetoxy-3β, 5α-dihydroxypregnan-20-one	(III)	6,19	4.7
333							
316	1469	A	$C_{23}FH_{34}BrO_5$	6β-fluoro-21-acetoxy-5α-bromo-16α,17α-epoxy-3β-hydroxypregnan-20-one	(III)	6,19	4.0
316	1470	A	$C_{23}FH_{34}O_4$	6β-fluoro-5α-hydroxypregnan-3,20-dione 3-ethylene ketal	(III)	6,19	5
333							
316	1471	A	$C_{23}FH_{34}O_5$	6β-fluoro-3β,17β-diacetoxy-5α-hydroxyandrostane	(II)	6,19	4.5
317							
316	1472	G	$C_{23}F_2H_{32}O_3$	3β,6β-difluoro-17α-acetoxypregn-4-en-20-one	(III)	6,19	1.9
313	1473	A	$C_{23}F_2H_{34}O_3$	3β,6β-difluoro-17α-acetoxypregn-4-en-20-one	(III)	6,19	1.9
313	1474	A	$C_{23}F_3H_{31}O_3$	17α,21,21-trifluoro-3β-acetoxypregn-5-en-20-one	(III)	17,19	1-2
334	1475	A	$C_{23}F_4H_{28}O_2$	16α,17α-terafluoroethylene pregn-4-en-3,20-dione	(III)	,21	2.2
334	1476	A	$C_{23}F_4H_{30}O$	16α,17α-tetrafluoroethylene-3β-hydroxypregn-5-en-20-one	(III)	,21	2.4
332	1477	A	$C_{24}FH_{35}O_6$	17α-fluoro-3α,16α-diacetoxypregnan-11,20-dione	(III)	17,16	16.2
316	1478	A	$C_{25}FH_{33}O_6$	6β-fluoro-17α,21-diacetoxypregn-4-en-3,20-dione	(III)	6,19	1.6
333							
316	1479	A	$C_{25}FH_{33}O_8$	6β-fluoro-17α,21-diacetoxy-5α-hydroxypregnan-3,11,20-trione	(III)	6,19	2.5
313	1480	A	$C_{25}FH_{35}O_6$	17α-fluoro-3α,21-diacetoxy-5β-pregnan-11,20-dione	(III)	17,18	1
321							
332	1481	A	$C_{25}FH_{35}O_6$	14β-fluoro-3α,16α-diacetoxy-17 methyl-18-nor-17-isopregnan-11,20-dione	(V)	14,13	35
313	1482	A	$C_{25}FH_{35}O_8$	6β-fluoro-5α-hydroxy-17α,20:20,21-bismethylenedioxy-pregnan-3,11-dione 3-ethylene ketal	(III)	6,19	4.6

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.	J	
313 329	1483	A	$C_{25}FH_{36}BrO_6$	6β-fluoro-17α,21-diacetoxy-5α-bromo-3β-hydroxypregnan-20-one	III	6,19	4.3
313 335	1484	A	$C_{25}FH_{37}O_6$	6β-fluoro-21-acetoxy-5α,11β-dihydroxypregn-17(20)-en-3-one 3-ethylene ketal	III	6,19	7
313	1485	A	$C_{25}FH_{37}O_6$	6β-fluoro-5α,21-dihydrxypregnan-3,20-dione 3,20-bisethylene ketal	III	6,19	5.2
334	1486	A	$C_{25}F_4H_{32}O_3$	16α,17α-tetrafluoroethylene-3β-acetoxypregn-5-en-20-one	III	,21	2.3
334	1487	A	$C_{25}F_4H_{32}O_3$	16β,17β-tetrafluoroethylene-3β-acetoxypregn-5-en-20-one	III	,21	2.6
						,18	3.7
313	1488	A	$C_{26}FH_{38}BrO_6$	6β-fluoro-3β-acetoxy-5α-bromo-16α,17α,21-trihydroxypregnan-20-one 16α,17α-acetonide	III	6,19	4.5
313	1489	A	$C_{26}FH_{38}BrO_6$	6β-fluoro-21-acetoxy-5α-bromo-3β,16α,17α-trihydroxypregnan-20-one 16α,17α-acetonide	III	6,19	4.8
313 336	1490	A	$C_{26}FH_{39}O_7$	6β-fluoro-21-acetoxy-3β,5α,16α,17α-tetrahydroxypregnan-20-one 16α,17α-acetonide	III	6,19	4.7
332	1491	A	$C_{26}FH_{40}NO_6$	17α-fluoro-3α,16α-diacetoxy-11β-hydroxypregnan-20-one 20-methoxime	III	17,16	22
332	1492	A	$C_{26}FH_{40}NO_6$	17α-fluoro-3α,16β-diacetoxy-11β-hydroxypregnan-20-one 20-methoxime	III	17,16	24
							1.3
313	1493	A	$C_{27}FH_{37}O_7$	6β-fluoro-3β,17α,21-triacetoxypregn-4-en-20-one	III	6,19	1.7
313 337	1494	A	$C_{27}FH_{37}O_9$	6β-fluoro-17α,21-diacetoxy-5α-hydroxypregnan-3,11,20-trione 3-ethylene ketal	III	6,19	4.2
313	1495	A	$C_{27}FH_{39}O_8$	6β-fluoro-3β,17α,21-triactoxy-5α-hydroxypregnan-20-one	III	6,19	4.5
338	1496	A	$C_{27}FH_{43}$	3β-fluoro-5β,19(5β)-cyclocholest-6-ene	VI		50
328	1497	A	$C_{27}FH_{43}$	(R)-3β-fluoro-5-methylene-4(5:6)-abeo cholest-9(6β)-ene	VII		46
338	1498	A	$C_{27}FH_{43}$	3β-fluoro-5β,6β-cyclocholest-9-ene	VIII		50
324	1499	A	$C_{27}FH_{43}O$	3β-fluorocholest-5-en-4-one	VIII		48

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.		J
324	1500	A	$C_{27}FH_{43}O$	3β-fluorocholest-4-en-6-one	VIII		46
						3,4	12
339	1501	A	$C_{27}FH_{44}O_2$	3β-fluoro-6β:5β-epoxy-19-hydroxy-5α-cholestane	VIII		51
339	1502	A	$C_{27}FH_{44}BrO$	3β-fluoro-5α-bromo-6β:19-epoxycholestane	VIII		51
328	1503	A	$C_{27}FH_{44}Cl$	(R)-3β-fluoro-5-chloro-5-methyl 4(5:6)-abeo-6β-cholest-9-ene	VII		45.5
339	1504	A	$C_{27}FH_{44}ClO$	3β-fluoro-5α-chloro-6β:19-epoxy cholestane	VIII		50
318	1505	A	$C_{27}FH_{45}$	3β-fluorocholest-5-ene	VIII		50
339							
324							
328	1506	A	$C_{27}FH_{45}$	3β-fluoro-5-methyl-6α,10-cyclo-19-nor-5β,9β,10α-cholestane	VIII		49.5
324	1507	A	$C_{27}FH_{45}O$	3β-fluoro-4β-hydroxycholest-5-ene	VIII		48
						3,4	4.5
339	1508	A	$C_{27}FH_{45}O$	3β-fluoro-19-hydroxycholest-5-ene	VIII		51
340	1509	A*	$C_{27}FH_{45}O$	2α-fluorocholestan-3-one	VIII	2α,2β	48
						2,1α	11.5
						2,1β	4.5
						2,4α	7.3
						2,4β	-2.0
						2,5α	0
341	1510	G	$C_{27}FH_{45}O$	2β-fluorocholestan-3-one	VIII		50
341	1511	G	$C_{27}FH_{45}O$	2α-fluorocholestan-3-one	VIII		47.5
341	1512	G	$C_{27}FH_{45}O$	3β-fluorocholestan-2-one	VIII		50.5
341	1513	G	$C_{27}FH_{45}O$	3α-fluorocholestan-2-one	VIII		51
242	1514	A	$C_{27}FH_{45}O$	5α-fluoro-3β-hydroxycholest-7-ene	VIII		42
						5, ?	38
							20

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.	J	
242	1515	A	$C_{27}FH_{45}O$	5α-fluoro-3β-hydroxycholest-8(14)-ene	VIII		44
						5, ?	
							44
338	1516	A	$C_{27}FH_{45}O$	3β-fluoro-7β-hydroxy B-homo-19-cholest-5(10)-ene	IX		50
339	1517	A	$C_{27}FH_{45}O$	3β-fluoro-6β:19-epoxycholestane	VIII		50
318	1518	A	$C_{27}FH_{45}O$	3β-fluoro-6β-hydroxy-5-methyl 19-nor 5β-cholest-9-ene	X		47
						3,2	40
						3,4	40
328	1519	A	$C_{27}FH_{45}O$	(R) 3β-fluoro-5-hydroxy-5-methyl 4(5:6)-abeo-6β-cholest-9-ene	VII		46
324	1520	A	$C_{27}FH_{45}O_2$	3β-fluoro-5α-hydroxycholestan-6-one	VIII		52
339	1521	A	$C_{27}FH_{45}O_2$	3β-fluoro-5α-hydroxy-6β:19-epoxycholestane	VIII		48
341	1522	G	$C_{27}FH_{47}O$	2α-fluoro-3α-hydroxycholestane	VIII		48
341	1523	G	$C_{27}FH_{47}O$	2α-fluoro-3β-hydroxycholestane	VIII		50
341	1524	G	$C_{27}FH_{47}O$	2β-fluoro-3α-hydroxycholestane	VIII		47
341	1525	G	$C_{27}FH_{47}O$	2β-fluoro-3β-hydroxycholestane	VIII		51.5
							29
341	1526	G	$C_{27}FH_{47}O$	3α-fluoro-2α-hydroxycholestane	VIII		52.5
							31
341	1527	G	$C_{27}FH_{47}O$	3α-fluoro-2β-hydroxycholestane	VIII		46.5
341	1528	G	$C_{27}FH_{47}O$	3β-fluoro-2β-hydroxycholestane	VIII		47
318	1529	A	$C_{27}FH_{47}O_2$	3β-fluoro-5,6β-dihydroxy-5α-cholestane	VIII		49
328	1530	A	$C_{27}F_2H_{44}$	(R) 3β,5-difluoro-5-methyl 4(5:6)-abeo-19-nor-6β-cholest-9-ene	VII	3β,3α	45
318						5,19	23
						5,6	12
338	1531	A	$C_{27}F_2H_{44}$	3β,7β-difluoro B-homo-19-cholest-5(10)-ene	IX		50
339	1532	A	$C_{27}F_2H_{44}O$	5β,5α-difluoro-6β,19-epoxycholestane	VIII		50
343	1533		$C_{27}F_2H_{44}O$	4α,5α-difluorocholestan-3-one	VIII	4α,4β	47
						5α,4β	32.6

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Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.	J	
339	1534	A	$C_{27}F_2H_{46}O$	3β,5α-difluoro-6β-hydroxycholestane	VIII	3β,3α	50
						5α ?	50
342	1537	A	$C_{27}F_3H_{45}O$	5α,8,8-trifluoro-B-nor-C-homo-(7α)-cholestan-3-one	XI	5,4	43
						5,6	43
						8β,7α	31
						8β,14	31
324	1538	A	$C_{29}FH_{47}O_2$	3β-fluoro-4β-acetoxycholest-5-ene	VIII		48
318	1539	A	$C_{29}FH_{47}O_2$	3β-fluoro-6β-acetoxy-5-methyl 19-nor-5β-cholest-9-ene	X	3β,3α	49
						3,2	45
						3,4	45
328	1540	A	$C_{29}FH_{47}O_2$	(R) 3β-fluoro-5-acetoxy-5-methyl 4-abeo (5:6)-6β-cholest-9-ene	VII		45.5
388	1541	A	$C_{29}FH_{47}O_2$	3β-fluoro-7β-acetoxy B-homo-19-cholest-5(10)-ene	IX		50
338	1542	A	$C_{29}FH_{47}O_2$	3β-fluoro-6β-acetoxy-5β,19(5β)-cyclocholestane	VI		50
334	1543	G	$C_{29}FH_{49}O$	2α-fluoro-4,4-dimethylcholestan-3one	VIII		48.5
344	1544	G	$C_{29}FH_{49}O$	2β-fluoro-4,4-dimethylcholestan-3-one	VIII		50.5
342	1545	A	$C_{29}FH_{49}O_2$	5α-fluoro-3α- and 5α-fluoro-3β-hydroxycholestane	VIII	5,4	46
						5,6	46
342	1546	A	$C_{29}FH_{49}O_2$	5β-fluoro-3α- and 5β-fluoro-3β-hydroxy-5α-cholestane	VIII		45.1
							45.1
						5, ?	11.8
							11.8
							11.8
341	1547	G	$C_{29}FH_{49}O_2$	2α-fluoro-3α-acetoxycholestane	VIII		49
341	1548	G	$C_{29}FH_{49}O_2$	2α-fluoro-3β-acetoxycholestane	VIII		48
341	1549	G	$C_{29}FH_{49}O_2$	2β-fluoro-3α-acetoxycholestane	VIII		46
341	1550	G	$C_{29}FH_{49}O_2$	2β-fluoro-3β-acetoxycholestane	VIII		52
						2,3	29
341	1551	G	$C_{29}FH_{49}O_2$	3α-fluoro-2α-acetoxycholestane	VIII		49.5

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						3,2	26

Table A.2.i. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	Structure No.	J
341	1552	G	$C_{29}FH_{49}O_2$	3α-fluoro-2β-acetoxycholestane	(VIII)	46.5
341	1553	G	$C_{29}FH_{49}O_2$	3β-fluoro-2β-acetoxycholestane	(VIII)	45
318	1554	A	$C_{29}FH_{49}O_3$	3β-fluoro-6β-acetoxy-5α-hydroxycholestane	(VIII)	49
344	1555	G	$C_{29}FH_{51}O$	2α-fluoro-3α-hydroxy-4,4-dimethylcholestane	(VIII)	46.5
344	1556	G	$C_{29}FH_{51}O$	2α-fluoro-3β-hydroxy-4,4-dimethylcholestane	(VIII)	52
344	1557	G	$C_{29}FH_{51}O$	2β-fluoro-3α-hydroxy-4,4-dimethylcholestane	(VIII)	49
344	1558	G	$C_{29}FH_{51}O$	2β-fluoro-3β-hydroxy-4,4-dimethylcholestane	(VIII)	51.5
345	1559	A	$C_{31}FH_{46}O_4$	2β-fluoro-3α-hydroxy-18α-glycyrrhetic acid	(XII)	50
344	1560	G	$C_{31}FH_{53}O_2$	2α-fluoro-3α-acetoxy-4,4-dimethylcholestane	(VIII)	46
344	1561	G	$C_{31}FH_{53}O_2$	2α-fluoro-3β-acetoxy-4,4-dimethylcholestane	(VIII)	45
344	1562	G	$C_{31}FH_{53}O_2$	2β-fluoro-3α-acetoxy-4,4-dimethylcholestane	(VIII)	44.6
344	1563	G	$C_{31}FH_{53}O_2$	2β-fluoro-3β-acetoxy-4,4-dimethylcholestane	(VIII)	52

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Table A.2.j. Fluorine bonded to carbon in seven membered ring, hydrogen bonded to carbon in the same ring.

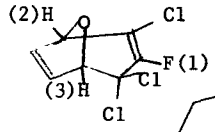
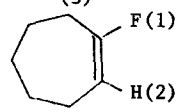
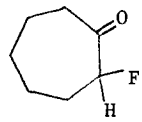
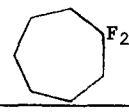
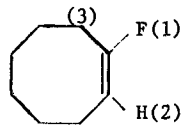
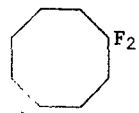
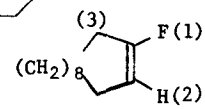
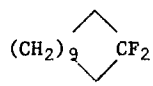
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
269	1564		$C_7FH_4Cl_3O$			1,2	7
						1,3	7
291	1565		C_7FH_{11}			1,2	21.5
						1,3	11.5
90	1566		$C_7FH_{11}O$		49		
291	1567	A	$C_7F_2H_{12}$			16.0	

Table A.2.k. Fluorine bonded to carbon in larger rings, hydrogen bonded to carbon in the same ring.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J
291	1568	A	C_8FH_{13}		1,2	18.0
348					1,3	22.5
291	1568a	A	$C_8F_2H_{14}$			15.0
291	1568b	A	$C_{12}FH_{21}$		1,2	37.0
					1,3	16.0
291	1569	A	$C_{12}F_2H_{22}$			14.5

A.3. Fluorine bonded to carbon in non-aromatic heterocyclic system, hydrogen bonded to carbon in either acyclic or cyclic system.

Table A.3.a. Fluorine bonded to carbon in non-aromatic nitrogen heterocyclic, hydrogen bonded to carbon in the same ring.

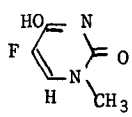
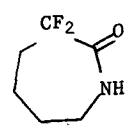
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
463	1570	A^2	$C_5FH_5N_2O_2$			6.0	
349	1571 (4027)	E	$C_6F_2H_9NO$			14.1	

Table A.3.a. (contd.)

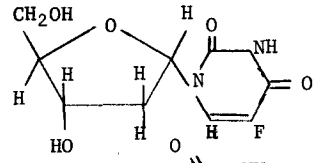
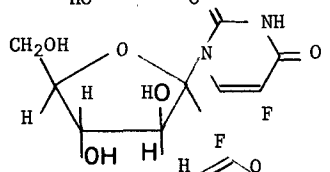
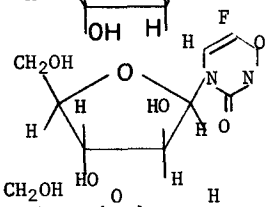
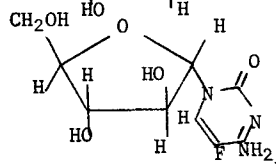
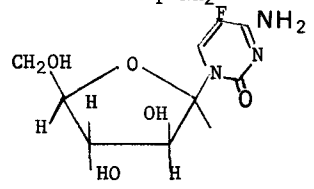
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
463	1572 (1578)	F	$C_9FH_{11}N_2O_5$			7.2	
463	1573	F	$C_9FH_{11}N_2O_5$			7.2	
463	1574 (1580)	F	$C_9FH_{11}N_2O_6$			7.5	
463	1575 (1581)	A^2	$C_9FH_{12}N_3O_5$			6.4	
463	1576 (1582)	F	$C_9FH_{12}N_3O_5$			7.1	

Table A.3.b. Fluorine bonded to carbon in non-aromatic nitrogen heterocycle, hydrogen bonded to carbon outside this ring.

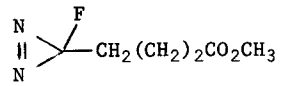
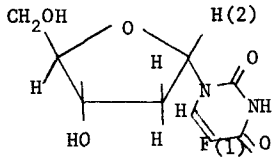
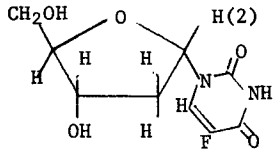
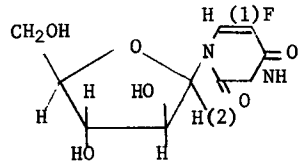
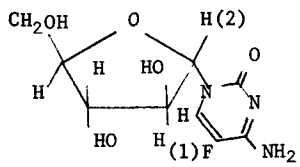
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^nJ	
351	1577		$C_6FH_9N_2O_2$		8		
463	1578 (1572)	F	$C_9FH_{11}N_2O_5$			1,2	1.8
463	1579 (1573)	F	$C_9FH_{11}N_2O_5$			1,2	~2
463	1580 (1574)	F	$C_9FH_{11}N_2O_6$			1,2	1.8
463	1581 (1575)	A^2	$C_9FH_{12}N_3O_5$			1,2	1.3

Table A.3.b. (contd.)

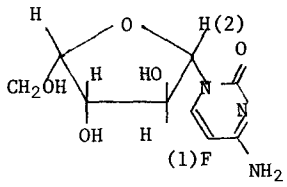
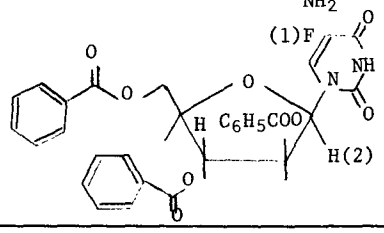
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^nJ
463	1582 (1576)	F	$C_9FH_{12}N_3O_5$		1,2		2
463	1583	F H^2	$C_{30}FH_{23}N_2O_9$		1,2 1,2		∿1.3 2.0

Table A.3.c. Fluorine bonded to carbon in non-aromatic oxygen heterocycle other than carbohydrate, hydrogen bonded to carbon in the same ring.

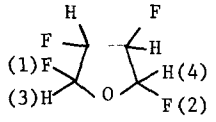
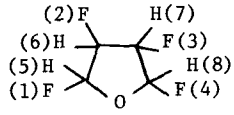
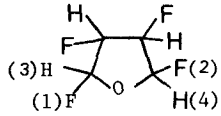
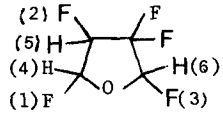
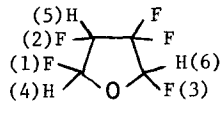
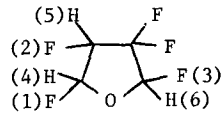
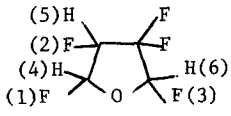
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J
188	1584		$C_4F_4H_4O$		1,3 2,4	62.3 62.3
188	1585		$C_4F_4H_4O$		1,5 2,6 3,7 4,8	61.9 50.8 51.8 60.9
188	1586		$C_4F_4H_4O$		1,3 2,4	63.3 63.3
188	1587 (4032)		$C_4F_5H_3O$		1,4 2,5 3,6	58.6 50.5 59.8
180	1588 (4033)		$C_4F_5H_3O$		1,4 2,5 3,6	59.8 50.9 60.0
188	1589 (4034)		$C_4F_5H_3O$		1,4 2,5 3,6	62.1 52.0 62.7
188	1590 (4035)		$C_4F_5H_3O$		1,4 2,5 3,6	62.1 50.1 61.0

Table A.3.c. (contd.)

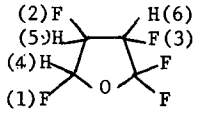
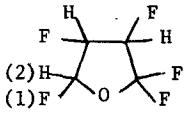
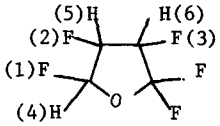
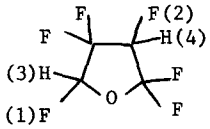
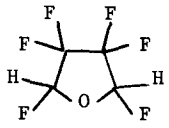
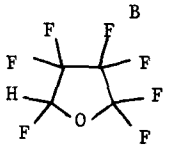
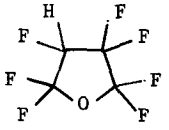
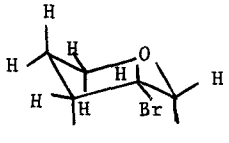
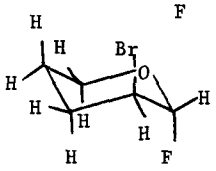
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
188	1591 (4036)		$C_4F_5H_3O$		1,4 2,5 3,6	58.3 48.5 47.9		
188	1592 (4037)		$C_4F_5H_3O$		1,2	59.4		
188	1593 (4038)		$C_4F_5H_3O$		1,4 2,5 3,6	60.6 51.6 49.4		
188	1594 (4039)		$C_4F_6H_2O$		1,3 2,4	60 48.9		
188	1595 (4040)		$C_4F_6H_2O$					
188	1596 (4042)		C_4F_7HO		A B	57.0 58.7 58.4		
188	1597 (4043)		C_4F_7HO			49.5		
354	1598	A	C_5FH_8BrO			52.2	26.3	
354	1599	A	C_5FH_8BrO			51.3	4.6	

Table A.3.c. (contd.)

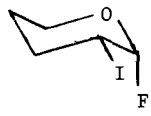
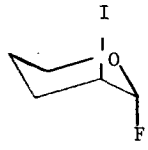
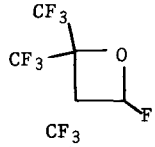
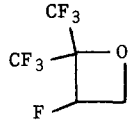
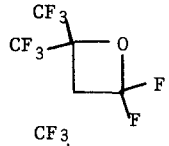
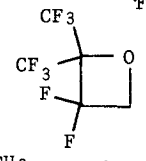
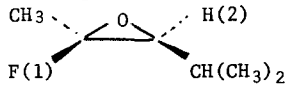
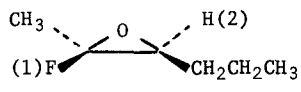
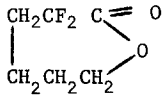
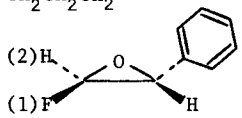
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
354	1600	A	C_5FH_8IO		51.1	27.2	
354	1601	A	C_5FH_8IO		51.3	5.2	
352	1602		$C_5F_7H_3O$		70		
352	1603		$C_5F_7H_3O$		55		
352	1604		$C_5F_8H_2O$			7.0	
352	1605		$C_5F_8H_2O$			12.2	
193	1606 (1626)	G	$C_6FH_{11}O$			1,2 2	
193	1607 (1628)	G	$C_6FH_{11}O$			1,2 2	
349	1608 (4045)	E	$C_6F_2H_8O_2$			14.5	
193	1609	G	C_8FH_7O		1,2	84.7	

Table A.3.c. (contd.)

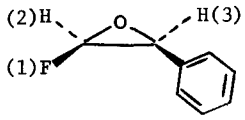
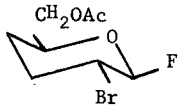
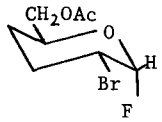
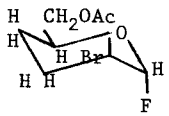
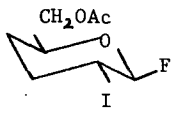
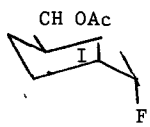
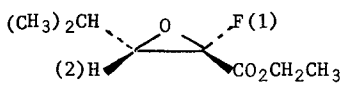
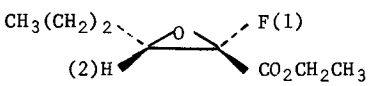
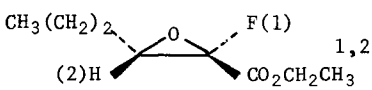
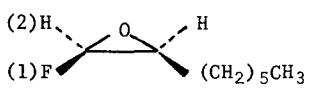
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
193	1610	G	C_8FH_7O		1,2	88.2	1,3	2	
354	1611	A	$C_8FH_{12}BrO_3$			ν52			
354	1612	A	$C_8FH_{12}BrO_3$			51.6		26.0	
354	1613	A	$C_8FH_{12}BrO_3$			51.1		4.0	
354	1614	A	$C_8FH_{12}IO_3$			ν50			
354	1615	A	$C_8FH_{12}IO_3$			51.4		5.0	
193	1616	G	$C_8FH_{13}O_3$				1,2	3	
193	1617	G	$C_8FH_{13}O_3$				1,2	3	
193	1618	G	$C_8FH_{15}O$		1,2	87.5	1,3	0.4	
193	1619	G	$C_8FH_{15}O$		1,2	91.7	1,3	1.6	

Table A.3.c. (contd.)

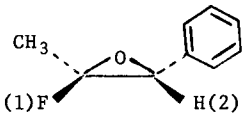
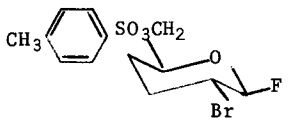
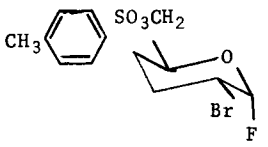
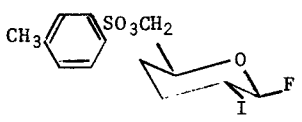
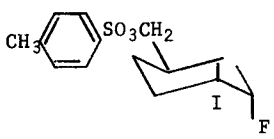
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
193	1620 (1631)	G	C_9FH_9O			1,2 1	
354	1621	A	$C_{13}FH_{16}BrO_4S$		~51		
354	1622	A	$C_{13}FH_{16}BrO_4S$		52.0	26.0	
354	1623	A	$C_{13}FH_{16}IO_4S$		~50		
354	1624	A	$C_{13}FH_{16}IO_4S$		51.5		

Table A.3.d. Fluorine bonded to carbon in non-aromatic oxygen heterocycle other than carbohydrate, hydrogen bonded to carbon outside this ring.

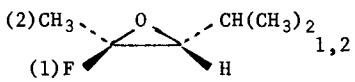
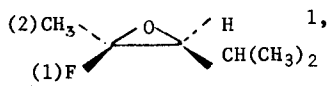
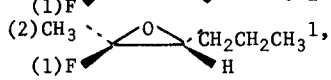
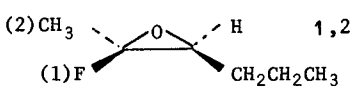
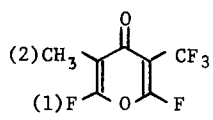
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J
193	1625	G	$C_6FH_{11}O$	 1,2	16.6	
193	1626 (1606)	G	$C_6FH_{11}O$	 1,2	15.4	
193	1627	G	$C_6FH_{11}O$	 1,2	16.0	
193	1628 (1607)	G	$C_6FH_{11}O$	 1,2	15.4	
125	1629 (4046)	A	$C_7F_5H_3O_2$	 1,2	2.4	

Table A.3.d. (contd.)

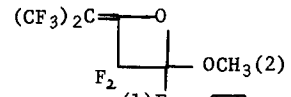
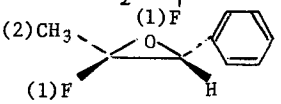
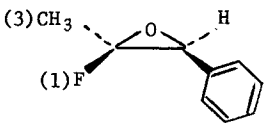
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J	
117	1630	B	$C_7F_9H_3O_2$				1,2	0.7
193	1631 (1620)	G	C_9FH_9O		1,2	15.6		
193	1632	G	C_9FH_9O		1,2	14.6		

Table A.3.e. Fluorine bonded to carbon in carbohydrates

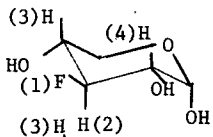
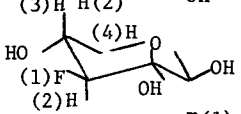
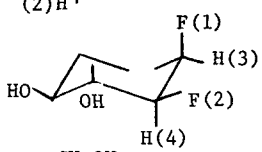
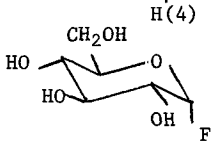
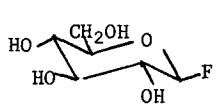
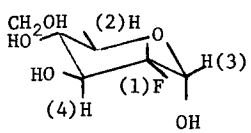
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
358	1633		$C_5FH_9O_4$		1,2	57	1,3 1,4	12.6 13.6	
358	1634	A^2	$C_5FH_9O_4$		1,2	55	1,3 1,4	13 13	
356	1635	A^2	$C_5F_2H_8O_3$		1,3 2,4	53.0 45.5	1,4 2,3	22 4.5	
357	1636	A^2	$C_6FH_{11}O_5$			53.2		27.2	
357	1637	A^2	$C_6FH_{11}O_5$			52.0		12.0	
357	1638	A^2	$C_6FH_{11}O_5$		1,2	49.0	1,3 1,4	<0.5 14.5	

Table A.3.e. (contd.)

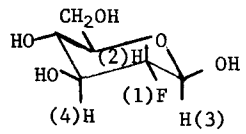
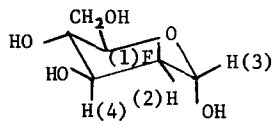
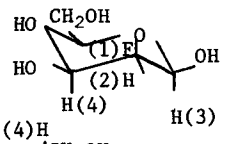
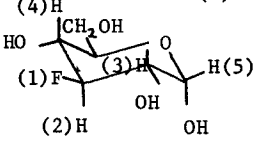
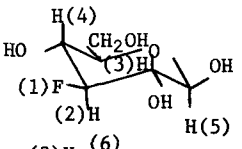
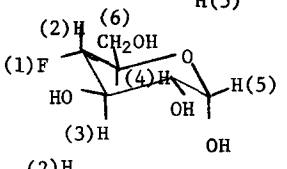
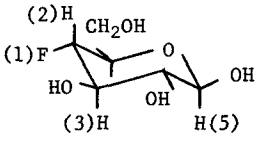
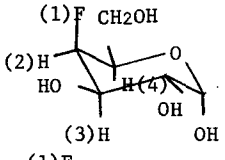
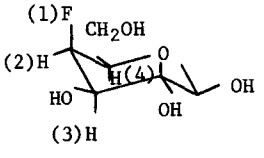
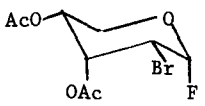
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
357	1639	A^2	$C_6FH_{11}O_5$		1,2	50.0	1,3 1,4	2.5 14.5		
357	1640	A^2	$C_6FH_{11}O_5$		1,2	49.0	1,3 1,4	7.5 30.0		
357	1641	A^2	$C_6FH_{11}O_5$		1,2	52.0	1,3 1,4	20.0 32.0		
357	1642	A^2	$C_6FH_{11}O_5$		1,2	53.0	1,3 1,4	12.0 12.0	1,5	3.9
357	1643	A	$C_6FH_{11}O_5$		1,2	52.0	1,3 1,4	13.5 13.5	1,5	<0.5
357 359	1644	A^2	$C_6FH_{11}O_5$		1,2	49.0	1,3 1,4	15.0 ∿ 4.5	1,5 1,6	3.5 ∿ 3.0
357	1645	A^2	$C_6FH_{11}O_5$		1,2	49.5	1,3 1,4	16.0 ∿ 4.5	1,5 1,6	0 ∿ 2.0
360	1646	A^2	$C_6FH_{11}O_5$		1,2	50	1,3 1,4	∿30 ∿30		
360	1647	A^2	$C_6FH_{11}O_5$		1,2	50	1,3 1,4	∿30 ∿30		
354	1648	A	$C_9FH_{11}BrO_5$			51.3		25.1		

Table A.3.e. (contd.)

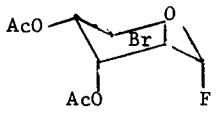
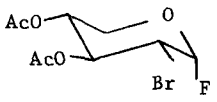
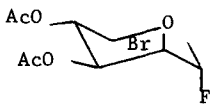
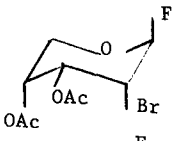
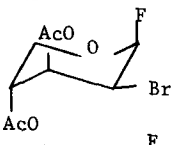
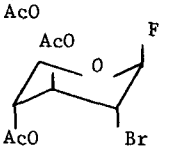
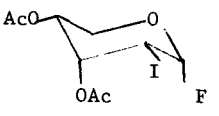
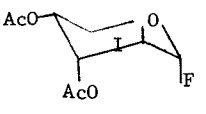
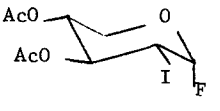
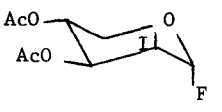
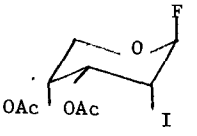
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
354	1649	A	$C_9FH_{12}BrO_5$		50.5	3.5	
354	1650	A	$C_9FH_{12}BrO_5$		50.8	26.8	
354	1651	A	$C_9FH_{12}BrO_5$		50.1	3.5	
354	1652	A	$C_9FH_{12}BrO_5$		50.4	3.4	
354	1653	A	$C_9FH_{12}BrO_5$		50.3	25.1	
354	1654	A	$C_9FH_{12}BrO_5$		51.0	9.0	
354	1655	A	$C_9FH_{12}IO_5$		50.7	27.6	
354	1656	A	$C_9FH_{12}IO_5$		~ 50	~ 5	
354	1657	A	$C_9FH_{12}IO_5$		50.8	29	
354	1658	A	$C_9FH_{12}IO_5$		50.0	3.5	
354	1659	A	$C_9FH_{12}IO_5$		51.0	6.5	

Table A.3.e. (contd.)

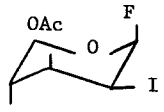
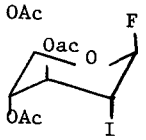
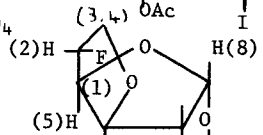
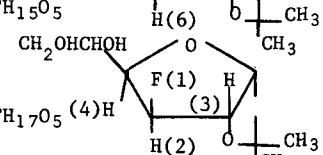
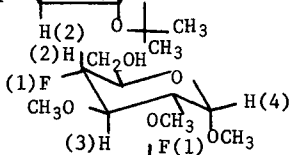
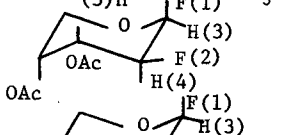
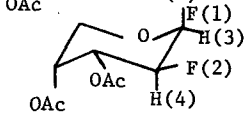
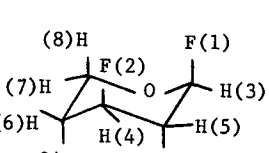
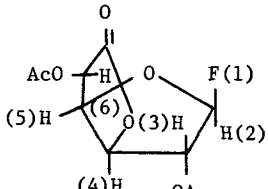
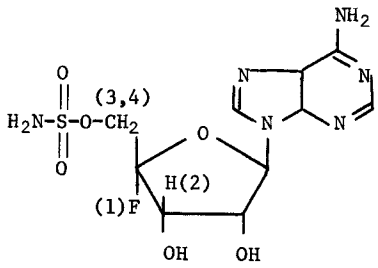
Ref. No.	Serial No.	Solvent	Molecular formula		^2J		^3J		^nJ
354	1660	A	$C_9FH_{12}IO_5$ 		50.8		29		
354	11661	A	$C_9FH_{12}IO_5$ 		51.1		9.2		
363	1662	A*	$C_9FH_{13}O_4$ 	1,2	50.4	1,3	38.3	1,6	1.5
						1,4	26.1	1,7	<0.5
						1,5	7.5	1,8	1.5
364	1663	A	$C_9FH_{15}O_5$ 	1,2	50.0	1,3	10.5		
						1,4	28.8		
359	1664		$C_9FH_{17}O_5$ 	1,2	49.5	1,3	15	1,4	3.8
358	1665	A	$C_9F_2H_{12}O_5$ 	1,3	53	1,4	25		
	(4050)			2,4	47	2,3	4		
356	1666	A	$C_9F_2H_{12}O_5$ 	1,3	55	1,4	24.2		
				2,4	43.5	2,3	∿1		
365	1667	A	$C_9F_2H_{12}O_5$ 	1,3	49.8	1,5	7.7	1,4	0.1-
	(4051)			2,4	+45.5	2,5	+12		0.2
						2,6	+12	1,8	0.5
								1,7	0
								2,3	0
								2,8	+2.5
								2,7	0.3
366	1668	E	$C_{10}FH_{11}O_7$ 	1,2	60.1	1,3	4.5	1,4	<0.5
								1,5	4.4
								1,6	<0.5
367	1669	F	$C_{10}FH_{13}N_6O_6S$			1,2	18.0	1,3	9
								1,4	9
		H^2						1,3	∿9.6
								1,4	∿12.6

Table A.3.e. (contd.)

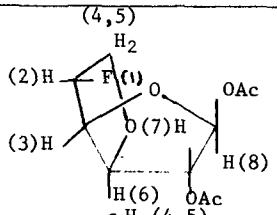
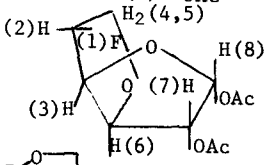
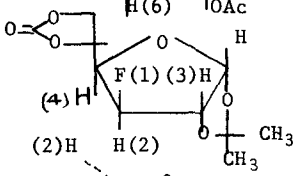
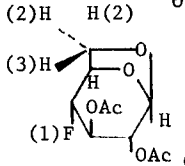
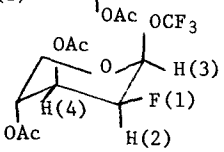
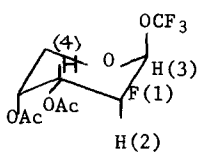
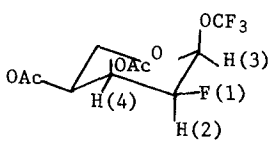
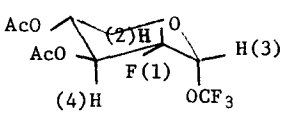
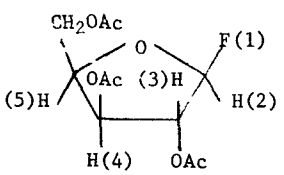
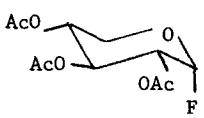
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
363	1670	E	$C_{10}FH_{13}O_6$		1,2	50.6	1,4	39.8	1,6	∿1.0
							1,5	25.5	1,7	<0.5
							1,3	10.8	1,8	2.7
363	1671	E	$C_{10}FH_{13}O_6$		1,2	50.6	1,4	38.1	1,6	< 1.0
							1,5	22.3	1,7	<0.5
							1,3	8.1	1,8	2.0
364	1672	A	$C_{10}FH_{13}O_6$		1,2	49.9	1,3	10.8		
							1,4	29.2		
368	1673	A	$C_{10}FH_{13}O_6$						1,2	4.4
									1,3	0.7
358	1674	A	$C_{10}F_4H_{12}O_6$		1,2	46	1,3	6		
							1,4	0		
358	1675	A	$C_{10}F_4H_{12}O_6$		1,2	46	1,3	6		
							1,4	8		
356	1676	A	$C_{10}F_4H_{12}O_6$		1,2	44.2	1,3	∿3		
							1,4	8.5		
356	1677	A	$C_{10}F_4H_{12}O_6$		1,2	48	1,3	0.5		
							1,4	∿1		
369	1678	A	$C_{11}FH_{15}O_7$		1,2	60.5	1,3	5.2	1,4	∿ 0.5
									1,5	5.2
370	1679	A	$C_{11}FH_{15}O_7$			53.5		23.7		
371		E				53.3		24.1		
		H				53.2		24.0		

Table A.3.e. (contd.)

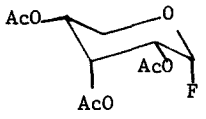
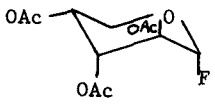
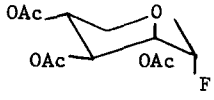
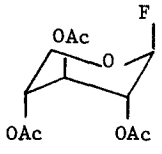
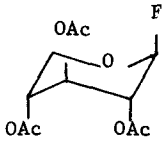
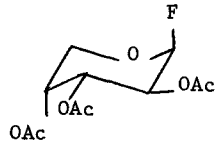
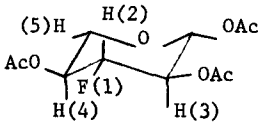
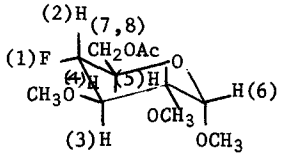
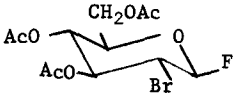
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
370	1680	A	$C_{11}FH_{15}O_7$		52.1	26.3	
370	1681	A	$C_{11}FH_{15}O_7$		49.2	5.3	
		E			50.0	9.5	
		H			50.2	5.0	
370	1682	A	$C_{11}FH_{15}O_7$		49.1	< 2	
		E			48.9	< 2	
		H			48.0	< 2	
370	1683	A	$C_{11}FH_{15}O_7$		50.4	6.8	
		E			52.1	7.9	
		H			∿ 52	7.0	
370	1684	A	$C_{11}FH_{15}O_7$		∿ 49	< 3	
371		E			49.5	∿ 5	
		H			49.2	∿ 3	
370	1685	A	$C_{11}FH_{15}O_7$		53.4	22.2	
371		E			54.0	23.9	
		H			∿ 54	∿ 25	
364	1686	H	$C_{11}FH_{15}O_7$		1,2 49.4	1,3 12.4 1,4 12.4	1,5 4.2
359	1687	A	$C_{11}FH_{19}O_6$		1,2 51.2	1,3 +16.0 1,4 3.6	1,5 -0.9 1,6 +3.3 1,7 1.9 1,8 1.3 1,OCH_3 0.8
372							
354	1688	A	$C_{12}FH_{16}BrO_7$		50.3	10.0	
373							

Table A.3.e. (contd.)

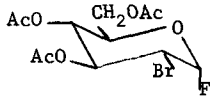
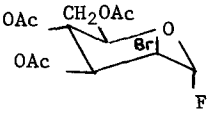
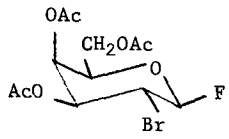
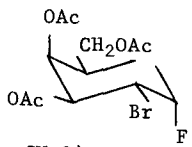
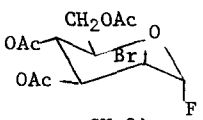
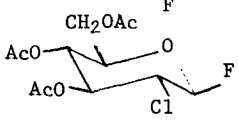
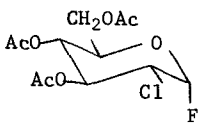
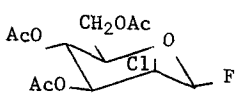
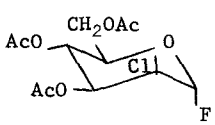
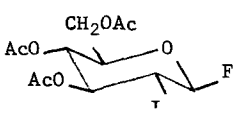
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
354 373	1689	A	$C_{12}FH_{16}BrO_7$		51.5	25.2	
354 371 373	1690	A	$C_{12}FH_{16}BrO_7$		50.2	2.85	
354	1691		$C_{12}FH_{16}BrO_7$		49.7	10.0	
354	1692	A	$C_{12}FH_{16}BrO_7$		50.5	25.1	
354	1693	A	$C_{12}FH_{16}BrO_7$		49.8	4.6	
374 373	1694	A	$C_{12}FH_{16}ClO_7$		51.0	10.6	
374 373	1695	A	$C_{12}FH_{16}ClO_7$		51.2	24.0	
374	1696	A	$C_{12}FH_{16}ClO_7$		49.4	3.6	
374 373	1697	A	$C_{12}FH_{16}ClO_7$		49.5	~ 2	
354 373	1698	A	$C_{12}FH_{16}IO_7$		49.9	9.3	

Table A.3.e. (contd.)

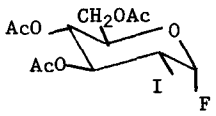
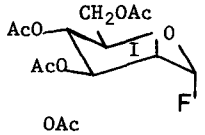
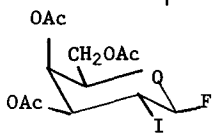
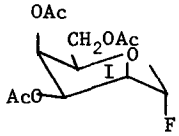
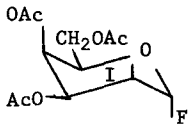
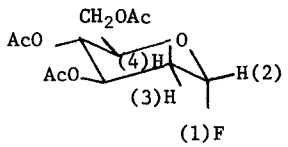
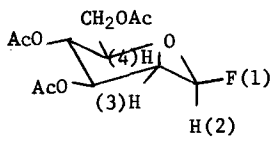
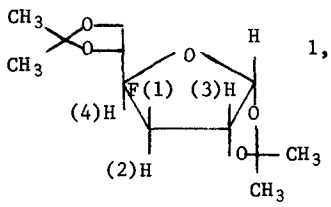
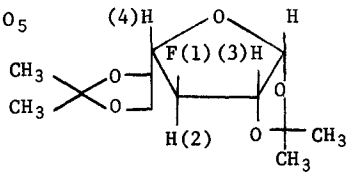
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
354 373	1699	A	$C_{12}FH_{16}IO_7$		50.5	27.8	
354 373	1700	A E	$C_{12}FH_{16}IO_7$		51.7	3.9 4.3	
354	1701	A	$C_{12}FH_{16}IO_7$		49.8	10.2	
354	1702	A	$C_{12}FH_{16}IO_7$		50.0	27.6	
354	1703	A	$C_{12}FH_{16}IO_7$		50.5	6.3	
371 373 375	1704	A	$C_{12}FH_{17}O_7$		1,2 +51.4	1,3 +5.0 1,4 +38.0	
373	1705	A	$C_{12}FH_{17}O_7$			1,3 10.7 1,4 15.3	
376 364	1706	A	$C_{12}FH_{19}O_5$		1,2 49.8	1,3 10.8 1,4 29.8	
377	1707	A	$C_{12}FH_{19}O_5$		1,2 51.6	1,3 15 1,4 23.7	

Table A.3.e. (contd.)

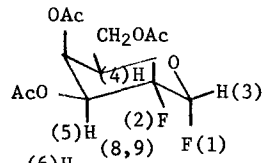
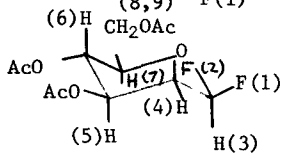
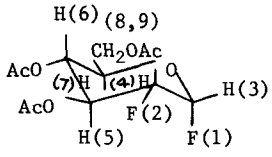
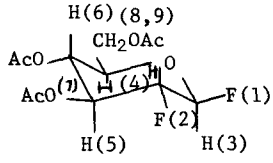
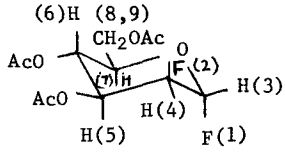
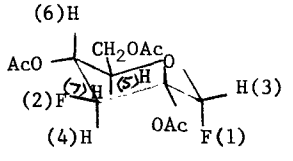
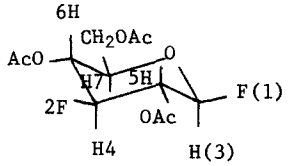
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
358	1708 (4052)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	53 47	1,4 2,5	23 12		
379 380 381	1709 (4053)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+48.5 +49.0	1,4 2,3 2,5	+8.0 +13.5 +22.4	1,5 1,7 2,6 2,7 (1,8+ 1,9)	0.5 0.8 +2.0 0.5 2.0
379 380 381	1710 (4054)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+53.3 +48.3	1,4 2,3 2,5	+23.8 0 +12.3	1,5 1,7 2,6 2,7 (1,8+ 1,9)	0.5 0 0 0 0
381	1711 (4055)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+51.7 +49.0	1,4 2,3 2,5	+11.2 +4.0 +15.0	1,5 1,7 2,6 2,7 (1,8+ 1,9)	-1.0 0 0 0 1.5
381	1712 (4056)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+48.0 +48.5	1,4 2,3 2,5	0 +4.0 +27.0	1,5 1,7 2,6 2,7 (1,8+ 1,9)	+2.5 0 0 0 0
365	1713 (4057)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+52.2 51.5	1,5 2,5 2,6	+22.6 +14.5 13.5	1,4 2,3 2,7 1,7	1.0 +4.0 1.0 0.5
365	1714 (4058)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+51.5 +51.3	1,5 2,5 2,6	+10.8 +15.0 +13.5	1,4 2,3 2,7 1,7	0 0 -1.0 0

Table A.3.e. (contd.)

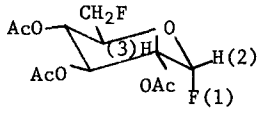
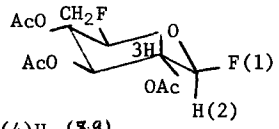
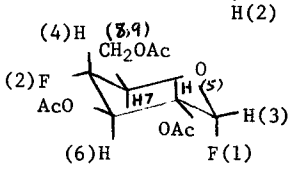
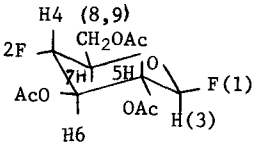
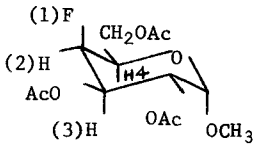
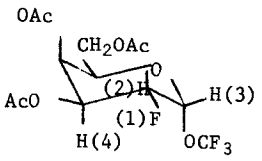
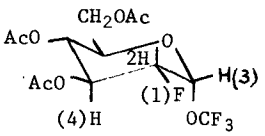
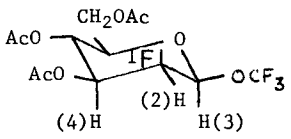
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
378	1715 (699 / 3118)	A	$C_{12}F_2H_{16}O_7$		1,2	52.4	1,3	23.8		
378	1716 (698 / 3119)	A	q $C_{12}F_2H_{16}O_7$		1,2	52.7	1,3	10.4		
372	1717 (4059)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+52.0 48.5	1,5 2,6	+23.7 14.6	2,5 2,3	−0.8 +3.0
372	1718 (4060)	A	$C_{12}F_2H_{16}O_7$		1,3 2,4	+50.7 +49.5	1,5 2,6 2,7	10.2 15.8 4.9	1,6 1,4 1,7 1,8 1,9 2,3 2,5 2,8 2,9	−0.8 0.8 0.9 0.6 0.6 +0.5 0 1.6 1.9
360	1719	A	$C_{13}FH_{19}O_8$		1,2	50	1,3 1,4	∼26 ∼26		
358	1720	A	$C_{13}F_4H_{16}O_8$		1,2	47	1,3 1,4	0.5 11.3		
379 380	1721	A	$C_{13}F_4H_{16}O_8$				1,2 1,3	<0.5 11.5		
379 380	1722	A	$C_{13}F_4H_{16}O_8$				1,2 1,3	16 ∼25		

Table A.3.e. (contd.)

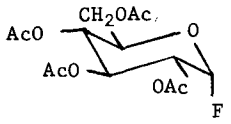
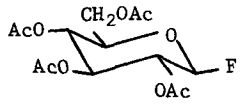
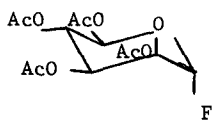
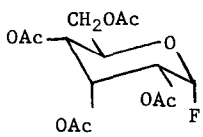
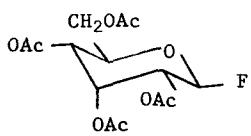
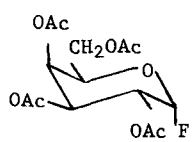
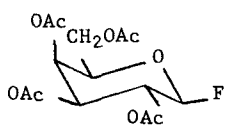
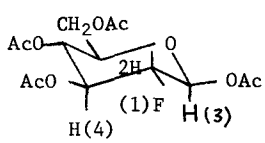
Ref. No.	Serial No.	Solvent	Molecular formula		^2J	^3J	^nJ
375	1723	A	$C_{14}FH_{19}O_9$		52.8	23.8	
371		E			53.0	24.1	
373		H			52.9	23.9	
382							
375	1724	A	$C_{14}FH_{19}O_9$		52.5	12.0	
371		E			52.6	12.0	
373		H			∿53	∿9	
382							
373	1725	A	$C_{14}FH_{19}O_9$		48.6	∿1.5	
382		E			48.5	∿1.5	
					48.1	∿1.5	
382	1726	A	$C_{14}FH_{19}O_9$		53.4	26.1	
		E			53.4	26.3	
		H			53.5	26.0	
382	1727	A	$C_{14}FH_{19}O_9$		1,2 53.0	1,3 11.9	1,4 +3.7
		E			53.4	12.0	
		H			52.7	12.0	
382	1728	A	$C_{14}FH_{19}O_9$		53.0	22.2	
		E			53.0	21.7	
		H			53.0	21.8	
382	1729	A	$C_{14}FH_{19}O_9$		53.8	10.0	
		E			∿52	∿12.5	
		H			52.0	12.6	
380	1730	A	$C_{14}FH_{19}O_9$		1,2 50.5	1,3 3.3	
						1,4 14.2	

Table A.3.e. (contd.)

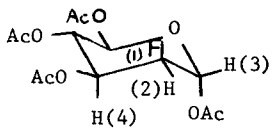
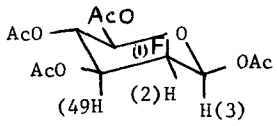
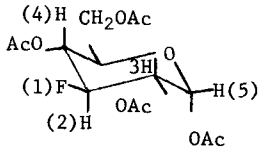
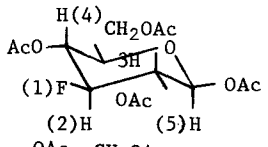
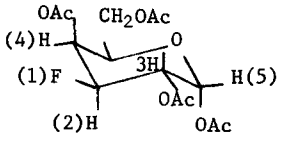
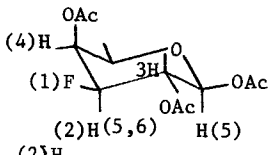
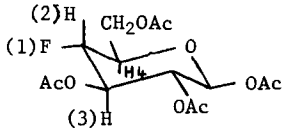
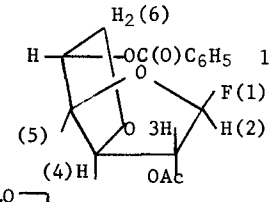
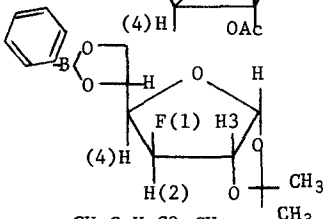
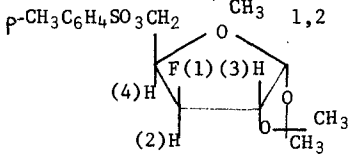
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
380	1731	A	$C_{14}FH_{19}O_9$		1,2	48.9	1,3 1,4	6.6 24.5		
380	1732	A	$C_{14}FH_{19}O_9$		1,2	50.7	1,3 1,4	18.9 25.6		
364	1733	A	$C_{14}FH_{19}O_9$		1,2	52.0	1,3 1,4	12.5 12.5	1,5	4.0
364	1734	A	$C_{14}FH_{19}O_9$		1,2	51.2	1,3 1,4	12.8 12.8	1,5 1,6 1,7	0 1.1 1.5
377	1735	A	$C_{14}FH_{19}O_9$		1,2	47.5	1,3 1,4	11.4 ∿6.4	1,5	∿4.8
377	1736	A	$C_{14}FH_{19}O_9$		1,2	47.4	1,3 1,4	11.5 5.6		
368	1737	A	$C_{14}FH_{19}O_9$		1,2	49.5	1,3 1,4	14.5 ∿2.6	1,5 ∿1,6	∿1.6 ∿1.5
366	1738	E	$C_{15}FH_{15}O_6$		1,2	62.3	1,3	5.8	1,4 1,5 1,6	<0.5 4.8 1.5
364	1739	A	$C_{15}FH_{18}BO_5$		1,2	50.0	1,3 1,4	10.5 28.9		
364	1740	A	$C_{15}FH_{19}O_6S$		1,2	50.5	1,3 1,4	10.5 ∿25		

Table A.3.e. (contd.)

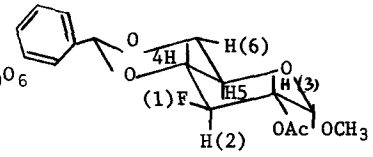
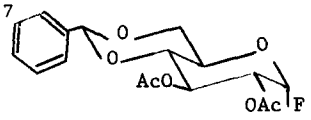
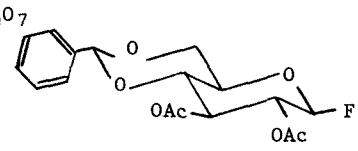
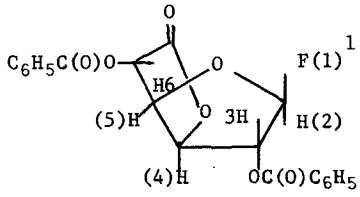
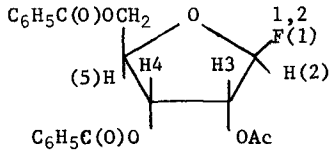
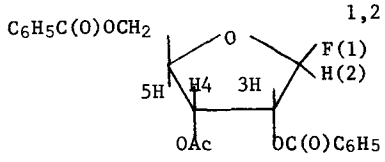
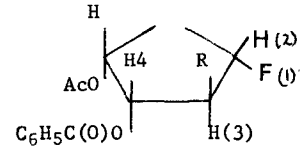
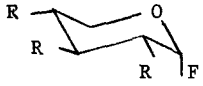
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
364	1741	H	$C_{16}FH_{19}O_6$		1,2	53.0	1,3	14.1	1,5	1.5
							1,4	15.1	1,6	2.0
382	1742	A	$C_{17}FH_{19}O_7$			53.1		24.3		
371		E				53.0		24.6		
		H				53.0		24.4		
382	1743	A	$C_{17}FH_{19}O_7$			52.6		10.2		
371		E				53.4		11.6		
		H				≈52		≈10		
366	1744	E	$C_{20}FH_{15}O_7$		1,2	60.1	1,3	4.0	1,4	< 0.5
									1,5	4.6
									1,6	0.3
369	1745	A	$C_{21}FH_{19}O_7$		1,2	61.4	1,3	4.8	1,4	1.9
									1,5	6.8
		E				60.9		4.7		2.4
										6.7
369	1746	A	$C_{21}FH_{19}O_7$		1,2	61.1				
		E				61.6	1,3	4.5	1,4	1.7
									1,5	7.9
369	1747	A	$C_{21}FH_{19}O_7$		1,2	61.4				
		E				61.3	1,3	4.9	1,4	2.1
									1,5	7.2
				R = $C_6H_5C(O)OCH_2$						
370	1748	A	$C_{26}FH_{21}O_7$			53.1		23.5		
		E				53.2		23.7		
		H				53.1		23.6		
				R = $C_6H_5C(O)O$						

Table A.3.e. (contd.)

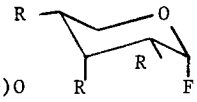
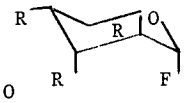
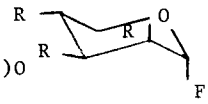
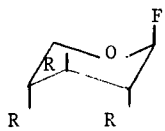
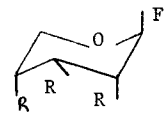
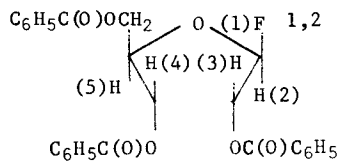
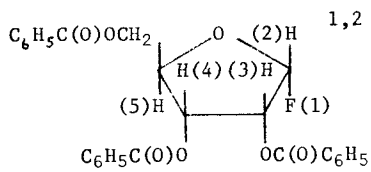
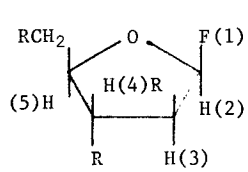
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
370	1749	A	$C_{26}FH_{21}O_7$	 R = $C_6H_5C(O)O$	53.5	25.3	
370	1750	A	$C_{26}FH_{21}O_7$	 R = $C_6H_5C(O)O$	∿49	3.9	
		E			50.9	6.1	
		H			49.5	4.3	
370	1751	A	$C_{26}FH_{21}O_7$	 R = $C_6H_5C(O)O$	48.6	< 2	
		E			48.6	< 2	
		H			48.6	< 2	
370	1752	A	$C_{26}FH_{21}O_7$	 R = $C_6H_5C(O)O$	49	∿ 6	
		E			49.8	6.7	
		H			49.0	6.0	
370	1753	A	$C_{26}FH_{21}O_7$	 R = $C_6H_5C(O)O$	∿49	< 3	
					∿48	< 3	
					48.5	< 3	
369	1754	A	$C_{26}FH_{21}O_7$		1,2 61.2	1,3 4.9	1,4 2.2 1,5 7.3
		E			61.5	4.8	2.2 6.6
369	1755	A	$C_{26}FH_{21}O_7$		1,2 63.6	1,3 20.6	1,4 ∿ 0 1,5 1.8
		E			64.4	20.6	∿ 0 1.0
369	1756	A	$C_{26}FH_{21}O_7$	 R = $C_6H_5C(O)O$	1,2 58.1	1,3 6.1	1,4 0.5 1,5 1.0
					58.4	6.4	< 0.7 1.5

Table A.3.e. (contd.)

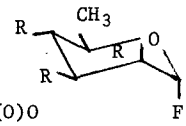
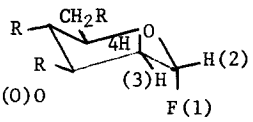
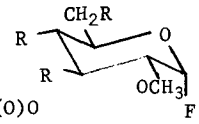
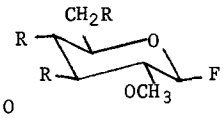
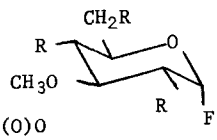
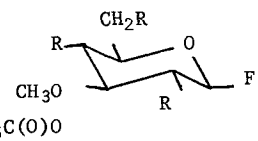
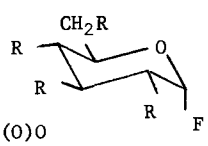
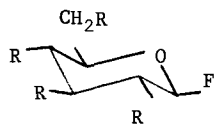
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	n_J
382	1757	A	$C_{27}FH_{23}O_7$		~49.0	1.0	
		E			48.5		
		H			48.4		
			R = $C_6H_5C(O)O$				
375	1758	A	$C_{27}FH_{23}O_7$		1,2 51.1	1,3 5.3	
						1,4 38.3	
			R = $C_6H_5C(O)O$				
382	1759	A	$C_{28}FH_{25}O_8$		52.0	24.3	
		E			52.5	25.0	
		H			52.2	24.3	
			R = $C_6H_5C(O)O$				
382	1760	A	$C_{28}FH_{25}O_8$		52.4	10.4	
		E			52.8	11.5	
		H			52.3	11.0	
			R = $C_6H_5C(O)O$				
382	1761	A	$C_{28}FH_{25}O_8$		53.4	24.2	
		E			53.4	24.1	
		H			53.4		
			R = $C_6H_5C(O)O$				
382	1762	A	$C_{28}FH_{25}O_8$		51.2	7.5	
		E			51.8	11.1	
		H			53.5	8.0	
			R = $C_6H_5C(O)O$				
382	1763	A	$C_{34}FH_{27}O_9$		52.6	23.6	
		E			53.2	23.7	
		H			53.0	23.6	
			R = $C_6H_5C(O)O$				
382	1764	A	$C_{34}FH_{27}O_9$		52.5	8.0	
		E			51.2	12.0	
		H			51.5	10.3	
			R = $C_6H_5C(O)O$				

Table A.3.f. Fluorine bonded to carbon in non-aromatic di-oxygen heterocycle, hydrogen bonded to carbon in the same ring.

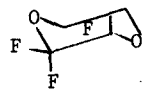
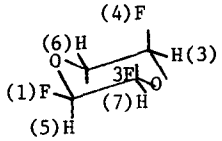
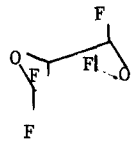
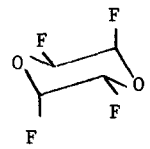
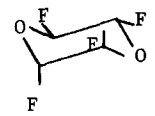
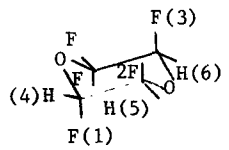
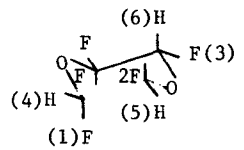
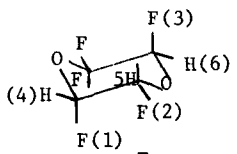
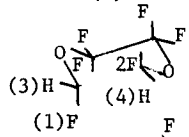
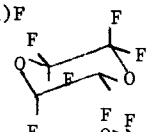
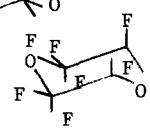
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
353	1765 (4076)	G	$C_4F_3H_5O_2$			52		
353	1766	G	$C_4F_4H_4O_2$		1,5 2,6 3,7 4,8	59 51 53 51		
353	1767	G	$C_4F_4H_4O_2$			53		
353	1768	G	$C_4F_4H_4O_2$			48		
353	1769	G	$C_4F_4H_4O_2$			53		
353	1770 (4079)	G	$C_4F_5H_3O_2$		1,4 2,5 3,6	49 49 51		
353	1771 (4078)	G	$C_4F_5H_3O_2$		1,4 2,5 3,6	51 52 53		
353	1772 (4077)	G	$C_4F_5H_3O_2$		1,4 2,5 3,6	49 50 53		
353	1773 (4080)	G	$C_4F_6H_6O_2$		1,3 2,4	51 51		
353	1774 (4081)	G	$C_4F_6H_2O_2$			51 51		
353	1775 (4082)	G	$C_4F_6H_2O_2$			51		

Table A.3.f. (contd.)

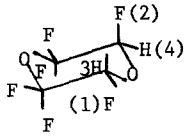
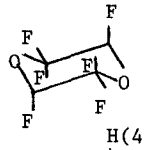
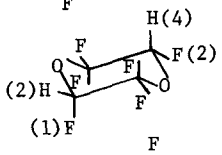
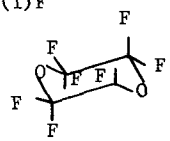
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
353	1776 (4083)	G	$C_4F_6H_2O_2$		1,2 3,4	47 47		
353	1777 (4084)	G	$C_4F_6H_2O_2$			51		
353	1778 (4085)	G	$C_4F_6H_2O_2$		1,3 2,4	51 51		
353	1779		$C_4F_7HO_2$			51		

Table A.3.g. Fluorine bonded to carbon in non-aromatic heterocyclic systems with more than one heteroatom, hydrogen bonded to carbon in the same ring.

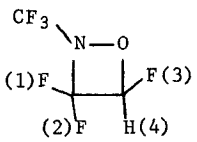
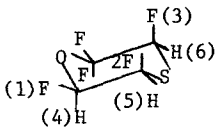
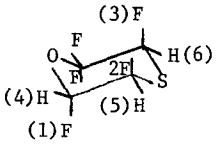
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
988	1780 [229 2732 4096]		C_3F_6HNO					
					Isomer I	3,4	65.2	2,4 < 1
				(-79°)				1,4 < 1
					Isomer II	3,4	65.2	2,4 < 1
								1,4 < 1
353	1781 (4105)	G	$C_4F_5H_3OS$			1,4 2,5 3,6	47 48 48	
353	1782 (4106)	G	$C_4F_5H_3OS$			1,4 2,5 3,6	47 45 45	

Table A.3.g. (contd.)

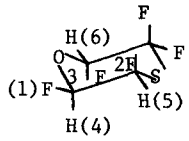
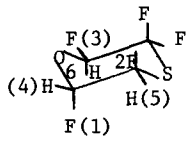
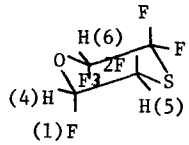
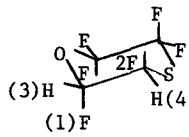
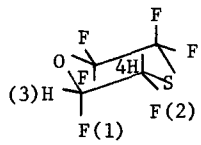
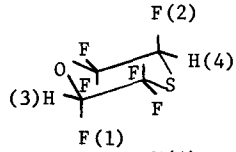
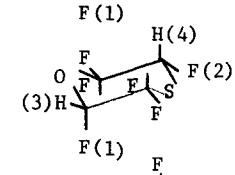
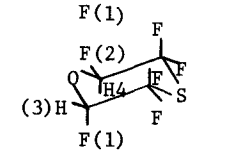
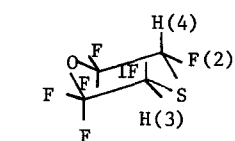
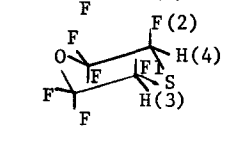
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
353	1783 (4107)	G	$C_4F_5H_3OS$		1,4 2,5 3,6	47 49 47		
353	1784 (4108)	G	$C_4F_5H_3OS$		1,4 2,5 3,6	49 45 50		
353	1785 (4109)	G	$C_4F_5H_3OS$		1,4 2,5 3,6	54 49 50		
353	1786 (4110)	G	$C_4F_6H_2OS$		1,3 2,4	45 45		
353	1787 (4111)	G	$C_4F_6H_2OS$		1,3 2,4	47 47		
353	1788 (4112)	G	$C_4F_6H_2OS$		1,3 2,4	51 46		
353	1789 (4113)	G	$C_4F_6H_2OS$		1,3 2,4	51 48		
353	1790 (4114)	G	$C_4F_6H_2OS$		1,3 2,4	51 51		
353	1791 (4115)	G	$C_4F_6H_2OS$		1,3 2,4	51 51		
353	1792 (4116)	G	$C_4F_6H_2OS$		1,3 2,4	45 45		

Table A.3.g. (contd.)

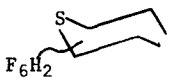
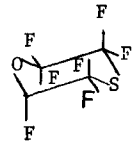
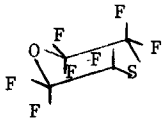
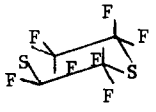
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
353	1793 (4088)	G	$C_4F_6H_2S_2$				
				Isomer 1	48		
				Isomer 2	60		
				Isomer 3	48		
				Isomer 4	45		
				Isomer 5	~30 ~45		
353	1794	G	C_4F_7HOS		50		
353	1795 (4117)	G	C_4F_7HOS		47		
353	1796	G	$C_4F_7HS_2$		45		

Table A.4. Fluorine bonded to carbon in alicyclic aromatic systems, hydrogen bonded to carbon in either aromatic or non-aromatic systems.

Table A4.a. Fluorine bonded to carbon in substituted monofluorobenzenes, hydrogen bonded to carbon in the same ring.

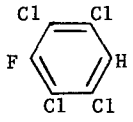
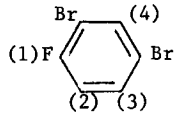
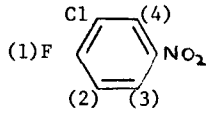
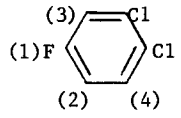
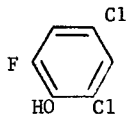
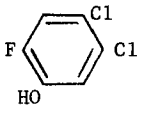
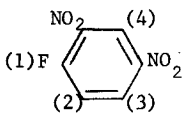
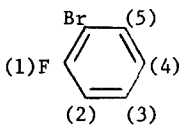
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
383	1797		C_6FHCl_4							2.1
384	1798	E*	$C_6FH_3Br_2$		1,2	8.54	1,4 1,3	6.13 4.33		
384	1799	E*	$C_6FH_3ClNO_2$		1,2	8.43	1,4 1,3	6.36 4.11		
384	1800	E*	$C_6FH_3Cl_2$		1,3 1,2	8.35 7.93	1,4	5.41		
383	1801		$C_6FH_3Cl_2O$			+9.6				-2.1
383	1802		$C_6FH_3Cl_2O$			+10.1		+8.3		
383	1803		$C_6FH_3N_2O_4$		1,2	10.19	1,4 1,3	6.49 3.72		
384 385	1804 (5469)	E*	C_6FH_4Br		1,2	9.10	1,3 1,5	4.97 7.10	1,4	-0.52
		S^{2*}			1,2	8.58	1,3 1,5	4.82 6.82	1,4	-0.63

Table A.4.a. (contd.)

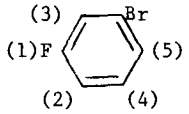
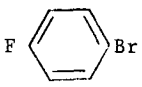
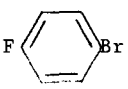
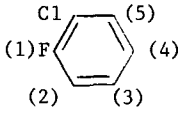
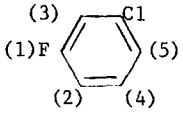
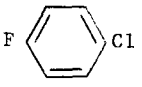
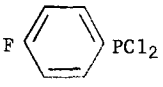
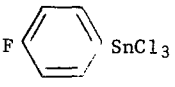
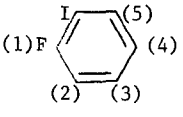
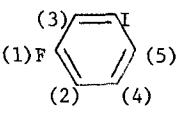
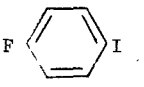
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
384	1805	E*	C_6FH_4Br		1,2	8.69	1,4	6.45	1,5	-0.63
385	(5470)				1,3	8.61				
		S^2*			1,2	8.31	1,4	5.99	1,5	-0.46
					1,3	8.38				
384	1806	E*	C_6FH_4Br			8.62		4.90		
385	(5471)									
		S^2*				8.18		4.83		
35	1807		C_6FH_4Br			8.1		4.9		
	(5471)									
384	1808	E*	C_6FH_4Cl		1,2	9.64	1,3	5.01	1,4	-0.85
385	(5473)						1,5	7.62		
		S^2*			1,2	9.06	1,3	4.72	1,4	-0.85
							1,5	7.29		
384	1809	E*	C_6FH_4Cl		1,2	8.63	1,4	6.30	1,5	-0.47
385	(5475, 5476)				1,3	9.02				
		S^2*			1,2	8.23	1,4	6.08	1,5	-0.59
					1,3	8.66				
384	1810	E*	C_6FH_4Cl			8.48		4.79		
385	(5477)									
		S^2*				8.08		4.66		
386	1811		$C_6FH_4Cl_2P$			8.5		5.4		
	(6106)									
387	1812	Q*	$C_6FH_4Cl_3Sn$			8.40		5.46		
385	1813	S^2*	C_6FH_4I		1,2	7.97	1,3	4.99	1,4	-0.24
	(5478)						1,5	6.29		
385	1814	S^2*	C_6FH_4I		1,2	8.42	1,4	5.85	1,5	-0.27
	(5479)				1,3	8.14				
385	1815	S^2*	C_6FH_4I			8.39		5.10		
	(5480)									

Table A.4.a. (contd.)

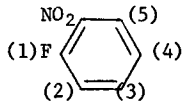
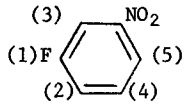
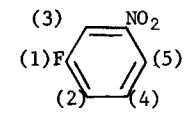
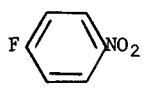
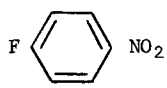
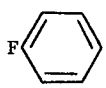
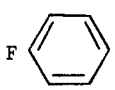
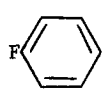
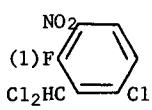
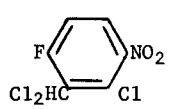
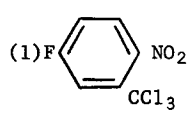
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
384	1816 (5484)	E*	$C_6FH_4NO_2$		1,2	11.40	1,3 1,5	4.61 7.46	1,4	-0.86
384	1817 (5485)	E*	$C_6FH_4NO_2$		1,2 1,3	8.28 8.82	1,4	5.60	1,5	-0.53
388	1818 (5485)	B*	$C_6FH_4NO_2$		1,2 1,3	8.2 8.8	1,4	5.7	1,5	-0.3
384	1819 (5486, 5487)	E*	$C_6FH_4NO_2$			8.13		4.71		
35	1820 (5486, 5487)		$C_6FH_4NO_2$			8.2		4.8		
389	1821 (5489)		C_6FH_5			9.4		5.8		0.0
390	1822	S2*	C_6FH_5		(10%)	8.90		5.57		0.20
384					(50%)	9.02		5.70		0.25
					(80%)	9.13		5.72		0.28
		B*				9.14		5.70		0.29
		E*				9.31		5.79		0.34
391	1823 (5490)	B* D*	C_6FH_5			9.08 9.16		5.82 5.90		0.35 0.12
393	1824 (1990)	T2*	$C_7FH_3Cl_3NO_2$					7.77		-1.83
393	1825 (1991)	T2*	$C_7FH_3Cl_3NO_2$			9.44		4.90		
394	1826		$C_7FH_3Cl_3NO_2$		1,2 1,3	7.0 13.0	1,4	5.2		

Table A.4.a. (contd.)

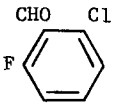
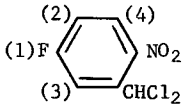
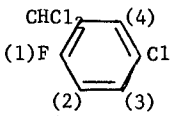
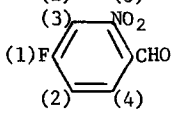
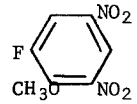
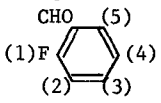
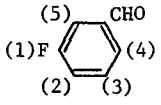
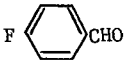
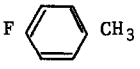
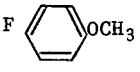
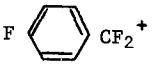
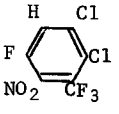
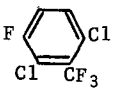
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^5J
395	1827 (1135)	E*	C_7FH_4ClO			10.47		5.85		-1.07
394	1828 (1992)		$C_7FH_4Cl_2NO_2$		1,2 1,3	7.0 9.2	1,4	5.0		
393	1829 (1993)	T^{2*}	$C_7FH_4Cl_3$		1,2	9.56	1,3 1,4	4.43 6.32		
395	1830	E*	$C_7FH_4NO_3$		1,2 1,3	8.2 7.72	1,4	5.60		
408	1831	F*	$C_7FH_5N_2O_5$			+11.58				-1.83
395	1832 (5521)	E*	C_7FH_5O		1,2	10.80	1,3 1,5	5.40 7.09	1,4	-0.18
395	1833 (5523)	E*	C_7FH_5O		1,2 1,5	8.58 8.88	1,3	5.35	1,4	0.23
395	1834 (5525)	E*	C_7FH_5O			8.69		5.50		
396 397	1835		C_7FH_7			8.7		5.8		
35	1836		C_7FH_7O			7.8		4.8		
61	1837 (1090 / 3354)	C^2	$C_7F_3H_4^+$			8.4		4.6		
383	1838		$C_7F_4HCl_2NO_2$			8.4				
383	1839		$C_7F_4H_2Cl_2$			+6.2		+6.2		

Table A.4.a. (contd.)

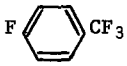
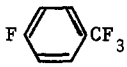
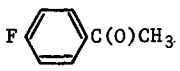
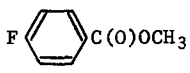
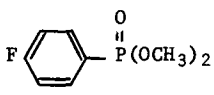
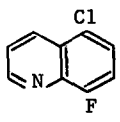
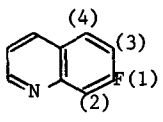
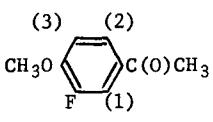
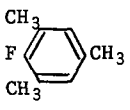
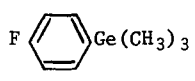
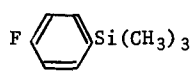
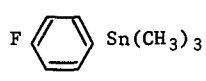
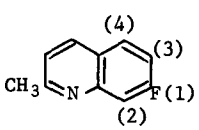
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J	^5J
35	1840		$C_7F_4H_4$			8.5		5.1	
61	1841 (846 3355)		$C_7F_4H_4$			8.5		4.8	
35	1842		C_8FH_7O			8.7		5.5	
147	1843		$C_8FH_7O_2$			10.3		5.5	
400	1844 (6219)	B	$C_8FH_{10}OP$			8.97		5.64	
469	1845 (1995)		C_9FH_5ClN			8.7		4.2	
470	1846		C_9FH_6N		1,2 1,3	10.0 8.2	1,4	6.5	
402	1847		$C_9FH_9O_2$			±12.3		±8.6	±1.0
383	1848		C_9FH_{11}					7.0	
404	1849	G	$C_9FH_{13}Ge$			9.35		6.55	
404	1850	G	$C_9FH_{13}Si$			9.11		6.39	
404 405	1851	G	$C_9FH_{13}Sn$			9.36		6.48	
470	1852		$C_{10}FH_8N$		1,2 1,3	10.0 8.4	1,4	6.5	

Table A.4.a. (contd.)

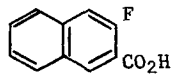
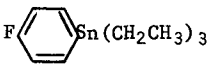
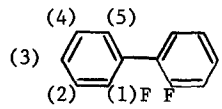
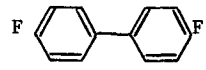
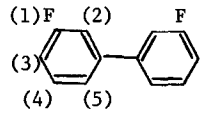
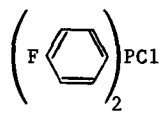
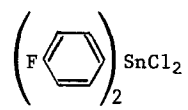
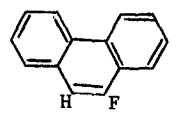
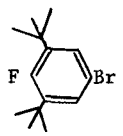
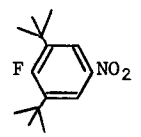
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
452	1853	V[2]	$C_{11}FH_7O_2$			7				
405	1854		$C_{12}FH_{19}Sn$			9.26		6.74		
454	1855	H*	$C_{12}F_2H_8$		1,2	10.02	1,3	4.96	1,4	-0.16
							1,5	8.34		
		J*				10.07		5.13		-0.15
								8.36		
454	1856 (4157)	G*	$C_{12}F_2H_8$			8.39		5.21		
		H*				8.56		5.21		
		J*				8.66		5.36		
454	1857 (4155)	G*	$C_{12}F_2H_8$		1,2	9.92	1,4	5.87	1,5	0.02
					1,3	8.35				
		H*				10.19		6.10		0.10
						8.61				
		J*				10.14		6.04		0.08
						8.48				
386	1858 (6316)		$C_{12}F_2H_8ClP$			8.6		5.4		
387	1859		$C_{12}F_2H_8Cl_2Sn$			8.64		5.70		
458	1860	A	$C_{14}FH_9$			11.6				
406	1861 (2004)	G	$C_{14}FH_{20}Br$					6.6		
406	1862 (2005)	G	$C_{14}FH_{20}NO_2$					6.3		

Table A.4.a. (contd.)

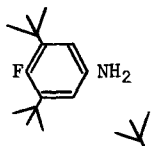
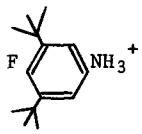
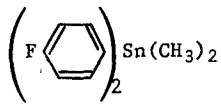
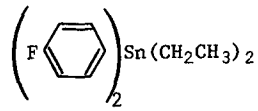
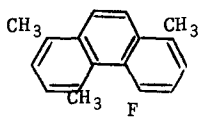
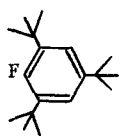
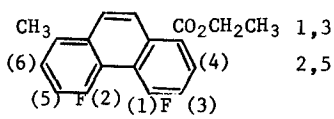
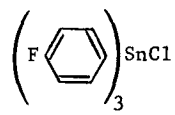
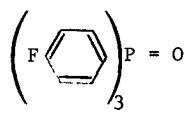
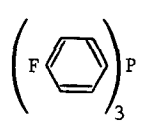
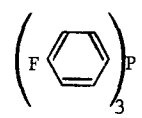
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
406	1863 (2006)	G	$C_{14}FH_{22}N$			6.2	
406	1864 (2007)	K^2	$C_{14}FH_{23}N^+$			6.1	
405	1865		$C_{14}F_2H_{14}Sn$		9.22	6.40	
405	1866		$C_{16}F_2H_{18}Sn$		9.19	6.56	
460	1867 (2018)		$C_{17}FH_{15}$		12.4	5.4	
406	1863 (2022)	G	$C_{18}FH_{29}$			7.4	
461	1869 (2026 4594)	E*	$C_{18}F_2H_{14}O_2$		1,3 11.81 2,5 12.71	1,4 4.98 2,6 4.76	
387	1870	Q*	$C_{18}F_3H_{12}ClSn$		8.96	5.96	
400	1871 (6404)	E	$C_{18}F_3H_{12}OP$		8.99	5.66	
386	1872 (6405)		$C_{18}F_3H_{12}P$		8.8	5.9	
407	1873 (6406)	J	$C_{18}F_3H_{12}P$		+8.5	+5.5	

Table A.4.a. (contd.)

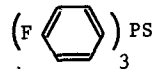
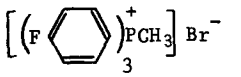
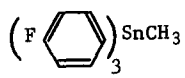
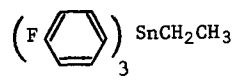
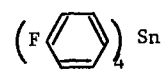
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
407	1874 (6407)	J	$C_{18}F_2H_{12}PS$		+8.7	+5.5	
407	1875 (6436)	J	$C_{19}F_2H_{15}BrP$		+8.8	+4.8	
405	1876		$C_{19}F_3H_{15}Sn$		9.12	6.13	
405	1877		$C_{20}F_3H_{17}Sn$		9.23	6.27	
387	1878	Q*	$C_{24}F_4H_{16}Sn$		9.35	6.18	

Table A.4.b. Fluorine bonded to carbon in substituted difluorobenzenes, hydrogen bonded to carbon in the same ring.

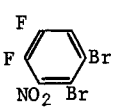
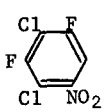
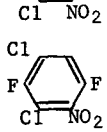
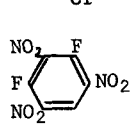
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
383	1879 (4119)		$C_6F_2HBr_2NO_2$		8.7	6.8	
383	1880 (4120)		$C_6F_2HCl_2NO_2$		8.0		2.3
383	1881 (4121)		$C_6F_2HCl_2NO_2$		8.2	6.3	
383	1882 (4122)		$C_6F_2HCl_3$		+8.4	+6.3	
409	1883		$C_6F_2HN_3O_6$			8.2	

Table A.4.a. (contd.)

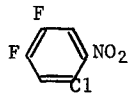
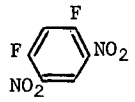
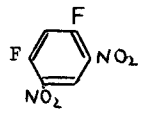
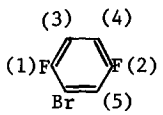
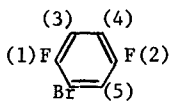
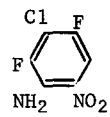
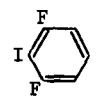
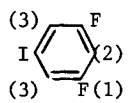
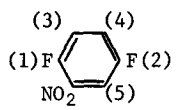
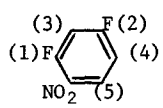
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
383	1884 (4125)		$C_6F_2H_2ClNO_2$			9.5		7.1		
				Assignments ambiguous						
384	1885	E*	$C_6F_2H_2N_2O_4$			10.56		7.62		
410	1886	A	$C_6F_2H_2N_2O_4$			9.71		7.54		
		E				10.61		7.66		
		H				10.01		7.00		
		J				9.93		7.61		
		M				10.53		7.70		
		D^2				10.62		7.71		
		U^2				10.58		7.65		
384	1887 (4126)	E*	$C_6F_2H_3Br$		1,3	8.23	1,4	3.72		
					2,4	7.91	2,3	4.68		
					2,5	7.81	1,5	5.40		
411	1888 (4127)	G*	$C_6F_2H_3Br$		1,3	7.71	1,4	3.64		
					2,4	7.51	2,3	4.61		
					2,5	7.51	1,5	5.30		
383	1889 (4128)		$C_6F_2H_3ClN_2O_2$			+9.4				-2.2
412 413	1890 (4129)		$C_6F_2H_3I$			7.40		6.35		-1.30
411	1891 (4130)		$C_6F_2H_3I$		1,2	8.89			1,3	-1.26
					1,3	7.61				
384	1892 (4131a)	E*	$C_6F_2H_3NO_2$		1,3	10.59	1,4	3.49		
					2,4	7.48	1,5	5.80		
					2,5	7.91	2,3	4.34		
384	1893 (4131)	E*	$C_6F_2H_3NO_2$		1,3	11.26	1,5	8.64	1,4	-1.58
					2,3	8.68	2,5	5.73		
					2,4	7.70				

Table A.4.b. (contd.)

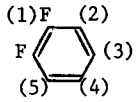
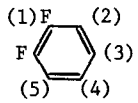
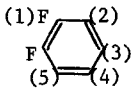
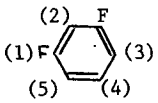
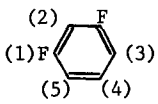
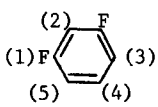
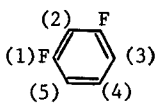
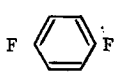
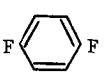
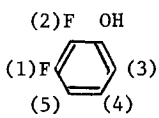
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
414	1894 (4132 5507)	B*	$C_6F_2H_4$		1,2	10.44	1,3 1,5	4.33 7.87	1,4	-1.39
384	1895 (4132)	E*	$C_6F_2H_4$		1,2	10.93	1,3 1,5	4.51 8.17	1,4	-1.31
415	1896 (4133)	G*	$C_6F_2H_4$		1,2	10.38	1,3 1,5	4.43 7.93	1,4	-1.45
384	1897 (5509 5510)	E*	$C_6F_2H_4$		1,2 1,5	9.60 8.70	1,4	6.69	1,3	-0.88
385	1898 (5509 5510)	S*	$C_6F_2H_4$		1,2 1,5	9.14 8.22	1,4	6.45	1,3	-0.93
416	1899 (4134)	B*	$C_6F_2H_4$		1,2 1,5	9.6 9.2	1,4	5.8	1,3	-1.0
417	1900 (4135)	G*	$C_6F_2H_4$		1,2 1,5	+9.23 +8.19	1,4	+6.46	1,3	-0.86
384	1901 (5511)	E*	$C_6F_2H_4$			8.19		4.16		
418	1902 (4137 5513)	*	$C_6F_2H_4$			8.03		4.17		
413	1903 (4140)	*	$C_6F_2H_4O$			10.4		6.0		-1.9
415	1904 (4139)	G*	$C_6F_2H_4O$		1,5	9.96	1,4 2,3 2,5	5.79 7.43 6.97	1,3 2,4	-1.85 -2.31
412 413	1905 (4142)	*	$C_6F_2H_5N$			10.40		6.25		-1.50

Table A.4.b. (contd.)

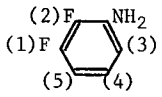
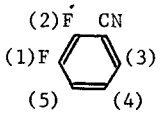
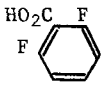
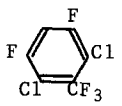
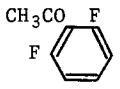
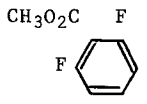
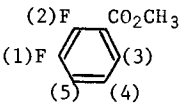
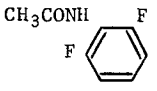
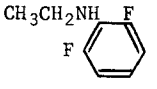
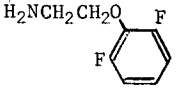
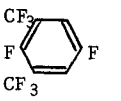
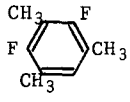
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
415	1906 (4141)	G*	$C_6F_2H_5N$		1,5	9.98	1,4 2,3 2,5	5.49 7.54 7.04	1,3 2,4	-1.67 -2.04
412 413	1907 (4144)	*	$C_7F_2H_3N$			9.10		6.60		-0.85
415	1908 (4143)	G*	$C_7F_2H_3N$		1,5	9.92	1,4 2,3 2,5	4.52 5.21 7.63	1,3 2,4	-1.65 -1.69
412 413	1909 (4145)	*	$C_7F_2H_4O_2$			9.50		6.40		-1.40
383	1910		$C_7F_5HCl_2$			7.8				
412 413	1911 (4146)	*	$C_8F_2H_6O$			9.60		6.35		-1.40
412 413	1912 (4148)	*	$C_8F_2H_6O_2$			9.35		6.20		-1.30
415	1913 (4147)	G*	$C_8F_2H_6O_2$		1,5	9.92	1,4 2,3 2,5	4.59 5.91 7.12	1,3 2,4	-1.72 -1.75
412 413	1914 (4149)	*	$C_8F_2H_7NO$			9.50		6.10		-1.90
412 413	1915 (4150)	*	$C_8F_2H_9N$			11.50		6.00		-1.70
412 413	1916 (4151)	*	$C_8F_2H_9NO$			10.35		5.88		-1.90
876	1917		$C_8F_8H_2$			7.4		5.1		
383	1918		$C_9F_2H_{10}$					7.7		

Table A.4.c. Fluorine bonded to carbon in substituted trifluoro-benzenes, hydrogen bonded to carbon in the same ring.

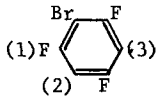
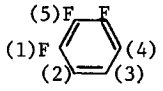
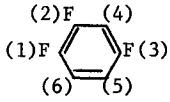
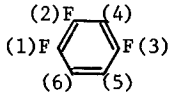
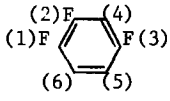
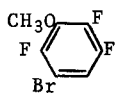
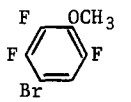
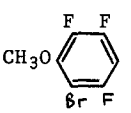
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^5J
383	1919 (4162)		$C_6F_3HCl_2$			8.6			2.2
420	1920 (4163)		$C_6F_3HCl_2$			8.6			2.3
421	1921 (4164)	B	$C_6F_3HCl_2$			8.6			2.3
422	1922		$C_6F_3H_2Br$		1,2	8.5			2.05
413	1923 (4170)		$C_6F_3H_3$		1,2	10.0	1,3 5,2	6.9 5.7	1,4 -2.1 5,3 -2.5
384	1924 (4173)	E*	$C_6F_3H_3$		1,6 2,4 3,4 3,5	10.25 10.77 8.45 8.01	1,4 1,5 2,6 3,6	6.39 3.33 9.10 5.12	2,5 -2.02
423	1925 (4172)	B*	$C_6F_3H_3$		1,6 2,4 3,4 3,5	9.94 10.54 8.32 7.77	1,4 1,5 2,6 3,6	6.31 3.27 8.88 5.07	2,5 -2.03
424	1926 (4171)	G*	$C_6F_3H_3$		1,6 2,4 3,4 3,5	9.69 10.36 8.17 7.64	1,4 1,5 2,6 3,6	6.24 3.26 8.71 5.03	2,5 -2.00
425	1927 (4174)	*	$C_6F_3H_3$			±8.96			∓1.68
426	1928	B	$C_7F_3H_4BrO$			9.7		8.0 6.2	
426	1929	B	$C_7F_3H_4BrO$			10.2		6.2	2.7
426	1930 (2037)	B	$C_7F_3H_4BrO$			10.5 8.5		6.6	

Table A.4.c. (contd.)

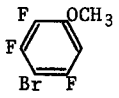
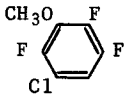
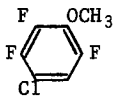
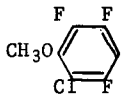
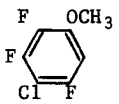
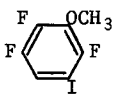
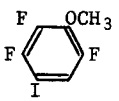
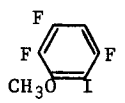
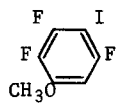
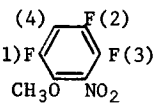
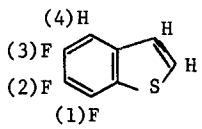
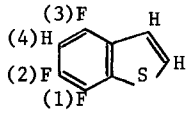
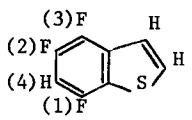
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
426	1931	B	$C_7F_3H_4BrO$		10.3	6.9	2.3
426	1932 (2038)	B	$C_7F_3H_4ClO$		10.0	7.8 6.6	
426	1933 (2039)	B	$C_7F_3H_4ClO$		10.6	6.8	2.6
426	1934 (2040)	B	$C_7F_3H_4ClO$		10.4 9.0	6.7	
426	1935	B	$C_7F_3H_4ClO$		10.7	7.0	2.4
426	1936 (2041)	B	$C_7F_3H_4IO$		9.3	8.2 5.4	
426	1937 (2042)	B	$C_7F_3H_4IO$		10.2	5.5	2.7
426	1938	B	$C_7F_3H_4IO$		10.5 7.8	6.2	
426	1939 (2043)	B	$C_7F_3H_4IO$		9.6	6.5	2.3
427	1940 (2044)		$C_7F_3H_4NO$		1,4 {10.9 2,4 {10.2	3,4 7.3	
451	1941 (2047 4182)	G	$C_8F_3H_3S$		3,4 8.8	2,4 6.05	1,4 1.7
451	1942 (2048 4183)	G	$C_8F_3H_3S$		2,4 10.2 3,4 8.7	1,4 5.75	
451	1943 (2049 4184)	G	$C_8F_3H_3S$		1,4 8.85 2,4 10.3	3,4 5.45	

Table A.4.c. (contd.)

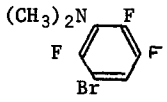
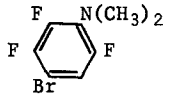
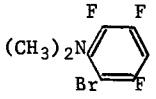
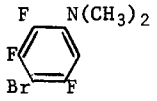
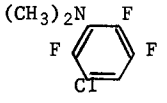
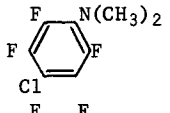
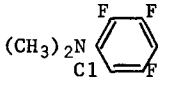
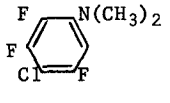
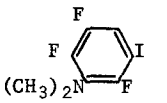
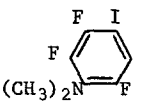
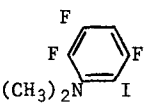
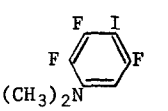
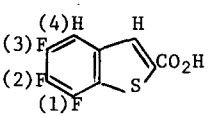
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
426	1944	B	$C_8F_3H_7BrN$		9.3	8.0 6.2	
426	1945	B	$C_8F_3H_7BrN$		11.6	6.2	2.6
426	1946 (2053)	B	$C_8F_3H_7BrN$		10.4 8.5	6.8	
426	1947 (2054)	B	$C_8F_3H_7BrN$		11.2	7.4	2.4
426	1948 (2055)	B	$C_8F_3H_7ClN$		9.8	8.0 6.6	
426	1949 (2056)	B	$C_8F_3H_7ClN$		11.8	7.7	2.3
426	1950 (2057)	B	$C_8F_3H_7ClN$		10.0 8.8	6.8	
426	1951 (2058)	B	$C_8F_3H_7ClN$		11.9	7.5	2.3
426	1952 (2059)	B	$C_8F_3H_7IN$		9.1	8.2 5.5	
426	1953 (2060)	B	$C_8F_3H_7IN$		11.5	5.6	2.6
426	1954 (2061)	B	$C_8F_3H_7IN$		10.5 9.5	7.5	
426	1955 (2062)	B	$C_8F_3H_7IN$		11.0	7.2	2.2
451	1956 (2065 4192)	E	$C_9F_3H_3O_2S$		3,4 10.0	2,4 6.55	1,4 1.55

Table A.4.c. (contd.)

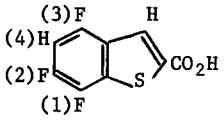
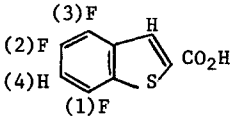
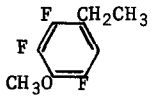
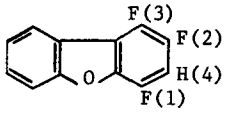
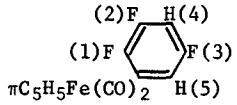
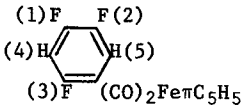
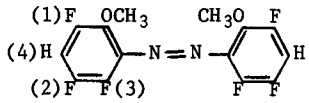
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
451	1957 (2066 / 4193)	E	$C_9F_3H_3O_2S$		2,4 3,4	10.81 9.22	1,4	5.58		
451	1958 (2067 / 4194)	E	$C_9F_3H_3O_2S$		1,4 2,4	9.4 10.7	3,4	6.2		
430	1959 (2069 / 4197)		$C_9F_3H_9O$			11.4		6.5		2.5
455	1960 (4200)	G	$C_{12}F_3H_5O$		1,4 2,4	9.6 10.6	3,4	6.3		
434	1961 (4206)	U[2]	$C_{13}F_3H_7FeO_2$		2,4 3,4 3,5	10.4 8.15 8.15	1,4 1,5	6.15 2.4	2,5	1.75
434	1962 (4207)	U[2]	$C_{13}F_3H_7FeO_2$		1,4 2,5 3,4	10.65 11.1 7.2	2,4 1,5 3,5	6.55 9.65 4.35		
459	1963 (2080)	E	$C_{14}F_6H_8N_2O_2$		1,4 2,4	11.1 11.1	3,4	7.6		

Table A.4.d. Fluorine bonded to carbon in substituted tetrafluoro-benzenes, hydrogen bonded to carbon in the same ring.

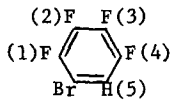
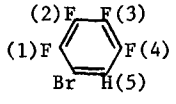
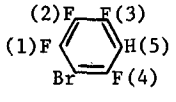
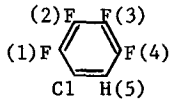
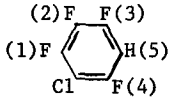
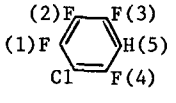
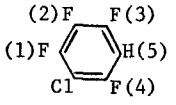
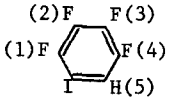
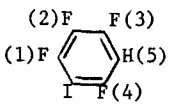
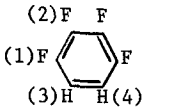
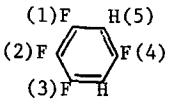
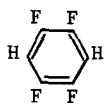
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
426	1964	B	C_6F_4HBr		4,5	10.0	1,5 3,5	6.2 7.9	2,5	2.7
435	1965		C_6F_4HBr		4,5	9.8	1,5 3,5	5.8 8.0	2,5	2.7
426	1966	B	C_6F_4HBr		3,5 4,5	10.3 8.4	2,5	6.3	1,5	2.5
426	1967	B	C_6F_4HCl		4,5	10.0	1,5 3,5	6.4 7.4	2,5	2.7
426	1968	B	C_6F_4HCl		3,5 4,5	10.7 9.3	2,5	6.8	1,5	2.7
420	1969 (4221)		C_6F_4HCl		3,5 4,5	10.0 8.8	2,5	6.4	1,5	2.8
421	1970 (4222)	G	C_6F_4HCl		3,5 4,5	10.1 8.8	2,5	6.5	1,5	2.4
426	1971	B	C_6F_4HI		4,5	9.2	1,5 3,5	5.2 7.7	2,5	2.7
426	1972	B	C_6F_4HI		3,5 4,5	10.1 7.8	2,5	6.0	1,5	2.5
436	1973 (4229)	B*	$C_6F_4H_2$		1,3	+9.65	1,4 2,3	+4.41 +7.99	2,4	-2.69
893	1974 (4231)	*	$C_6F_4H_2$		4,5 1,5	8.6 10.4	2,5	5.6	3,5	2.46
437	1975		$C_6F_4H_2$			7.6		4.6		

Table A.4.d. (contd.)

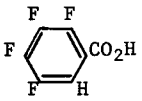
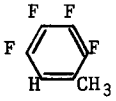
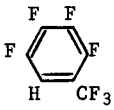
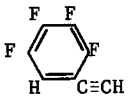
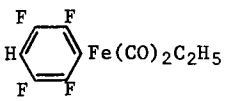
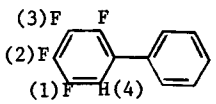
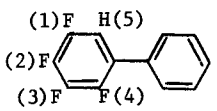
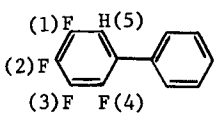
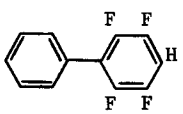
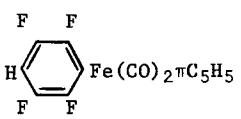
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
440	1976	B	$C_7F_4H_2O_2$			10.1		6.5 8.3		2.6
440	1977 (4245)	B	$C_7F_4H_4$			10.7	F(?)	1.5		2.4
440	1978	B	C_7F_7H			9.2		5.5 7.4		2.6
440	1979 (4257)	B	$C_8F_4H_2$			9.7		5.6 7.4		2.24
447	1980		$C_{10}F_4H_6FeO_2$			10		7		
440	1981 (4275)	B	$C_{12}F_4H_6$			11.0	F(?)	7.9		2.4
896	1982		$C_{12}F_9H$		1,5	10.3				
435	1983		$C_{12}F_9H$		1,5	10.3	2,5 4,5	8.0 6.0	3,5	2.7
456	1984		$C_{12}F_9H$			10.1		7.8		
434	1985		$C_{13}F_4H_6FeO_2$			9.35		7.3		

Table A.4.e. Fluorine bonded to carbon in pentafluorobenzene, hydrogen bonded to carbon in the same ring.

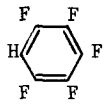
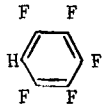
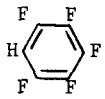
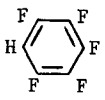
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
434	1986 (5517)	A	C_6F_5H		11.25	8.0	2.7
438	1987 (4344 5517)		C_6F_5H		10.2	6.9	2.7
439	1988 (4345 5517)	G	C_6F_5H		+9.98	+6.79	-2.64
905	1989 (4348 5517)	G	C_6F_5H		+10.4	+7.0	-2.7

Table A.4.f. Fluorine bonded to carbon in substituted monofluoro-benzenes, hydrogen bonded to carbon outside this ring.

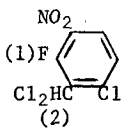
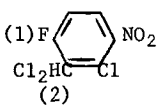
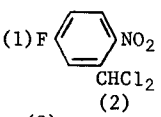
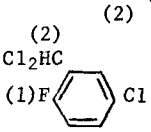
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^4J		^nJ
393	1990 (1824)	T^{2*}	$C_7FH_3Cl_3NO_2$		1,2	-2.48		
393	1991 (1825)	T^{2*}	$C_7FH_3Cl_3NO_2$		1,2	-2.58		
394	1992 (1828)		$C_7FH_4Cl_2NO_2$				1,2	1.2
393	1993 (1829)	T^{2*}	$C_7FH_4Cl_3$		1,2	-0.30		

Table A.4.f. (contd.)

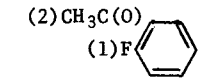
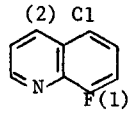
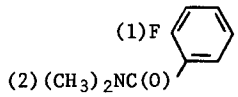
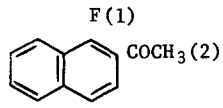
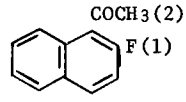
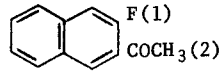
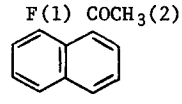
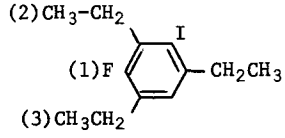
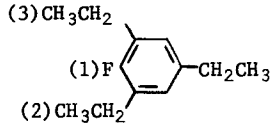
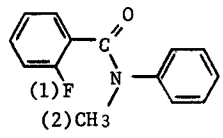
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^nJ
399	1994	A	C_8FH_7O		1,2	4.80
		F				4.20
		H				4.80
469	1995 (1845)		C_9FH_5ClN		1,2	1.5
403	1996		$C_9FH_{10}NO$		1,2	1.2
399	1997	A	$C_{12}FH_9O$		1,2	5.40
		F				5.10
		H				5.60
399	1998	A	$C_{12}FH_9O$		1,2	3.40
		F				2.80
		H				3.20
399	1999	A	$C_{12}FH_9O$		1,2	4.60
		F				3.60
		H				4.60
399	2000	A	$C_{12}FH_9O$		1,2	3.50
		F				2.70
		H				3.20
406	2001	G	$C_{12}FH_{16}I$		1,2	≤0.3
						≤0.3
406	2002	G	$C_{12}FH_{17}$		1,2	≤0.3
					1,3	≤0.3
403	2003		$C_{14}FH_{12}NO$		1,2	1.3

Table A.4.f. (contd.)

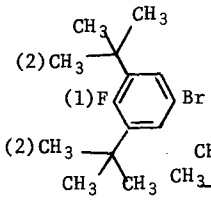
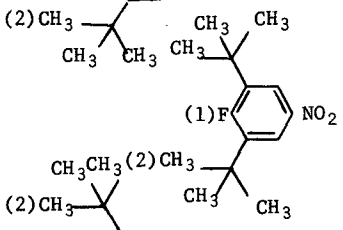
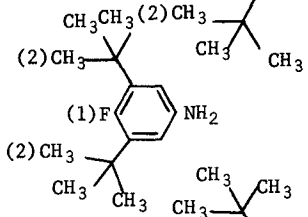
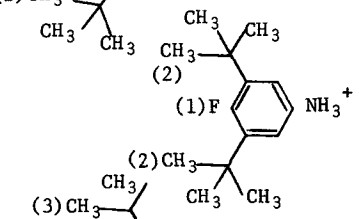
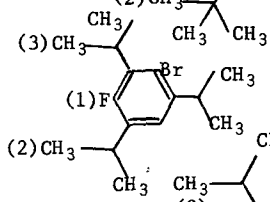
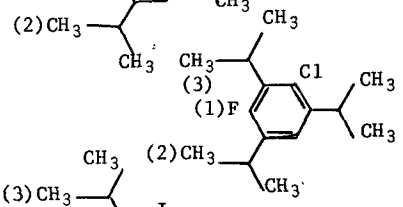
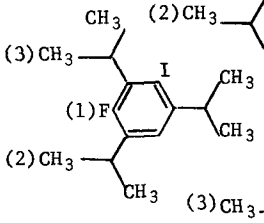
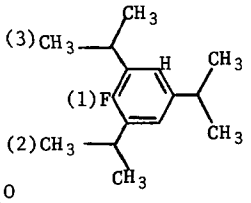
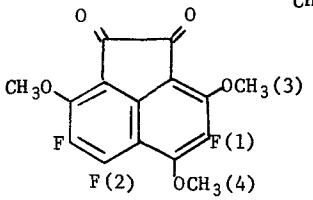
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^nJ
406	2004 (1861)	G	$C_{14}FH_{20}Br$		1,2	1.10
406	2005 (1862)	G	$C_{14}FH_{20}NO_2$		1,2	1.15
406	2006 (1863)	G	$C_{14}FH_{22}N$		1,2	0.93
406	2007 (1864)	KK	$C_{14}FH_{23}N^+$		1,2	1.03
406	2008	G	$C_{15}FH_{22}Br$		1,2 1,3	0.3 1.89
406	2009	G	$C_{15}FH_{22}Cl$		1,2 1,3	0.3 1.84
406	2010	G	$C_{15}FH_{22}I$		1,2 1,3	0.3 1.94
406	2011	G	$C_{15}FH_{23}$		1,2 1,3	≤ 0.3
453	2012		$C_{15}F_3H_9O_5$		1,3 1,4 2,4	1.2 3.5 0.4

Table A.4.f. (contd.)

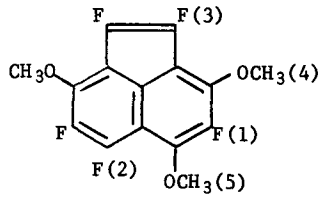
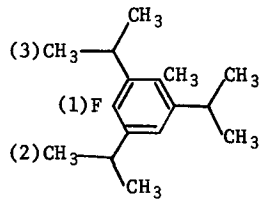
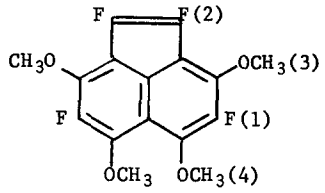
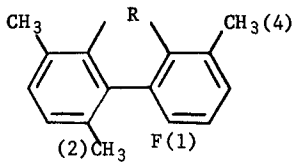
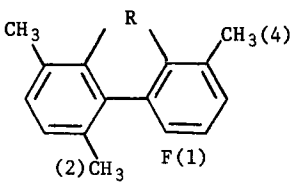
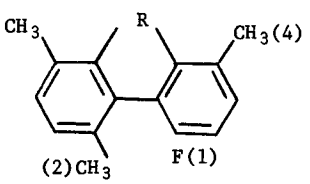
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^nJ
454	2013		$C_{15}F_5H_9O_3$		1,4 3,4 [or 1,5 2,5	3.6 1.6 3.9 1.3] 2.6 0.5
406	2014	G	$C_{16}FH_{25}$		1,2 1,3	0.3 1.68
453	2015		$C_{16}F_4H_{12}O_4$		1,3 2,3 1,4	3.4 1.4 1.4
460	2016		$C_{17}FH_{13}O_2$	 R = -C(O)-C(O)-	1,2	8.2
460	2017		$C_{17}FH_{13}O_3$	 R = -C(O)-O-C(O)-	1,2	3.7
460	2018		$C_{17}FH_{15}$	 R = -CH=CH- (3)	1,2 1,3 1,4	11.9 2.1 1.1

Table A.4.f. (contd.)

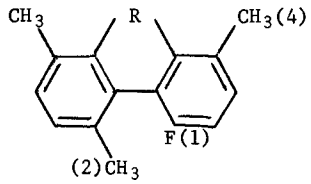
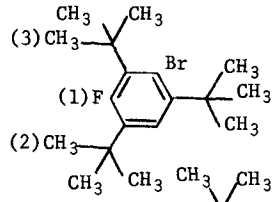
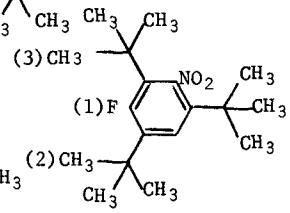
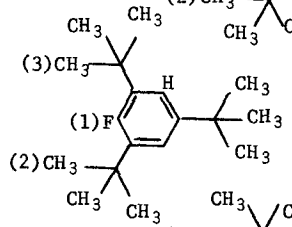
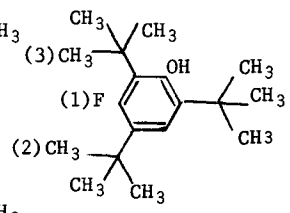
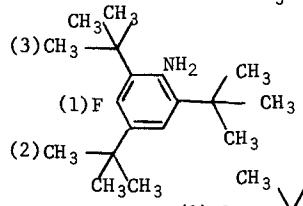
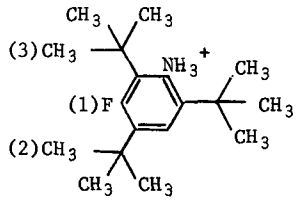
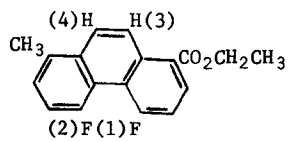
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^nJ
460	2019		$C_{17}FH_{17}O_2$	 R = -CH(OH)-CH(OH)- (hydroxyl groups cis)	1,2	7.7
406	2020	G	$C_{18}FH_{28}Br$		1,2 1,3	1.22 4.22
406	2021	G	$C_{18}FH_{28}NO_2$		1,2 1,3	1.29 1.92
406	2022 (1868)	G	$C_{18}FH_{29}$		1,2 1,3	0.93
406	2023	G	$C_{18}FH_{29}O$		1,2 1,3	1.28 2.90
406	2024	G	$C_{18}FH_{30}N$		1,2 1,3	1.33 3.52
406	2025	K^2	$C_{18}FH_{31}N^+$		1,2 1,3	1.09 1.64
461	2026 (1869 / 4594)	E*	$C_{18}F_2H_{14}O_2$		1,3 2,4	2.22 2.22

Table A.4.g. Fluorine bonded to carbon in substituted difluoro-benzenes, hydrogen bonded to carbon outside this ring.

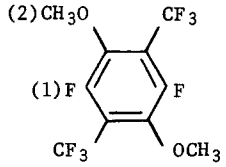
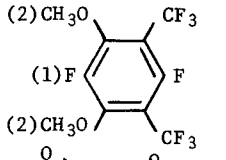
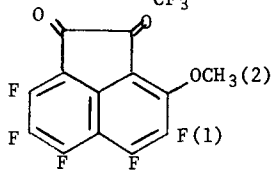
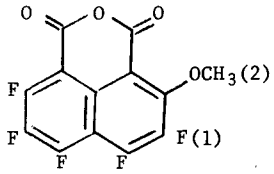
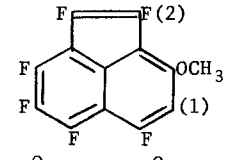
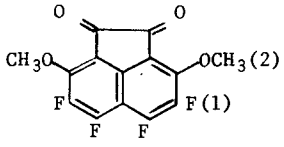
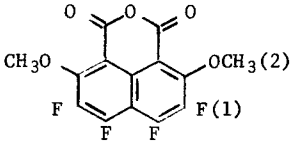
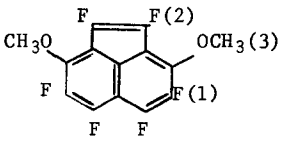
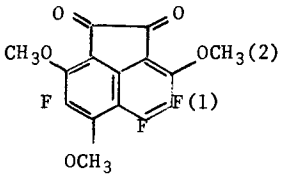
Ref. No.	Serial No.	Solvent	Molecular No.	Structure	^nJ
419	2027 (3380 4153)		$C_{10}F_8H_6O_2$		1,2 1.5
431	2028		$C_{10}F_8H_6O_2$		1,2 2.9
453	2029		$C_{13}F_5H_3O_3$		1,2 1.0
453	2030		$C_{13}F_5H_3O_4$		1,2 2.5
453	2031 (4576)		$C_{13}F_7H_3O$		1,3 4.6 2,3 1.2
453	2032 (4577)		$C_{14}F_4H_6O_4$		1,2 1.0
453	2033		$C_{14}F_4H_6O_5$		1,2 2.7
453	2034		$C_{14}F_6H_6O_2$		1,3 3.8 2,3 1.5
453	2035		$C_{15}F_3H_9O_5$		1,2 1.0

Table A.4.g. (contd.)

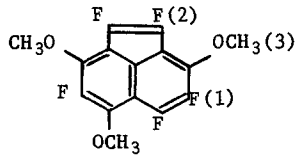
Ref. No.	Serial NO.	Solvent	Molecular formula	Structure	n_J
453	2036		$C_{15}F_5H_9O_3$		1,3 {1.3 2,3 {3.9 [or 1.6 3.6]

Table A.4.h. Fluorine bonded to carbon in substituted trifluoro-benzenes, hydrogen bonded to carbon outside this ring.

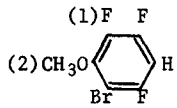
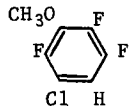
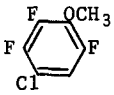
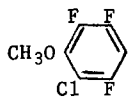
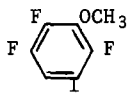
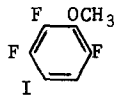
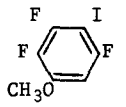
Ref. No.	Serial NO.	Solvent	Molecular formula	Structure	n_J
426	2037 (1930)	B	$C_7F_3H_4BrO$		1,2 2.3
426	2038 (1932)	B	$C_7F_3H_4ClO$		1.4
426	2039 (1933)	B	$C_7F_3H_4ClO$		1.3
426	2040 (1934)	B	$C_7F_3H_4ClO$		2.1
426	2041 (1936)	B	$C_7F_3H_4IO$		1.4
426	2042 (1937)	B	$C_7F_3H_4IO$		1.4
426	2043 (1939)	B	$C_7F_3H_4IO$		2.4

Table A.4.h. (contd.)

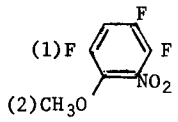
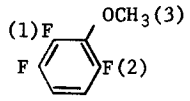
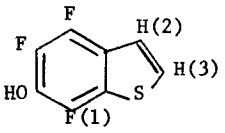
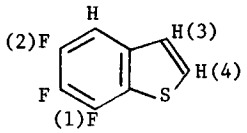
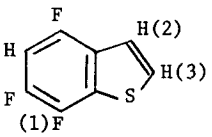
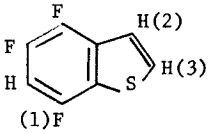
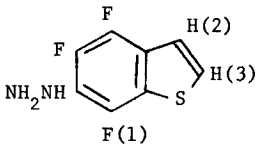
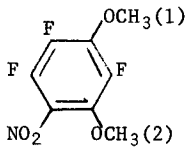
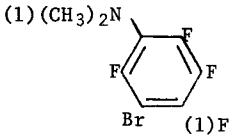
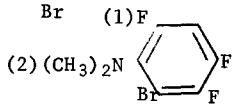
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^nJ
427	2044 (1940)		$C_7F_3H_4NO_3$		1,2	2.0
428	2045		$C_7F_3H_5O$		1,3 2,3	1.2 1.2
451	2046 (4181)	G	$C_8F_3H_3OS$		1,2 1,3	2.1 2.1
451	2047 (1941 / 4182)	G	$C_8F_3H_3S$		1,4 2,4 1,3	0.7 0.75 3.4
451	2048 (1942 / 4183)	G	$C_8F_3H_3S$		1,2 1,3	1.9 1.9
451	2049 (1943 / 4184)	G	$C_8F_3H_3S$		1,2 1,3	2.75 1.45
451	2050 (4185)	G	$C_8F_3H_5N_2S$		1,2 1,3	2.2 2.2
429	2051		$C_8F_3H_6NO_4$		F,1 F,2	1.7 1.7
426	2052 (1944)	B	$C_8F_3H_7BrN$		F,1	2.0
426	2053 (1946)	B	$C_8F_3H_7BrN$		1,2	2.6

Table A.4.h. (contd.)

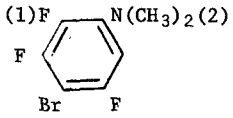
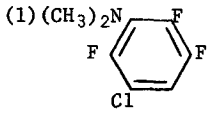
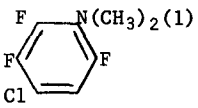
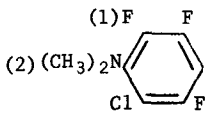
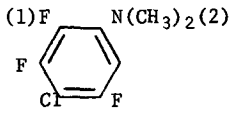
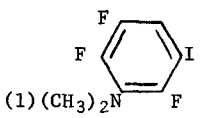
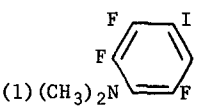
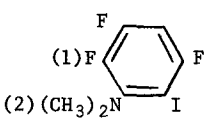
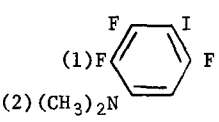
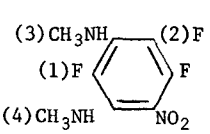
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^nJ
426	2054 (1947)	B	$C_8F_3H_7BrN$		1,2	1.6
426	2055 (1948)	B	$C_8F_3H_7ClN$		F,1	2.1
426	2056 (1949)	B	$C_8F_3H_7ClN$		F,1	1.6
426	2057 (1950)	B	$C_8F_3H_7ClN$		1,2	2.8
426	2058 (1951)	B	$C_8F_3H_7ClN$		1,2	1.8
426	2059 (1952)	B	$C_8F_3H_7IN$		F,1	2.2
426	2060 (1953)	B	$C_8F_3H_7IN$		F,1	2.2
426	2061 (1954)	B	$C_8F_3H_7IN$		1,2	2.4
426	2062 (1955)	B	$C_8F_3H_7IN$		1,2	1.7
429	2063	E	$C_8F_3H_8N_3O_2$		1,4 1,3 2,3	3.2 7.0 7.0

Table A.4.h. (contd.)

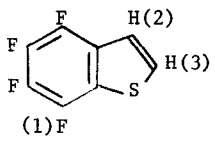
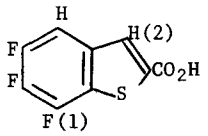
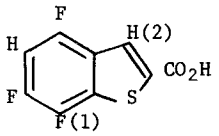
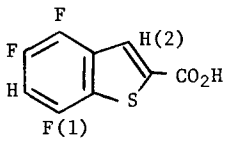
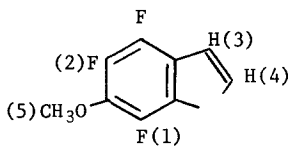
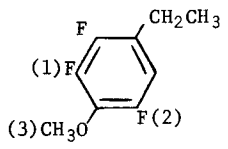
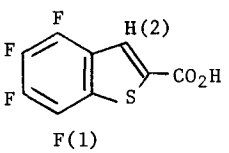
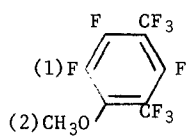
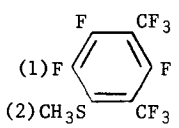
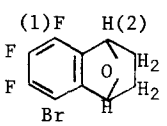
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^nJ
451	2064 (4259)	G	$C_8F_4H_2S$		1,2 1,3	2.8 0.95
451	2065 (1956, 4192)	E	$C_9F_3H_3O_2S$		1,2	3.28
451	2066 (1957, 4193)	E	$C_9F_3H_3O_2S$		1,2	3.35
451	2067 (1958, 4194)	E	$C_9F_3H_3O_2S$		1,2	3.47
451	2068 (4195)	G	$C_9F_3H_5OS$		1,3 1,4 1,5 2,5	4.35 0.0 1.8 0.75
430	2069 (1959, 4197)		$C_9F_3H_9O$		1,3 2,3	1.0 1.0
451	2070 (2096, 4266)	G	$C_9F_4H_2O_2S$		1,2	3.29
431	2071		$C_9F_9H_3O$		1,2	3.4
431	2072		$C_9F_9H_3S$		1,2	2.1
432	2073	J^2	$C_{10}F_3H_6BrO$		1,2	2.5

Table A.4.h. (contd.)

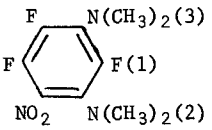
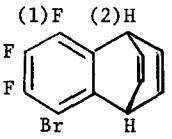
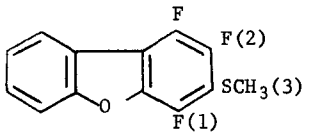
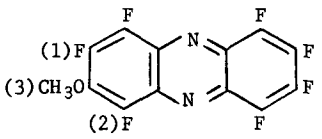
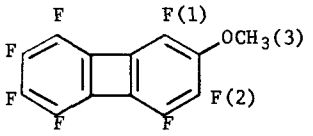
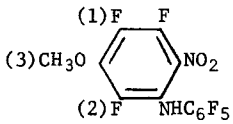
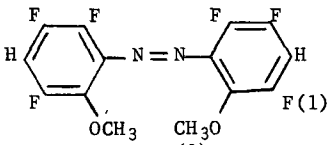
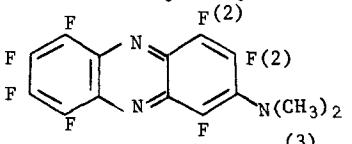
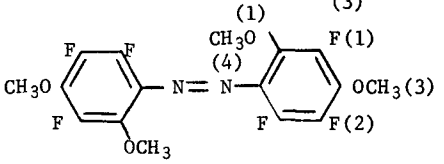
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^nJ	
429	2074	E	$C_{10}F_3H_{12}N_3O_2$		1,2 F,3	1.6 3.0
433	2075		$C_{12}F_3H_6Br$		1,2	1.9
455	2076 (4208)	G	$C_{13}F_3H_7S$		1,3 2,3	0.7 0.7
449	2077		$C_{13}F_7H_3N_2O$		1,3 2,3	3.6 0.8
457	2078 (4209 4289)	H	$C_{13}F_7H_3O$		1,3 2,3	1.0 1.5
449	2079		$C_{13}F_8H_4N_2O_3$		1,3 2,3	2.0 2.0
459	2080 (1963)	E	$C_{14}F_6H_8N_2O_2$		1,2	1.0
449	2081		$C_{14}F_7H_6N_3$		1,3 2,3	2.0 2.0
459	2082	E	$C_{16}F_6H_{12}N_2O_4$		1,4 1,3 2,3	0.7 1.6 1.6

Table A.4.i. Fluorine bonded to carbon in substituted tetrafluoro-benzenes, hydrogen bonded to carbon outside this ring.

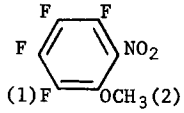
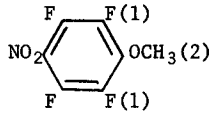
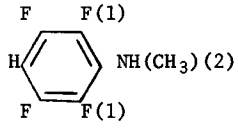
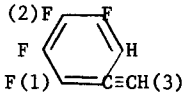
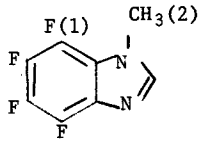
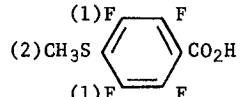
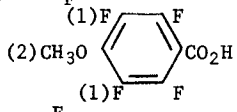
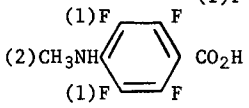
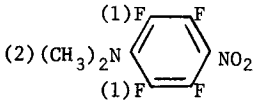
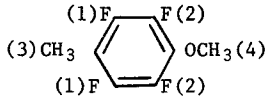
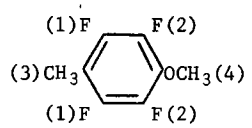
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^nJ	
429	2083	E	$C_7F_4H_3NO_3$				1,2	2.05
429	2084	E	$C_7F_4H_3NO_3$				1,2	2.0
441	2085		$C_7F_4H_5N$				1,2	2.5
440	2086	B	$C_8F_4H_2$				1,3 ∿ 0.9 2,3 ∿ 0.9	
442	2087		$C_8F_4H_4N_2$				1,2	1.4
441	2088		$C_8F_4H_4O_2S$				1,2	1.2
441	2089		$C_8F_4H_4O_3$				1,2	1.8
441	2090		$C_8F_4H_5NO_2$				1,2	3.0
429	2091	E	$C_8F_4H_6N_2O_2$				1,2	1.8
429	2092	E	$C_8F_4H_6N_2O_2$				1,2	2.7
443	2093		$C_8F_4H_6O$		1,3	2.15	2,4	1.2
444	2094		$C_8F_4H_6O$		1,3	2.2	2,4	1.2

Table A.4.i. (contd.)

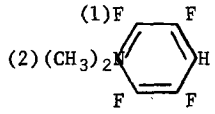
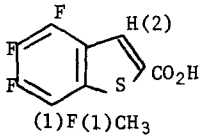
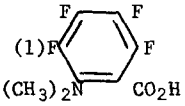
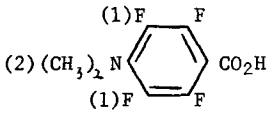
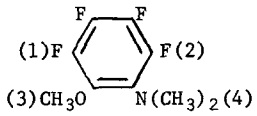
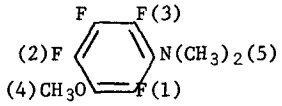
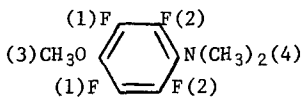
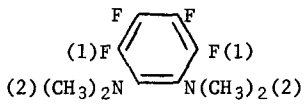
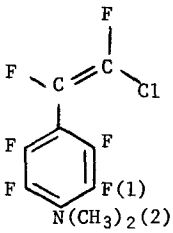
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^nJ
441	2095		$C_8F_4H_7N$		1,2	2.2
451	2096 (2070 4266)	E	$C_9F_4H_2O_2S$		1,2	3.29
441	2097		$C_9F_4H_5NO_2$		1,2	1.3
441	2098		$C_9F_4H_7NO_2$		1,2	2.6
441	2099		$C_9F_4H_7NO_2$		1,2	1.7
442	2100		$C_9F_4H_9NO$		1,3 2,4	2.0 1.2
442	2101		$C_9F_4H_9NO$		1,4 2,4 1,5 3,5	0.9 0.9 1.7 1.7
442	2102		$C_9F_4H_9NO$		1,3 2,4	1.0 1.7
442	2103		$C_{10}F_4H_{12}N_2$		1,2	0.9
896	2104 (3378 3597)		$C_{10}F_6H_6ClN$		1,2	2.5

Table A.4.i. (contd.)

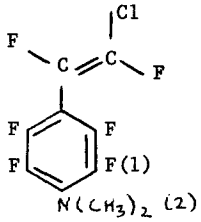
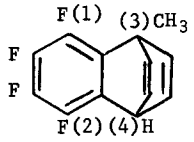
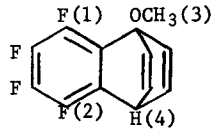
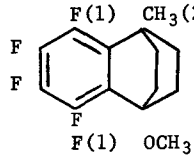
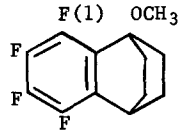
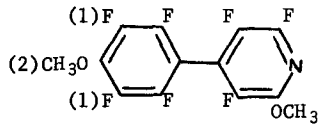
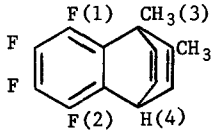
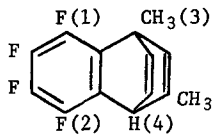
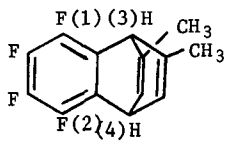
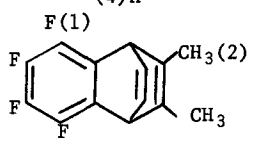
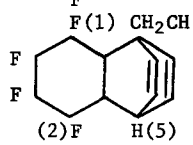
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^nJ	
896	2105 (3379; 3598)		$C_{10}F_6H_6ClN$				1,2	2.5
433	2106	G	$C_{13}F_4H_8$		2,4	1.8	1,3	5.1
433	2107	G	$C_{13}F_4H_8O$		2,4	1.8	1,3	2.6
448	2108	G	$C_{13}F_4H_{12}$				1,2	6.0
448	2109	G	$C_{13}F_4H_{12}O$				1,2	2.6
897	2110 (4291; 4667)	E	$C_{13}F_7H_6NO_2$				1,2	1.8
448	2111	G	$C_{14}F_4H_{10}$		2,4	1.8	1,3	5.1
448	2112	G	$C_{14}F_4H_{10}$		2,4	1.8	1,3	5.1
448	2113	G	$C_{14}F_4H_{10}$		1,3 2,4	1.8 1.8		
433	2114		$C_{14}F_4H_{10}$				1,2	0
448	2115	G	$C_{14}F_4H_{10}$		2,5	1.8	1,4 1,3	0.95 3.4

Table A.4.i. (contd.)

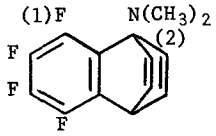
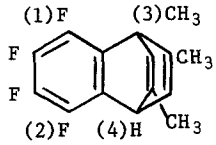
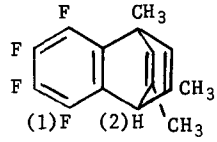
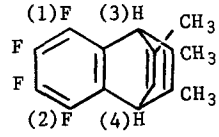
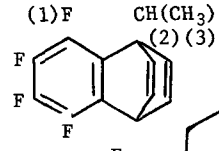
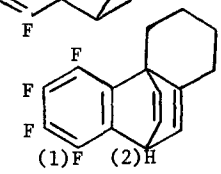
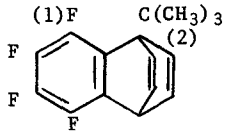
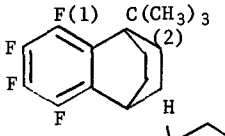
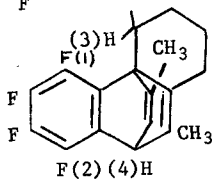
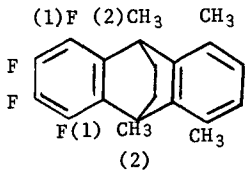
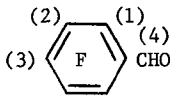
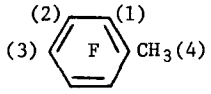
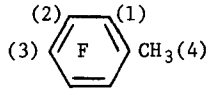
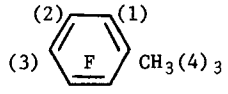
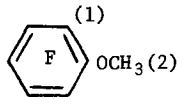
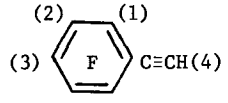
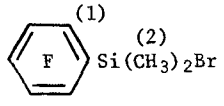
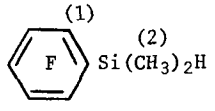
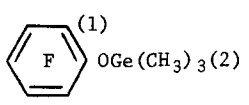
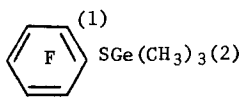
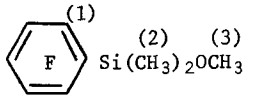
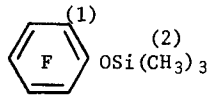
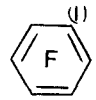
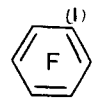
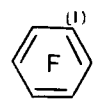
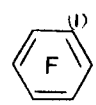
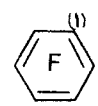
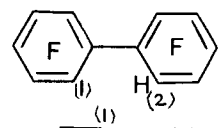
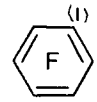
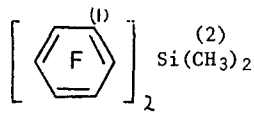
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^4J	^nJ	
433	2116		$C_{14}F_4H_{11}N$				1,2	3.8
448	2117	G	$C_{15}F_4H_{12}$		2,4	2.0	1,3	5.0
448	2118	G	$C_{15}F_4H_{12}$		1,2	1.9		
448	2119	G	$C_{15}F_4H_{12}$		1,3 2,4	1.8 1.8		
448	2120	G	$C_{15}F_4H_{12}$				1,2 1,3	2.1 2.1
448	2121	G	$C_{16}F_4H_{12}$		1,2	1.8		
433 448	2122	G	$C_{16}F_4H_{14}$				1,2	2.9
448	2123	G	$C_{16}F_4H_{18}$				1,2	4.5
448	2124	G	$C_{18}F_4H_{16}$		2,4	1.9	1,3	4.8
448	2125	G	$C_{20}F_4H_{18}$				1,2	7.5

Table A.4.j. Fluorine bonded to carbon in substituted pentafluoro-benzenes, hydrogen bonded to carbon outside this ring.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^nJ	
905	2126 (4381)	G	C_7F_5HO		1,4	+1.0	2,4 3,4	-1.3 +0.2
434	2127 (4391)	A	$C_7F_5H_3$		1,4	2.2	2,4 3,4	≈0 1.3
905	2128 (4392)	G	$C_7F_5H_3$		1,4	+2.3	2,4 3,4	0.2 +1.4
438	2129		$C_7F_5H_3$		1,4	2.3	2,4 3,4	0.6 1.4
438	2130		$C_7F_5H_3O$				1,2	1.1
434	2131 (4406)	U[2]	C_8F_5H				1,4 2,4 3,4	≈0.8 0 ≈0.7
445	2132	H	$C_8F_5H_6BrSi$				1,2	2.0
445	2133 (4416)	H	$C_8F_5H_7Si$				1,2	1.0
445	2134	H	$C_9F_5H_9GeO$				1,2	0.8
445	2135	H	$C_9F_5H_9GeS$				1,2	0.6
445	2136 (4428)	H	$C_9F_5H_9OSi$				1,2 1,3	1.7 0.5
445	2137	H	$C_9F_5H_9OSi$				1,2	0.9

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^nJ
446	2138		$C_9F_5H_9Pb$		1,2	0.5	
445	2139	H	$C_9F_5H_9SSi$		1,2	0.6	
445	2140	H	$C_9F_5H_9Si$		1,2	1.5	
445	2141	H	$C_9F_5H_{10}NSi$		1,2	1.4	
445	2142 (2500)	H	$C_9F_5H_{10}NSn$		1,2	1.1	
445	2143 (4434)	H	$C_{10}F_5H_{12}NSi$		1,2 1,3	1.7 0.9	
435	2144 4285 4450		$C_{12}F_9H$		1,2	0.7	
445	2145 (4466)	H	$C_{14}F_5H_{12}NSi$		1,2	1.7	
445	2146 (4469)	H	$C_{14}F_{10}H_6Si$		1,2	1.6	

A.5. Fluorine bonded to carbon in hetercyclic aromatic system, hydrogen bonded to carbon in either heterocyclic aromatic or non-aromatic systems.

Table A.5.a. Fluorine bonded to carbon in aromatic heterocycle containing nitrogen, hydrogen bonded to carbon in the same ring.

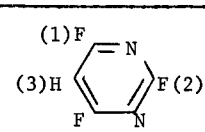
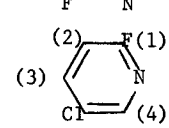
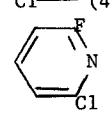
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J				^nJ
228	2147	B	$C_4F_3HN_2$		1,3	1.8		2,3	1.1
462	2148	A*	C_5FH_3Cl		1,2	-3.26	1,3 1,4	+6.77 1.38	
462	2149	A*	C_5FH_3Cl			-2.69		+7.97	+1.54

Table A.5.a. (contd.)

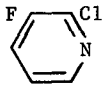
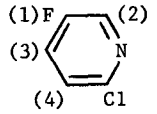
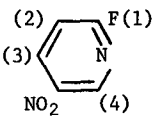
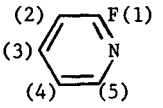
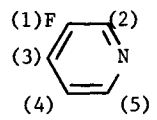
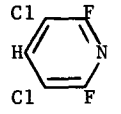
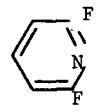
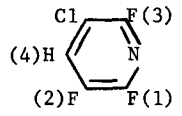
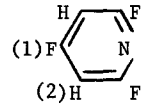
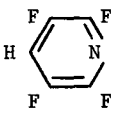
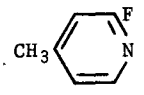
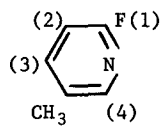
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^5J
462	2150	A*	C_5FH_3Cl			+8.27		+3.67		+0.76
462	2151	A*	C_5FH_3Cl		1,2 1,3	+1.16 +7.92	1,4	+4.82		
462	2152	A*	$C_5FH_3NO_2$		1,2	-2.96	1,3 1,4	+6.41 0		
462	2153	B*	C_5FH_4		1,2	-2.63	1,3 1,5	+8.19 ∿ 0	1,4	+2.49
462	2154	A*	C_5FH_4		1,2 1,3	+0.66 +8.79	1,4	+4.83	1,5	+1.97
464	2155	B	$C_5F_2HCl_2N$					7.5		
462	2156 (4611)	A*	$C_5F_2H_3N$			-2.47		+7.97		+1.19
465	2157		C_5F_3HClN		2,4	7	1,4 3,4	7 7		
466	2158 (4616)		$C_5F_3H_2N$		1,2	7.6				
942	2159 (4624)		C_5F_4HN			7.8		7.0		
467	2160 (2177)	Q*	C_6FH_6N			-2.18		-0.7		2.13
467	2161 (2178)	Q*	C_6FH_6N		1,2	-2.81	1,3 1,4	7.63 -0.7		

Table A.5.a. (contd.)

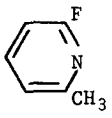
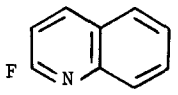
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
467	2162 (2179)	Q*	C_6FH_6N		-3.12	8.32	2.48
469	2163	C	C_9FH_6N		8.5	2.9	

Table A.5.b. Fluorine bonded to carbon in aromatic heterocycle containing sulphur, hydrogen bonded to carbon in the same ring.

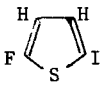
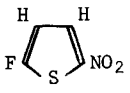
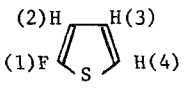
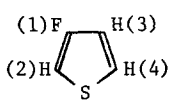
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^5J
471	2163	W[2]	C_4FH_2IS			2.1		3.6
471	2164	W[2]	$C_4FH_2NO_2S$			2.0		4.6
472	2165 (5451)	B-H* (50%)	C_4FH_3S		1,2 1,4	1.62 3.10	1,3	3.07
		B-D* (41%)				1.54 3.08		3.07
		D* (5%)				1.43 2.87		2.95
472	2166 (5452)	B-H* (46%)	C_4FH_3S		1,2 1,3	1.08 -0.81	1,4	3.30
		B-D* (77%)				1.06 -0.34		3.23
		B-D* (22%)				0.94 -0.88		3.17

Table A.5.b. (contd.)

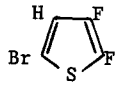
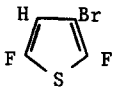
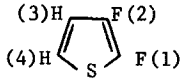
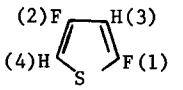
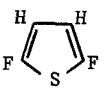
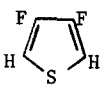
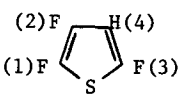
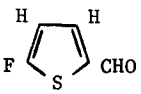
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^5J	
		D* (6%)				0.92 -0.88		3.16		
473	2167 (4672)	B-D	C_4F_2HBrS			~ 0.0		3.56		
473	2168 (4673)	B-D	C_4F_2HBrS			2.81		3.43		
		H				2.89		3.52		
							^4J			
473	2169 (4674)	D	$C_4F_2H_2S$		2,3	-0.09	1,3 1,4	3.08 4.28	2,4	4.41
		H			2,3	-0.12	1,3 1,4	3.12 4.47	2,4	4.61
473	2170 (4675)	B-D	$C_4F_2H_2S$		1,3 2,3 2,4	1.29 -0.33 2.81	1,4	3.40		
		B-H			1,3 2,3 2,4	1.35 -0.27 2.92	1,4	3.45		
473	2171 (4677)	H	$C_4F_2H_2S$			0.5		3.66		
473	2172 (4676)	B-D	$C_4F_2H_2S$			1.23		3.17		
		B-H				1.35		3.26		
473	2173 (4678)	B	C_4F_3HS		2,4 3,4	0.88 3.40	1,4	3.62		
		G				0.80 3.30		3.60		
471	2174 (2193)	W[2]	C_5FH_3OS			1.4		3.8		

Table A.5.b. (contd.)

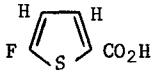
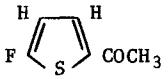
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
471	2175	W[2]	$C_5FH_3O_2S$		1.8	4.0	
471	2176 (2196)	W[2]	C_6FH_5OS		1.4	3.6	

Table A.5.c. Fluorine bonded to carbon in aromatic heterocycle containing nitrogen, hydrogen bonded to carbon outside this ring.

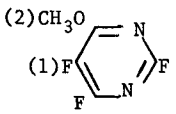
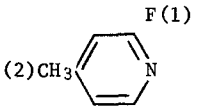
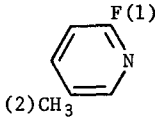
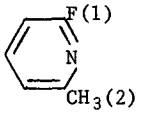
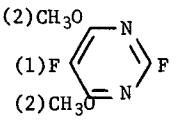
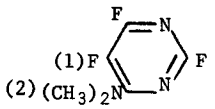
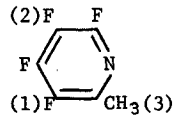
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^nJ	
228	2176a (4620)	A	$C_5F_3H_3N_2O$				1,2	≤ -0.3
467	2177 (2160)	Q*	C_6FH_6N				1,2	-0.24
467	2178 (2161)	Q*	C_6FH_6N				1,2	1.25
467	2179 (2162)	Q*	C_6FH_6N				1,2	-0.61
228	2180 (4631)	A	$C_6F_2H_6N_2O_2$				1,2	≤ 0.3
228	2181 (4635)	A	$C_6F_3H_6N_3$				1,2	2.2
942	2182 (4637)		$C_6F_4H_3N$		1,3	17.0	2,3	1.6

Table A.5.c. (contd.)

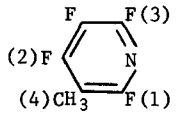
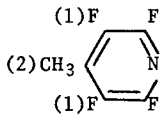
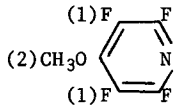
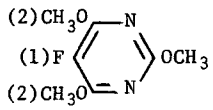
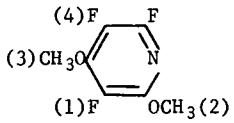
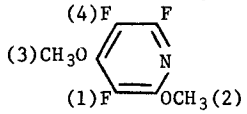
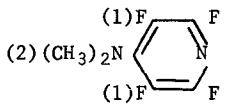
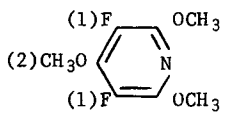
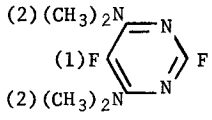
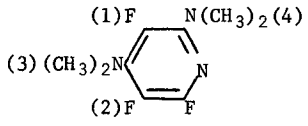
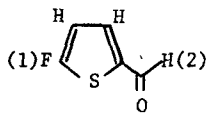
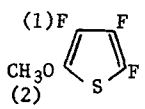
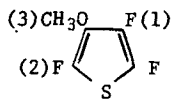
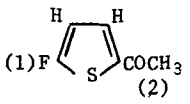
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^nJ	
942	2183 (4638)		$C_6F_4H_3N$		1,4 2,4	20.4 20.4	3,4	1.1
942	2184 (4639)		$C_6F_4H_3N$		1,2	20.9		
942	2185 (4640)		$C_6F_4H_3NO$				1,2	2.7
228	2186	L	$C_7FH_9N_2O_3$				1,2	≤0.3
468	2187 (4644)	B	$C_7F_3H_6NO_2$				1,2 1,3	0 2.5
942	2188 (4643)		$C_7F_3H_6NO_2$				1,3 4,3	2.2 2.2
942	2189 (4645)		$C_7F_4H_6N_2$				1,2	3.4
942	2190		$C_8F_2H_9NO_3$				1,2	2.2
228	2191 (4647)	A	$C_8F_2H_{12}N_4$				1,2	3.0
942	2192 (4652)		$C_9F_3H_{12}N_3$				1,4 1,3 2,3	2.4 2.7 2.7

Table A.5.d. Fluorine bonded to carbon in aromatic heterocycle containing sulphur, hydrogen bonded to carbon outside this ring.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^nJ
471	2193 (2174)	X[2]	C_5FH_3OS		1,2	4.6
229	2194 (4680)		$C_5F_3H_3OS$		1,2	0.6
229	2195 (4681)		$C_5F_3H_3OS$		1,3 2,3	2.1 ~0.2
471	2196 (2176)	W[2]	C_6FH_5OS		1,2	0.45

A.6. Fluorine bonded to element, M, other than carbon, hydrogen bonded to carbon.

Table A.6.a. M = arsenic (As)

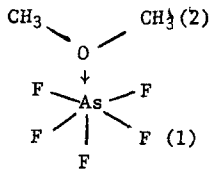
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
474	2197	J	$C_2F_5H_6AsO$		1,2	0.82	

Table A.6.b. M = boron (B)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J
476	2198	E	$C_3F_3H_9BN$	$(CH_3)_3NBF_3$		0.8
475	2199 (5338 5928)		$C_3F_3H_9BP$	$(CH_3)_3PBF_3$		0.65
477	2200		$C_4F_4H_4B_3$	$(BF_2CH{=}CH)_2BF$ (1)(3)(4)(2)	1,3 7 2,4 11	

Table A.6.b. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
475	2201 (5351)		$C_6F_3H_{15}BN$	$(CH_3CH_2)_3NBF_3$		0.79	

Table A.6.c. M = germanium (Ge)

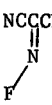
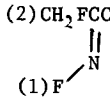
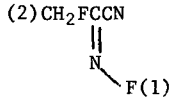
Ref. No.	Serial NO.	Solvent	Molecular formula	Structure		^3J	^4J	^nJ
478	2202		C_3FH_9Ge	$(CH_3)_3GeF$		7		
479	2203		CF_2H_3N	CH_3NF_2		22		
480	2204	A	CF_2H_3NO	$CH_2(NF_3)OH$		23		
10 11	2205 (17)	A	CF_3H_2N	FCH_2NF_2		22		
480	2206 (4891)	A	$C_2F_2H_5NO$	$CH_3CH(NF_2)OH$	1,3	16		
				(3)(1,2)	1,2	24		
481	2207		$C_2F_2H_6N$	$(CH_3)_2NF_2$		35		
11	2208	A	$C_2F_3H_4N$	$FCH_2CH_2NF_2$		25		
480	2209	A	$C_2F_4H_4N_2O$	$O(CH_2NF_2)_2$		21		
499	2210		$C_3FH_3N_2$				4	
499	2211		$C_3FH_3N_2$				~0	
482	2212		$C_3FH_7N_2O$	$CH_3NFC(O)NHCH_3$		32.7		
64	2213 (148 4700)		$C_3F_2H_2N_2$				1,2 4.2	
64	2214 (149 4701)		$C_3F_2H_2N_2$				1,2 2.9	

Table A.6.d. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		3	4	n_J
483	2215	B	$C_3F_2H_4IN$	$CH_2{=}ClCH_2NF_2$		26.3		
484	2216		$C_3F_2H_5N$	$CH_2{=}CHCH_2NF_2$		29		
483	2217	B	$C_3F_2H_5N$	$CH_2{=}CHCH_2NF_2$		29		
485	2218 (4702)		$C_3F_2H_5NO$	$CH_3CH_2NFCF(O)$		30		
480	2219	A	$C_3F_2H_5NO_2$	$F_2NCH_2CO_2CH_3$		24		
486	2200		$C_3F_2H_7NO_2$	$(CH_3O)_2CHNF_2$		28		
11	2221 (193)	A	$C_3F_3H_6N$	$FCH_2CH_2CH_2NF_2$		28		
64	2222 (202, 4703)		$C_3F_4H_4N_2$	(3) (4) $CH_2FCCH_2NF_2$ (2); N; (1)F	2,4	29	1,3 1,4	4.8 0
64	2223 (203, 4704)		$C_3F_4H_4N_2$	(3) (4) $CH_2FCCH_2NF_2$ (2); N; F(1)	2,4	28	1,3 1,4	2.3 2.4
487	2224 (4893)	B	$C_3F_4H_6N_2$	$NF_2CH_2CH(NF_2)CH_3$ (1,2)(5)(6)(3,4) (at -75^{o})	1,5 2,5 3,6 4,6	27.0 31.0 23.0 23.4		
479	2225 (4894)		$C_3F_4H_6N_2O$	$NF_2CH_2CH_2CH(NF_2)OH$ (1)(4) (5)(2,3)	1,4 2,5 3,5	27 10 30		
484	2226		$C_3F_6H_5N_3$	$NF_2CH_2CH(NF_2)CH_2NF_2$ (2)(1)	1,2	27		
488	2227		C_4FH_9N	(4)H, F(1), C=N, (3)H, $CH_2CH_2CH_3$ (2)	1,2 1,3 1,4	19 23 48		

Table A.6.d. (contd.)

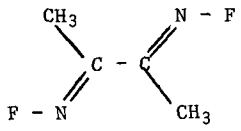
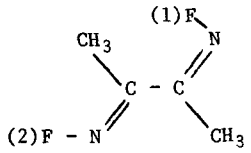
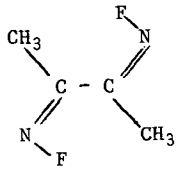
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J	^5J
484	2228		$C_4F_2H_4N_2$	$CH_2=C(CN)CH_2NF_2$		28		
489	2229		$C_4F_2H_5N$	$CH_3C\equiv CCH_2NF_2$		28		
490	2230		$C_4F_2H_6N_2$				2.5	
						(1) or (2)	2.8 4.6	
						(1) or (2)	3.5	
								1.75
489	2231		$C_4F_2H_7N$	$CH_3CH=CHCH_2NF_2$		28		
485	2232 (4712)		$C_4F_2H_7NO$	$CH_3(CH_2)_2NFCF(O)$		31		
491	2233		$C_4F_2H_9N$	$CH_3(CH_2)_3NF_2$		28		
488	2234	S	$C_4F_2H_9N$	$[(CH_3)_2C=\overset{+}{N}FCH_3]F^-$		18.7		
492	2235 (4898)		$C_4F_3H_8N_3O$	$CH_3\overset{(3)}{C}H\overset{(1,2)}{(NF_2)}CH_3$ $O\leftarrow N=NF$	1,3 2,3	33 9		
492	2236		$C_4F_3H_8N_3O$	$CH_3C(CH_3)CH_2NF_2$ $O\leftarrow N=NF$		27		
493	2237	P	$C_4F_4H_6N_2$	$CH_3C(NF_2)_2CH=CH_2$			2.0	
487	2238 (4901)	K	$C_4F_4H_8N_2$	$[CH_3CH(NF_2)]_2$ (3)(1,2)	1,3 2,3	22.2 25.6		

Table A.6.d. (contd.)

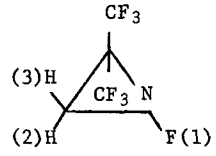
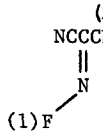
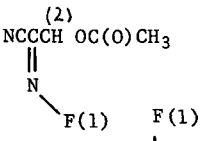
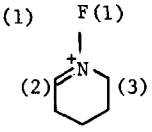
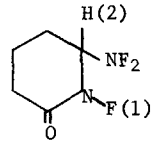
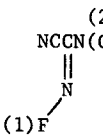
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J	^nJ
487	2239 (4900)	B	$C_4F_4H_8N_2$	$NF_2CH_2CH(NF_2)CH_2CH_3$ (1,2)(5)(6)(3,4) (at -78°)	1,5 2,5 3,6 4,6	24.5 27.0 14.7 30.3			
496	2240	S	$C_4F_5H_9NB$	$[(CH_3)_2C{=}N^+FCH_3]BF_4^-$		18.5			
114	2241 [311 2807 4717]	K	$C_4F_7H_2N$		1,2 1,3	29.0 40.0			
499	2242		$C_5FH_5N_2O_2$				1,2	3	
499	2243		$C_5FH_5N_2O_2$				1,2	3.8	
494	2244	K	$C_5FH_9N^+$		1,2 1,3	24.1 2.8			
482	2245 (2523)		$C_5FH_{11}N_2O$	$CH_3CH_2NFC(O)NHCH_2CH_3$		38.7			
485	2246 (4723)		$C_5F_2H_9NO$	$CH_3(CH_2)_3NFCF(O)$		28			
351	2247 (4903)		$C_5F_3H_7N_2O$		1,2	~25			
479	2248 (4904)		$C_5F_4H_8N_2O_2$	$CH_3C(NF_2)_2CO_2CH_2CH_3$				~2.5	
487	2249 (4905)	K	$C_5F_4H_{10}N_2$	$CH_3CH(NF_2)C(NF_2)(CH_3)_2$ (3)(1,2)	1,3 2,3	15.8 34.6			
499	2250		$C_6FH_{10}N_3$						1,2 ~0

Table A.6.d. (contd.)

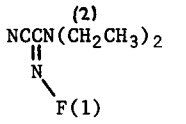
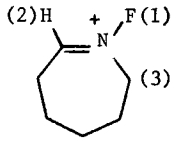
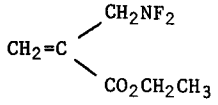
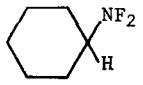
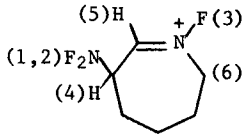
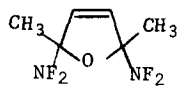
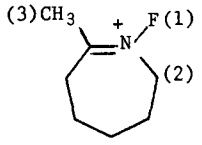
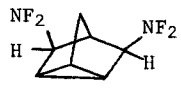
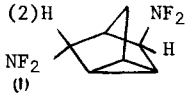
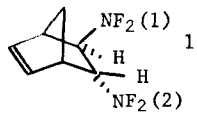
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ
499	2251		$C_6FH_{10}N_3$						1,2 1.5
494	2252	S	$C_6FH_{11}N^+$		1,2 1,3	24 12			
484	2253		$C_6F_2H_9NO_2$			30			
491	2254		$C_6F_2H_{11}N$			25			
494	2255 (4906)		$C_6F_3H_{10}N_2^+$		1,4 2,4 3,5 3,6	11.8 3.31 25.6 18			
495	2256	B	$C_6F_4H_8N_2O$					2.5	
491	2257		$C_6F_4H_{12}N_2$	$NF_2(CH_2)_6NF_2$		30			
484	2258		$C_6F_6H_9N_3O_2$	$(F_2NCH_2)_2C(NF_2)CO_2CH_2CH_3$		27			
494	2259	S	$C_7FH_{13}N^+$		1,2	∿16	1,3	5	
495	2260 (4911)		$C_7F_4H_8N_2$			∿30			
495	2261 (4912)		$C_7F_4H_8N_2$		1,2	∿30			
495	2262 (4913)		$C_7F_4H_8N_2$		1 or 2	∿30			

Table A.6.d. (contd.)

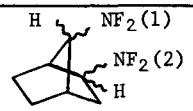
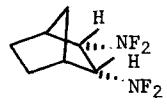
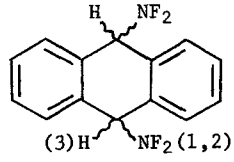
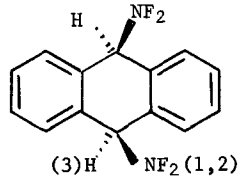
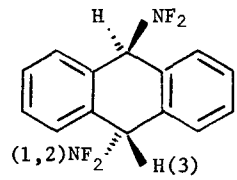
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
495	2263 (4910)		$C_7F_4H_{10}N_2$		1 or 2 ∿30		
495	2264 (4914)		$C_7F_4H_{10}N_2$		30		
234	2265 (4730)		$C_{10}F_3H_{12}N$	$C_6H_5CF_2NFCH(CH_3)_2$	37		
234	2266 (3107 4732)		$C_{11}F_3H_{14}N$	$C_6H_5CF_2NFCH(CH_3)CH_2CH_3$	38		
234	2267 (4733)		$C_{11}F_3H_{14}N$	$C_6H_5CF_2NFCH_2CH(CH_3)_2$	43		
234	2268 (4734 3120)		$C_{12}F_3H_{16}N$	$C_6H_5CF_2NFCH(CH_3)(CH_2)_2CH_3$	39		
486	2269		$C_{13}F_2H_{11}N$	$(C_6H_5)_2CHNF_2$	7		
496	2270	A	$C_{14}F_4H_{10}N_2$		1,3 2,3	24.0 25.8	
497	2271		$C_{14}F_4H_{10}N_2$			∿30	
497	2272		$C_{14}F_4H_{10}N_2$			∿30	
496	2273	A	$C_{14}F_4H_{12}N_2$	$[C_6H_5CH(NF_2)]_2$ (3)(1,2)	1,3 2,3	23.5 24.5	

Table A.6.d. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J	^nJ
				(3)(1,2)				
498	2274		$C_{14}F_4H_{12}N_2$	$[C_6H_5CH(NF_2)]_2$	1,3	13.8		
	(4922)			(dl)	2,3	33.8		
234	2275		$C_{15}F_3H_{14}N$	$C_6H_5CF_2NFCH(CH_3)C_6H_5$		31		
	(3153, 4737)							

Table A.6.e. M = phosphorus (P)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
501	2276	B	CF_2H_2ClOP	$ClCH_2P(O)F_2$	4.6		
	(5758)						
500	2277	B	CF_2H_2ClP	$ClCH_2PF_2$	12.5		
501	(5760)						
501	2278	B	CF_2H_2ClPS	$ClCH_2P(S)F_2$	4.6		
502	2279		CF_2H_3ClPS	$ClCH_2P(S)F_2$	5.5		
	(5761)						
84	2279a		CF_2H_3DNPS	$F_2P(S)N(D)CH_3$		~1.0	
	(5764)						
501	2280	B	CF_2H_3OP	$CH_3P(O)F_2$	6.3		
502	(5765)						
502	2281		CF_2H_3OPS	$CH_3OP(S)F_2$		0.7	
	(5768)						
503	2282		CF_2H_3OPS	$CH_3SP(O)F_2$		1	
	(5767)						
502	2283		$CF_2H_3O_2P$	$CH_3OP(O)F_2$		0.5	
	(5769)						
504	2284		CF_2H_3P	CH_3PF_2	20.0		
	(5770)						
501	2285	B	CF_2H_3P	CH_3PF_2	20.0		
501	2286						
502	(5772)	B	CF_2H_3PS	$CH_3P(S)F_2$	6.3		

Table A.6.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J	^nJ
84	2287 (2547, 5773)		CF_2H_4NOP	$F_2P(O)N(H)CH_3$ (1) (2)		1,2	1.2	
505	2288 (2548, 5775)	B	CF_2H_4NP	F_2PNHCH_3			2.0	
84	2289 (5744)	P HH	CF_2H_4NP	F_2PNHCH_3			2.0 2.4	
84	2290 (2549, 5776)		CF_2H_4NPS	$F_2P(S)N(H)CH_3$ (1) (2)		1,2	1.0	
506	2291 [2550, 4933, 5791]	B	CF_3H_4P	CH_3PF_3H (1)	Fa,1 Fe,1	12 4		
507	2292 (5794)		CF_4H_2ClP	$ClCH_2PF_4$		6-7		
508	2293	B	$CF_4H_3NP_2$	$CH_3N(PF_2)_2$			1.6	
501	2294	B	CF_4H_3P	CH_3PF_4		7.2		
507 509 510	(5796)	P				+7.0		
511	2295 (4936, 5802)		$CF_5H_3P^-$	$CH_3PF_5^-$		8		
512	2296 (5812)	B	$C_2FH_4O_2P$				2.0	
501 502	2297 (5814)	B	C_2FH_6OP	$(CH_3)_2P(O)F$		8.9 9.0		
503	2298 (5815)		$C_2FH_6OPS_2$	$(CH_3S)_2P(O)F$			1.2	
502	2299 (5816)		$C_2FH_6O_2P$	$(CH_3O)_2PF$			0.6	
502	2300 (5817)		$C_2FH_6O_2P$	$CH_3P(O)F(OCH_3)$		6.1	0.8	
501	2301 (5818)	H	$C_2FH_6O_2PS$	$(CH_3O)_2P(S)F$			0.57	

Table A.6.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
513	2302 (5819)		C_2FH_6P	$(CH_3)_2PF$	18.5		
501 502	2303 (5820)	B	C_2FH_6PS	$(CH_3)_2P(S)F$	8.0		
502	2304 (5821)		C_2FH_7NPS	$CH_3P(S)F(NHCH_3)$	6.4	3.0	
502	2305 (5836)		$C_2F_2H_5PS$	$CH_3CH_2P(S)F_2$	4.5		
501	2306 (5839)	B B-G	$C_2F_2H_6NOP$	$(CH_3)_2NP(O)F_2$		1.4 1.3	
514	2307 (5840)		$C_2F_2H_6NOP$	$(CH_3)_2NP(O)F_2$		1.70	
501 515 512	2308 (5841)	B	$C_2F_2H_6NP$	$(CH_3)_2NPF_2$		3.7	
516	2309 (5842)		$C_2F_2H_6NP$	$(CH_3)_2NPF_2$		3.6	
502	2310 (5843)		$C_2F_2H_6NPS$	$(CH_3)_2NP(S)F_2$		2.1	
517	2311 (5845)	B	$C_2F_2H_6NPS$	$(CH_3)_2NP(S)F_2$		2.0	
518	2312 (5844)		$C_2F_2H_6NPS$	$(CH_3)_2NP(S)F_2$		2.1	
519	2313 (5846)		$C_2F_2H_{13}B_3NP$	$(CH_3)_2NPF_2B_3H_7$		3.2	
520	2314 (5847)	B	$C_2F_2H_{14}B_4ND$	$(CH_3)_2NPF_2B_4H_8$		3.0	
507	2315 (4940 5853)		$C_2F_3H_6P$	$(CH_3)_2PF_3$ (1)	F_e,1 ∿2		
510	2316 (4940 5853)	P	$C_2F_3H_6P$	$(CH_3)_2PF_3$ (1)	F_e,1 +3.05 F_a,1 +12.6		
506	2317 (4941 5854)	B	$C_2F_3H_6P$	$CH_3CH_2PF_3H$ (1)	F_e,1 4.4 F_a,1 (95?)		1.3

Table A.6.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
512	2318 (5858)	B	$C_2F_4H_4O_2P_2$	$(F_2POCH_2)_2$				2.0		
507	2319 (5860)		$C_2F_4H_5P$	$CH_3CH_2PF_4$		6-7				
521	2320 (5862)		$C_2F_4H_6NP$	$(CH_3)_2NPF_4$				2		
522	2321 (4945, 5867)	M	$C_2F_5H_6CsNP$	$Cs^+[(CH_3)_2NPF_5]^-$ (1)			F_e,1 F_a,1	1.8 ~0		
523	2322 [2555, 4948, 5867]	J	$C_2F_5H_7P_2$	$(CH_3)_2HPPF_5$ (1)			F_e,1	0.5		
501 502	2323 (5903)		$C_3FH_8PS_2$	$CH_3P(S)F(SCH_2CH_3)$ (3) (1) (2)	1,3	6.4	1,2	1.8		
501 502	2324 (5904)		C_3FH_9NOP	$CH_3P(O)F[N(CH_3)_2]$		6.0		2.4		
501 515	2325 (5906)	B	C_3FH_9NP	$CH_3PF[N(CH_3)_2]$		8.3		5.1		
502	2326 (5908)		C_3FH_9NPS	$CH_3P(S)F[N(CH_3)_2]$		6.2		3.1		
512	2327 (5912)	B	$C_3F_2H_5OP$	$CH_2=CHCH_2OPF_2$ (3)(2)(1)			1,2	0.5	1,3	0.5
512	2328 (5913)	B	$C_3F_2H_7OP$	$CH_3CH_2CH_2OPF_2$				0.5		
503	2329 (5916)		$C_3F_2H_9N_2OP$	$F_2P(O)NCH_3N(CH_3)_2$				3		
502 507 510	2330 (5445, 5919)	B-S[2]	$C_3F_2H_9P$	$(CH_3)_3PF_2$		+12.17				
524	2331	Y[2]	$C_3F_2H_9P$	$(CH_3)_3PF_2$		12.8				
515	2332 (4953, 5929)		$C_3F_3H_9NP$	$CH_3PF_3[N(CH_3)_2]$ (1)	F_e,1 F_a,1	1.7 12.3		2.6		
75	2333 (4769, 5933)		$C_3F_4H_6NP$	$CF_3PFN(CH_3)_2$				5.6		

Table A.6.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
76	2334 (5934)	P	$C_3F_4H_6NPS$	$CF_3P(S)F[N(CH_3)_2]$ (1) (2)		1,2 2.5	
474	2335 (4954 5935)	J	$C_3F_5H_9NP$	$(CH_3)_3NPF_5$ (1)		F_a,1 <0.5 F_e,1 2.04	
523	2336 (4955 5936)	M	$C_3F_5H_9P_2$	$(CH_3)_3PPF_5$ (1)		F_e,1 1.1	
525	2337 (4956 5937)		$C_3F_5H_{11}NP$	$[(CH_3)_2NH_2]^+[CH_3PF_5]^-$ (1)	F_e,1 9.0		
502	2338 (5978)		$C_4FH_{10}OPS$	$CH_3CH_2P(S)F(OCH_2CH_3)$	3.9		
501	2339	B B-G	$C_4FH_{12}N_2OP$	$[(CH_3)_2N]_2P(O)F$		1.55 1.50	
514	2340 (5985)		$C_4FH_{12}N_2OP$	$[(CH_3)_2N]_2P(O)F$		1.45	
501 512 515	2341 (5986)		$C_4FH_{12}N_2P$	$[(CH_3)_2N]_2PF$		3.0	
516	2342 (5986)		$C_4FH_{12}N_2P$	$[(CH_3)_2N]_2PF$		3.2	
502	2343 (5989)		$C_4FH_{12}N_2PS$	$[(CH_3)_2N]_2P(S)F$		1.6	
518	2344 (5988)		$C_4FH_{12}N_2PS$	$[(CH_3)_2N]_2P(S)F$		1.70	
527	2345 (5995)		$C_4F_2H_8NP$			3.3	
501 526	2346 (5997)	H	$C_4F_2H_9OP$	$(CH_3)_3CP(O)F_2$		1.07	
512	2347 (5998)		$C_4F_2H_9OP$	$CH_3(CH_2)_3OPF_2$		<0.5	
526	2348 (6001)	B	$C_4F_2H_9P$	$(CH_3)_3CPF_2$		~1.8	
526	2349 (6002)	B	$C_4F_2H_9PS$	$(CH_3)_3CP(S)F_2$		0.8	
512	2350 (6004)	B	$C_4F_2H_{10}NP$	$(CH_3CH_3)_2NPF_2$		3.0	

Table A.6.e. (contd.)

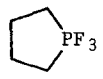
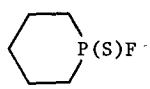
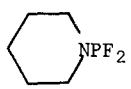
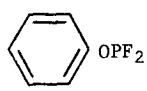
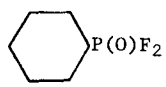
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ
527	2351 (6005)		$C_4F_2H_{10}NP$	$(CH_2CH_2)_2NPF_2$			3.2		
522	2352 (6009)	B	$C_4F_2H_{12}NP$	$(CH_3)_2PF_2[N(CH_3)_2]$	13.1		2.6		
507	2353 (4957, 6011)		$C_4F_3H_8P$		8.6				
507	2354 (4959, 6015)		$C_4F_3H_{10}P$	$(CH_3CH_2)_2PF_3$	12				
521	2355		$C_4F_3H_{12}N_2P$	$[(CH_3)_2N]_2PF_3$ (1)		F_e,1 F_a,1	1.5 2.8		
507	2356 (6022)		$C_4F_4H_9P$	$CH_3(CH_2)_3PF_4$	6				
519	2357 (6027)		$C_4F_4H_{16}B_2N_2P_2$	$[(CH_3)_2NPF_2]_2B_2H_4$			2.6		
227	2357a		$C_4F_4H_6NP$	CF_2=CFPF$[N(CH_3)_2]$ (1) (2)		1,2	6.2		
502	2358		$C_5FH_{10}PS$		13.3				
501	2359	B	$C_5FH_{12}O_2P$	$(CH_3)_3CP(O)F(OCH_3)$ (2) (1) (3)		1,2 1,3	0.88 1.3		
502	2360 (6073)		$C_5FH_{13}NOP$	$(CH_3CH_2)_2NPF(OCH_3)$ (2) (1)(3)		1,2 1,3	3.1 0.6		
527	2361 (6078)		$C_5F_2H_{10}NP$				2.9		
529	2362 (6116)	B-H	$C_6FH_{14}O_3P$	$[(CH_3)_2CHO]_2P(O)F$ (3) (2) (1)		1,2	0	1,3	+0.8
512	2363 (6123)		$C_6F_2H_5OP$						<0.5
502	2364		$C_6F_2H_{10}NP$	$(CH_2$=$CHCH_2)_2NPF_2$			2.5		
502	2365 (6133)		$C_6F_2H_{11}OP$				2.5		

Table A.6.e. (contd.)

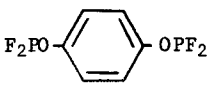
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J	^nJ
507	2366 (6136)		$C_6F_2H_{15}P$	$(CH_3CH_2)_3PF_2$		11		
522	2367 (6137)		$C_6F_2H_{16}NP$	$(CH_3)_2PF_2[N(CH_2CH_3)_2]$ (2) (1)	1,2	12.7		
528	2368 (6138)		$C_6F_2H_{18}N_3P$	$[(CH_3)_2N]_3PF_2$			2.8	
530	2369 (4971, 6144)		$C_6F_3H_{15}NP$	$CH_3CH_2PF_3[N(CH_2CH_3)_2]$		11		
507	2370 (6150)		$C_6F_4H_4ClP$	meta-$ClC_6H_4PF_4$			<0.5	
507	2371 (6151)		$C_6F_4H_4ClP$	para-$ClC_6H_4PF_4$			<0.5	
512	2372 (6153)		$C_6F_4H_4O_2P_2$					<0.5
507	2373 (6158)		$C_6F_4H_5P$	$C_6H_5PF_4$			<0.5	
510 515 525	2374 (4981, 6175)	B-H-M	$C_6F_6H_{18}N_2P_2$	$[CH_3PF(N(CH_3)_2)_2]^+[CH_3PF_5]^-$ (1)	F_a,1 F_e,1	0.0 +8.9		
501 502	2375 (6190)	B	C_7FH_8OP	$CH_3P(O)F(C_6H_5)$		8.34		
501	2376	B	C_7FH_8OPS	$CH_3OP(S)F(C_6H_5)$			1.14	
501 502	2377 (6193)	G	$C_7FH_8O_2P$	$CH_3OP(O)F(C_6H_5)$			0.5	
501 502	2378 (6194)	A	C_7FH_8PS	$CH_3P(S)F(C_6H_5)$		7.0		
502	2379 (6195)		$C_7FH_{10}ClNO_2$	$[C_6H_5NH_3]^+[ClCH_2P(O)FO]^-$		4.2		
502	2380 (6196)		$C_7FH_{11}NO_2P$	$[C_6H_5NH_3]^+[CH_3P(O)FO]^-$		6.0		
531	2381 (6201)	B	$C_7F_2H_7PS_2$	$C_6H_5CH_2SP(S)F_2$			1	
501 507	2382 (4982, 6206)	B	$C_7F_3H_8P$	$CH_3PF_3(C_6H_5)$ (1)	F_e,1 F_a,1	1.8 13.0		

Table A.6.e. (contd.);

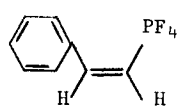
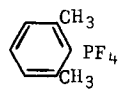
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
507	2383 (6213)		$C_7F_4H_7P$	$C_6H_5CH_2PF_4$	6-7		
507	2384 (6211)		$C_7F_4H_7P$	m$CH_3C_6H_4PF_4$		<0.5	
507	2385 (6212)		$C_7F_4H_7P$	p-$CH_3C_6H_4PF_4$		<0.5	
501 502	2386 (6222)	G	$C_8FH_{11}NOP$	$C_6H_5P(O)F[N(CH_3)_2]$		2.3	
501	2387 (6223)	B	$C_8FH_{11}NP$	$C_6H_5PF[N(CH_3)_2]$		5.5	
502	2388 (6226)		$C_8FH_{18}OP$	$[CH_3(CH_2)_3]_2P(O)F$	7		
526	2389 (6227)		$C_8FH_{18}OP$	$[(CH_3)_3C]_2P(O)F$		<1	
526	2390 (6229)		$C_8FH_{18}P$	$[(CH_3)_3C]_2PF$		2.1	
502	2391 (6230)		$C_8FH_{18}PS$	$[CH_3(CH_2)_3]_2P(S)F$	7		
526	2392 (6231)		$C_8FH_{18}PS$	$[(CH_3)_3C]_2P(S)F$		<1	
532	2393 (6239)	A	$C_8F_2H_{11}P$	$(CH_3)_2PF_2(C_6H_5)$	12.5		
501	2394	B	$C_8F_3H_{11}NP$	$C_6H_5PF_3[N(CH_3)_2]$		2.7	
507	2395		$C_8F_3H_{18}P$	$[CH_3(CH_2)_3]_2PF_3$ (1)	F_a,1 F_e,1	14 ∿2	
526	2396 (4991 6245)	B	$C_8F_3H_{18}P$	$[(CH_3)_3C]_2PF_3$		∿2	
507	2397 (6250)		$C_8F_4H_7P$		6-7		
502 507	2398 (6251)		$C_8F_4H_9P$				1.2
507	2399 (6253)		$C_8F_4H_{15}P$	$C_8H_{15}PF_4$			
				isomer A	6.5		
				isomer B	6.5		

Table A.6.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
507	2400 (6275)		$C_9F_4H_{11}P$	meta-$C_3H_7C_6H_4PF_4$		<0.5	
507	2401 (6276)		$C_9F_4H_{11}P$	para-$C_3H_7C_6H_4PF_4$		<0.5	
515	2402 (6279)		$C_{10}FH_{15}NP$	$C_6H_5PF[N(CH_2CH_3)_2]$		4.4	
501	2403	M	$C_{10}FH_{17}NP^+$	$[C_6H_5PF(N(CH_3)_2)_2]^+$ (1) (2)		3.1	
522	2404 (6303)	M	$C_{11}F_2H_{18}NP$	$C_6H_5PF(CH_3)[N(CH_2CH_3)_2]$	13.0		
507	2405 (6318)		$C_{12}F_2H_{27}P$	$[CH_3(CH_2)_3]_3PF_2$	16		
533	2406 (6335)	H	$C_{12}F_4H_{18}MoO_4P_2$	$[(CH_3)_3CPF_2]_2Mo(CO)_4$		1.2	
522	2407 (6360)	B	$C_{14}F_2H_{16}NP$	$(C_6H_5)_2PF_2[N(CH_3)_2]$ (1) (2)		2.5	
533	2408 (6375)	H	$C_{15}F_6H_{27}MoO_3P_3$	$[(CH_3)_3CPF_2]_3Mo(CO)_3$		0.8	
533	2409 (6440)	H	$C_{20}F_2H_{36}MoO_4P_2$	$[((CH_3)_3C)_2PF]_2Mo(CO)_4$		1.2	
533	2410	H	$C_{27}F_3H_{54}MoO_3P_3$	$[((CH_3)_3C)_2PF]_3Mo(CO)_3$		0.7	

Table A.6.f. M = sulphur (S)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
534	2411		CFH_3OS	CH_3OSF		46.5	
534	2412		CFH_3OS_2	$CH_3OS(S)F$		1.0	
535 182	2413		CFH_3O_2S	$CH_3OS(O)F$		1.3	
534	2414		CFH_3O_2S	$CH_3OS(O)F$		1.2	
536	2415		CFH_3O_2S	$CH_3S(O_2)F$	6.0		
537	2416		CFH_3O_2S	$CH_3S(O_2)F$	5.8		

Table A.6.f. (contd.)

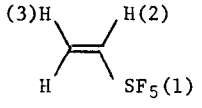
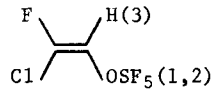
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
538	2417		$CF_2H_3NO_3S_2$	$CH_3S(O_2)N{=}S(O)F_2$			0.3
539	2418 (5034)	B	$CF_2H_4N_2O_3S_2$	$FS(O_2)N{=}S(O)F(NHCH_3)$		3.0	
12	2419		CF_6H_2S	SF_5CH_2F (1) (2)	1_e,2 7.0		
538	2420		$C_2FH_2Cl_4NO_2S$	$(CHCl_2)_2NS(O_2)F$		1.6	
534	2421		C_2FH_5OS	CH_3CH_2OSF		46.5	25.8
534	2422		$C_2FH_5OS_2$	$CH_3CH_2OS(S)F$ (2,3) (1)		1,2 0.8 1,3 1.3	
534	2423		$C_2FH_5O_2S$	$CH_3CH_2OS(O)F$ (2,3) (1)		1,2 1.5 1,3 1.0	
535	2424		$C_2FH_5O_2S$	$CH_3CH_2OS(O)F$ (2,3) (1)		1.3	
539	2425 (5045)		$C_2F_2H_6N_2O_3S_2$	$FSO_2N{=}S(O)FN(CH_3)_2$			3.4
20	2426 [101 2635 4810]	B	$C_2F_4HBrO_2S$	$FS(O_2)CHFCF_2Br$	1.6		
20	2427 [117 2650 4813]	B	$C_2F_5HO_2S$	$FS(O_2)CHFCF_3$	2.6		
541	2428 (5046)		$C_2F_5H_3S$		1,2 6.1	1,3 2.3	
541	2429 (5047)		$C_2F_5H_4Cl$	$ClCH_2CH_2SF_5$	8.0		
187	2430 [1007 5051 4817]		C_2F_6HClOS			1,3 0.4 2,3 1.1	
20	2431 [204 2695 4833]	B	$C_3F_4H_4O_3S$	$FS(O_2)CHFCF_2OCH_3$	1.1		
541	2432 (5073)		$C_3F_5H_6ClS$	$CH_3CHClCH_2SF_5$	8.1		

Table A.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular Structure	Structure		^3J	^4J	^nJ
54	2433	B	$C_3F_8H_4OS$	$SF_5CFHCF_2OCH_3$	$1_e,3$	4.7		
	[250 2769 4837 5074]			(1,2)(3)	$2_a,3$	0.0		
539	2434 (5076)		$C_4F_2H_{10}N_2O_3S_2$	$FS(O_2)N{=}S(O)F[N(CH_2CH_3)_2]$			2.8	
541	2435 (5077)		$C_4F_5H_8ClS$	$Cl(CH_2)_4SF_5$		8.0		

Table A.6.g. M = selenium (Se)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
542	2436 (6550)		CFH_3O_3Se	$FSe(O_2)OCH_3$		1.40	
542	2437		$C_2FH_5O_3Se$	$FSe(O_2)OCH_2CH_3$		1.45	0.82

Table A.6.h. M = silicon (Si)

543	2438 (2580 6676)		CF_2H_5Si	CH_3SiF_2H	6.63
14	2439 (6677)		CF_3HCl_2Si	$CHCl_2SiF_3$	1.2
14	2440 (6678)		CF_3H_2ClSi	CH_2ClSiF_3	2.6
543	2441 (6681)		CF_3H_3Si	CH_3SiF_3	3.17
544	2442 (5402 6680)		CF_3H_3Si	CH_3SiF_3	+4.13
545	2443 (6683)		CF_3H_3Si	CH_3SiF_3	4.0
546	2444 (6684)	P	$CF_6H_3NSi_2$	$(F_3Si)_2NCH_3$	0.4

Table A.6.h. (contd.)

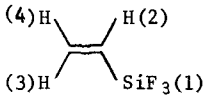
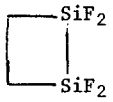
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J	^nJ
547	2445	B	$C_2FH_6ClO_3SiS$	$(CH_3)_2SiF(OSO_2Cl)$		6.6			
547	2446	G	C_2FH_6ClSi	$(CH_3)_2SiFCl$		6.63			
543	2447 (2581, 6685)		C_2FH_7Si	$(CH_3)_2SiFH$		7.63			
543	2448 (2582)		$C_2FH_8OSi_2$	$(CH_3SiFH)_2O$		6.61			
548	2449	Z^2	$C_2F_2H_5ClO_3SSi$	$CH_3SiF(OSO_2F)CH_2Cl$ (2) (1) (3)	1,2 1,3	6.4 3.2			
548	2450	Z^2	$C_2F_2H_5ClSi$	$CH_3SiF_2CH_2Cl$ (2)(1)(3)	1,2 1,3	6.1 3.8			
548	2451	Z^2	$C_2F_2H_6O_3SSi$	$(CH_3)_2SiF(OSO_2F)$		6.6			
547	2452	B	$C_2F_2H_6O_3SSi$	$(CH_3)_2SiF(OSO_2F)$		6.76			
543	2453 (6687)		$C_2F_2H_6Si$	$(CH_3)_2SiF_2$		6.13			
545	2454 (6686)	B	$C_2F_2H_6Si$	$(CH_3)_2SiF_2$		6.0			
548	2455	Z^2	$C_2F_2H_6Si$	$(CH_3)_2SiF_2$		6.7			
547	2456	G	$C_2F_2H_6Si$	$(CH_3)_2SiF_2$		6.50			
14	2457	B	$C_2F_3H_3Si$		1,2	2.5	1,3 1,4	1.1 2.6	
546	2458 (6692)	P	$C_2F_3H_6NSi$	$SiF_3N(CH_3)_2$				1.1	
549	2459 (6694)		$C_2F_4H_4Si_2$			4.4			
14	2460 (122, 2669, 4853)		$C_2F_6H_2Si$	$CH_2FCF_2SiF_3$				1.4	
14	2461 (122a, 4854, 6696, 2672)		C_2F_7HSi	$CHF_2CF_2SiF_3$				2.5	
548	2462	Z	C_3FH_8ClSi	$(CH_3)_2SiFCH_2Cl$ (2) (1)(3)	1,2 1,3	8.0 3.1			

Table A.6.h. (contd.)

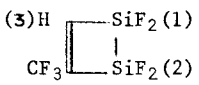
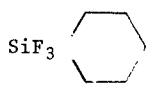
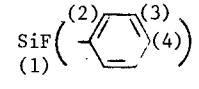
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
550	2463 (6697)		C_3FH_9Si	$(CH_3)_3SiF$		+7.51				
547	2464	G	C_3FH_9Si	$(CH_3)_3SiF$		7.48				
543	2465 (6698)		C_3FH_9Si	$(CH_3)_3SiF$		7.15				
545	2466 (6699)	B	C_3FH_9Si	$(CH_3)_3SiF$		7.0				
548	2467	Z[2]	C_3FH_9Si	$(CH_3)_3SiF$		7.4				
546	2468 (6704)	P	$C_3F_6H_9N_3Si_3$	$(F_2SiNCH_3)_3$				<0.3		
203	2469 (785 4855)		$C_3F_7HSi_2$		1,3	16.5	2,3	1.6		
94	2470	B	$C_4FH_{11}Si$	$CH_3CH_2SiF(CH_3)_2$ (1)(2)	1,2	7.2				
546	2471 (6707)	P	$C_4F_2H_{12}N_2Si$	$SiF_2[N(CH_3)_2]_2$				1.1		
545	2472 (6710)	B	$C_4F_3H_9Si$	$CH_3(CH_2)_3SiF_3$		2.8				
546	2473 (6711)	P	$C_4F_3H_{10}NSi$	$SiF_3N(CH_2CH_3)_2$				1.1		
546	2474 (6715)	P	$C_5F_3H_{10}NSi$					<1		
551	2475	B	$C_6F_3H_{18}NSi_3$	$SiF_3N[Si(CH_3)_3]_2$						0.75
552	2476	G	$C_9FH_{24}AlSi$	$(CH_3)_3SiF.Al(CH_2CH_3)_3$		9.4				
553	2477	G	$C_{10}F_2H_{24}Si_2$	$(CH_3)_2SiFC(CH_3)_2SiF(CH_3)C(CH_3)_3$ (3) (1) (2) (4)	1,3	7.5				
					2,4	7.5				
545	2478 (6722)	J	$C_{13}F_4H_{31}NSi$	$[(CH_3CH_2CH_2)_4N][SiF_4CH_3]$		4.8				
545	2479 (6723)	J	$C_{16}F_4H_{37}NSi$	$[(CH_3CH_2CH_2)_4N][SiF_4(CH_2)_3CH_3]$		3.5				
545	2480 (6724)	J	$C_{17}F_4H_{39}NSi$	$[(CH_3(CH_2)_3)_4N][SiF_4CH_3]$		4.8				
554	2481	R*	$C_{18}FH_{15}Si$				1,2	-0.07	1,3 1,4	0.52 -0.22

Table A.6.i. M = tin (Sn)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
555	2482 (6845)		$C_{30}FH_{39}Sn$	$SnF[CH_2C(CH_3)_2C_6H_5]_3$	5.0		

Table A.6.j. M = tellurium (Te)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
556	2483 (5198)	B	$C_2F_5H_6NTe$	$TeF_5N(CH_3)_2$		3.5	
556	2484 (5199)	B	$C_4F_4H_{12}N_2Te$	$TeF_4[N(CH_3)_2]_2$		2.3	
557	2485	B	$C_4F_5H_{10}NTe$	$TeF_5N(CH_2CH_3)_2$ (1) (2)		F_e,1 +3.5 F_a,1 <0.5	F_e,2 0.3
556	(5201 6847)						
556	2486 (5202)	B	$C_4F_5H_{12}NSiTe$	$TeF_5N(CH_3)Si(CH_3)_3$		2.5	

Table A.6.k. M = tungsten (W)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
535	2487	A^3	CF_5H_3OW	WF_5OCH_3		1	
558 182	(6859 5268)						
182'	2488	B	$C_2F_4H_6O_2W$	cis $WF_4(OCH_3)_2$		1	
558	(5269 6860)						
558	2489 (6864)	A^3	$C_3F_3H_9O_3W$	cis $WF_3(OCH_3)_3$		1	
558	2490 (5270 6863)	A^3	$C_3F_3H_9O_3W$	trans $WF_3(OCH_3)_3$		1	

A.7. Fluorine bonded to carbon, hydrogen bonded to element, M, other than carbon.

Table A.7.a. M = nitrogen (N)

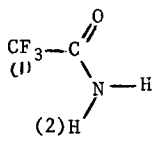
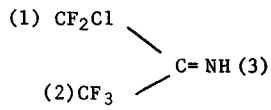
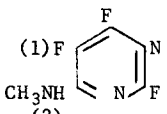
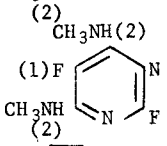
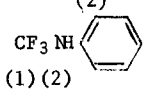
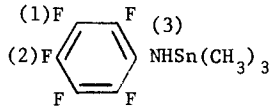
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
559	2491		CF_4HNO_2S	CF_3NHSO_2F	3		
72	2492	U[2]	$C_2F_3H_2NO$	 (−45°C)	1,2	1.8	
72	2493 (184)	E	$C_3F_3H_4NO$	$CF_3C(O)NHCH_3$ (1) (2)		1.1	
85	2494 (2702)		C_3F_5HClN				
				Isomer A	1,3	1.8	
				Isomer B	1,3	2	
					1,2	2.3	
560	2495 (2716)		$C_3F_5H_4NSe$	$CF_3CF_2SeNHCH_3$ (1) (2)	1,2	1.0	
85	2496 (2731)		C_3F_6HN	$(CF_3)_2C{=}NH$ (1,2) (3)	1,3	2.5	
228	2497 (4621)	E	$C_5F_3H_4N_3$		1,2	1.7	
228	2498 (4632)	E	$C_6F_2H_8N_4$		1,2	1.7	
561	2499		$C_7F_3H_6N$		1,2	5.4	
445	2500 (2142)	H	$C_9F_5H_{10}NSn$				1,3 1.0 2,3 0.9

Table A.7.a. (contd.)

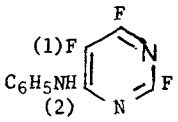
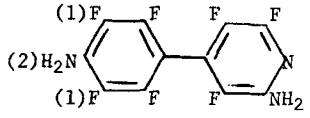
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
228	2501 (4645)	E	$C_{10}F_3H_6N_3$		1,2	2.8	
897	2502 (4660)	E	$C_{11}F_7H_4N_3$		1,2	1.4	

Table A.7.b. M = oxygen (O)

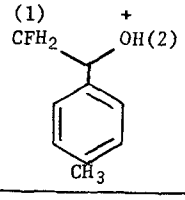
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
221	2503	C[2]	$C_9FH_{10}O^+$		1,2	7	

Table A.7.c. M = phosphorus (P)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
36	2504 (5784)	B	CF_3H_2P	CF_3PH_2	12.2		
562	2505 [2552 4938 4759 5805]	M	CF_7HKP	trans $K^+[CF_3PF_4H]^-$	~0		
				cis $K^+[CF_3PF_4H]^-$	8.2		
563	2506	A	C_2F_6HP	$(CF_3)_2PH$	9.8		
	(5884)	B			9.9		
		E			10.3		
		G			9.7		
		H			9.9		
		M			10.1		

Table A.7.c. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
		P			9.7		
		R			10.0		
		S^2			9.7		
36	2507 (5883)	B	C_2F_6HP	$(CF_3)_2PH$	9.8		
100	2508		C_2F_6HP	$(CF_3)_2PH$	9.7		
562 564	2509 [2556 4950 5899 4767]	M	C_2F_9HKP	K^+ [F, F, H, F, P, CF_3, CF_3]$^-$	9.5		
565	2510		$C_5F_4H_6ClP$	$CH_3CH_2PHCF_2$, $C{=}CF_2$, Cl	~18		
565	2511		$C_9F_4H_6ClP$	$C_6H_5PHCF_2$, $C{=}CF_2$, Cl	~17		

Table A.7.d. M = sulphur (S)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
45	2512	G	$C_3F_4H_2Cl_2OS$	$(CF_2Cl)_2C(OH)SH$		1	
45	2513	G	$C_3F_6H_2OS$	$(CF_3)_2C(OH)SH$		1	

Table A.7.e. M = silicon (Si)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
566	2514		CF_3H_3SeSi	CF_3SeSiH_3		1.6	
50	2515 (112 2642)		$C_2F_4H_4Si$	$CF_2HCF_2SiH_3$	10.5	3.2	

Table A.7.d. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^5J
566	2516		$C_3F_7H_3SeSi$	$CF_3CF_2CF_2SeSiH_3$		3.0	1.5
50	2517 (359)		$C_5F_4H_{13}NSi$	$CF_2HCF_2SiH_3.N(CH_3)_3$	11.1	3.0	

A.8. Fluorine bonded to element, M, other than carbon, hydrogen bonded to element other than carbon.

Table A.8.a. M = boron (B)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J
567	2518 (5306)		F_2HB	HBF_2	108	
568	2519		F_3H_2BO	BF_3H_2O		2.9

Table A.8.b. Coupling in hydrogen fluoride

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J
1144	2520		HF	HF	615

Table A.8.c. M = nitrogen (N)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
482	2521		$C_3FH_6NO_2$	$NFHCO_2CH_2CH_3$	51		
569	2522 (4716)		$C_4F_7HN_2$	$(CF_3)_2C(CN)NFH$	45.6		
482	2523 (2245)		$C_5FH_{11}N_2O$	$CH_3CH_2NFC(O)NHCH_2CH_3$		5.4	
569	2524 (4724)		$C_5F_4H_6N_2O$	$(CF_3C(CN)(OCH_2CH_3)NFH$	49.3		
569	2525 (4225)		$C_5F_7H_6NO$	$(CF_3)_2C(OCH_2CH_3)NFH$	50.7		

Table A.8.d. M = phosphorus (P)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
570	2526 (5621)		FH_2O_2P	H_2PO_2F	114		
570	2527		F_2HOP	$HPOF_2$	116		
571	2528 (5650)		F_2HOP	$HPOF_2$	116		
544	2529 (5657)		F_2HP	HPF_2	41.7		
572	2530 (5656)		F_2HP	HPF_2	41.7		
571 573	2531 (5658)		F_2HPS	$HPSF_2$	99.0		
574	2532 (5662)		$F_2H_2P_2$	H_2PPF_2		22	
519	2533 (5664)		$F_2H_8B_3P$	$HPF_2.B_3H_7$	56		
520	2354 (5665)	B	$F_2H_9B_4P$	$HPF_2.B_4H_8$	60		
575	2535 (4925 5689)		$F_3H_4N_2P$	$PF_3(NH_2)_2$ (1) (2)		$1a,2$ 20 $1_e,2$ 1.7	
576	2536		F_4HP	HPF_4	92		
519	2537 (5709)		$F_4H_6B_2P_2$	$(HPF_2)_2B_2H_4$	50.3		
562 577 578	2538 (5719)	M	F_5HKP	$K^+[HPF_5]^-$ (2)(1)	$1_a,2$ 0 $1_e,2$ 127		
579	2539	W	$F_9HFeNOP_3$	$HFe(NO)(PF_3)_3$			10.4
580	2540	E	$F_{12}HCoP_4$	$HCo(PF_3)_4$			9.75
580	2541	E	$F_{12}HIrP_4$	$HIr(PF_3)_4$			14.75
581	2542		$F_{12}HIrP_4$	$HIr(PF_3)_4$			14.93
580	2543	E	$F_{12}HOsP_4^-$	$HOs(PF_3)_4^-$			15.0
580	2544	E	$F_{12}HP_4Rh$	$HRh(PF_3)_4$			16.5
580	2545	E	$F_{12}HP_4Ru^-$	$HRu(PF_3)_4^-$			16.5
582	2546 (5742)		CFH_4O_2P	$HFPO_2CH_3$	115		
84	2547 (2287 5773)		CF_2H_4NOP	$PF_2(O)NH(CH_3)$ (1) (2)		1,2 1.5	

Table A.8.d. (contd.)

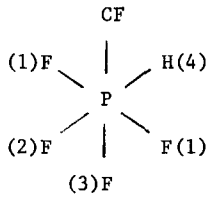
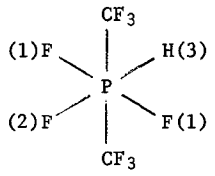
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
84	2548	P	CF_2H_4NP	$PF_2NH(CH_3)$		1,2 10.35	
	(2288)			(1)(2)		11.0	
	(5755)	HH					
84	2549		CF_2H_4NPS	$PF_2(S)NH(CH_3)$		1,2 5.2	
	(2290)			(1) (2)			
	(5770)						
506	2550		CF_3H_4P	HPF_3CH_3	1_a,2 115		
	[2291]			(2)(1)	1_e,2 26		
	[4933]						
	[5791]						
523	2551	A	$CF_5H_5P_2$	$(CH_3)H_2PPF_5$		1_e,2 7.7	
	(5803)			(2) (1)			
	(4937)			(−75°C)			
562	2552		CF_7HKP	trans $K^+[CF_3PF_4H]^-$	1_e,2 123		
583	[2505]			(1)(2)			
	[4938]						
	[5805]			cis $K^+[CF_3PF_4H]^-$	1,4 96		
	[4759]				3,4 125		
					2,4 ∿0		
							
582	2553		$C_2FH_9NO_2P$	$(CH_3)_2NH_2^+HFPO_2^-$	125		
	(5822)						
506	2554	B	$C_2F_3H_6P$	$CH_3CH_2PF_3H$	1_a,2 118.5		
				(1)(2)	1_e,2 28.7		
523	2555		$C_2F_5H_7P_2$	$(CH_3)_2HPPF_5$		1_e,2 6.5	
	[2322]			(2)(1)			
	[4948]						
	[5867]						
562	2556		C_2F_9HKP	$K^+[(CF_3)_2PF_3H]^-$	1,3 69.5		
564	[2509]				2,3 18.0		
	[4950]						
	[5899]						
	[4767]						

Table A.8.d. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
590	2557 (5910)		$C_3FH_{10}ClNPSSi$	$(CH_3)_3SiNHP(S)FCl$		2.5	
671	2558 (5909)		$C_3FH_{10}ClNPSSi$	$(CH_3)_3SiNHP(S)FCl$		2	
582	2559 (5911)		$C_3FH_{11}NO_2P$	$(CH_3)_3NH^+HFPO_2^-$	129		
590	2560 (5924)		$C_3F_2H_{10}NPSSi$	$(CH_3)_3SiNHP(S)F_2$		4	
773 517	2561 (6131)	T^2	$C_6F_2H_7N_2PS$	$C_6H_5NHNHP(S)F_2$		4.3	
530	2562 (6142 4970)		$C_6F_3H_6P$	$C_6H_5PF_3H$ (1)(2)	^1J_a,2 124 ^1J_e,2 31.5		
584	2562 (4948 6207)		$C_7F_3H_8P$	para $CH_3C_6H_4PF_3H$ (1)(2)	^1J_a,2 118 ^1J_e,2 34		

Table A.8.e. M = sulphur (S)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
539	2564 (5012)	B	$F_2H_2N_2O_3S_2$	$FSO_2N{=}S(O)FNH_2$		4.8	
559	2565 (4795)		CF_4HNO_2S	FSO_2NHCF_3		4	

Table A.8.f. M = silicon (Si)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
585	2566		FH_4ClSi_2	$SiH_3SiFHCl$	51.5	5.8	
586	2567		FH_5Si_2	SiH_3SiFH_2	43.2	6.6	
587	2568		FH_7Si_3	$SiH_3SiH_2SiFH_2$	45.2		
588	2569		F_2H_2SSi	SiF_2HSH	75.2	5.6	

Table A.8.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	2	3	n_J
589	2570		F_2H_4GeSi	SiF_2HGeH_3	54.5	8.0	
585 586	2571		$F_2H_4Si_2$	SiH_3SiF_2H	53	6.0	
585	2572 (5099)		$F_2H_4Si_2$	$SiFH_2SiFH_2$	45.0	7.0	
587	2573		$F_2H_6Si_3$	$SiH_3SiH_2SiF_2H$	53.2	6.2	
544	2574 (6662)		F_3HSi	SiF_3H	96.2		
585 586	2575 (6663)		$F_3H_3Si_2$	SiH_3SiF_3		6.0	
587	2576		$F_3H_5Si_3$	$SiH_3SiH_2SiF_3$		4.9	0.9
588	2577 (5100)		$F_4H_2SSi_2$	SiF_2HSiF_2SH	54.9		
585	2578 (5101)		$F_4H_2Si_2$	SiF_2HSiF_2H	52.0	9.0	
588	2579 (5102)		F_5HSi_2	SiF_2HSiF_3	53.2	12.7	
543	2580 (2438 6676)		CF_2H_4Si	CH_3SiF_2H	67.5		
543	2581 (2447 6685)		C_2FH_7Si	$(CH_3)_2SiFH$	52.1		
543	2582 (2448)		$C_2F_2H_8OSi_2$	$(CH_3SiFH)_2O$	68.2		

B. Fluorine-fluorine coupling.

1. One fluorine bonded to carbon in acyclic system, the other fluorine bonded to carbon in either acyclic or cyclic system.

Table B.1.a. Both fluorines bonded to sp^3 carbon.

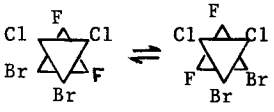
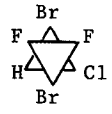
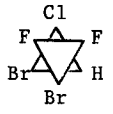
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
920	2583 (4687)	B	CF_3Cl_2N	$CF_2ClNFCl$	128		
800	2584 (-80°C)	Q	$C_2F_2Br_2Cl_2$		154.1		
801	2585	Q	$C_2F_2Br_2Cl_2$	as above	153.9		
801	2586 (41)	Q	$C_2F_2Br_2Cl$	$CF_2BrCHBrCl$	154.		
183	2587 (42)		$C_2F_2HBr_2Cl$		160.8		
					159.0		
31	2588 (43)		$C_2F_2HCl_3$	$CFHClCFCl_2$		24	
20	2589 (46, 47)	B	$C_2F_2H_2Br_2$	CFHBrCFHBr (rac.)		37.8	
				(meso)		24.8	
20	2590 (54)		$C_2F_2H_2Cl_2$	CF_2ClCH_2Cl	170		
34	2591 (50)		$C_2F_2H_2Cl_2$	$CFCl_2CFH_2$		22.4	
34	2592 (51, 52)		$C_2F_2H_2Cl_2$	CFHClCFHCl (dl)		26.5	
				(meso)		20.6	
34	2593 (56)		$C_2F_2H_3Br$	CFH_2CFHBr		22.1	

Table B.1.a. (contd.)

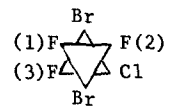
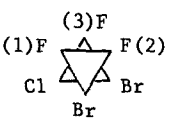
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
38	2594 (64)		$C_2F_2H_4$			-30	
						-10.9	
		W*	(2% v/v)	CFH_2CFH_2		-12.26	
		W*	(5% v/v)	(averaged coupling)		-11.97	
		W*	(10% v/v)			-11.50	
		T*	(2% v/v)			-12.14	
		T*	(10% v/v)			-11.57	
		D*	(2% v/v)			-11.95	
		D*	(10% v/v)			-11.56	
		G*	(10% v/v)			-11.53	
		X*	(10% v/v)			-11.20	
		Y*	(10% v/v)			-11.21	
		R*	(10% v/v)			-11.02	
		A*	(10% v/v)			-11.32	
		J*	(10% v/v)			-10.96	
		Z*	(10% v/v)			-11.03	
		E*	(10% v/v)			-10.56	
		B*	(10% v/v)			-10.70	
		M*	(10% v/v)			-10.53	
26	2595		$C_2F_3Br_2Cl$	$CF_2BrCFClBr$	168	15.0	
						14.0	
843	2596		$C_2F_3Br_2Cl$	$CF_2BrCFClBr$	159	13	
						14	
841	2597		$C_2F_3Br_2Cl$			1,3 12 2,3 14	
						1,3 21 2,3 21	

Table B.1.a. (contd.)

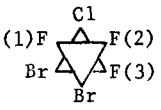
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
						1,2 17 2,3 18	
842	2598	Q	$C_2F_3Br_2Cl$	(1,2)(3) $CF_2BrCFBrCl$ (Average coupling)	165.0	1,2 + 2,3 28.4	
		B			166.6	27.6	
		R			169.3	27.6	
		Z^3			169.7	27.8	
		J^2			169.8	27.7	
		D^2			170.7	28.1	
		A^4			170.7	27.9	
		E^2			170.9	27.6	
		M			171.2	27.8	
		E	(10% v/v)		171.5	27.8	
		E	(20% v/v)		171.1	27.8	
		E	(30% v/v)		170.7	27.8	
		E	(40% v/v)		170.2	27.8	
		E	(50% v/v)		169.7	27.8	
		E	(60% v/v)		169.0	27.8	
		E	(70%)		168.5	27.8	
		E	(80% v/v)		167.8	27.8	
		E	(90% v/v)		167.3	27.8	
		E	(100% v/v)		166.6	27.6	
		B^4	(-123°C)	Rotamer I (lower energy)	169.2	-26.3	
				Rotamer II	169.2	-13.3	
		C^4	(-123°C)	I	170.6	-26.6	
				II	170.6	-13.6	
		P	(-123°C)	I	170.0	-26.6	
				II	170.0	-14.0	
		D^4	(123°C)	I	170.2	-25.5	
				II	170.2	-13.3	
843	2599		$C_2F_3Br_2Cl$	$CF_2BrCFBrCl$	150	13 14	

Table B.1.a. (contd.)

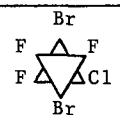
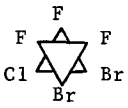
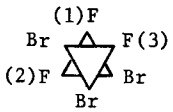
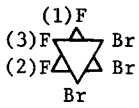
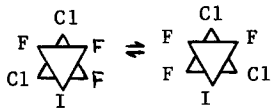
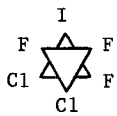
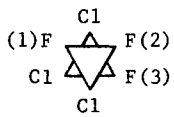
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
844	2600	P	$C_2F_3Br_2Cl$ (50% v/v @ -125°C)		169.5	14.7 11.9	
						20.8 19.5	
183	2601		$C_2F_3Br_3$ (-123°C)		1,2 168.1	1,3 -16.1 2,3 -18.4	
						-21.5	
849	2602		$C_2F_3Br_3$	$CF_2BrCFBr_2$		19	
20	2603		$C_2F_3Cl_2I$	CF_2ICFCl_2		14.2	
844	2604		$C_2F_3Cl_2I$ (-120°C)		190	14.0 14.2	
844	2605		$C_2F_3Cl_2I$		145	12.9 12.7	
20	2606		$C_2F_3Cl_2I$	$CF_2ClCFICl$ (Average coupling)	165	15.5 15.2	
850	2607		$C_2F_3Cl_3$		1,3	1.3 ∓40.4 ±21.2	
847	2608		$C_2F_3Cl_3$	$CF_2ClCFCl_2$		9.5	
20	2609		$C_2F_3Cl_3O_2S$	$CF_2ClCFClSO_2Cl$	170	8.1 13.5	
186	2610		$C_2F_3Cl_3O_2S$	$CF_2ClCFClSO_2Cl$		8.1 13.5	
20 186	2611		$C_2F_3Cl_3S$	$CF_2ClCFClSCl$	170	8.6 16.6	
20	2612		$C_2F_3Cl_3S$	$CFCl_2CF_2SCl$		12.2	

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
845	2613		C_2F_3HBrCl	$CF_2BrCFHCl$	177	18	
846	(71)					18	
32							
42							
847	2614		C_2F_3HBrCl	$CF_2ClCFHBr$	173	20	
33	(70)					19	
847	2615		$C_2F_3HBr_2$	$CF_2BrCFHBr$	174	24	
33	(72)					21	
20	2616		$C_2F_3HCl_2$	$CF_2ClCFHCl$	174	15.4	
	(74)					15.4	
185	2617		$C_2F_3HCl_2$	$CF_2ClCFHCl$	175	15.5	
	(73)					15.4	
185	2618		$C_2F_3HCl_4Si$	CF_2SiCl_3CFHCl	343	15.7	
	(76)					16.3	
848	2619		$C_2F_3HCl_4Si$	CF_2SiCl_3CFHCl	343	16.8	
	(75)					16.8	
14	2620		$C_2F_3HCl_4Si$	CF_2SiCl_3CFHCl	305	14.5	
	(77)					15.5	
20	2621		$C_2F_3H_2Br$	CF_2BrCFH_2		22.8	
	(78)						
20	2622		$C_2F_3H_2Cl$	CF_2ClCFH_2		20.7	
	(81)						
36	2623	B	$C_2F_3H_2Cl_2P$	$CFH_2CF_2PCl_2$		18.4	
	(851, 5849)						
36	2624	B	$C_2F_3H_2Cl_2P$	$CF_2HCFHPCl_2$		16.6	
	(86, 5850)						
14	2625		$C_2F_3H_2Cl_3Si$	$CFHSiCl_3CF_2H$	305*	17.0	
	(88)					21.2	
14	2626		$C_2F_3H_2Cl_3Si$	$CF_2SiCl_3CFH_2$		18.8	
	(87)						
20	2627		$C_2F_3H_2I$	CF_2ICH_2F		24.6	
	(89)						

Table B.1.a. (contd.)

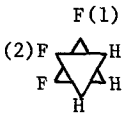
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
38	2628 (91)		$C_2F_3H_3$			1,2 -5.2	
						1,2 -13.7	
		W*	(10% v/v)	CF_2HCH_2F		18.16	
		T*	(10% v/v)	(averaged coupling)		18.32	
		G*	(10% v/v)			18.25	
		Q*	(10% v/v)			18.20	
		Y*	(10% v/v)			17.44	
		X*	(10% v/v)			17.44	
		R*	(10% v/v)			18.58	
		A*	(10% v/v)			17.39	
		J*	(10% v/v)			17.12	
		Z*	(10% v/v)			16.94	
		E*	(10% v/v)			16.00	
		M*	(10% v/v)			15.38	
		F*	(10% v/v)			15.10	
		B*	(10% v/v)			16.49	
20	2629 (90)	B	$C_2F_3H_3$	CF_2HCH_2F (averaged coupling)			16.2
185	2630 (94)		$C_2F_3H_3ClP$	CF_2PH_2CFHCl	289		14.3 15.0
20	2631 (4807)		$C_2F_4Br_2O_2S$	$CF_2BrCFBrSO_2F$ (1,2)(3)	176	1,3 15.7 2,3 15.8	
841	2632	-65°C	$C_2F_4Cl_2$	CF_3CFCl_2			6.1
857		+90°C					5.6
842	2633		$C_2F_4Cl_2$	CF_3CFCl_2			
		B	(20°C)				5.7
			(-60°C)				6.0
		E[4]	(20°C)				5.8
		P	(20°C)				5.8
			(-60°C)				6.2
		B[4]	(20°C)				5.8
			(-60°C)				6.2

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
		F^4	(20°C)					5.9	
			(-60°C)					6.2	
		G^4	(20°C)					5.9	
			(-60°C)					6.2	
		E^2	(20°C)					5.9	
			(-60°C)					6.2	
		E	(20°C)					5.9	
			(-60°C)					6.2	
20	2634		$C_2F_4Cl_2O_2S$	$CF_2ClCFClSO_2F$		168	1,3	8.1	
186	(4808)			(1,2) (3)			2,3	12.2	
20	2635		$C_2F_4HBrO_2S$	$CF_2BrCHFSO_2F$	1,2	188	1,3	22.3	
186	(101, 2426)			(1,2) (3)			2,3	10.7	
36	2636	B	$C_2F_4HCl_2P$	$CF_2HCF_2PCl_2$				5.4	
	(102, 5857)								
14	2637		$C_2F_4HCl_3Si$	$CF_2HCF_2SiCl_3$				3.5	
	(103)								
38	2638	W	$C_2F_4H_2$	CF_3CH_2F				16.10	
	(107)	D						16.08	
		G						16.05	
		Q						16.00	
		X						16.02	
		Y						15.87	
		B						15.49	
		R						15.69	
		A						15.72	
		Z						15.85	
		E						15.14	
		M						15.23	
						^3J			
851	2639	T*	$C_2F_4H_2$	CF_2HCF_2H		-4.95		-1.75	
		D*				-4.99		-1.95	
		G*				-5.02		-2.0	
		H*				-5.11		-3.66	
		Q*				-5.26		-2.77	
		A*				-4.96		-2.80	
		B*				-4.46		-2.88	
		U*				-4.88		-4.02	

Table B.1.a. (contd.)

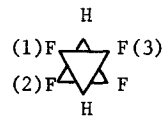
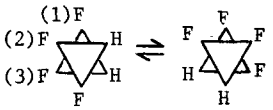
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
						$\leftarrow {}^3J \rightarrow$		
		V*				-4.46	-5.74	
		E*				-4.38	-5.89	
		L*				-4.59	-7.28	
38	2640 (105)				1,2	-5.4		
					2,3	-0.6		
					1,2	-9.2		
					2,3	-8.8		
25 852	2641		$C_2F_4H_2$	CF_3CFH_2			15.5	
50	2642 (2515, 112)		$C_2F_4H_4Si$	$CF_2HCF_2SiH_3$			1.6	
51	2643 (113, 6632)		$C_2F_4H_{15}N_4O_5SRh$	$[Rh(CF_2HCF_2)(NH_3)_4(H_2O)]^{2+}(SO_4)^{2-}$			5.2	
51	2644 (114, 6633)		$C_2F_4H_{16}N_5O_4SRh$	$[Rh(CF_2HCF_2)(NH_3)_5]^{2+}(SO_4)^{2-}$			1.2	
560	2645		C_2F_5BrSe	CF_3CF_2SeBr			3.4	
560	2646		C_2F_5ClSe	CF_3CF_2SeCl			3.5	
862	2647		C_2F_5I	CF_3CF_2I			4.6	
863	2648 (4746)		$C_2F_5NO_3$	$CF_2NO_2CF_2OF$ (1) (2)			1.5	
25	2649 (115)		C_2F_5H	CF_3CF_2H			2.8	
20 186	2650 [117, 4813, 2427]		$C_2F_5HO_2S$	CF_3CFHSO_2F (1)(2)		1,2	11.5	
40	2651 (118)		$C_2F_5HO_3S$	$CF_3SO_3CF_2H$				3.2

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
623	2652	B (-80^oC)	C_2F_6	CF_3CF_3		3.50	
864	2653		C_2F_6AsCl	$(CF_3)_2AsCl$		7.85	
865	2654 (4814)		C_2F_6ClNOS	$CF_2ClCF_2NS(O)F_2$ (1) (2)		3.7	
864	2655		C_2F_6ClP	$(CF_3)_2PCl$			8.93
864	2656		C_2F_6Hg	$(CF_3)_2Hg$			5.3
864	2657		$C_2F_6HgS_2$	$(CF_3S)_2Hg$			<0.2
864	2658		$C_2F_6HgSe_2$	$(CF_3Se)_2Hg$			<0.2
864	2659		$C_2F_6N_2O_2$	$(CF_3)_2NNO_2$			10.8
863	2660 (4747)		C_2F_6O	CF_3CF_2OF (1)(2)	1,2	1.67	
35	2661		C_2F_6O	$(CF_3)_2O$			8.0
867	2662		C_2F_6OS	CF_3S-OCF_3			3.4
868	2663 (4748)		$C_2F_6O_2$	$CF_3CF(OF)_2$ (1)(2)	1,2	<1	
869	2664 (4749)		$C_2F_6O_3$	CF_3OOCF_2OF (1) (2)			1,2 3.4
864	2665		C_2F_6S	$(CF_3)_2S$			9.68
864	2666		$C_2F_6S_2$	$(CF_3S)_2$			4.47
864	2667		C_2F_6Se	$(CF_3)_2Se$			8.48
864	2668		$C_2F_6Se_2$	$(CF_3Se)_2$			3.08
14	2669 [122, 2460, 4853]		$C_2F_6H_2Si$	$CFH_2CF_2SiF_3$		18.5	
734	2670 (4763, 5893)		C_2F_7P	$(CF_3)_2PF$			3.46
76	2671 (5894)		C_2F_7PS	$(CF_3)_2PSF$			1.6
14	2672 [122a, 2461, 4554, 6696]	B	C_2F_7HSi	$CF_2HCF_2SiF_3$		3.5^+	

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
54	2673 (4819 5057)		C_2F_8BrClS	$CF_2ClCFBrSF_5$ (1,2)(3)		1,3 13 2,3 13	
54	2674 (4818 5058)		C_2F_8BrClS	$CF_2BrCFClSF_5$ (1,2)(3)		1,2 11 2,3 11	
54	2675 (4820 5059)		$C_2F_8Br_2S$	$CF_2BrCFBrSF_5$ (1,2) (3)		1,3 13 2,3 13	
54	2676 (4821 5060)		$C_2F_8Cl_2S$	$CF_2ClCFClSF_5$ (1,2) (3)		1,3 11 2,3 11	
54	2677 (4822 5061)		$C_2F_8Cl_2S$	$CFCl_2CF_2SF_5$ (1) (2)		1,2 8.2	
54	2678 [123 4825 5064]		C_2F_8HBrS	$CF_2BrCFHSF_5$ (1,2) (3)	1,2 183.9	1,3 22.3 2,3 16.6	
187	2679 [124 4826 5065]		C_2F_8HClOS	$CF_2ClCFHOSF_5$ (1) (2)		1,2 9.0	
54	2680 (126 4827)		C_2F_8HClS	$CF_2ClCFHSF_5$ (1,2) (3)	1,2 184.6	1,3 15.2 2,3 14.9	
54	2681 (125 4828)		C_2F_8HClS	$CFHClCF_2SF_5$ (1) (2,3)	2,3 221.0	1,2 15.0 1,3 14.6	
507	2682 (5898)		C_2F_9P	$(CF_3)_2PF_3$			16
870	2683 (4830 5070)		$C_2F_{10}S$	$CF_2CF_2SF_5$ (1)(2)		1,2 <1	
874	2684		$C_3F_3Cl_5$	$CF_2CCl_3CFCl_2$ (1) (2)		1,2 4.9	
20	2685 [159 983 3645]		$C_3F_3HBr_2O$	$CF_2BrCHBrCOF$ (1,2)	1,2 165		

Table B.1.a. (contd.)

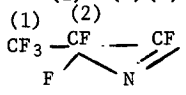
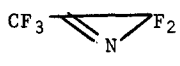
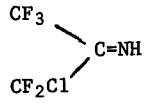
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
185	2686 (177)		$C_3F_3H_4ClO$	CF_2OCH_3CFHCl (1,2) (3)	1,2 142	1,3 12.0 2,3 11.2	
185	2687 (178)		$C_3F_3H_4ClS$	CF_2SCH_3CFHCl (1,2) (3)	1,2 222	1,3 18.8 2,3 18.1	
188	2688 (187)		$C_3F_3H_5$	$CF_2HCH_2CH_2F$ (1) (2)			1,2 1.2
20	2689 (189)		$C_3F_3H_5O$	$CF_2(OCH_3)CH_2F$ (1) (2)		1,2 15.9	
20	2690 (192)		$C_3F_3H_5S$	$CF_2SCH_3CH_2F$ (1) (2)		1,2 22.4	
874	2691		$C_3F_4Cl_4$	$CFCl_2CF_2CFCl_2$ (1) (2)		1,2 6.1	
74	2692 (197)		C_3F_4HClO	$CF_2HC(O)CF_2Cl$		7	
85	2693		$C_3F_4HCl_2N$	$(CF_2Cl)_2C{=}NH$			7
188	2694 (200)		$C_3F_4H_4$	$CF_3CH_2CH_2F$			6.2
186 20	2695 (204, 4833)		$C_3F_4H_4O_3S$	$CF_2(OCH_3)CFHSO_2F$ (1,2) (3)	1,2 147	1,3 11.5 2,3 13.4	
874	2696		$C_3F_5Cl_3$	$CF_2ClCF_2CFCl_2$ (1) (2) (3)		1,2 <1 2,3 7.2	1,3 13.6
904	2697 (3227, 4019)		C_3F_5N			1,2 5.9	
904	2698		C_3F_5N				0.9
77	2699 (207)		$C_3F_5HBr_2$	$CF_3CHBrCF_2Br$			11.0
184	2700 (208)		C_3F_5HClI	$CF_3CHClCF_2I$ (1) (2,3)			1,2 11.6 1,3 11.0
184	2701		C_3F_5HClI	CF_3CF_2CHClI (1,2)	1,2 265		
189	2702 (2494)		C_3F_5HClN	 (Both isomers)			7

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
184	2703 (209)		$C_3F_5HCl_2$	$CF_3CF_2CHCl_2$		0.4	
884	2704		$C_3F_5HO_2$	CF_3CF_2COOH		1.38	
804	2705		$C_3F_5HO_2$ (-29°C)	CF_3CF_2COOH		1.7	
841			(+85°C)			1.3	
73	2706 (212)		$C_3F_5H_2Br$	$CF_2BrCF_2CH_2F$ (1) (2) (3)		1,2 3.9 2,3 15.5	1,3 7.7
73	2707 (211)		$C_3F_5H_2Br$	CF_2HCF_2CHFBr (1) (2) (3)		2,3 16.7	
73	2708 (216)		$C_3F_5H_2Cl$	$CF_2ClCF_2CH_2F$ (1) (2) (3)		1,2 2.8 2,3 15.1	1,3 7.7
947	2709	B	$C_3F_5H_2ClOS$	(1) CF_3, SH, CF_2Cl, OH; C; (2,3)	2,3 168	1,2 10.1 1,3 12.5	
73	2710 (217)		$C_3F_5H_3$	$CF_2HCF_2CH_2F$ (1) (2) (3)		2,3 13.9	
188	2711 (218)		$C_3F_5H_3$	$CF_2HCFHCF_2H$ (1) (2)		1,2 12.8	
188	2712 (219)		$C_3F_5H_3$	$CF_3CH_2CF_2H$ (1) (2)		1,2 6.2	
78	2713 (220)		$C_3F_5H_3O$	$CF_2HCFHOCF_2H$ (1,2)(3) (4)	1,2 166	1,3 5.5 2,3 7.0 3,4 7.5	
40	2714 (221)		$C_3F_5H_3O$	$CF_3CH_2OCF_2H$			2.0
560	2715 (223)		$C_3F_5H_3Se$	$CF_3CF_2SeCH_3$		4.2	
560	2716 (2495)		$C_3F_5H_4NSe$	$CF_3CF_2SeNHCH_3$		3.0	
85	2717		C_3F_6BrN	$(CF_3)_2C{=}NBr$			7
906	2718		C_3F_6ClI	CF_3CF_2CFICl (1,2)	1,2 270.4		
907	2719		C_3F_6ClI	CF_3CF_2CFICl (1)(2)(3)		1,2 <1 2,3 14.6	1,3 10.8

Table B.1.a. (contd.)

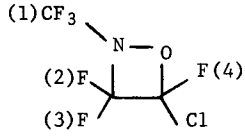
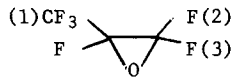
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ	
208	2720		C_3F_6ClI	CF_3CF_2CFICl	2,3	270.4	2,4	13.3	1,4	10.7
				(1)(2,3)(4)			3,4	14.5		
909	2721		C_3F_6ClI	CF_3CFICF_2Cl			1,2	11.8	1,3	9.4
				(1)(2)(3,4)			2,3	18.8	1,4	11.8
							2,4	18.1		
208	2722		C_3F_6ClI	$CF_3CFClCF_2I$	3,4	201.0	1,2	6.7	1,3	11.9
				(1)(2) (3,4)			2,3	13.0	1,4	10.1
							2,4	9.0		
988	2723 (4095)		C_3F_6ClNO							
				Isomer I					1,2	13.0
									1,3	<1
									1,4	<1
				Isomer II					1,2	<1
				(-79^o)					1,3	14.1
									1,4	3.7
874	2724		$C_3F_6Cl_2$	$CF_2ClCF_2CF_2Cl$			1,2	1.1		
				(1) (2)						
911	2725		$C_3F_6Cl_2O$	$CF_3OCF_2CFCl_2$			1,2	9.5	1,3	0.7
				(1) (2)(3)			2,3	7.0		
1118	2726 (4031)		C_3F_6O						1,2	8.8
									1,3	8.8
916	2727		$C_3F_6O_4S$	$CF_3CF_2C(O)OSO_2F$			1,2	1.7		
				(1) (2)						
916	2728 (4834)		$C_3F_6O_7S$	$FO_2SOC(O)CF_2CF_2OSO_2F$			1,2	2.0		
				(1)(2)						
20	2729 (228)		C_3F_6HI	$CF_2ICFHCF_3$	1,2	210	1,3	25.9	1,4	11.0
				(1,2)(3)(4)			2,3	19.4	2,4	8.4
							3,4	11.5		
20	2730 (227)		C_3F_6HI	CF_3CF_2CFHI	2,3	279	2,4	31.5	1,4	9.6
				(1)(2,3)(4)			1,2	1.0		
							1,3	0.0		
							3,4	19.1		
85	2731 (2496)		C_3F_6HN	$(CF_3)_2C{=}NH$						6

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
988	2732 [229 1780 4096]		C_3F_6HNO	(1)CF_3, N—O, (2)F, F(4), (3)F, H			
				Isomer I			1,2 <1
				(−79°)			1,3 12.4
							1,4 4.6
				Isomer II			1,2 13.3
							1,3 <1
							1,4 <1
73	2733 (230)		$C_3F_6H_2$	$CF_3CF_2CFH_2$ (1)(2)(3)	2,3 15.2		1,3 7.9
188	2734 (231)		$C_3F_6H_2$	CF_3CFHCF_2H (1)(2)(3)	1,2 11.8 2,3 11.8		1,3 7.3
78	2735 (238)		$C_3F_6H_2S$	$CF_3SCFHCF_2H$ (1) (2)(3)	2,3 21		1,2 4
917	2736		C_3F_7Br	$(CF_3)_2CFBr$ (1) (2)	1,2 8.9		
806 918	2737		C_3F_7Cl	$CF_3CF_2CF_2Cl$ (1)(2)(3)	2,3 1.6		1,3 9.0
874	2738		C_3F_7Cl	$CF_3CF_2CF_2Cl$ (1)(2)(3)	1,2 <1 2,3 1.8		1,3 8.9
911	2739		C_3F_7ClO	$CF_3OCF_2CF_2Cl$ (1) (2)(3)	1,2 9.23 2,3 1.90		1,3 0.58
919	2740		$C_3F_7ClO_3S$	$(CF_3)_2CFOSO_2Cl$ (1) (2)	1,2 2.0		
920	2741		$C_3F_7Cl_2N$	$(CF_3)_2CFNCl_2$ (1) (2)	1,2 3		
917	2742		C_3F_7I	$(CF_3)_2CFI$ (1) (2)	1,2 12.5		
917	2743		C_3F_7I	$CF_3CF_2CF_2I$ (1)(2)(3)	1,2 0.8 2,3 4.7		1,3 9.4
862	2744		C_3F_7I	$CF_3CF_2CF_2I$ (1)(2)(3)	1,2 0 2,3 4.6		1,3 9.3
909	2745		C_3F_7I	$CF_3CF_2CF_2I$ (1)(2)(3)	2,3 4.7		1,3 9.4

Table B.1.a. (contd.)

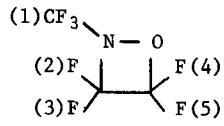
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
712	2746 (5955)		$C_3F_7Cl_2P$	$CF_3CF_2CF_2PCl_2$ (1) (2)			1,2 9.6
712	2747 (5956)		$C_3F_7I_2P$	$CF_3CF_2CF_2PI_2$ (1) (2)			1,2 9.7
569	2748 (4707)		C_3F_7N	$(CF_3)_2C{=}NF$ (1,2)			1,2 6.5
988	2749 (4097)		C_3F_7NO				
				Isomer I			1,2 14.1
							1,3 <1
				(-75^o)			1,4 <1
							1,5 <1
				Isomer II			1,2 <1
							1,3 14.1
							1,4 <1
							1,5 <1
913	2750 (4708)		C_3F_7NO	$CF_3CF_2C(O)NF_2$ (1) (2)	1,2	1.3	
64	2751 (256 / 4708a)		$C_3F_7HN_2$	$CF_3C(NF)CFHNF_2$ (1) (2)			1,2 5
857	2752 (5957)		$C_3F_7O_2P$	$CF_3CF_2C(O)OPF_2$ (1) (2)	1,2	1.5	
73	2753 (253)		C_3F_7H	$CF_3CF_2CF_2H$ (1) (2) (3)	2,3	4.5	1,3 7.3
907	2754		C_3F_7H	$CF_3CF_2CF_2H$ (1) (2) (3)	1,2 2,3	⩽1 4.5	1,3 ⩽1
73	2755		C_3F_7H	$CF_3CF_2CF_2H$ (1) (2) (3)	2,3	4.5	1,3 7.3
87	2756 (254)		C_3F_7H	CF_3CFHCF_3		11	
925	2757		$C_3F_7HO_2S$	$(CF_3)_2CFS(O)OH$ (1) (2)	1,2	8.0	

Table B.1.a. (contd.)

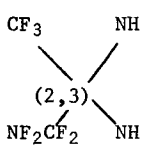
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
				(1)			
881	2758		$C_3F_7H_2N_3$		2,3 206		1,2 5.6 1,3 4.8
874	2759		C_3F_8	$CF_3CF_2CF_3$ (1)(2)(3)		1,2 <1	1,3 7.3
920	2760 (4709)		C_3F_8ClN	$(CF_3)_2CFNFCl$ (1,2) (3)		1,3 2.8 2,3 3.8	1,2 9.4
863	2761		C_3F_8O	$CF_3CF_2CF_2OF$ (1)(2)(3)		1,2 <1 2,3 2.9	1,3 7.0
863	2762 (4750)		C_3F_8O	$(CF_3)_2CFOF$ (1) (2)		1,2 1.6	
1146	2763		C_3F_8O	$CF_3CF_2OCF_3$ (1)(2) (3)		1,2 2.2	2,3 9.2
935	2764 (4835)		C_3F_8OS	$(CF_3)_2CFS(O)F$ (1) (2)		1,2 8.5	
1146	2764		$C_3F_8O_2$	$CF_3OOCF_2CF_3$ (1) (2)(3)		2,3 1.5	1,2 4.3
952	2765 (4752)		$C_3F_8O_3$	$CF_3OOCF(OF)CF_3$ (1) (2)(3)(4)			1,2 5.3
1146	2766		$C_3F_8O_3$	$CF_3CF_2OOOCF_3$ (1)(2) (3)		1,2 1.5	2,3 <1
869	2767 (4753)		$C_3F_8O_5$	$(CF_3OO)_2CFOF$ (1) (2)			1,2 3.5
925	2768 (4836)		C_3F_8S	$(CF_3)_2CFSF$ (1) (2)		1,2 9.3	
54	2769 [257 2433 4837 5074]	B	$C_3F_8H_4OS$	$CH_3OCF_2CFHSF_5$	150.7	{ 9.5 12.1	
907	2770 (4771)		C_3F_9N	$CF_3CF_2CF_2NF_2$ (1)(2)(3)(4		1,2 ≤1 2,3 1	1,3 8.6
35	2771 (5450)		C_3F_9N	$(CF_3)_3N$			10.8
800	2772		C_3F_9NO	$(CF_3)_2NOCF_3$ (1) (2)			1,2 5.2

Table B.1.a. (contd.)

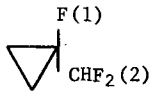
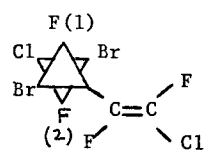
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
801	2773		C_3F_9NO	$(CF_3)_2NOCF_3$ (1) (2)			1,2 5
1025	2774		$C_3F_9N_3O$	$(CF_3)_2NN(CF_3)NO$ (1) (2)			1,2 3.0
12	2775		C_3F_9NS	$(CF_3)_2NSCF_3$ (1) (2)			1,2 3.4
712	2776 (5964)		C_3F_9P	$CF_3CF_2CF_2PF_2$ (1)(2)(3)		2,3 7.9	1,3 9.3
734	2777 (5968)		C_3F_9PS	$(CF_3)_2PSCF_3$ (1) (2)			1,2 1.11
925	2778 (4838)		$C_3F_{10}S$	$(CF_3)_2CFSF_3$ (1) (2)		1,2 0.4	
54	2779 ( )	B	$C_3F_{11}IS$	$CF_3CF_2CFISF_5$ (1,2)(3)	1,2 283.7	1,3 12 2,3 19	
953	2780		$C_4F_2H_3Br_2N$	$CF_2BrCBr(CN)CH_3$	155		
95	2781 (284, 5994)		$C_4F_2H_7Cl_3NP$	$CCl_2HCF_2PCl(N(CH_3)_2)$	266		
204	2782 (786)	*	$C_4F_3H_2BrCl_2$	$CF_2BrCFClCCl{=}CH_2$ (1,2) (3)	1,2 +171	1,2 -10 1,3 -12	
262	2783 (288, 1185)		$C_4F_3H_5$			1,2 12	
185	2784 (291)		$C_4F_3H_7ClP$	$CF_2P(CH_3)_2CFHCl$ (1,2) (3)	1,2 278	1,3 17.2 2,3 15.9	
20	2785 (293)	B	$C_4F_3H_7O$	$CF_2(OC_2H_5)CH_2F$		15.7	
20	2786 (294)	B	$C_4F_3H_7S$	$CF_2(SC_2H_5)CH_2F$		22.5	
954	2787 (3238, 3475)	*	$C_4F_4Br_2Cl$ erythro			1,2 -26.83	

Table B.1.a. (contd.)

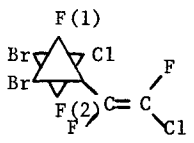
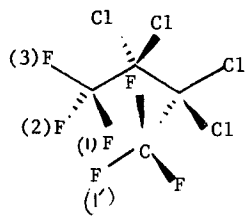
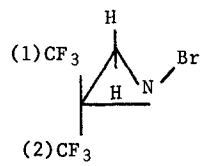
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
			threo			1,2 -28.06	
67	2788		$C_4F_4H_4N_2O_4$	$CF_3CH_2CH_2CF(NO_2)_2$			1,2 1.9
50	2789		$C_4F_4H_{13}Si$	$CF_2HCF_2(SiH_3)N(CH_3)_2$		0.7	
947	2790		$C_4F_5H_4ClOS$	$CF_3C(CF_2Cl(OH)SCH_3$	2,3 173	1,2 10.6	
				(1) (2,3)		1,3 11.6	
950	2791	P	$C_4F_5H_5$	$CF_3CH_2CF_2CH_3$			8.90
	(296)	H^2					9.02
		F					9.08
560	2792		$C_4F_5H_5Se$	$CF_3CF_2SeCH_2CH_3$		3.9	
35	2793		C_4F_6	$CF_3.C\equiv C.CF_3$			2.2
955	2794	C	C_4F_6	$CF_3.C\equiv C.CF_3$			+2.2
625	2795		$C_4F_6Cl_2$	$CF_3.CCl=CCl.CF_3$			
	(5460 5461)			cis			13.4
				trans			1.44
956	2796	T^3	$C_4F_6Cl_4$		1,2 105 1,3 124 2,3 116		1,1' 75
	(5462)	(-150°C)					
757	2797	B	$C_4F_6D_6PS$	$[CD_3(CF_3)P]_2S$			
	(6033)						
				Isomer I			0.3
				Isomer 2			2.0
206	2798	B	C_4F_6HCl	$CF_3CCl=CHCF_3$			1,2 1.3
	(794)			(1) (2)			
				(trans)			
114	2799	G	$C_4F_6H_2BrN$				1,2 7.5
	(297)						

Table B.1.a. (contd.)

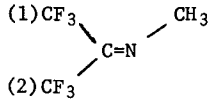
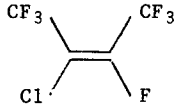
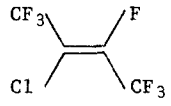
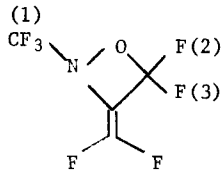
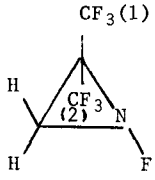
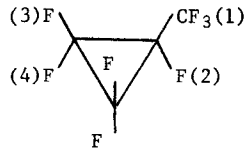
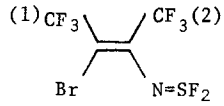
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
85	2800 (298)		$C_4F_6H_3N$						1,2	8
907	2801		$C_4F_6H_4$	$CF_3CF_2CFHCH_3$ (1)(2,3)(4)	2,3	270.4	1,2 1,3 2,4 3,4	≤1 ≤1 14.6 14.6	1,4	10.8
1068	2802 (3246)		C_4F_7Cl							11.32
1068	2803 (3247)		C_4F_7Cl							1.27
919	2804		$C_4F_7ClO_2$	$(CF_3)_2CFOCOCl$ (1) (2)			1,2	1.9		
988 989	2805 [3249 3494 4098 4099]		C_4F_7NO						1,2 1,3	3.4 3.4
907	2806		$C_4F_7HO_2$	$CF_3CF_2CF_2COOH$ (1)(2)(3)			1,2 2,3	≤1 ≤1	1,3	9.9
114	2807 [311 4717 2241]		$C_4F_7H_2N$						1,2	7.0
37	2808 (313)		$C_4F_7H_3ClN$	$(CF_3)_2NCH_2CFHCl$ (1) (2)					1,2	8.4
261	2809 (3678)	B	C_4F_8				1,2	9.2	1,3 1,4	7.7 6.0
975	2810 (4842)		C_4F_8BrNS						1,2	13.5

Table B.1.a. (contd.)

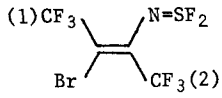
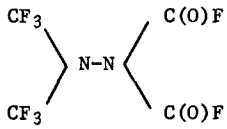
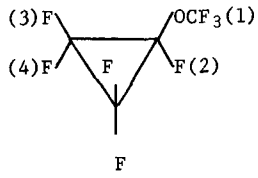
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
975	2811 (4843)		C_4F_8BrNS						1,2	1.4
975	2812 (4844)		$C_4F_8Br_3NS$	$CF_3CBr_2CBr(CF_3)NSF_2$ (1) (2) (1)					1,2	9.7
991	2813		$C_4F_8N_2O_2$	 (2)					1,2	15.5
261	2814 (3679)	B	C_4F_8O						1,2 1,3 1,4	4.9 4.6 1.2
992	2815		$C_4F_8O_3S$	$CF_3CF_2C(O)OS(O)CF_3$ (1) (2)			1,2	1.75		
961	2816		$C_4F_8O_4S$	$(CF_3)_2CFC(O)OSO_2F$				7.3		
77	2817 (317)	*	C_4F_8HI	$(CF_3)_2CHCF_2I$ (1) (2)					1,2	10.9
77	2818 (318)	*	C_4F_8HI	$CF_3CF_2CHICF_3$ (1) (2,3) (4)	2,3	277			1,4	5.4
20	2819		C_4F_9I	$(CF_3)_2CFCF_2I$ (1) (2) (3)			1,2 2,3	6.1 15.4	1,3	10.5
20	2820		C_4F_9I	$CF_3CF_2CFICF_3$ (1) (2,3) (4) (5)	2,3	289	2,4 1,2 3,4 1,3 4,5	15.6 0.0 16.1 0.0 12.7	2,5 3,5 1,4 1,5	7.1 11.7 10.8 6.4
994	2821 (3257, 3504)	-63°C	C_4F_9N	$(CF_3)_2CFN{=}CF_2$ (1) (2)			1,2	4.4		
708	2822 (6056)		$C_4F_9O_2P$	$CF_3CF_2CF_2C(O)OPF_2$ (1) (2)					1,2	8.5
102	2823 (320)		C_4F_9HBrN	$(CF_3)_2NCF_2CFHBr$ (1,2)	1,2	229				

Table B.1.a. (contd.)

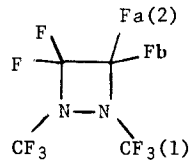
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ	
102	2824 (321)		C_4F_9HClN	$(CF_3)_2NCF_2CFHCl$ (1,2)	1,2	240				
102	2825 (322)		C_4F_9HClN	$CF_2ClCHFN(CF_3)_2$ (1,2)	1,2	172				
102	2826 (324)		C_4F_9HIN	$CF_2ICFHN(CF_3)_2$ (1,2)	1,2	200				
102	2827 (323)		C_4F_9HIN	$(CF_3)_2NCF_2CFHI$ (1,2)	1,2	240				
995	2828	*	C_4F_{10}	$CF_3CF_2CF_2CF_3$ (1)(2)(3)(4)			1,2 2,3	±0.1 4.6	1,3 1,4	±9.9 0.1
907	2829		C_4F_{10}	$(CF_3)_3CF$ (1) (2)			1,2	4.0		
996	2830 (5465)	B	C_4F_{10}	$CF_3CF_2CF_2CF_3$ (1)(2,2')(3,3')(4)	2,2' 3,3'	280‡	1,2 2,33' 2',33'	-0.2 +12.2 -5.4	1,33' 1,4	+9.9 +2.0
‡ Assumed										
560	2831		$C_4F_{10}HgSe_2$	$(CF_3CF_2Se)_2Hg$ (1)(2)				4.1		
997	2832 (4065)	65°	$C_4F_{10}N_2$						1,2	5.0
		-86°					1,2a	15.7	1,2a	15.7
907	2833		$C_4F_{10}O$	$CF_3CF_2OCF_2CF_3$ (1)(2,2')			|1,2+1,2'|	3.4		
961	2834 (4755)		$C_4F_{10}O$	$(CF_3)_2CFCF_2OF$ (1) (2)(3)			1,2	7	1,3	9
856	2835 (6714)		$C_4F_{10}O_2Si$	$CF_3CF_2CF_2C(O)OSiF_3$ (1) (2)					1,2	8.5
560	2836		$C_4F_{10}Se$	$(CF_3CF_2)_2Se$ (1)(2)			1,2	4.4		
560	2837		$C_4F_{10}Se_2$	$(CF_3CF_2)_2Se_2$ (1)(2)			1,2	1.8		
560	2838		$C_4F_{10}HNSe_2$	$(CF_3CF_2Se)_2NH$ (1)(2)			1,2	3.7		
998	2839		$C_4F_{11}N$	$(CF_3)_2NCF_2CF_3$ (1) (2)(3)			2,3	≤1	1,2 1,3	16 6

Table B.1.a. (contd.)

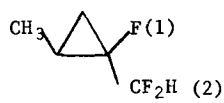
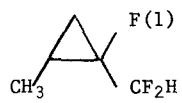
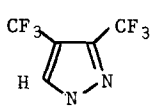
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
764	2840		$C_4F_{12}AsN$	$(CF_3)_2NAs(CF_3)_2$ (1) (2)			1,2 3.7
999	2841		$C_4F_{12}AsNO$	$(CF_3)_2NOAs(CF_3)_2$ (1) (2)			1,2 1.4
99	2842 (6058)		$C_4F_{12}AsP$	$(CF_3)_2PAs(CF_3)_2$ (1) (2)			1,2 3.4
764	2843 (6059)	P	$C_4F_{12}NP$	$(CF_3)_2NP(CF_3)_2$ (1) (2)			1,2 4.7
765	2844 (6064)		$C_4F_{12}P_2S_2$	$(CF_3)_2PSP(S)(CF_3)_2$ (1) (2)			1,2 0.5
925	2845 (4849)		$C_4F_{12}S$	$(CF_3)_2CFSF_2CF_3$ (1) (2) (3)		1,2 7.2	1,3 4.1
870	2846 (4851 5079)		$C_4F_{14}S$	$CF_3CF_2CF_2CF_2SF_5$ (1) (2) (3) (4)		1,2 10.80 2,3 ≤1 3,4 ≤1	1,3 2.42
870	2847 (4850)		$C_4F_{14}S$	$(CF_3CF_2)_2SF_4$ (1) (2)		1,2 ≤1	
109	2848 (347)	G*	$C_5F_2H_8O_2$	$CFH_2CFHC(O)OC_2H_5$ (1) (2)		1,2 -11.6	
262	2849 (351 1187)		$C_5F_3H_7$			1,2 10	
262	2850 (352 1188)		$C_5F_3H_7$	 (2,3)	2,3 295	1,2 10 1,3 10	
20	2851 (354)		$C_5F_3H_9S$	$(CH_3)_2CHSCF_2CH_2F$ (1) (2)		1,2 22.5	
185	2852 (355)		$C_5F_3H_{10}ClSi$	$(CH_3)_3SiCF_2CFHCl$ (1,2) (3)	1,2 338	2,3 14.9 1,3 14.8	
68	2853		$C_5F_5H_5O$	$CF_3CF_2C(O)CH_2CH_3$ (1) (2)		1,2 1	
68	2854		$C_5F_5H_6O^+$	$CF_3CF_2{}^+C(OH)CH_2CH_3$ (1) (2)		1,2 2.5	
1129	2855		$C_5F_6HN_2$				0.9

Table B.1.a. (contd.)

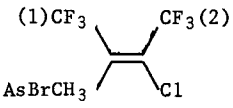
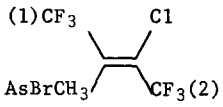
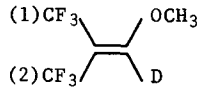
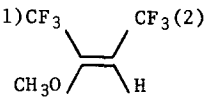
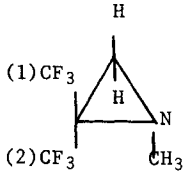
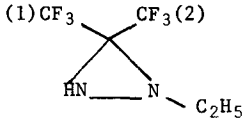
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
218	2856		$C_5F_6H_3AsBrCl$				1,2 14
218	2857		$C_5F_6H_3AsBrCl$				1,2 1.4
210	2858	H	$C_5F_6H_3DO$				1,2 6.4
205	2859 (810)		$C_5F_6H_4O$				1,2 11
114	2860 (365)		$C_5F_6H_5N$				1,2 7.0
569	2861		$C_5F_6H_6N_2$				1,2 8.7
192	2862		C_5F_7Cl	$(CF_3)_2CFC\equiv CCl$ (1) (2)	1,2	10.0	
907	2863		$C_5F_7H_3O_2$	$CF_3CF_2CF_2C(O)OCH_3$ (1)(2)(3)	1,2 2,3	≤1 ≤1	1,3 9.0
925	2864		$C_5F_7H_5O_2S$	$(CF_3)_2CFS(O)OCH_2CH_3$ (1) (2)	1,2	8.0	
208	2865 (3270 3513)	P -80°C	C_5F_8	$CF_3CF_2CF=C=CF_2$ (1) (2)	1,2	2.9	
190	2866		C_5F_8	$CF_3CF_2C\equiv CCF_3$ (1)(2) (3)	1,2	3.3	2,3 3.3

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ	
190	2867		$C_5F_8Cl_4$	$CF_3CF_2CFClCCl_2CF_2Cl$	2,3	277.0	3,4	6.5	1,4	13.5
				(1)(2,3) (5,6)	5,6	163.0	1,3	1.5	2,5	10.0
									2,6	10.0
									3,6	18.0
									3,5	16.9
									4,5	9.8
				(1)(2)					4,6	10.9
991	2868		$C_5F_8O_2$	$CF_2=CFOCF_2CF_2C(O)F$			1,2	3.7		
	3517									
	3655									
190	2869	P	C_5F_8HBr	$CF_3CF_2CFHCBr=CF_2$	2,3	285	2,4	14.5	1,4	9.3
	371			(1)(2,3)(4)			3,4	13.8		
	3272									
	3518									
208	2870	P	C_5F_8HCl	$CF_3CF_2CFClCH=CF_2$	2,3	279			1,4	11.1
				(1)(2,3)(4)						
208	2871		C_5F_8HCl	CF_3CF_2 H			1,2	1.9	2,3	2.0
	814			(1)(2)						
	1046			F CF_2Cl(3)						
	3273									
209	2872		$C_5F_8H_2$	$(CF_3)_2CF$ F			1,2	7.6		
	815			(1) (2)						
	1047			C C						
	3274			H H						
209	2873		$C_5F_8H_2$	(CF_2) CF H			1,2	7.6		
	816			(1) (2)						
	1048			C C						
	3275			H F						
208	2874	P	$C_5F_8H_2ClI$	$CF_3CF_2CFClCH_2CF_2I$	3,4	178			1,2	11.2
				(1) (2) (3,5)						
991	2875		$C_5F_8H_2O_3$		1,2	238				
					3,4	132				
1000	2876	B*	C_5F_9Cl	$CF_3.C(CF_2Cl)F.CF=CF_2$			2,4	11.8	1,2	10.5
	3276			(1) (2,3) (4)			3,4	10.9	1,3	11.5
	3519									

Table B.1.a. (contd.)

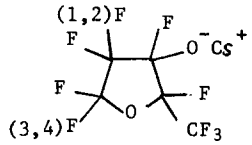
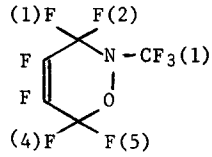
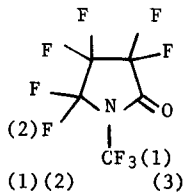
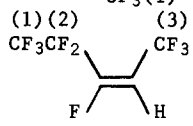
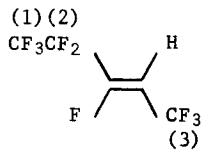
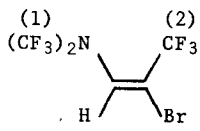
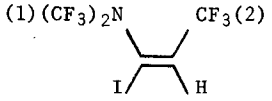
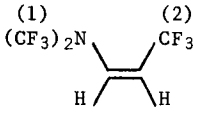
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
991	2877		$C_5F_9CsO_2$		1,2 248 3,4 128		
988	2878		C_5F_9NO				1,2 11.7 1,3 11.7 1,4 <0.5 1,5 <0.5
991	2879		C_5F_9NO				1,2 8.2
190	2880 [817 1049 3279]		C_5F_9H			1,2 1.9	2,3 15.0
190	2881 [818 1050 3280]		C_5F_9H			1,2 1.9	2,3 1.9
120	2882 (820)		C_5F_9HBrN				1,2 3.7
119	2883 (822)		C_5F_9HIN				1,2 2.4
40	2884 (377)		$C_5F_9HO_2$	$CF_3CF_2CF_2C(O)OCF_2H$ (1) (2)			1,2 8.8
120	2885 (823)		$C_5F_9H_2N$				1,2 2.2
1000	2886 (3281 3521)	*	C_5F_{10}	$(CF_3)_2CFCF=CF_2$ (1) (2)		1,2 8.0	

Table B.1.a. (contd.)

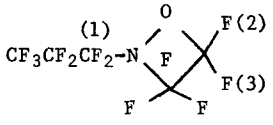
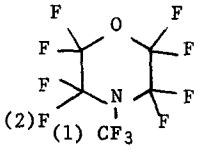
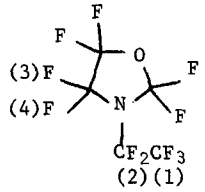
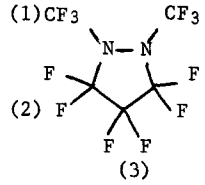
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1001	2887 (3282 / 3522)		$C_5F_{10}N_2$	$CF_2{=}NCF_2CF(CF_3)N{=}CF_2$ (1)(2)(3)	2,3 0	1,3	10.6
992	2888		$C_5F_{10}O_3S$	$CF_3CF_2CF_2C(O)OS(O)CF_3$ (1) (2)		1,2	8.6
560	2889		$C_5F_{10}H_2Se_2$	$(CF_3CF_2Se)_2CH_2$ (1)(2)	1,2 3.7		
560	2890		$C_5F_{10}H_3NSe_2$	$(CF_3CF_2Se)_2NCH_3$ (1)(2)	1,2 3.4		
1002	2891 (3523)		$C_5F_{11}N$	$CF_3CF_2CF_2CF_2N{=}CF_2$ (1)(2)(3)	1,2 1.8	1,3	9.0
988	2892 (4102)		$C_5F_{11}NO$			1,2 1,3	2.4 2.4
907	2893		$C_5F_{11}NO$			1,2	13.6
907	2894		$C_5F_{11}NO$		1,2 ≤1	1,3 1,4 2, 2,3	6.5 6.5 9.9 ≤1
1003	2895		$C_5F_{12}BrN$	$(CF_3)_2NCF_2CFBrCF_3$ (1) (2)		1,2	1.7
997	2896	84°C	$C_5F_{12}N_2$			1,2 1,3	20.2 2.0
907	2897		$C_5F_{13}N$	$(CF_3CF_2)_2NCF_3$ (1)(2) (3)	1,2 + 1,2' 10.2	1,3 2,3	6.8 15.8

Table B.1.a. (contd.)

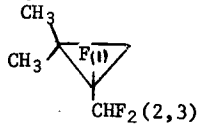
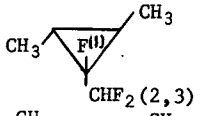
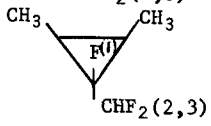
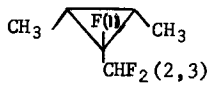
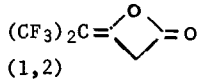
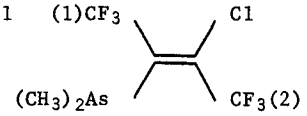
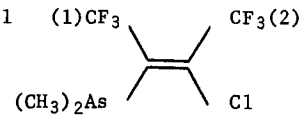
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
764	2898	P	$C_5F_{15}AsN$	$[(CF_3)_2N]_2AsCF_3$ (1) (2)					1,2	4.8
764	2899 (6104)	P	$C_5F_{15}N_2P$	$[(CF_3)_2N]_2PCF_3$ (1) (2)					1,2	5.5
108	2900 (398)		$C_6F_2H_9NO$	$CH_3CH_2CF_2C(OH)(CN)CH_3$ (1,2)	1,2	243				
262	2901 (404 1189)		$C_6F_3H_9$		2,3	301	1,2 1,3	9 11		
262	2902 (407 1192)		$C_6F_3H_9$		2,3	291	1,2 1,3	11 10		
262	2903 (405 1190)		$C_6F_3H_9$				1,2 1,3	9 9		
262	2904 (406 1191)		$C_6F_3H_9$				1,2 1,3	11 11		
20	2905 (408)		$C_6F_3H_{11}S$	$(CH_3)_3CSCF_2CH_2F$ (1) (2)			1,2	22.3		
124	2906 (412)		$C_6F_4HCoO_4$	$CF_2HCF_2Co(CO)_4$ (1)(2)			1,2	4.7		
67	2907		$C_6F_4H_7NO_4$	$CF_3CF(NO_2)CH_2CH_2C(O)OCH_3$ (1)(2)			1,2	4.4		
862	2908		$C_6F_5FeIO_4$	$CF_3CF_2Fe(CO)_4I$ (1)(2)			1,2	1.8		
125	2909		$C_6F_6H_2O_2$	 (1,2)					1,2	6.6
1021	2910		$C_6F_6H_4O_2$	$(CF_3)_2C{=}CHC(O)OCH_3$ (1,2)					1,2	8
218	2911		$C_6F_6H_6AsCl$						1,2	1.4
218	2912		$C_6F_6H_6AsCl$						1,2	15

Table B.1.a. (contd.)

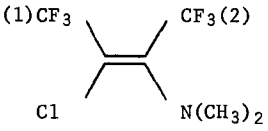
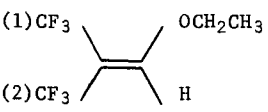
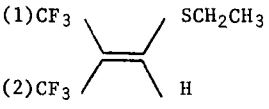
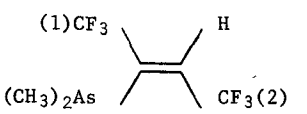
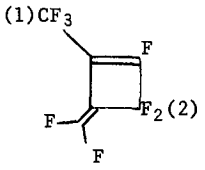
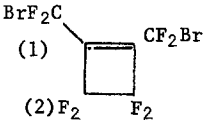
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
206	2913	B	$C_6F_6H_6ClN$						1,2	13.5
210	2914 (825)	H/J[2]	$C_6F_6H_6O$						1,2	6.4
210	2915 (826)	H	$C_6F_6H_6S$						1,2	6.2
127	2916 (828)		$C_6F_6H_7As$						1,2	1.9
74	2917 (418)	B	$C_6F_6H_8O$	$CF_3CH(CH_3)C(OH)(CH_3)CF_3$ (1) (2)					1,2	8
112	2918 [423 6812 5519]		$C_6F_6H_{10}Sn$	$CF_3CFHCF_2Sn(CH_3)_3$ (1)(2)(3,4)	3,4	340.0	1,2 2,3 2,4	11.75 7.1 6.5	1,3 1,4	6.5 11.0
190	2919		$C_6F_7H_3O$	$CF_3CF_2C{\equiv}CCF_2OCH_3$ (1)(2) (3)			1,2	3.3	2,3	3.3
1052	2920 [3287 3543 3754]		C_6F_8						1,2	2.4
1022	2921		$C_6F_8Br_2$						1,2	2.0

Table B.1.a. (contd.)

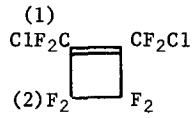
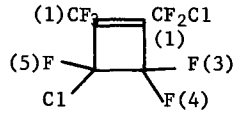
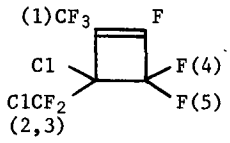
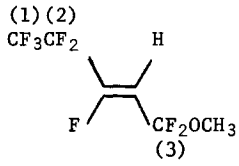
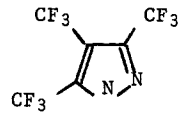
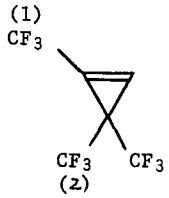
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1022	2922		$C_6F_8Cl_2$			1,2	2.4
1052	2923		$C_6F_8Cl_2$			1,2	6.3
	(3755)					2,5	2.2
						2,3	2.7
						2,4	2.6
						1,5	1.9
						1,3	2.6
						1,4	2.6
1052	2924		$C_6F_8Cl_2$		2,3 179	1,2	4.6
	(3288 3756)					1,3	2.2
						2,4	3.4
						3,4	3.2
						2,5	13.3
						3,5	18.5
						1,4	2.6
						1,5	2.8
190	2925	P	$C_6F_8H_4O$		1,2	1,3	2,3 1.9
	[831 1082 3290]						
1129	2926		$C_6F_9N_2$				0.94
115	2927		C_6F_9H				1,2 1.2
	(832)						

Table B.1.a. (contd.)

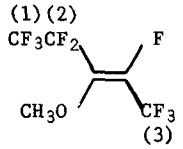
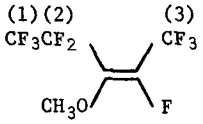
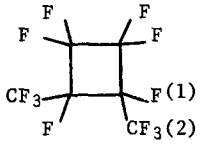
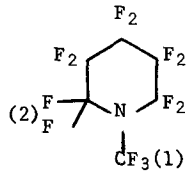
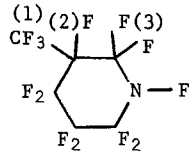
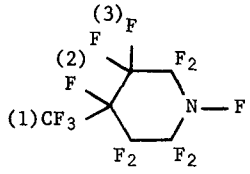
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
194	2928 (952 3289)		$C_6F_9H_3O$		1,2 1.9		2,3 1.6
194	2929 (426 3291)		$C_6F_9H_3O$				1,3 2.8 2,3 17.5
952	2930 (3656)		$C_6F_{10}O_4$	$CF_3OOC(O)CF_2CF_2CF_2C(O)F$ (1) (2)			1,2 10
1024	2931		C_6F_{12}		1,2 7.1		
1001	2932		$C_6F_{12}N_2$	$CF_2=NCF(CF_3)CF(CF_3)N=CF_2$ (1) (2)			1,2 7.5
920	2933		$C_6F_{13}ClN_2$	$(CF_3)_2CFN=NCCl(CF_3)_2$ (1) (2)	1,2 4.9		
907	2934		$C_6F_{13}N$				1,2 16.4
1122	2935 (4029)		$C_6F_{13}N$		1,2 6.6		1,3 13.8
1122	2936 (4030)		$C_6F_{13}N$		1,2 6.2		1,3 12.9
780	2937 (6180)		$C_6F_{13}H_3P_2$	$(CF_3)_2PCH_2CFHP(CF_3)_2$ (1) (2)			1,2 8

Table B.1.a. (contd.)

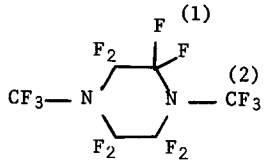
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
917	2938		C_6F_{14}	$(CF_3)_2CFCF(CF_3)_2$ (1) (2)		1,2 9.0	
862	2939 (6181)		$C_6F_{14}ClP$	$(CF_3CF_2CF_2)_2PCl$ (1) (2)			1,2 9.6
712	2940 (6182)		$C_6F_{14}ClP$	$(CF_3CF_2CF_2)_2PCl$ (1) (2)			1,2 9.9
780	2941 (6183)		$C_6F_{14}Cl_2P_2$	$(CF_3)_2PCF_2CCl_2P(CF_3)_2$ (1) (2) (3)			1,2 9 2,3 7
862	2942 (6185)		$C_6F_{14}IP$	$(CF_3CF_2CF_2)_2PI$ (1)(2)(3)		1,2 3.2	1,3 9.2
712	2942a (6184)		$C_6F_{14}IP$	$(CF_3CF_2CF_2)_2PI$ (1)(2)(3)			9.7
920	2944	B	$C_6F_{14}N_2$	$((CF_3)_2CFN)_2$ (1) (2)		1,2 5	
997	2945		$C_6F_{14}N_2$				1,2 12.6
925	2946		$C_6F_{14}OS$	$(CF_3)_2CFS(O)CF(CF_3)_2$ (1) (2) (2')(1')		1,2 1',2' } 11	2,2' 20 1',2 2',1 } 2
780	2947 (6186)		$C_6F_{14}H_2P_2$	$(CF_3)_2PCF_2CH_2P(CF_3)_2$ (1) (2) (3)			1,2 7.5 2,3 3.4
907	2948		$C_6F_{15}N$	$(CF_3CF_2)_3N$ (1)(2)		1,2 6.8	
780	2949		$C_6F_{16}P_2$	$(CF_3)_2PCF_2CF_2P(CF_3)_2$ (1) (2) (2')		2,2' 39	1,2 5.7
925	2950 (4852)		$C_6F_{16}S$	$[(CF_3)_2CF]_2SF_2$ (1) (2)		1,2 7.5	
1025	2951		$C_6F_{18}HgN_4$	$[(CF_3)_2NNCF_3]_2Hg$ (1) (2)			1,2 1.9
140	2952 (466)		$C_7F_3HClMnO_5$	$CFHClCF_2Mn(CO)_5$ (1) (2,3)	1,2	1,2 16.4 1,3 12.4	

Table B.1.a. (contd.)

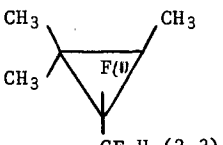
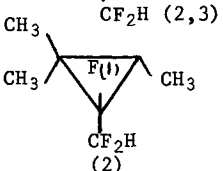
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
140	2953		$C_7F_3HClMnO_5$	$CF_2HCFClMn(CO)_5$		1,3 20.2	
	(467)			(1,2)(3)		2,3 10.0	
262	2954		$C_7F_3H_{11}$		2,3 301	1,2 10	
	(473 / 1197)					1,3 12	
				CF_2H (2,3)			
262	2955		$C_7F_3H_{11}$			1,2 13	
	(474 / 1198)			CF_2H (2)			
141	2956		$C_7F_4HCoN_5$	$[CF_2HCF_2Co(CN)_5]^{3-}$		1,2 5.4	
	(476)			(1) (2)			
141	2957		$C_7F_4HMnO_5$	$CF_2HCF_2Mn(CO)_5$		1,2 <1	
	(477)			(1) (2)			
142	2958		$C_7F_4HN_5Rh^{3-}$	$[CF_2HCF_2Rh(CN)_5]^{3-}$		1,2 5.4	
	(478)			(1) (2)			
145	2959		$C_7F_4HO_5Re$	$CF_2HCF_2Re(CO)_5$		1,2 <1	
	(479)			(1) (2)			
862	2960		$C_7F_4O_5Mn$	$CF_3CF_2Mn(CO)_5$		1,2 1.5	
				(1)(2)			
862	2961		$C_7F_5O_5Re$	$CF_3CF_2Re(CO)_5$		1,2 1.9	
				(1)(2)			
947	2962	B	$C_7F_5H_{12}ClOSSi$	$CF_3C(CF_2Cl)(SCH_3)OSi(CH_3)_3$			
				(1) (2,3)			
					2,3 167	1,2 12.0	
						1,3 10.8	
947	2963	B	$C_7F_5H_{12}ClO_2Si$	$CF_3C(CF_2Cl(OCH_3)OSi(CH_3)_3$			
				(1) (2)	2,3 172	1,2 10.2	
						1,3 11.8	
166	2964		$C_7F_7CoO_4$	$CF_3CF_2CF_2Co(CO)_4$			1,2 10
				(1)(2)			
862	2965	J	$C_7F_7FeIO_4$	$CF_3CF_2CF_2Fe(CO)_4I$			1,2 11
				(1) (2)			
111	2966		$C_7F_7H_6N$	$CF_3CF_2CF_2CH_2CH(CN)CH_3$			1,2 14
				(1) (2)			

Table B.1.a. (contd.)

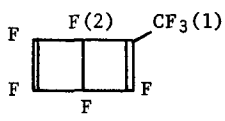
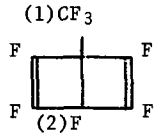
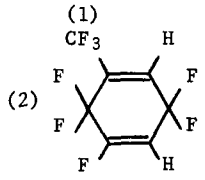
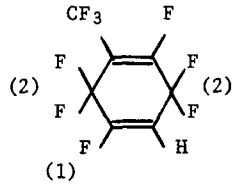
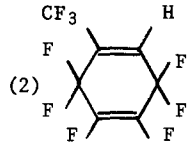
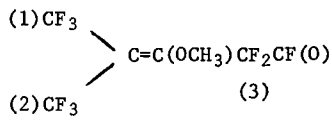
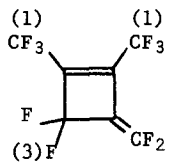
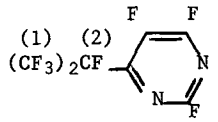
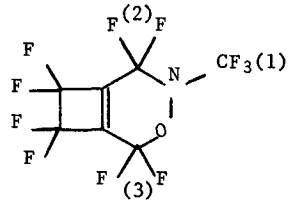
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ
284	2967 (3765 3297)		C_7F_8				1,2	2.8
284	2968 (3298)		C_7F_8				1,2	7.7
213	2969 [852 1333 3940 3299]		$C_7F_8H_2$				1,2	7.1
213	2970 [1334 3949 3300]		C_7F_9H				1,2 1,3	7.51 0.95
213	2971 (854)		C_7F_9H				1,2	2.55
117	2972 (3657)	B	$C_7F_9H_3O_2$				1,2 1,3	9.0 13.6
1023	2973 (3301 3553)		C_7F_{10}				1,2 1,3 2,3	5.6 1.2 2.3
945	2974 (4646 3387)	B	$C_7F_{10}N_2$		1,2	5.9		
988 1022	2975 (3767 4104)		$C_7F_{11}NO$				1,2 1,3	11.7 <0.5

Table B.1.a. (contd.)

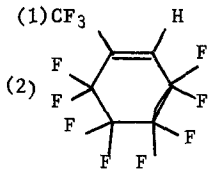
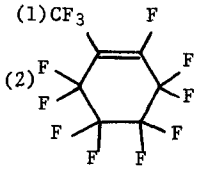
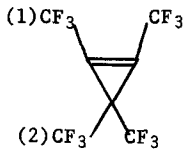
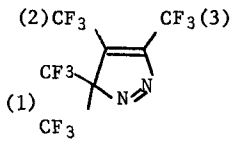
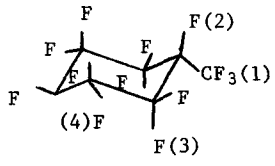
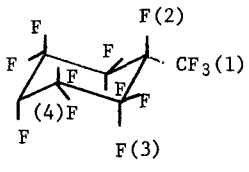
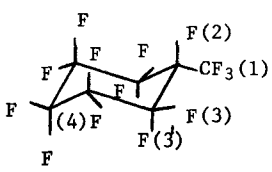
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
213	2976 (854)		$C_7F_{11}H$				1,2 7.1
213	2977 (3303 3957)		C_7F_{12}				1,2 2.4
115	2978		C_7F_{12}				1,2 1.15
115	2979		$C_7F_{12}N_2$				1,2 6 2,3 8.5
301	2980 (1340 3959)	P*	$C_7F_{13}H$		1,2	6.2	1,3 13.1 1,4 <1.5
301	2981 (1339 3958)	P*	$C_7F_{13}H$		1,2	6.2	1,3 13.5 1,4 1.4
194	2982 (494)		$C_7F_{13}HO$	$CF_3CF_2CFHC(O)CF_2CF_2CF_3$ (1,2)	1,2	290	
301	2983 (3960)	P*	C_7F_{14}		1,2	6.0	1,3 13.4 1,3' 13.4 1,4 0.9

Table B.1.a. (contd.)

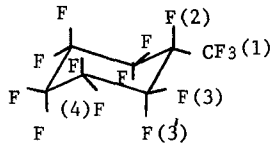
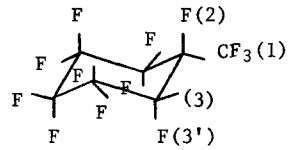
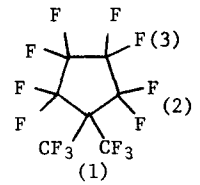
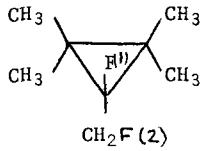
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
1069	2984 (3961)	B* (40°)	C_7F_{14}			1,2	6.0	1,3 13.9 1,3' 13.9 1,4 0.98
		R (-20°C)				1,2	6.7	1,3 13.9 1,3' 13.9 1,4 0.98
1070	2985		C_7F_{14}			1,2	6.1	1,3 14.2 1,3' 14.2
1071	2986 (3841)		C_7F_{14}					1,2 12.7 1,3 3.2
				(1,2)				
843	2987 (521)		$C_8F_2H_6Br_2$	$CF_2BrCHBrC_6H_5$	1,2	152		
843	2988 (522)		$C_8F_2H_6Cl_2$	$CF_2ClCHClC_6H_5$ (1,2)	1,2	158		
139	2989 (529)		$C_8F_2H_{15}Cl$	$CF_2HCHClCH_2CH_2CH_2CH_2CH_2CH_3$	1,2	279		
140	2990 (530)		$C_8F_3H_3ClMnO_5$	$CH_3CF_2CFClMn(CO)_5$			1,2 13.0 1,3 <1	
262	2991 (539 1201)	B	$C_8F_3H_{13}$	 $CH_2F(2)$			1,2 13	
187	2992 (544)		$C_8F_3H_{19}GeSn$	$(CH_3)_3GeCFHCF_2Sn(CH_3)_3$	2,3	271.3	1,2 11 1,3 13	
187	2993 (543)		$C_8F_3H_{19}GeSn$	$(CH_3)_3GeCF(Sn(CH_3)_3)CF_2H$ (1) (2,3)	2,3	277.6	1,2 19.2 1,3 24	

Table B.1.a. (contd.)

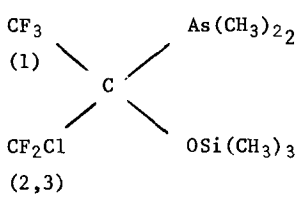
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
195	2994 (546)		$C_8F_3H_{19}SiSn$	$(CH_3)_3SiCFHCF_2Sn(CH_3)_3$ (1)(2,3)	2,3	312	1,2 1,3	8.4 9.6
195	2995 (545)		$C_8F_3H_{19}SiSn$	$(CH_3)_3SiCF(Sn(CH_3)_3)CF_2H$ (1) (2,3)				
					2,3	290	1,2 1,3	20 27
140	2996 (547)		$C_8F_4H_3MnO_5$	$CH_3CF_2CF_2Mn(CO)_5$ (1) (2)			1,2	4.2
137	2997 (548)		$C_8F_4H_3O_5Re$	$CH_3CF_2CF_2Re(CO)_5$ (1)(2)			1,2	4.5
152	2998 (553)		$C_8F_4H_{12}S$	CF_2HCF_2S  (1) (2)			1,2	10
862	2999	U[2]	$C_8F_5MnO_6$	$CF_3CF_2C(O)Mn(CO)_5$ (1)(2)			1,2	0.7
862	3000	U[2]	$C_8F_5O_6Re$	$CF_3CF_2C(O)Re(CO)_5$ (1)(2)			1,2	0.7
		J	$C_8F_5O_7Re$	$CF_3CF_2C(O)ORe(CO)_5$ (1)(2			1,2	1.5
142 833	3001		$C_8F_5H_5CoIO$	CF_3CF_2—Co(CO)I(πC_5H_5) (1)(2,3)	2,3	233	1,2 1,3	20 1.8
833 142	3002 (6635)		$C_8F_5H_5IORh$	CF_3CF_2—Rh(CO)I(πC_5H_5) (1)(2,3)	2,3	234	1,2 1,3	2.3 1.7
1056	3003		$C_8F_5H_5NiO$	CF_3CF_2—Ni(CO)(πC_5H_5) (1)(2)			1,2	2.2
947	3004	B	$C_8F_5H_{15}AsClO$	 (1) (2,3)	2,3	170	1,2 1,3	9.8 10.6

Table B.1.a. (contd.)

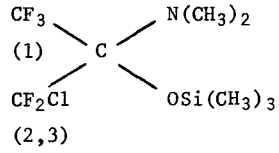
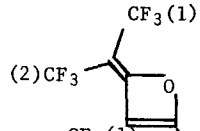
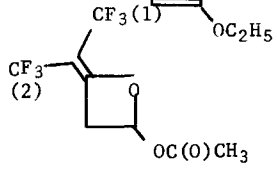
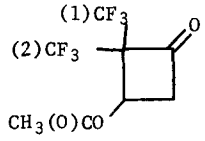
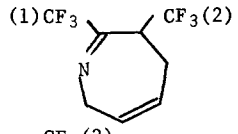
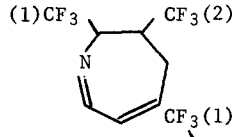
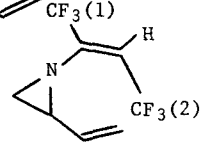
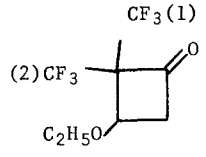
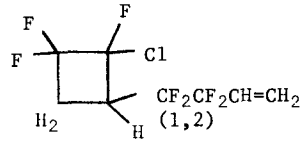
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
947	3005	B	$C_8F_5H_{15}ClNOSi$		2,3	168	1,2 1,3	12.9 9.7		
117	3006	B -80°C	$C_8F_6H_6O_2$						1,2	7.0
117	3007	B	$C_8F_6H_6O_3$						1,2	6.5
117	3008	B	$C_8F_6H_6O_3$						1,2	8.5
215	3009 (558)		$C_8F_6H_7N$						1,2	5
215	3010 (559)		$C_8F_6H_7N$						1,2	5
215	3011 (866)		$C_8F_6H_7N$						1,2	1.5
117	3012	B	$C_8F_6H_8O_2$						1,2	8.6
196	3013 (3770)	P	$C_8F_7H_6Cl$		1,2	276				

Table B.1.a. (contd.)

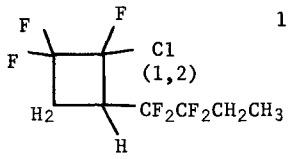
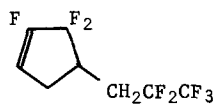
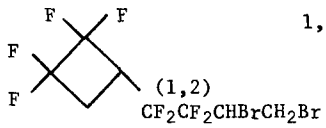
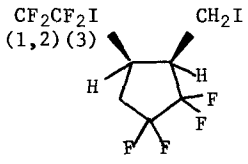
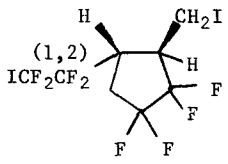
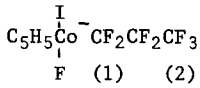
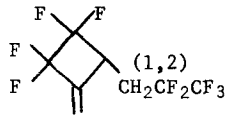
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ	
196	3014 (563 3771)	P	$C_8F_7H_8Cl$		1,2	276				
862	3015		$C_8F_7MnO_5$	$CF_3CF_2CF_2Mn(CO)_5$ (1)(2)(3)			2,3	0	1,3	12.4
862	3016		$C_8F_7ReO_5$	$CF_3CF_2CF_2Re(CO)_5$ (1)(2)(3)			2,3	0	1,3	12.3
198	3017 (3853)	P	$C_8F_8H_6$			268				
196	3018 (567 3774)		$C_8F_8H_6Br_2$		1,2	277				
1076	3019 (3854)		$C_8F_8H_6I_2$		1,2	266	1,3 2,3	5 5		
1076	3020 (3855)		$C_8F_8H_6I_2$		1,2	261				
1077	3021	E^2	$C_8F_8H_5CoI$						1,2	12.5
198	3022		$C_8F_9H_5$		1,2	266				
198	3023		$C_8F_9H_5$	$CF_3CF_2CH{=}CHCF_2CF_2CH{=}CH_2$ (1)(2)			1,2	1.8		
198	3024 (569)		$C_8F_9H_6I$	$CF_3CF_2CH_2CHICF_2CF_2CH{=}CH_2$ (1,2) (3,4) (5,6)		1,2 3,4 5,6	266 270 263			

Table B.1.a. (contd.)

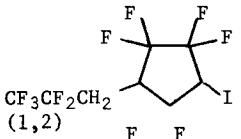
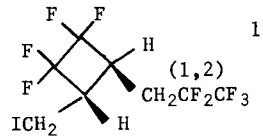
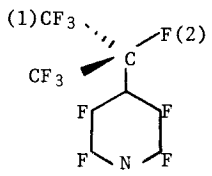
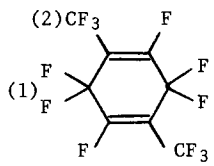
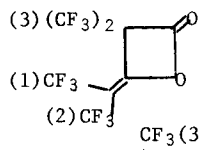
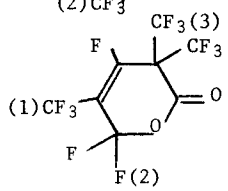
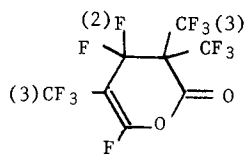
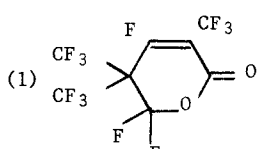
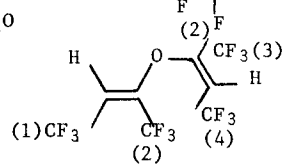
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
198	3025 (3858)		$C_8F_9H_6I$		1,2 266		
198	3026 (3778)		$C_8F_9H_6I$		1,2 260		
806	3027 (3778)	U[2]	$C_8F_{10}FeO_4$	$(CF_3CF_2)_2Fe(CO)_4$ (1)(2)		1,2 2.0	
933 949	3028	*	$C_8F_{11}N$			1,2 6	
213	3029 (3980 3310)		C_8F_{12}				1,2 6.6
113	3030		$C_8F_{12}O_2$				1,2 7 1,3 7.5 2,3 9
113	3031 (3311 4049)		$C_8F_{12}O_2$				1,2 7 1,3 0.5
113	3032 (3312 4048)		$C_8F_{12}O_2$				1,2 8 2,3 13
113	3033 (3313 4047)		$C_8F_{12}O_2$				1,2 11
206	3034 (868)	B	$C_8F_{12}H_2O$				1,2 10.2 3,4 <2
113	3035 (572)		$C_8F_{12}H_4O$	$(CF_3)_2CHC(OCH_3)=C(CF_3)_2$ (1,2)			1,2 10

Table B.1.a. (contd.)

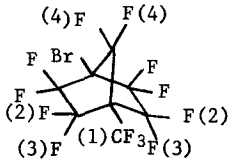
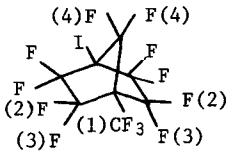
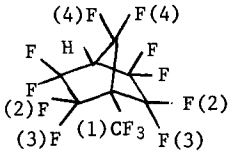
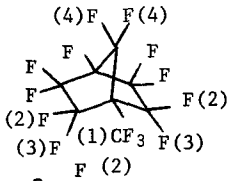
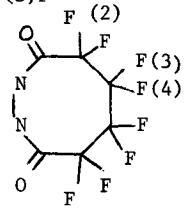
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
780	3036		$C_8F_{12}H_8P_2$	$(CF_3)_2PCH(CH_3)CH(CH_3)P(CF_3)_2$ (1,2)		1,2	9
1151	3037		$C_8F_{13}Br$			1,2 1,3 1,4	18.3 3.9 5.9
1151	3038		$C_8F_{13}I$			1,2 1,3 1,4	18.7 3.7 5.1
1151	3039		$C_8F_{13}H$			1,2 1,3 1,4	16.8 4.8 5.7
1151	3040		C_8F_{14}			1,2 1,3 1,4	16.5 5.5 5.5
991	3041 (4074)		$C_8F_{14}N_2O_2$		1,2 294 or 3,4		
154	3042 (596, 597)		$C_9F_2H_{10}$	$C_6H_5CHFCHFCH_3$ Erythro Threo			15-16 15
108	3043 (598)	G	$C_9F_2H_{10}O$	$C_6H_5CF_2CH(OH)CH_3$ (1,2)	1,2 249		
151	3044 (601)	B	$C_9F_3H_9O$	$C_6H_5CF(OCH_3)CF_2H$ (1) (2)		1,2	6

Table B.1.a. (contd.)

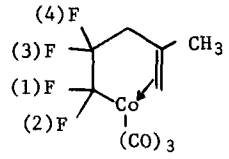
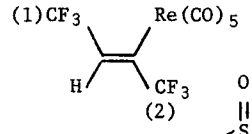
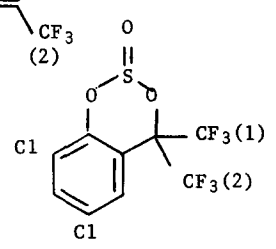
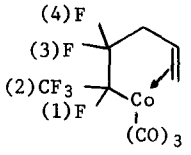
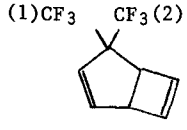
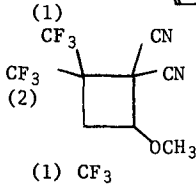
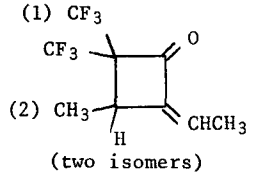
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
200	3045	A	$C_9F_4H_9CoO_3$		1,2 210	1,3 9.0	
1131	3046	A	$C_9F_5H_5FeO_5$	$CF_3CF_2C(O)OFe(CO)_3\pi C_3H_5$		1.5	
137	3047		$C_9F_6HO_5Re$				1,2 2.5
1083	3048	P	$C_9F_6H_2Cl_2O_3S$				1,2 9.6
1116	3049	H^2	$C_9F_6H_4ClN$	$(CF_3)_2C{=}NC_6H_4Cl$(para) (1,2)			1,2 6.9
1116	3050	H^2	$C_9F_6H_4N_2O_2$	$(CF_3)_2C{=}NC_6H_4NO_2$(para) (1,2)			1,2 6.6
200	3051	A	$C_9F_6H_5CoO_3$		3,4 240	1,2 23.0	2,3 12.0 2,4 12.0
1116	3052		$C_9F_6H_5N$	$(CF_3)_2C{=}NC_6H_5$ (1,2)			1,2 7.1
157	3053		$C_9F_6H_6$				1,2 9.5
201	3054		$C_9F_6H_6N_2O$				1,2 10
125	3055	B	$C_9F_6H_8O$	 (two isomers)			1,2 9.0 1,2 9.1

Table B.1.a. (contd.)

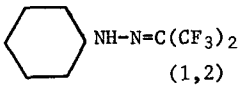
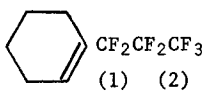
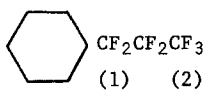
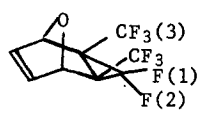
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
157	3056		$C_9F_6H_{12}N_2$	 NH-N=C(CF$_3$)$_2$ (1,2)			1,2 6
862	3057		$C_9F_7O_6Re$	$CF_3CF_2CF_2C(O)Re(CO)_5$ (1) (2)			1,2 9.3
1131	3058		$C_9F_7O_7Re$	$CF_3CF_2CF_2C(O)ORe(CO)_5$ (1)(2)(3)	2,3	1	1,3 8
1116	3059	H[2]	$C_9F_7H_4N$	$(CF_3)_2C{=}NC_6H_4F$(para) (1,2)			1,2 6.9
1077	3060	H	$C_9F_7H_5CoCl$	$CF_3CF_2CF_2Co(CO)(Cl)\pi C_5H_5$ (1) (2)			1,2 10.4
1132	3061	J	$C_9F_7H_5CoIO$	$\pi C_5H_5Co(CO)(CF(CF_3)_2)I$ (1)(2)			1,2 10.8
833	3062		$C_9F_7H_5CoIO$	$\pi C_5H_5Co(CO)(CF_2CF_2CF_3)I$ (1)(2,3)(4)	2,3 283		1,4 10.7
833	3063 (6636)		$C_9F_7H_5IORh$	$\pi C_5H_5Rh(CO)(CF_2CF_2CF_3)I$ (1,2)(3,4)(5)	1,2 239 3,4 284	(1,2)(3,4) 1.9	1,5 11.5 2,5 10.6
1056	3064		$C_9F_7H_5NiO$	$\pi C_5H_5Ni(CO)CF_2CF_2CF_3$ (1)(2)(3)		1,2 1.4 2,3 1.0	1,3 9.8
1134	3065		$C_9F_7H_9$	 $CF_2CF_2CF_3$ (1) (2)			1,2 10
1134	3066		$C_9F_7H_{11}$	 $CF_2CF_2CF_3$ (1) (2)			1,2 10
274	3067 (1203 3696)		$C_9F_8H_4O$				1,3 16 2,3 2.2
113	3068 (616)		$C_9F_9H_7O_3$	$(CF_3)_2C{=}C(OCH_3)CH(CF_3)C(O)OCH_3$ (1,2)			1,2 10

Table B.1.a. (contd.

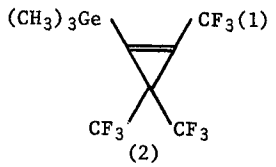
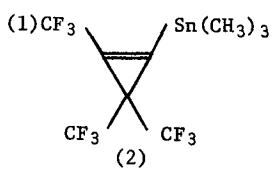
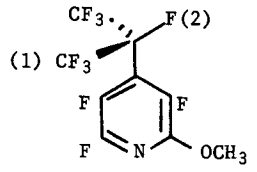
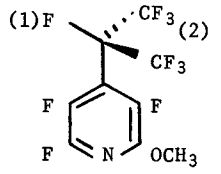
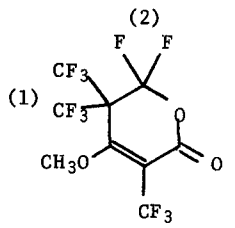
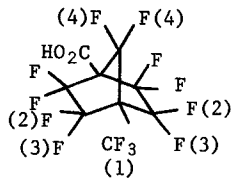
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^5J
1135 115	3069		$C_9F_9H_9Ge$			1,2	1.2
115	3070		$C_9F_9H_9Sn$			1,2	1.25
933 949	3071 (3389 4653)		$C_9F_{10}H_3NO$		1,2	5.5	
933 949	3072 (3389 4653)		$C_9F_{10}H_3NO$		1,2	5.5	
113	3073 (618)		$C_9F_{11}H_3O_3$			1,2	12
1151	3074		$C_9F_{13}HO_2$			1,2 1,3 1,4	1.2 4.8 5.4

Table B.1.a. (contd.)

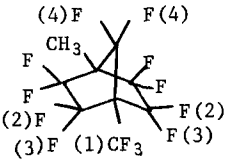
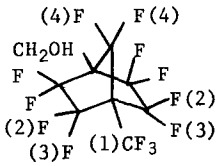
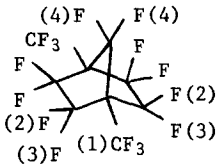
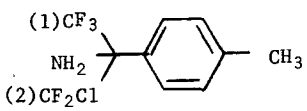
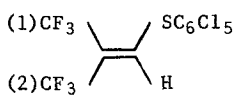
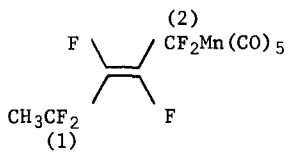
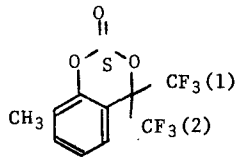
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1151	3075		$C_9F_{13}H_3$				1,2 17.6 1,3 4.4 1,4 5.2
1151	3076		$C_9F_{13}H_3O$				1,2 19.5 1,3 4.4 1,4 5.0
1151	3077		C_9F_{16}				1,2 17.2 1,3 4.1 1,4 6.1
1138	3078		$C_9F_{21}BO_3$	$((CF_3)_2CFO)_3B$ (1) (2)		1,2 2.8	
1139	3079		$C_9F_{21}NO$	$(CF_3CF_2CF_2)_2NOCF_2CF_2CF_3$ (1) (2,3) (4) (5)	2,3 230		1,2 } 10.1 1,3 } 4,5 6.1
1140	3080	P	$C_{10}F_5H_9NCl$				1,2 12
210	3081 (877)	A	$C_{10}F_6HCl_5S$				1,2 6.3
164	3082 [652 971 3331 3595]		$C_{10}F_6H_3MnO_5$				1,2 3.2
1083	3083	P	$C_{10}F_6H_6O_3S$				1,2 9.4

Table B.1.a. (contd.)

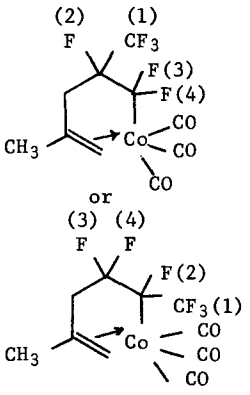
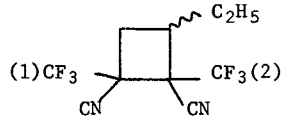
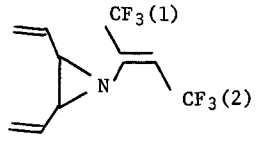
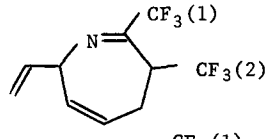
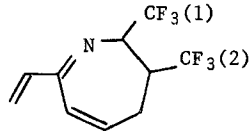
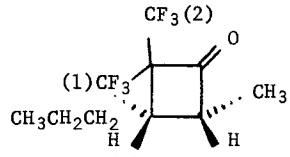
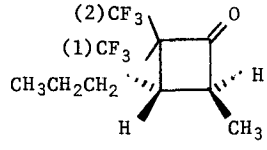
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
200	3084	A	$C_{10}F_6H_7CoO_3$	 or	3,4 230	1,2 16.0	1,3 / 1,4 } 10.0
1116	3085	H^2	$C_{10}F_6H_7N$	$(CF_3)_2C{=}NC_6H_4CH_3$(para) (1,2)			1,2 6.9
1116	3086	H^2	$C_{10}F_6H_7NO$	$(CF_3)_2C{=}NC_6H_4OCH_3$(para) (1,2)			1,2 7.2
1136	3087		$C_{10}F_6H_8N_2O$	 (two isomers)			1,2 13 1,2 10
215	3088 (879)		$C_{10}F_6H_9N$				1,2 1.5
215	3089 (654)		$C_{10}F_6H_9N$				1,2 5
215	3090 (655)		$C_{10}F_6H_9N$				1,2 5
117	3091 (657)	B	$C_{10}F_6H_{12}O$				1,2 8.8
117	3092 (656)	B	$C_{10}F_6H_{12}O$				1,2 8.6

Table B.1.a. (contd.)

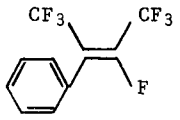
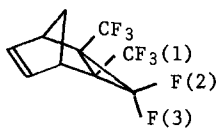
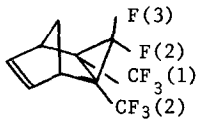
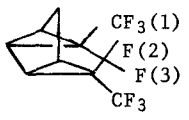
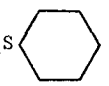
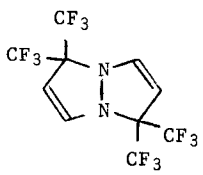
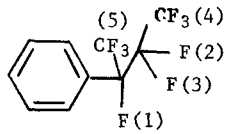
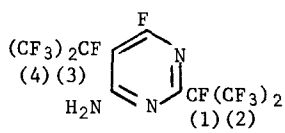
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1055	3093 (3335)		$C_{10}F_7H_5$							12
819	3094		$C_{10}F_7H_5FeO_2$	$(CF_3)_2CFFe(CO)_2\pi C_5H_5$			12			
274	3095 (1205 3699)	B	$C_{10}F_8H_6$						1,2 1,3	19.0 2.6
274	3096 (1206 3700)	B	$C_{10}F_8H_6$						1,2 1,3	19.0 2.6
274	3097 (1204 4002)	B	$C_{10}F_8H_6$						1,2 1,3	10.1 3.1
152	3098 (661)		$C_{10}F_8H_{12}S_2$	$CF_2HCF_2SCF_2CF_2S$ (1)(2) 			1,2	10.5		
1133	3099		$C_{10}F_{12}H_4N_2$							6.2
933	3100 (3381 4436)	P	$C_{10}F_{14}$		2,3	294	1,2 1,3 1,5 2,4 3,4	3.8 1.5 7 0 0	1,4 2,5 3,5 4,5	15.2 5 15.0 4.5
862	3101		$C_{10}F_{14}FeO_4$	$(CF_3CF_2CF_2)_2Fe(CO)_4$				~0		11.1
957	3102 (3391)	E	$C_{10}F_{15}H_2N_3$				1,2 3,4	10 11		

Table B.1.a. (contd.)

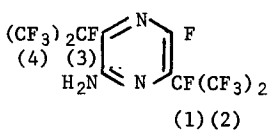
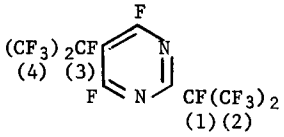
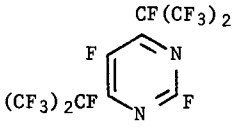
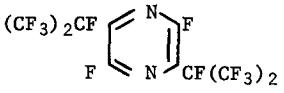
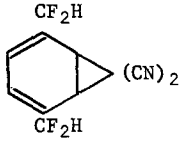
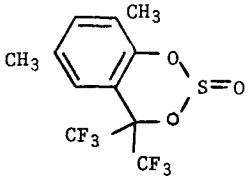
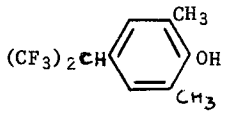
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
957	3103 (3392)	E	$C_{10}F_{15}H_2N_3$			1,2 6 3,4 6.5	
957	3104 (3395)	E	$C_{10}F_{16}N_2$			1,2 10 2,3 9	
945	3105 (3393 4657)		$C_{10}F_{16}N_2$			5.9	
957	3106 (3394)	E	$C_{10}F_{16}N_2$			7	
234	3107 (2266 4732)		$C_{11}F_3H_{14}N$	$C_6H_5CF_2NFCH(CH_3)CH_2CH_3$	190		
167	3108 (685)		$C_{11}F_4H_6N_2$		306		
1131	3109	E	$C_{11}F_5H_5MoO_5$	$CF_3CF_2CO_2Mo(CO)_3\pi C_5H_5$		1.5	
1083	3110	P	$C_{11}F_6H_8O_3S$				9.4
1083	3111 (687 884)		$C_{11}F_6H_{10}O$				8.4

Table B.1.a. (contd.)

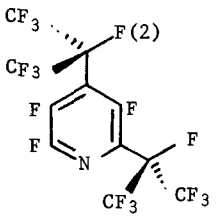
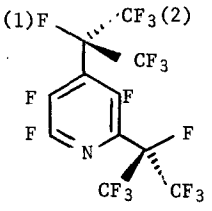
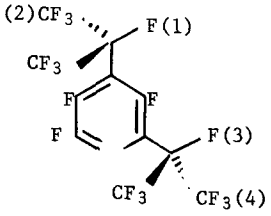
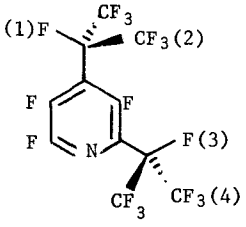
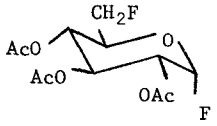
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1131	3112		$C_{11}F_7H_5FeO_4$	$CF_3CF_2CF_2Co_2Fe(CO)_2\pi C_5H_5$			8
1132	3113	E	$C_{11}F_7H_{16}FeIO_2P_2$	$CF_3CF_2CF_2Fe(CO)_2I[(CH_3)_2PCH_2CH_2P(CH_3)_2]$			12.2
933	3114		$C_{11}F_{13}N$	(1) 		1,2	6
933	3115		$C_{11}F_{13}N$			1,2	6
1132	3116	J	$C_{11}F_{15}FeIO_4$	$CF_3CF_2CF_2CF_2CF_2CF_2Fe(CO)_4I$ (1) (2) (3) (4)		1,2 3,4	11 17
949	3117 (3396, 4665)	E	$C_{11}F_{17}N$		1,2 3,4	6 6	
					1,2 3,4	6 6	
				(-40°)			
378	3118 (699, 1715)	A	$C_{12}F_2H_{16}O_7$				≤0.2

Table B.1.a. (contd.)

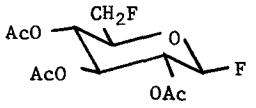
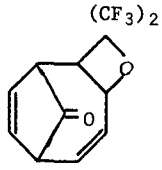
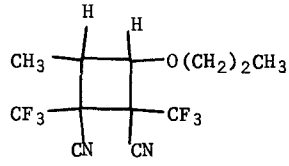
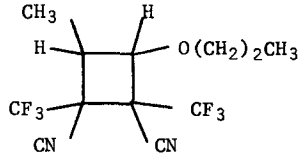
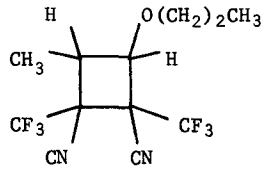
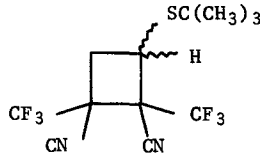
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
378	3119 (698 1716)	A	$C_{12}F_2H_{16}O_7$				0.9
234	3120 (2268 4734)		$C_{12}F_3H_{16}N$	$C_6H_5CF_2NFCH(CH_3)CH_2CH_2CH_3$ (1,2)	1,2 191		
202	3121 (702)		$C_{12}F_6H_8O_2$				10.5
1136	3122		$C_{12}F_6H_{12}N_2O$				12
1136	3123		$C_{12}F_6H_{12}N_2O$	 or 			12
1136	3124		$C_{12}F_6H_{12}N_2S$	 Both isomers			11

Table B.1.a. (contd.)

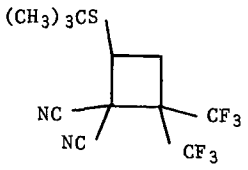
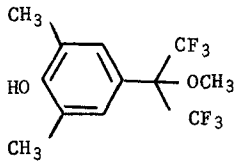
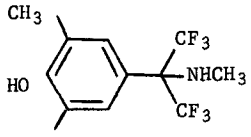
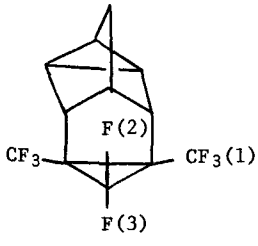
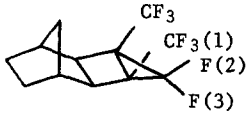
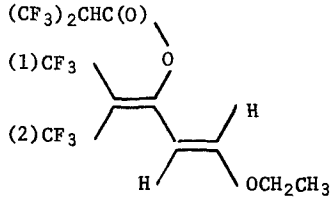
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
201	3125		$C_{12}F_6H_{12}N_2S$				10
1083	3126	P	$C_{12}F_6H_{12}O_2$				0.9
1083	3127	P	$C_{12}F_6H_{13}NO$				0.8
821	3128		$C_{12}F_7H_{11}ClCoN_2O_4$	$[CF_3CF_2CF_2Co(CH_3CN)_2\pi C_5H_5]^+ClO_4^-$			10.2
274	3129 (3701)	B	$C_{12}F_8H_8$			1,2 1,3	18.6 4.0
274	3130 (3702)	B	$C_{12}F_8H_{10}$			1,2 1,3	11.5 5.6
117	3131 (710)	B	$C_{12}F_{12}H_8O_3$			1,2	11.1

Table B.1.a. (contd.)

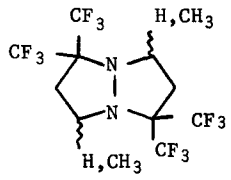
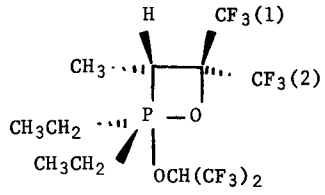
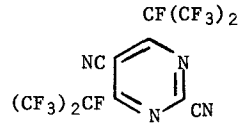
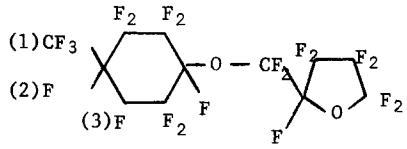
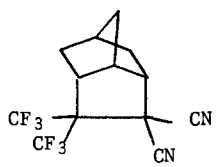
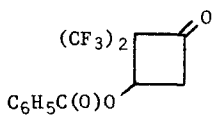
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1133	3132		$C_{12}F_{12}H_{12}N_2$				
				Isomer 1			10.0
				Isomer 2			10.0
158	3133 (711)	A	$C_{12}F_{12}H_{15}O_2P$	 (3,4)			1,2 10.2 3,4 7.2
945	3134	E	$C_{12}F_{14}N_4$			6.2	
1141	3135		$C_{12}F_{22}O_2$		1,2	8	1,3 13
140	3136		$C_{13}F_4H_5MnO_5$	$C_6H_5CF_2CF_2Mn(CO)_5$		<1	
201	3137		$C_{13}F_6H_8N_2$				13
117	3138	A	$C_{13}F_6H_8O_3$				9.0

Table B.1.a. (contd.)

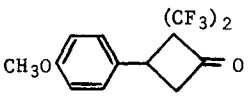
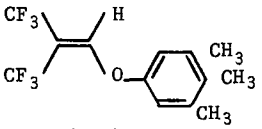
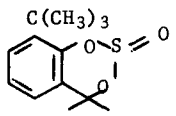
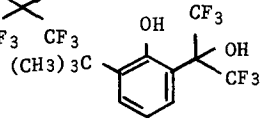
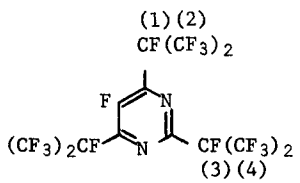
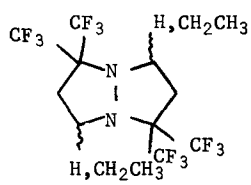
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
117	3139	E	$C_{13}F_6H_{10}O_2$				8.6
210	3140 (888)	A	$C_{13}F_6H_{12}O$				6.4
1083	3141	P	$C_{13}F_6H_{12}O_3S$				9
1083	3142	P	$C_{13}F_6H_{14}O_2$				1.0
1131	3142		$C_{13}F_{14}H_5CoO_3$	$CF_3CF_2CF_2CO_2Co(CO)(CF_2CF_2CF_3)(\pi C_5H_5)$ (1) (2) (3) (4)			1,2 9 3,4 11
1132	3143	E	$C_{13}F_{15}H_5CoIO$	$CF_3CF_2CF_2CF_2CF_2CF_2CF_2Co(CO)I(\pi C_5H_5)$ (1) (2) (3) (4)			1,2 10 3,4 17
945	3144 (3397)		$C_{13}F_{22}N_2$		1,2 3,4	5.9 6.8	
171	3145 (728)		$C_{14}F_2H_{12}$	$(C_6H_5)_2CFCH_2F$		20	
171	3146 (730)		$C_{14}F_3H_{11}$	$(C_6H_5)_2CFCHF_2$		12	
862	3147		$C_{14}F_5H_{27}Sn$	$CF_3CF_2Sn(C_4H_9)_3$		1.4	
1133	3148		$C_{14}F_{12}H_{16}N_2$	 Isomer 1 Isomer 2			10.0 10.0
1132	3149	E	$C_{14}F_{13}H_{21}CoP_3$	$[C_5H_5Co[(CH_3)_2PCH_2CH_2P(CH_3)_2]CF_2CF_2CF_3]PF_6$			12.4

Table B.1.a. (contd.)

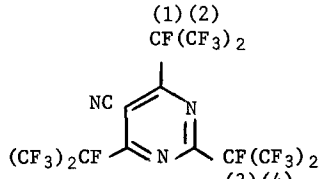
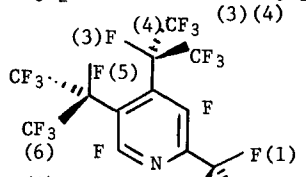
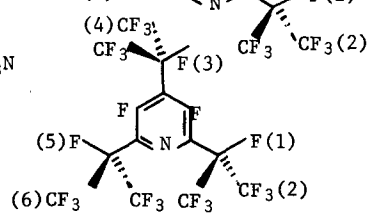
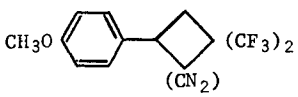
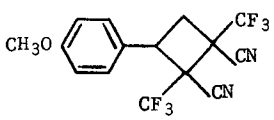
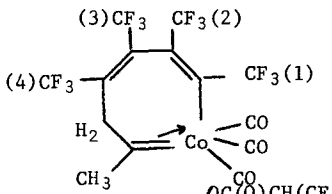
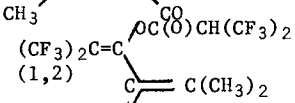
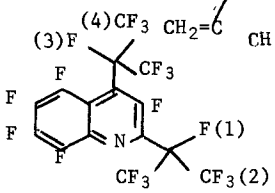
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
945	3150	E	$C_{14}F_{21}N_3$			1,2 5.6 3,4 6.8	
949	3151 (3398 4670)	E	$C_{14}F_{23}N$			1,2 6.5 3,4 7.5 5,6 7.5	
949	3152 (3399 4669)	P	$C_{14}F_{23}N$			1,2 5 3,4 4.5 5,6 5	
234	3153 (2275 4737)		$C_{15}F_3H_{14}N$	$C_6H_5CF_2NFCH(CH_3)C_6H_5$	192		
201	3154		$C_{15}F_6H_{10}N_2O$				10
1136	3155		$C_{15}F_6H_{10}N_2O$	 Isomer 1 Isomer 2			12 10
862	3156		$C_{15}F_7H_{27}Sn$	$CF_3CF_2CF_2Sn(C_4H_9)_3$		~0	9.5
200	3157	H	$C_{15}F_{12}H_7CoO_3$				1,2 14.0 2,3 14.0 3,4 14.0
125	3158 (735)	B	$C_{15}F_{12}H_{12}O_2$				1,2 8.2
933	3159 [3384 3400 4585]		$C_{15}F_{19}N$			1,2 -6.6 3,4 -4.1	

Table B.1.a. (contd.)

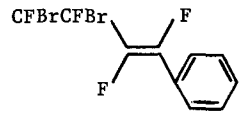
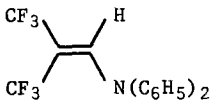
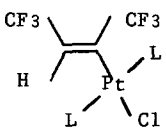
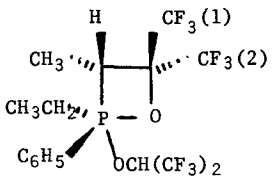
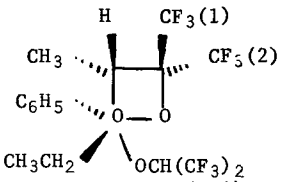
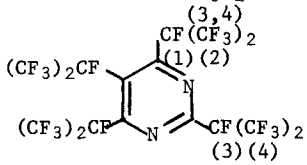
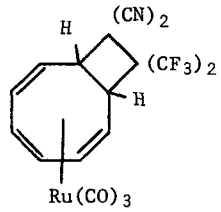
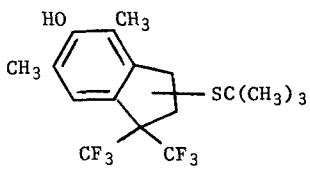
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
938	3160		$C_{16}F_3H_{30}Cl_3O_2Sn$	$CF_2ClC(OCH_3)[OSn(CH_2CH_2CH_2CH_3)_3]CFCl_2$			
					160		17
1137	3161 (3352 3617)		$C_{16}F_4H_{10}Br_2$			28	
210	3162 (893)	A	$C_{16}F_6H_{11}N$				7.9
173	3163 (896 6580)		$C_{16}F_6H_{31}ClP_2Pt$	 $L = P(CH_2CH_3)_3$			12.2
158	3164 (738)	A	$C_{16}F_{12}H_{15}O_2P$				1,2 9.6
158	3165	A	$C_{16}F_{12}H_{15}O_2P$				1,2 9.6 3,4 8.5
945	3166		$C_{16}F_{28}N_2$		1,2 3,4	2.6 3.1 6.9	
202	3167 (739)		$C_{17}F_6H_8N_2O_3Ru$				13
1083	3168	P	$C_{17}F_6H_{20}OS$				0.8

Table B.1.a. (contd.)

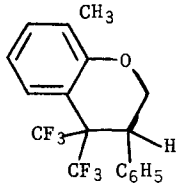
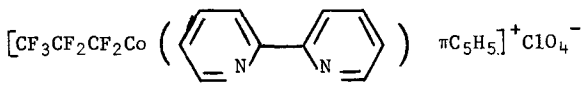
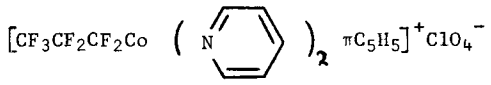
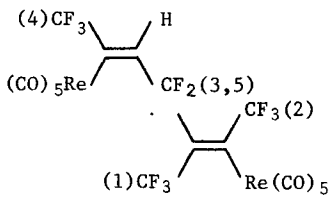
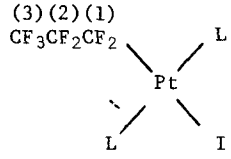
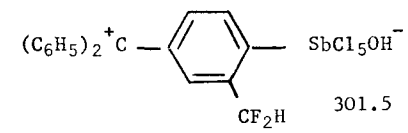
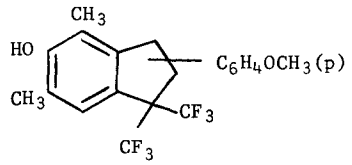
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1083	3169	P	$C_{18}F_6H_{14}O$				~9
821	3170		$C_{18}F_7H_{13}ClCoN_2O_4$				11.9
821	3171		$C_{18}F_7H_{15}ClCoN_2O_4$				15.9
219	3172 (899)		$C_{18}F_{11}HO_{10}Re_2$		3,5 176.0		1,2 1.8 1,3 4.0 3,4 3.7 4,5 1.7
1131	3173		$C_{18}F_{14}H_{10}O_4Ti$	$(C_5H_5)_2Ti(O_2CCF_2CF_2CF_3)_2$			9
1131	3174		$C_{18}F_{14}H_{10}O_4Zr$	$(C_5H_5)_2Zr(O_2CCF_2CF_2CF_3)_2$			9
1132	3175	E	$C_{18}F_{21}H_{21}CoP_3$	$[CF_3CF_2CF_2(CF_2)_4Co[(CH_3)_2PCH_2CH_2P(CH_3)_2]\pi C_5H_5]^+PF_6^-$ (1) (2)			1,2 10
177	3176 (6439 6589)		$C_{19}F_7H_{22}IP_2Pt$	 L = $P(CH_3)_2C_6H_5$	2,3	2.5	1,3 11
178	3177 (748)	M	$C_{20}F_2H_{16}Cl_5OSb$	 301.5			
1083	3178	P	$C_{20}F_6H_{18}O_2$				9.8

Table B.1.a. (contd.

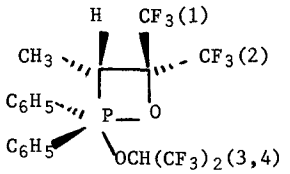
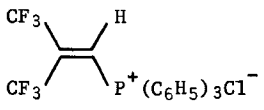
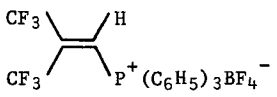
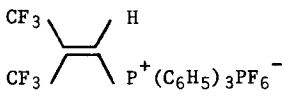
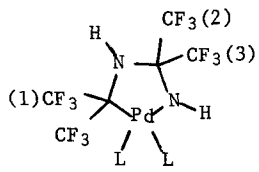
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ
158	3179 (752)	A	$C_{20}F_{12}H_{15}O_2P$				1,2 3,4	10.8 9.1
177	3180 (758 6596)		$C_{21}F_7H_{28}As_2IPt$	$(CH_3)_2PtI(CF_2CF_2CF_3)[As(CH_3)_2C_6H_5]_2$				13
177	3181 (6452 6597)		$C_{21}F_7H_{28}BrP_2Pt$	$(CH_3)_2PtBr(CF_2CF_2CF_3)[P(CH_3)_2C_6H_5]_2$				14
177	3182 (6453 6598)		$C_{21}F_7H_{28}IP_2Pt$	$(CH_3)_2PtI(CF_2CF_2CF_3)[P(CH_3)_2C_6H_5]_2$				14
210 817	3183 (6459)	A	$C_{22}F_6H_{16}ClP$					7.5
210	3184 (6462)	A	$C_{22}F_{10}H_{16}BP$					7.4
210	3185 (6463)	A	$C_{22}F_{12}H_{16}P_2$					7.5
813	3186		$C_{22}F_{12}H_{24}As_2N_2Pd$	 L = $As(CH_3)_2C_6H_5$			1,2 or 1,3	3.0
124	3187 (762 6464)		$C_{23}F_4H_{16}CoO_3$	$CF_2HCF_2Co(CO)_3P(C_6H_5)_3$		5.5		
1077	3188	H	$C_{24}F_7H_{41}CoNI_2$	$[CH_3(CH_2)_3]_4N^+\pi C_5H_5CoI_2(CF_3CF_2CF_2)^-$				10.8
1056	3189 (6487)		$C_{25}F_5H_{20}NiP$	$CF_3CF_2Ni[P(C_6H_5)_3]\pi C_5H_5$		2.3		
210	3190	A	$C_{25}F_6H_{17}N_2P$	$(C_6H_5)_3{}^+PCH_2C(CF_3)_2{}^-C(CN)_2$				1.5

Table B.1.a. (contd.)

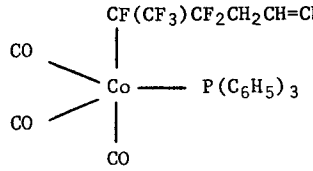
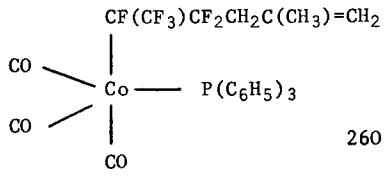
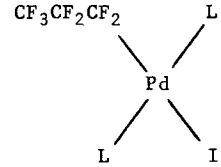
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
177	3191 (763 6602)		$C_{25}F_{15}H_{28}As_2IPt$	$(CH_3)_2PtI(CF_2CF_2CF_2(CF_2)_3CF_3)[As(CH_3)_2C_6H_5]_2$ (1) (2)	1,2		20
1077	3192	H	$C_{26}F_7H_{41}CoN_3$	$[CH_3(CH_2)_3]_4N^+[\pi C_5H_5Co(CN)_2CF_3CF_2CF_2]^-$			11.0
821	3193 (6503)		$C_{26}F_{11}H_{20}CoOP_2\pi C_5H_5Co(CO)[(C_6H_5)_3P]CF_3CF_2{}^+PF_6^-$	(1,2) 1,2 245			
210	3194 (6504)	A	$C_{26}F_{12}H_{17}O_4P$	$(CF_3)_2C{=}CHP^+(C_6H_5)_3(CF_3CO_2)_2^-H$			7.6
1131	3195	E	$C_{26}F_{28}H_{10}Mo_2N_2O_{10}$	$[\pi C_5H_5Mo(NO)(O_2CCF_2CF_2CF_3)_2]_2$			8
821	3196 (6506)		$C_{27}F_5H_{23}ClCoNO_4P$	$[\pi C_5H_5Co(CH_3CN)[(C_6H_5)_3P]CF_3CF_2]^+ClO_4^-$ 238			
200	3197	H	$C_{27}F_6H_{20}CoO_3P$	 270			
821	3198		$C_{27}F_7H_{20}ClCoO_5P$	$[\pi C_5H_5Co(CO)[(C_6H_5)_3P]CF_3CF_2CF_2]^+ClO_4^-$ 246			11.4
819	3199	J	$C_{27}F_7H_{20}FeOP$	$(CF_3)_2CFFe(CO)[P(C_6H_5)_3][\pi C_6H_5]$			6
210	3200	A	$C_{27}F_{12}H_{17}O_2P$	$(CF_3)_2C{=}CHP^+(C_6H_5)_3(CF_3CO)_2^-CH$			7.6
1077	3201	H	$C_{27}F_{21}H_{15}Co_3N_3S_3$	$[\pi C_5H_5Co(SCN)CF_3CF_2CF_2]_3$			{10.1 10.1
200	3202	A	$C_{28}F_6H_{22}CoO_3P$	 260			
823	3203 (6515)	A	$C_{29}F_7H_{26}IP_2Pd$	 L = $PCH_3(C_6H_5)_2$		2.0	

Table B.1.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
938	3204		$C_{30}F_6H_{54}Cl_6O_3Sn_2$	$[[CH_3(CH_2)_3]_3SnOC(CF_2Cl)(CFCl_2)-]_2O$ (1,2) (3)	1,2 160	1,3 / 2,3 } 13 (aw)	
823	3205 (6517)	A	$C_{30}F_7H_{26}IOP_2Pd$	$CF_3CF_2CF_2CO$, L, Pd, L, I; L = $PCH_3(C_6H_5)_2$		2.8	5.1
1132	3206	E	$C_{31}F_7H_{22}FeIO_2P_2$	$CF_3CF_2CF_2Fe(CO)_2I$ [$(C_6H_5)_2P$ $P(C_6H_5)_2$ H H]			12.6
1132	3207	J	$C_{31}F_7H_{22}FeIO_2P_2$	[$(C_6H_5)_2P$ $P(C_6H_5)_2$ H H]		8.0	
1132	3208	E	$C_{31}F_7H_{24}FeIO_2P_2$	$CF_3CF_2CF_2Fe(CO)_2I[(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2]$			12.6
1132	3209	J	$C_{31}F_7H_{24}FeIO_2P_2$	$(CF_3)_2CFFe(CO)I[C_6H_5PCH_2CH_2P(C_6H_5)_2]$		8.0	
819	3210	J	$C_{34}F_7H_{29}FeP_2$	$(CF_3)_2CFFe(\pi C_5H_5)[(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2]$			
1132	3211	E	$C_{34}F_{13}H_{27}CoP_3$	$[CF_3CF_2CF_2Co$ [$(C_6H_5)_2P$ $P(C_6H_6)_2$ H H] $\pi C_5H_5]^+PF_6^-$	12		11.6
1132	3212	E	$C_{34}F_{13}H_{29}CoP_3$	$[CF_3CF_2CF_2Co[(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2]\pi C_5H_5]^+PF_6^-$			13.0
1132	3213	E	$C_{38}F_{21}H_{27}CoP_3$	$[CF_3CF_2CF_2(CF_2)_4Co$ [$(C_6H_5)_2P$ H H $(C_6H_5)_2$] $\pi C_5H_5]^+PF_6^-$ (1) (2)	1,2 11		

Table B.1.a. (contd.)

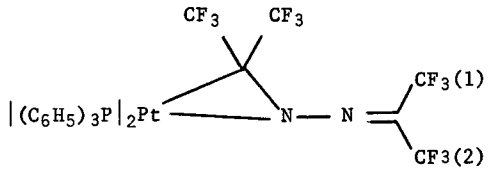
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1132	3214	E	$C_{38}F_{21}H_{29}CoP_3$	$[CF_3CF_2CF_2(CF_2)_4Co[(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2]\pi C_5H_5]^+PF_6^-$ (1) (2)		1,2	10
832	3215 (6556 6631)		$C_{42}F_{12}H_{30}N_2P_2Pt$			1,2	6.0

Table B.1.b. One fluorine bonded to sp^3 carbon, the other to sp^2 carbon

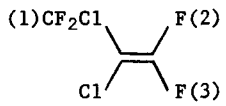
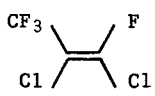
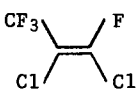
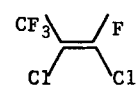
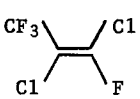
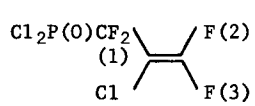
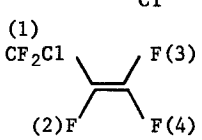
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
565	3216 (3440)		$C_3F_4Cl_2$			1,2 33.8 1,3 7.8	
1040	3217		$C_3F_4Cl_2$			23	
235	3218		$C_3F_4Cl_2$			20	
1041	3219		$C_3F_4Cl_2$			24.3	
1041	3220		$C_3F_4Cl_2$			10.4	
565	3221		$C_3F_4Cl_3OP$			1,2 28.4 1,3 7.2	
1043	3222 (3448)		C_3F_5Cl		1,2 19	1,3 31 1,4 6	

Table B.1.b. (contd.)

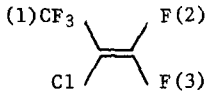
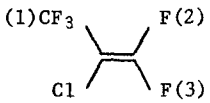
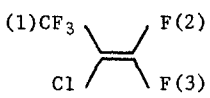
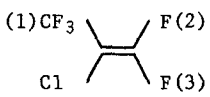
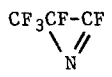
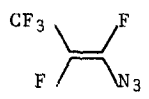
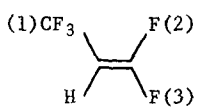
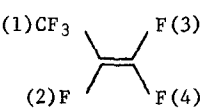
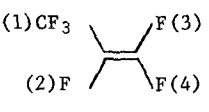
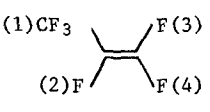
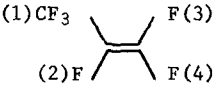
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
235	3223		C_3F_5Cl			1,2 21 1,3 12	
565	3224 (3453)		C_3F_5Cl			1,2 23.4 1,3 9.4	
1040	3225		C_3F_5Cl			1,2 21 1,3 12	
1041	3226 (3451)		C_3F_5Cl			1,2 23.83 1,3 9.20	
904	3227 (2697, 4019)		C_3F_5N		49.1	1.6	
904	3228 (3458)		$C_3F_5N_3$		12	21	
77	3229 [784, 1017, 3460]		C_3F_5H			1,2 17.5 1,3 11.4	
235	3230 (3461)		C_3F_6		1,2 13	1,3 22 1,4 8	
1040	3231 (3462)		C_3F_6		1,2 13	1,3 21 1,4 8	
1041	3232 (3461)		C_3F_6		1,2 13.2	1,3 22.0 1,4 8.7	
1044	3233 (3462)		C_3F_6		1,2 13	1,3 21	

Table B.1.b. (contd.)

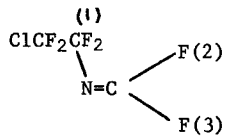
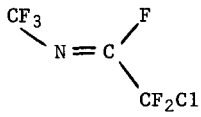
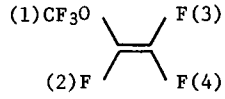
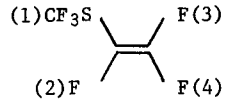
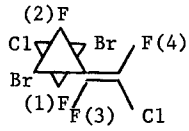
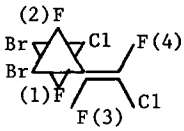
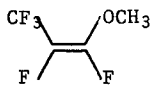
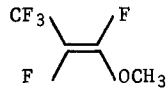
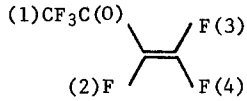
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
1045	3234 (3456)	P	C_3F_6ClN	 (-35°)		1,2 18.0 1,3 ~0	
1045	3235	P	C_3F_6ClN	 (-70°)	7.0	13.0	
1046	3236 (3467)		C_3F_6O			1,2 3.5	1,3 3.5 1,4 <0.5
1046	3237 (3468)		C_3F_6S			1,2 1.9	1,3 2.3 1,4 2.8
954	3238 (2787 3475)		$C_4F_4Br_2Cl_2$ erythro		2,3 -26.63	1,3 +12.15 2,4 +53.18	1,4 +3.18
			threo		2,3 -27.09	1,3 +15.58 2,4 +53.28	1,4 +3.69
1047	3239 (3481)		$C_4F_5H_3O$		12.9	9.4	
1047	3240 (3482)		$C_4F_5H_3O$		12.9	22.6	
1048	3241 (3488)	B	C_4F_6O			1,2 14	1,3 6 1,4 0

Table B.1.b. (contd.)

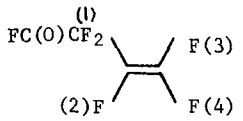
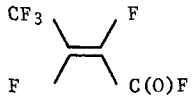
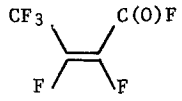
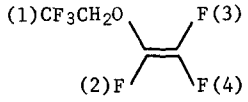
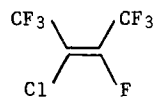
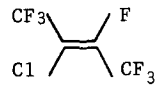
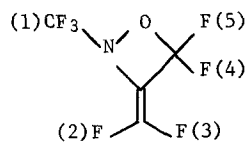
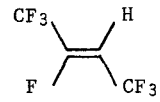
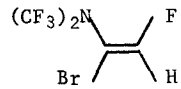
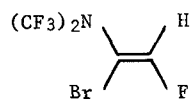
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
1049	3242 (3439 3649)	B	C_4F_6O		1,2	15.7	1,3 1,4	24.9 6.8		
1049	3243 (3490 3650)	B	C_4F_6O			7.7		21.1		
1049	3244 (3491 3651)	B	C_4F_6O			7.3		11.9		
1046	3245 (917 3492)		$C_4F_6H_2O$						1,2 1,3 1,4	1.5 2.2 <0.5
1068	3246 (2802)		C_4F_7Cl			7.74		8.67		
1068	3247 (2803)		C_4F_7Cl			5.49		24.72		
1050	3248		$C_4F_7ClN_2$	$CF_3N{=}CFCF{=}NCF_2Cl$ (1) (2) (3) (4)			1,2 4,3	14.1 15.6		
988 989	3249 [2805 3494 4089 4099]		C_4F_7NO				5,2 4,2 5,3 4,3	5.3 5.3 4.5 4.5	1,2 1,3	7.0 <0.5
206	3250 (798 1022)	B	C_4F_7H			9.25		17.0		
101	3251 (1023)		C_4F_7HBrN							3.4
101	3252 (1024)		C_4F_7HBrN							0.9

Table B.1.b. (contd.)

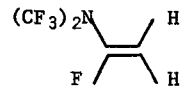
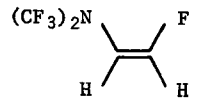
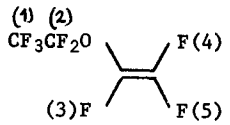
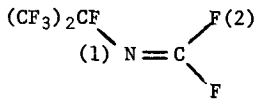
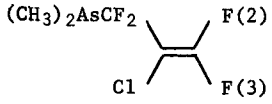
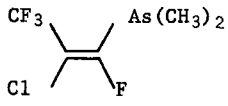
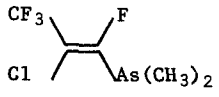
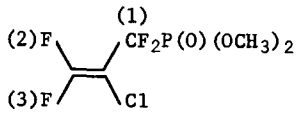
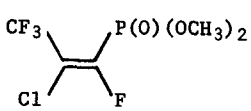
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
37	3253 (1027)		$C_4F_7H_2N$			2.5	
101	3254 (1025, 799)		$C_4F_7H_2N$				5.1
1050	3255		$C_4F_8N_2$	$CF_3N{=}CFCF{=}NCF_3$		14.2	
1046	3256 (3500)		C_4F_8O			2,3 6.0	1,3 0.7 1,5 <0.5 1,4 0.7 2,4 5.7 2,5 0.6
994	3257 (2827, 3504)		C_4F_9N			1,2 24.6	
1002	3258		C_4F_9N	$CF_3CF_2CF{=}NCF_3$ (1)(2)(3)(4)	1,3 13.3	2,3 5.0 4,3 13.4	
768	3259 (3510)		$C_5F_4H_6AsCl$			1,2 26.8 1,3 8.0	
768	3260		$C_5F_4H_6AsCl$			7.4	
768	3261		$C_5F_4H_6AsCl$			24.2	
565	3262 (3511, 6098)		$C_5F_4H_6ClO_3P$			1,2 27.3 1,3 7.4	
768	3263 (6100)		$C_5F_4H_6ClO_3P$			8.3	

Table B.1.b. (contd.)

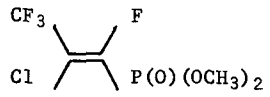
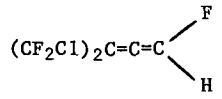
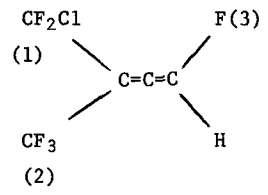
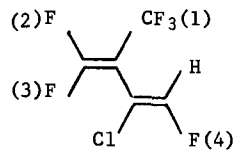
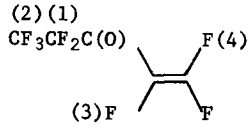
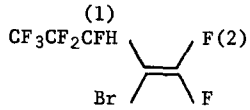
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J		^nJ
768	3264 (6099)		$C_5F_4H_6ClO_3P$			24.6		
192	3265 (803 1039)		$C_5F_5HCl_2$					5.8
192	3266 (806 1042)		C_5F_6HCl				1,3 2,3	5.8 5.5
192	3267 (1043)		C_5F_6HCl			1,2 1,3	21.1 10.3	1,4	0.7
192	3268		C_5F_7Cl	$(CF_3)_2C{=}C{=}CFCl$					3.5
192	3269 (893 1045)		C_5F_7H	$(CF_3)_2C{=}C{=}CFH$					5.4
208	3270 (2865 3513)	P	C_5F_8	$CF_3CF_2CF{=}C{=}CF_2$ (-80^o)	23.0	5.8			6.0
1048	3271 (3516)	B	C_5F_8O			1,3	22	1,4 2,3	8 7
190	3272 [371 2869 3518]	P	C_5F_8HBr			1,2	14		

Table B.1.b. (contd.)

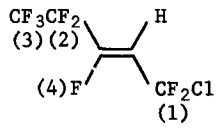
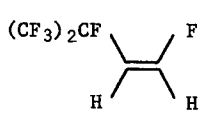
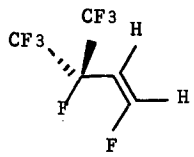
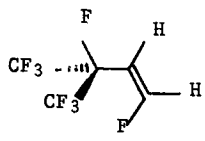
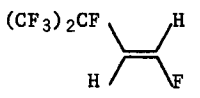
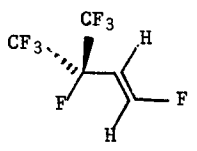
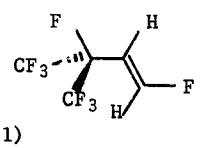
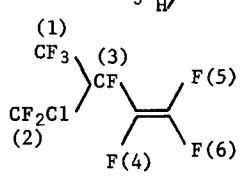
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
208	3273 [814 1046 2871]	P	C_5F_8HCl		2,4	12.7	1,4 3,4	21.7 6.2		
209	3274 [815 1047 2872]	*	$C_5F_8H_2$					30.8		5.8
								32.5		3.9
								2.6		39
209	3275	*	$C_5F_8H_2$					5.3		0.6
								∓9.8		
								±14.9		
1000	3276 (2876 3519)	B*	C_5F_9Cl		3,4	∓12.8	1,4 2,4 3,5 3,6	8.6 8.6 11.0 ±44.4 ±2.0	1,5 1,6 2,5 2,6	3.0 0.85 3.0 0.85

Table B.1.b. (contd.)

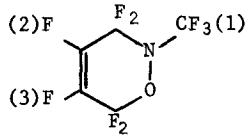
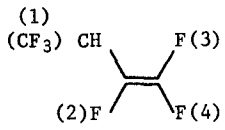
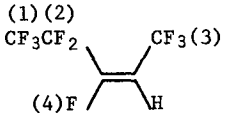
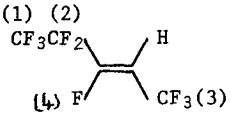
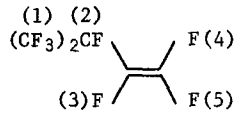
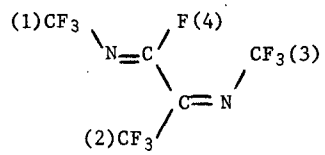
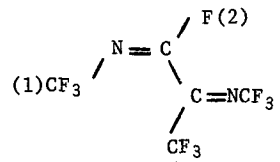
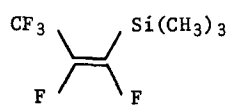
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
988	3277 (4101)		C_5F_9NO						1,2 1,3	0.8 <0.5
118	3278 (374 3520)	G	C_5F_9H				1,2	7.1	1,3 1,4	1.9 0.9
190	3279 [817 1049 2880]		C_5F_9H		2,4	10.5	1,4 3,4	7.9 11.4		
190	3280 [818 1050 2881]		C_5F_9H		2,4	12.6	1,4 3,4	6.6 18.0		
1000	3281 (2886 3521)	B*	C_5F_{10}		2,3	∓13.0	1,3 2,4 2,5	8.6 ±43.5 ±2.7	1,4 1,5	3.6 0.85
10	3282 (2887 3522)		$C_5F_{10}N_2$	$CF_3N{=}CFCF(CF_3)N{=}CF_2$ (1) (2)			1,2	13.3		
1050	3283		$C_5F_{10}N_2$				1,4 2,4	14.3 ∿0	3,4	7.7
1050	3284		$C_5F_{10}N_2$				1,2	6.0		
1051	3285 (3537)		$C_6F_5H_9Si$		13.5			7.3		

Table B.1.b. (contd.)

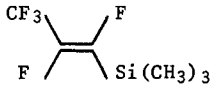
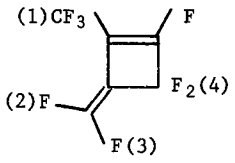
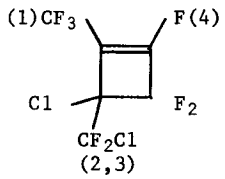
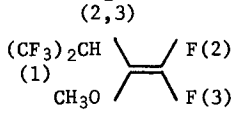
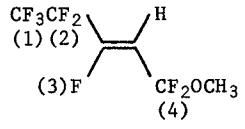
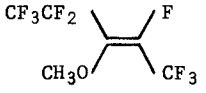
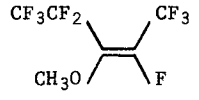
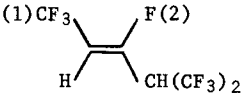
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
1051	3286 (3538)		$C_6F_5H_9Si$		22	10.5	
1052	3287 [2920, 3543, 3754]		C_6F_8				1,2 5.8 1,3 0.8 3,4 1.3
1052	3288 (2924, 3756)		$C_6F_8Cl_2$			1,4 9.5	2,4 1.4 3,4 1.4
118	3289 (952, 2928)	B	$C_6F_8H_4O$				1,2 2.2 1,3 1.0
190	3290 [831, 1082, 2995]	B-P	$C_6F_8H_4O$		2,3 13.6	1,3 6.4 4,3 17.4	
194	3291 (426, 2929)		$C_6F_9H_3O$		7.7	27.5	10.0
194	3292		$C_6F_9H_3O$		4.9		
634	3293 (3546, 5568)		$C_6F_{10}Hg$	$[CF_2=C(CF_3)]_2Hg$		{12.4, 16.6}	
113	3294 [427, 835, 953, 1083]		$C_6F_{10}H_2$			1,2 18	
634	3295 [431, 3547, 5569]		$C_6F_{11}HHg$	$CF_2=C(CF_3)HgCH(CF_3)_2$		{12.4, 16.6}	

Table B.1.b. (contd.)

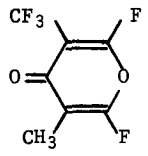
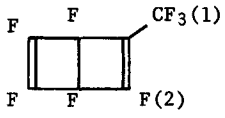
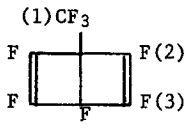
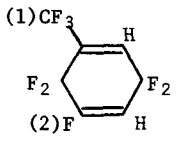
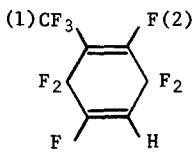
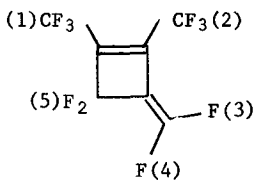
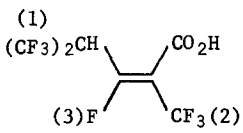
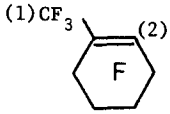
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
125	3296		$C_7F_5H_3O_2$			24.4	
284	3297 (2967, 3765)	P	C_7F_8				1,2 9.9
284	3298 (2968)	P	C_7F_8				1,2 2.9 1,3 0.9
213	3299 [852, 1333, 2969, 3940]		$C_7F_8H_2$				1,2 1
213	3300 [1334, 2970, 3949]		C_7F_9H				1,2 17.9
1023	3301 (2973, 3553)		C_7F_{10}				1,3 1.4 1,4 1.2 2,3 8.5 2,4 - 3,5 1.9 4,5 2.8
113	3302 (488, 955)		$C_7F_{10}H_2O_2$				1,3 7.9 2,3 31
213	3303 (2977, 3957)		C_7F_{12}				1,2 14.0

Table B.1.b. (contd.)

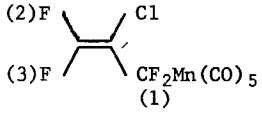
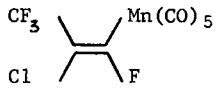
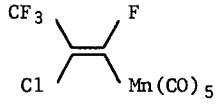
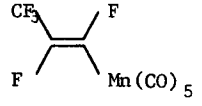
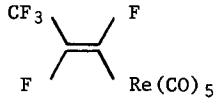
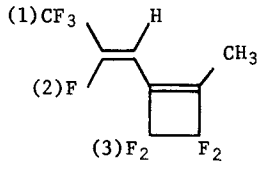
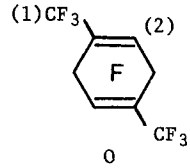
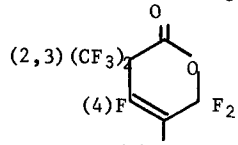
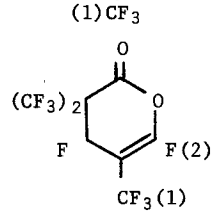
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J	^nJ
768	3304 (3561)		$C_8F_4ClMnO_5$			1,2 1,3	6.5 32.1	
768	3305		$C_8F_4ClMnO_5$	 (Tenative assignment)			8.8	
768	3306		$C_8F_4ClMnO_5$				24.3	
1040 1044	3307 (3563)		$C_8F_5MnO_5$		12		23	
1044	3308 (3565)		$C_8F_5O_5Re$		13		24	
198	3309 (956 1101)		$C_8F_8H_4$		9.8			2,3 12.8
213	3310 (3029 3980)		C_8F_{12}			1,2	18.8	
113	3311 (3031 4049)		$C_8F_{12}O_2$			1,4 2,4 3,4	20 13 13	
113	3312 (3032 4048)		$C_8F_{12}O_2$			1,2	22	

Table B.1.b. (contd.)

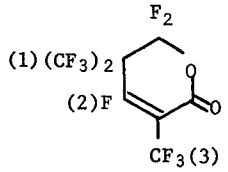
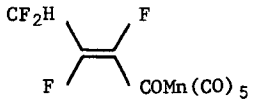
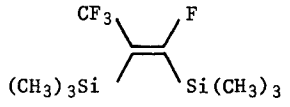
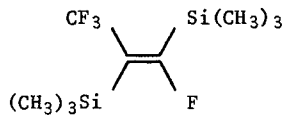
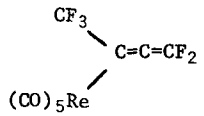
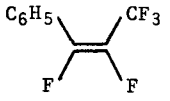
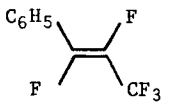
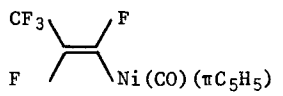
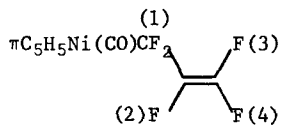
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J	^nJ
113	3313 (3033 4047)		$C_8F_{12}O_2$			1,2 2,3	10 28	
199	3314 [604 964 3580]	A	$C_9F_4HMnO_6$		18.6			
1051	3315		$C_9F_4H_{18}Si_2$				7.9	
1051	3316		$C_9F_4H_{18}Si_2$				8.4	
219	3317		$C_9F_5O_5Re$					4.0
1055	3318 (3584)		$C_9F_5H_5$			9	13	
1055	3319 (3585)		$C_9F_5H_5$			10	23	
1056	3320 (3587)		$C_9F_5H_5NiO$			12	20	
1056	3321 (3586)		$C_9F_5H_5NiO$		1,2	19	1,3 1,4	32 6

Table B.1.b. (contd.)

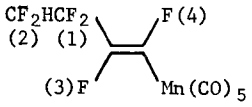
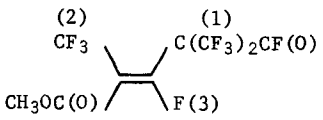
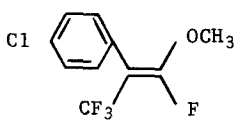
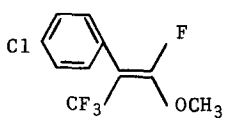
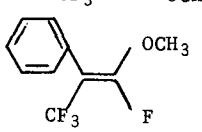
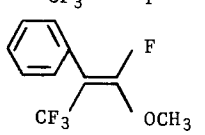
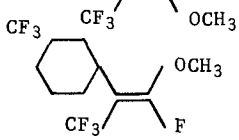
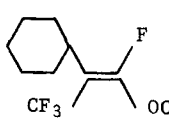
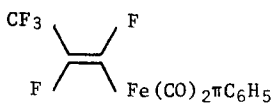
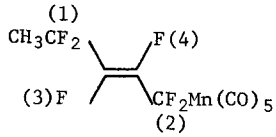
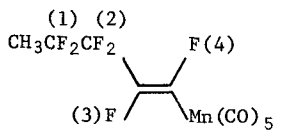
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
1057	3322	A	$C_9F_6HMnO_5$		1,3	12	1,4	27	2,4	6
	(608, 3588)						2,3	6		
113	3323		$C_9F_{11}H_3O_3$				1,3	12		
	(3661)						2,3	28		
233	3324	B	$C_{10}F_4H_7ClO$					24		
	(968)									
233	3325	B	$C_{10}F_4H_7ClO$					13		
	(968)									
233	3326	B	$C_{10}F_4H_8O$					24		
	(969)									
233	3327	B	$C_{10}F_4H_8O$					13		
	(969)									
233	3328	B	$C_{10}F_4H_{14}O$					27		
	(970)									
233	3329	B	$C_{10}F_4H_{14}O$					13		
	(970)									
1040	3330		$C_{10}F_5H_5FeO_2$			13		22		
1056	(3594)									
164	3331		$C_{10}F_6H_3MnO$		1,3	13.5	2,3	33.5		
	[652, 971, 3082, 3595]				2,4	20.0				
164	3332		$C_{10}F_6H_3MnO_5$		2,3	12.9	1,3	5.5	1,4	5.5
	[653, 972, 3596]						2,4	25.8		

Table B.1.b. (contd.)

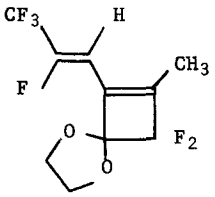
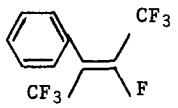
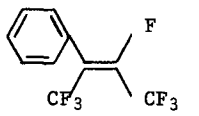
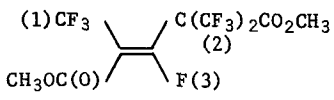
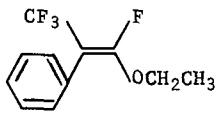
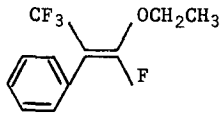
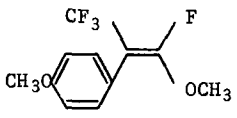
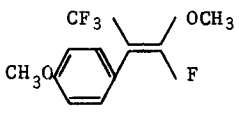
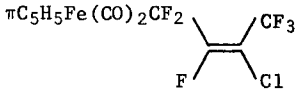
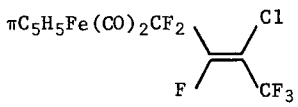
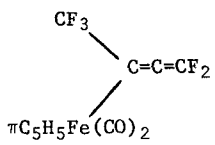
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
198	3333 (1117)		$C_{10}F_6H_8O_2$		10.8		
1055	3334		$C_{10}F_7H_5$		7	28	
1055	3335 (3093)		$C_{10}F_7H_5$		7	12	
113	3336		$C_{10}F_{10}H_6O_4$			1,3 24 2,3 12	
1058	3337		$C_{11}F_4H_{10}O$			25	
1058	3338		$C_{11}F_4H_{10}O$			13	
233	3339 (975)	B	$C_{11}F_4H_{10}O_2$			24	
233	3340 (975)	B	$C_{11}F_4H_{10}O_2$			13	
768	3341		$C_{11}F_5H_5ClFeO_2$			8.7	
768	3342		$C_{11}F_5H_5ClFeO_2$			23.6	
219	3343		$C_{11}F_5H_5FeO_2$				4.0

Table B.1.b. (contd.)

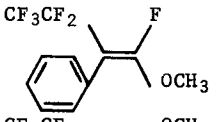
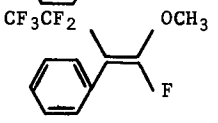
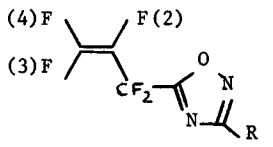
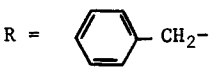
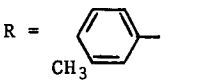
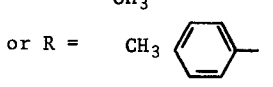
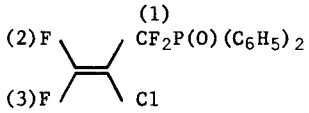
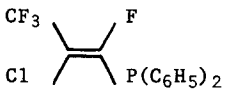
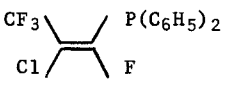
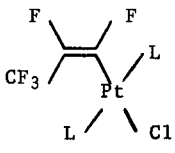
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
233	3344 (976)	B	$C_{11}F_6H_8O$			26	
233	3345 (976)	B	$C_{11}F_6H_8O$			10	
1000	3346 (3605)	B*	$C_{12}F_5H_7N_2O$	    same couplings to within ±0.2 Hz	1,2 ±18.7	1,4 ±26.2 1,3 ±6.6	
565	3347 (3613, 6370)		$C_{15}F_4H_{10}ClOP$			1,2 27.9 1,3 7.5	
768	3348 (6372)		$C_{15}F_4H_{10}ClP$			23.7	
768	3349 (6371)		$C_{15}F_4H_{10}ClP$			8.9	
173	3350 [3615, 6373, 6575]		$C_{15}F_5H_{30}ClP_2Pt$	 L = $P(CH_2CH_3)_3$	15.3		9.3

Table B.1.b. (contd.)

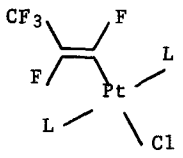
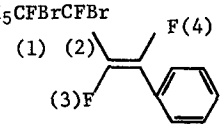
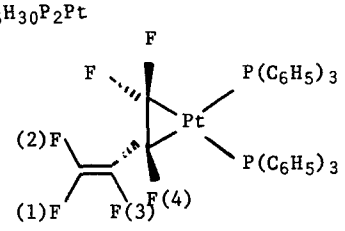
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
173	3351 [3616 6374 6576]		$C_{15}F_5H_{30}ClP_2Pt$			13.3		21.3		
				L = $P(CH_2CH_3)_3$						
1137	3352 (3161 3617)		$C_{16}F_4H_{10}Br_2$	$C_6H_5CFBrCFBr$ 	2,3	28	2,4 1,3	60 25	1,4	6
807	3353 (3642 6625)	A	$C_{40}F_6H_{30}P_2Pt$		3,4	23.0	1,4 2,4	7.2 29.5		

Table B.1.c. One fluorine bonded to sp^3 carbon, the other to an aromatic ring.

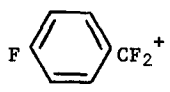
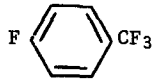
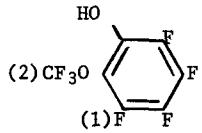
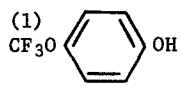
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^5J	^nJ
61	3354 (1090 1837)	C[2]	$C_7F_3H_4^+$				19.8
61	3355 (846 1841)		$C_7F_4H_4$				1.8
892	3356 (4253)	B	$C_7F_7HO_2$			1,2 9.2	
892	3357 (4255)	B	$C_7F_7HO_2$			1,2 9.0	

Table B.1.c. (contd.)

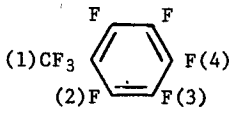
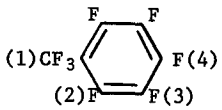
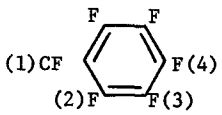
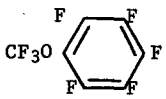
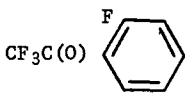
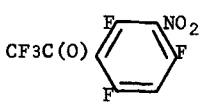
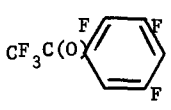
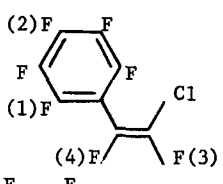
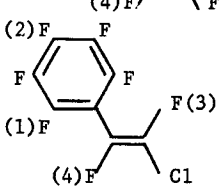
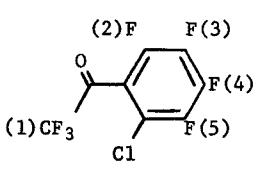
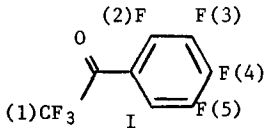
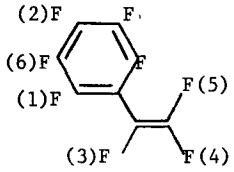
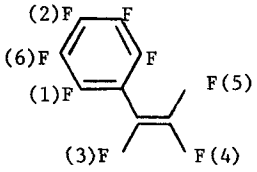
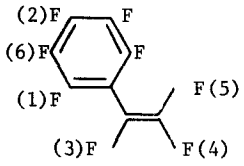
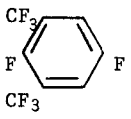
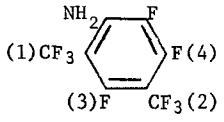
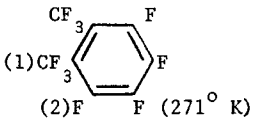
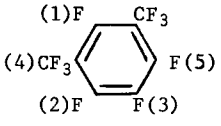
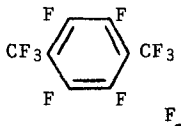
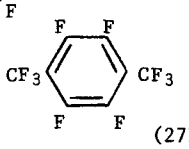
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^4J		^5J		^nJ
434	3358	A-B	C_7F_8		1,2	22.75	1,3	1.3	1,4	1.3
438	3359 (4399)		C_7F_8			22.5				
1053 1054	3360	B	C_7F_8	 (302°K)		22.71				
197	3361 (4405)	B	C_7F_8O					7.2		
401	3362 (862)		$C_8F_4H_4O$					12.70		
401	3363 (863)		$C_8F_6HNO_3$					22.62		1.2
401	3364 (864)		$C_8F_6H_2O$					13.30		0.6
896	3365 (3568)		C_8F_7Cl		1,4	4.9	1,3	2.6	2,4	3.7
896	3366 (3569)		C_8F_7Cl		1,4	7.2	1,3	11.7	2,4 2,3	2.8 1.9
401	3367		C_8F_7ClO				1,2	32.17	1,3 1,4 1,5	0.5 1.3 1.3

Table B.1.b. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^5J		^nJ	
401	3368		C_8F_7IO				1,2	34.18	1,3 1,4 1,5	0.5 1.6 1.2
896	3369 (3571)		C_8F_8		1,3	7.1	1,4	2.3	2,3	3.7
1073	3370 (3572 4418)	B	C_8F_8				1,4 1,5	2.5 10.5	2,4 2,5 2,3	1 1.5 3.5
929	3371 (3573 4417)	*	C_8F_8		1,3	+7.1	6,3 1,4 1,5	-0.8 +2.2 +10.4	2,3 6 4 2,4 6,5 2,5	+3.2 +0.2 +0.8 -0.4 +1.5
876	3372 (1917 4152)		$C_8F_8H_2$			13.9				
419	3373 (4191)		$C_8F_9H_2N$		1,3 2,3 2,4	26.3 22.9 21.8				
1054	3374 (4263)	B	C_8F_{10}		1,2	35.27				
876 419	3375 (4264)		C_8F_{10}		1,4 2,4	23.7 23.9			5,4	0.3
419	3376 (4265)		C_8F_{10}			22.7		0.4		
1054	3377	B	C_8F_{10}			22.40				

(271°K)

Table B.1.b. (contd.)

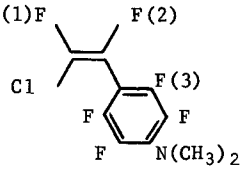
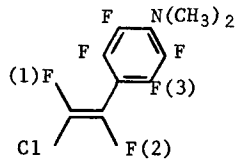
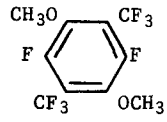
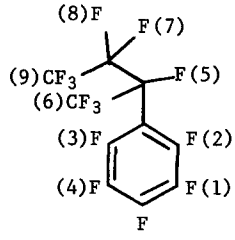
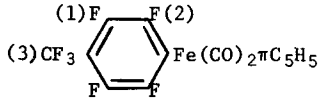
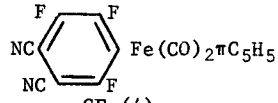
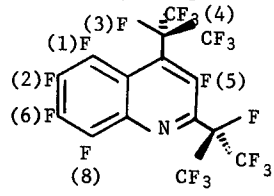
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^4J		^5J		^nJ
896	3378 (2104 3597)		$C_{10}F_6H_6ClN$		2,3	5.5	1,3	2.5		
896	3379 (2105 3598)		$C_{10}F_6H_6ClN$		2,3	7.2	1,3	11.7		
419	3380 (2027 4153)		$C_{10}F_8H_6O_2$			28.6		0.5		
933	3381 3100 4436		$C_{10}F_{14}$		2,5 3,5	+104 0	1,5 4,5 2,6 3,6	0 3.4 4 28.8	1,6 4,6 2,7 3,7 2,8 3,8 1,7 4,7 1,8 4,8 2,9 3,9 1,9 4,9	0 0 +3.8 +33.7 +1.8 +25.5 0 0 0 0 +2.2 1.0 0 0
434	3382 (4297)		$C_{14}F_7H_5FeO_2$		1,3	21.3	2,3	0		
434	3383		$C_{15}F_3H_5FeN_2O_2$			28.05		11.5		7.3
933	3384 [3159 3400 4585]	B-P	$C_{15}F_{19}N$		1,3	+196.4	1,4 2,3	+13.7 +1.4		

Table B.1.b. (contd.)

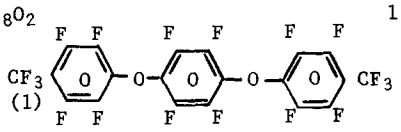
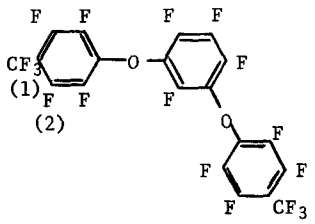
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^4J	^5J	^nJ
903	3385	E	$C_{20}F_{18}O_2$		1,2	22		
903	3386 (4306)	E	$C_{20}F_{18}O_2$		1,2	24		

Table B.1.d. One fluorine bonded to sp^3 carbon, the other to a heteroaromatic ring.

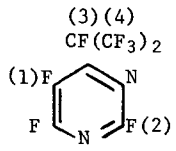
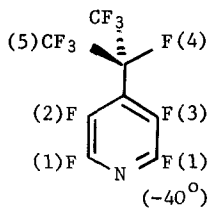
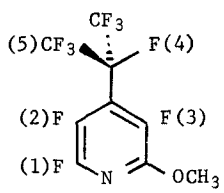
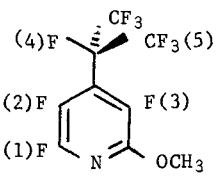
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^4J	^5J	^nJ
945	3387 (2974 4646)	B	$C_7F_{10}N_2$		1,3	50.0	1,4 2,4	5.1 2.3
933 949 1078	3388 (4651)	E	$C_8F_{11}N$		2,4 3,4	0 86	1,4 3,5 2,5	2.5 3.1 20
933 949	3389 [3071 3072 4653]	B	$C_9F_{10}H_3NO$		2,4 3,4	0 83	1,4 3,5	2.5 3.0
					2,4 3,4	86 0	1,4 3,5	0 22.0

Table B.1.d. (contd.)

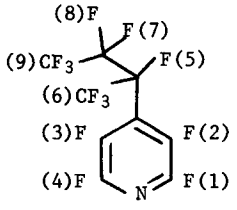
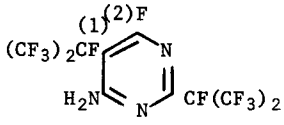
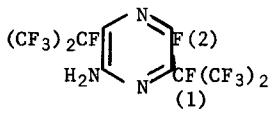
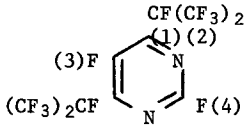
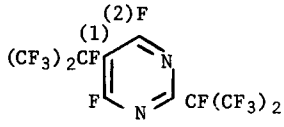
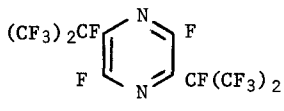
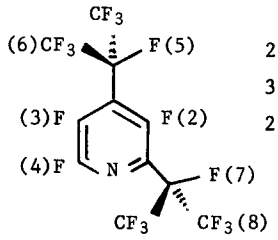
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^4J		^5J		^nJ
933	3390 (4655)		$C_9F_{13}N$		2,5	+94.5	1,5	0	1,6	0
					3,5	0	4,5	3.5	4,6	0
							2,6	4.2	2,7	4
							3,6	27.9	3,7	0
									2,8	2
									3,8	0
									1,7	0
									1,8	0
									2,9	+1.5
									3,9	1.0
									1,9	0
									4,9	0
957	3391 (3102)	E	$C_{10}F_{15}H_2N_3$		1,2	26				
957	3392 (3103)	E	$C_{10}F_{15}H_2N_3$		1,2	46	1,2	46	1,2	46
945	3393 (3105 4657)		$C_{10}F_{16}N_2$		1,3	56.0	2,3	5.6		
							1,4	1.7		
957	3394 (3106)	E	$C_{10}F_{16}N_2$		1,2	27				
957	3395 (3104)	E	$C_{10}F_{16}N_2$			47				
949 1078	3396 (3117 4665)	B-E	$C_{11}F_{17}N$		2,5	95	2,5	-		
					3,5	0	3,6	21		
					2,7	60	2,8	6		
							4,5	2.5		

Table B.1.d. (contd.)

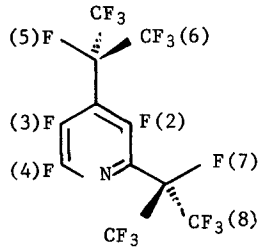
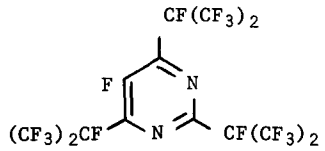
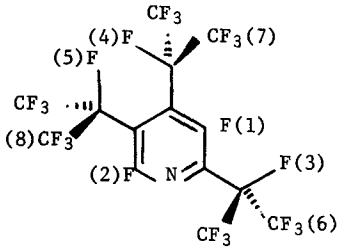
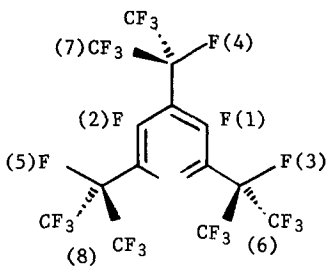
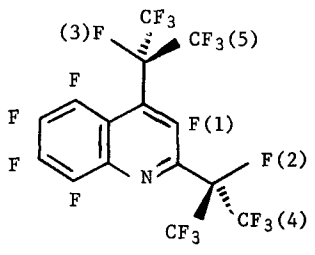
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^5J		^nJ
					2,5	0	2,6	20	
					3,5	83	3,6	-	
					2,7	60	2,8	6	
							4,5	0	
				(-40°)					
945	3397 (3144)		$C_{13}F_{22}N_2$			56.0			5.1
949 1078	3398 (3151 4670)	P	$C_{14}F_{23}N$		1,3	58	1,6	7	
					1,4	0	1,7	32	
					2,5	-	2,8	32	
							2,4	0	
949 1078	3399 (3152 4669)	B-E	$C_{14}F_{23}N$		1,3	57.5	1,6	4.5	
					1,4	92	2,8	4.5	
					2,4	0	2,7	19.8	
					2,5	57.5			
				(-30°)					
933	3400 [3159 3384 4585]	B-P	$C_{15}F_{19}N$		1,2	+61.0	1,4	+7.1	
					1,3	-5.0	1,5	+28.0	

Table B.1.e. One fluorine bonded to sp^3 carbon, the other to sp carbon.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J	^5J	^nJ
1049 1059	3401 (5448)		C_3F_4	$CF_3C{\equiv}CF$	4.3		

Table B.1.f. Both fluorines bonded to sp^2 carbon (both non carbonyl)

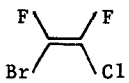
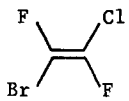
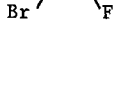
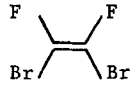
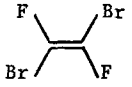
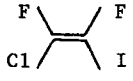
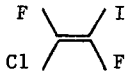
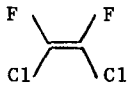
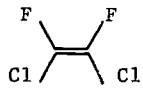
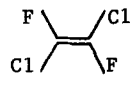
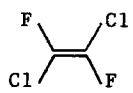
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
958	3402 (4688)		CF_3N	$CF_2{=}NF$	52.6		
805	3403		C_2F_2BrCl	$CF_2{=}CBrCl$	30.3		
1060	3404		C_2F_2BrCl			36.2	
1060	3405		C_2F_2BrCl			135.9	
240	3406 (5413)		$C_2F_2Br_2$	 		34.3	
240	3407 (5414)		$C_2F_2Br_2$			141.4	
1060	3408		C_2F_2ClI			30.5	
1060	3409		C_2F_2ClI			143.4	
620	3410 (5418)		$C_2F_2Cl_2$			37.50	
621	3411 (5420)	B	$C_2F_2Cl_2$			+37.9	
620	3412 (5421)		$C_2F_2Cl_2$			129.57	
621	3413 (5423)	B	$C_2F_2Cl_2$			-129.7	

Table B.1.f. (contd.)

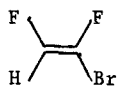
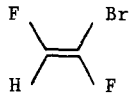
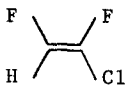
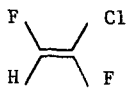
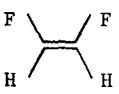
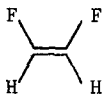
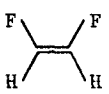
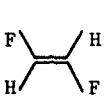
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
240 1061	3414 (996)		C_2F_2HBr	$CF_2=CHBr$	34.5		
240	3415 (995)		C_2F_2HBr			8.4	
240	3416		C_2F_2HBr			137.3	
235	3417 (997)		C_2F_2HCl	$CF_2=CHCl$	41		
184	3418 (998)	B	C_2F_2HCl	$CF_2=CHCl$	42.3		
1060	3419		C_2F_2HCl			11.5	
1060	3420		C_2F_2HCl			132.3	
184	3421 (999)		C_2F_2HI	$CF_2=CHI$	27.3		
235	3422 (1003)		$C_2F_2H_2$	$CF_2=CH_2$	37		
1061	3423		$C_2F_2H_2$	$CF_2=CH_2$	36.4		
242	3424 (1001)		$C_2F_2H_2$			18.6	
1062	3425		$C_2F_2H_2$			-18.7	
241	3426 (1000)		$C_2F_2H_2$			±18.7	
1062			$C_2F_2H_2$			132.7	

Table B.1.f. (contd.)

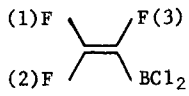
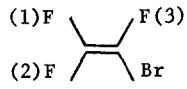
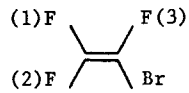
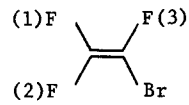
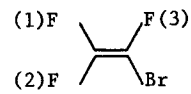
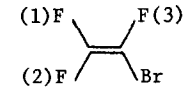
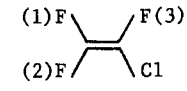
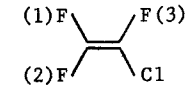
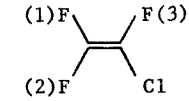
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
241	3427 (1002)		$C_2F_2H_2$					±124.8		
1063	3428		$C_2F_3BCl_2$		1,2	7	1,3 2,3	19 114		
235	3429		C_2F_3Br		1,2	75	1,3 2,3	57 124		
1061	3430		C_2F_3Br		1,2	71.3				
842	3431	B	C_2F_3Br	 (−105°)	1,2	73.7	1,3	56.6	2,3	122.8
		Q				71.7		56.4		123.1
		E^4				73.6		56.7		123.2
		P				73.3		56.8		123.4
		D^2				73.8		55.1		122.6
		Z^3				74.3		56.0		122.7
		R				73.8		56.0		123.1
		E^2				74.5		55.9		122.9
		J^2				73.9		55.9		122.9
		F^4				74.2		55.1		122.6
		E				74.9		54.9		122.5
		A^4				74.4		55.4		122.6
		M				74.6		54.9		121.9
		V^4				73.3		56.5		123.2
		W^4				74.3		53.7		122.5
		X^4				72.1		55.8		122.4
		Y^4				73.1		56.1		123.0
1046	3422		C_2F_3Br			73		57		123
235	3423		C_2F_3Cl		1,2	78	1,3 2,3	58 115		
1046	3424		C_2F_3Cl		1,2	78	1,3 2,3	58 115		
1061	3425		C_2F_3Cl		1,2	78				

Table B.1.f. (contd.)

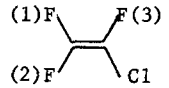
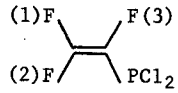
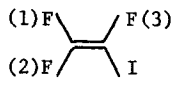
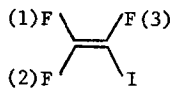
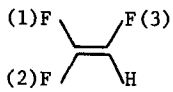
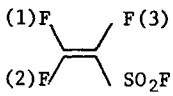
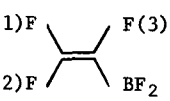
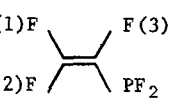
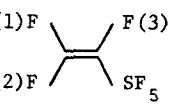
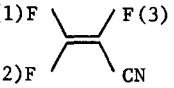
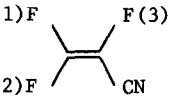
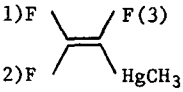
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1044	3426		C_2F_3Cl		1,2 78	1,3 58 2,3 115	
726 227	3427 (5848)		$C_2F_3PCl_2$		1,2 ±39.1	1,3 ±32.0 2,3 ∓123.4	
1060	3428		C_2F_3I			1,3 52.3 2,3 129.2	
1046	3429		C_2F_3I		1,2 65.3	1,3 52.2 2,3 127	
1046 1061	3430 (1004 1005)		C_2F_3H		1,2 87	1,3 33 2,3 119	
1001	3451		$C_2F_4N_2$	$CF_2=N-N=CF_2$	65		
186	3432 (4809)		$C_2F_4O_2S$		1,2 15.3	1,3 42.4 2,3 121.5	
1063	3433		C_2F_5B		1,2 18	2,3 117	
1001	3434		C_2F_5N	$CF_2=NCF_3$	82.0		
726 227	3435 (4761 5864)		C_2F_5P		1,2 ±42.5	1,3 ±31.0 2,3 ∓123.5	
972	3436 (4824 5036)	*	C_2F_8S		1,2 52.5	1,3 ±57.2 2,3 ∓117.6	
235	3437		C_3F_3N		1,2 27	1,3 35 2,3 118	
1046	3438		C_3F_3N		1,2 28.4	1,3 35.2 2,3 117	
243	3439		$C_3F_3H_3Hg$		1,2 +81.2	1,3 +36.5 2,3 -107.1	
565	3440 (3216)		$C_3F_4Cl_2$	$CF_2=CClCF_2Cl$	14.6		

Table B.1.f. (contd.)

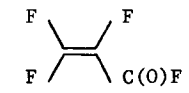
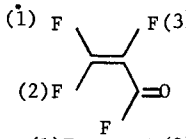
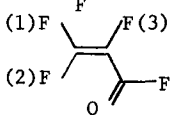
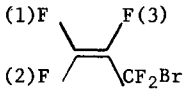
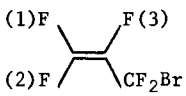
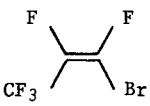
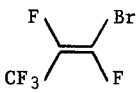
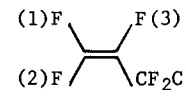
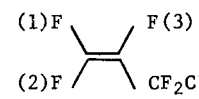
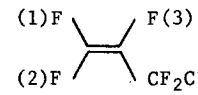
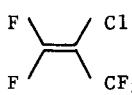
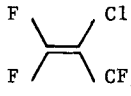
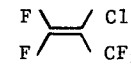
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
565	3441 (5932)		$C_3F_4Cl_3OP$	$CF_2=CClCF_2P(O)Cl_2$		6.6			
1061	3442		C_3F_4O			6.6			
857 1042 1046	3443 (3646)		C_3F_4O		1,2	4.0	1,3 2,3	33.7 111	
					1,2	<2	1,3 2,3	36.2 117	
1061	3444		C_3F_5Br		1,2	55.0			
1046	3445		C_3F_5Br		1,2	54.7	1,3 2,3	38.0 115	
1060	3446		C_3F_5Br						18.4
1060	3447		C_3F_5Br						141.6
1040 1043	3448 (3222)		C_3F_5Cl		1,2	56	1,3 2,3	39 118	
1061	3449		C_3F_5Cl		1,2	56			
1046	3450		C_3F_5Cl		1,2	57.0	1,3 2,3	39.0 116	
1041	3451 (3226)		C_3F_5Cl			16.65			
1061	3452		C_3F_5Cl			16.7			
565	3453 (3224)		C_3F_5Cl			17.2			

Table B.1.f. (contd.)

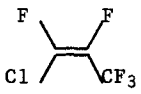
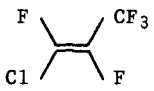
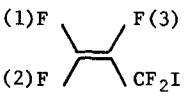
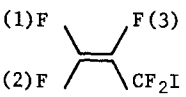
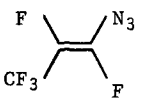
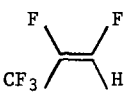
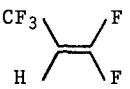
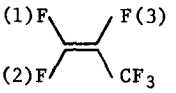
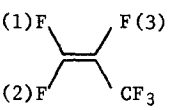
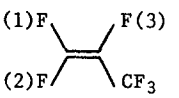
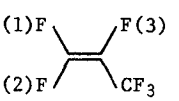
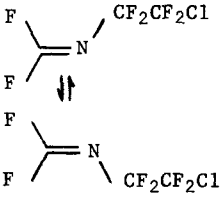
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
1060	3454		C_3F_5Cl					19.8	
1060	3455		C_3F_5Cl					134.6	
1061	3456		C_3F_5I			53.4			
1046	3457		C_3F_5I		1,2	53.4	1,3 2,3	36.2 115	
904	3458 (3228)		$C_3F_5N_3$					127	
1060	3459		C_3F_5H					5.7	
77 235 1041	3460 [784 1017 3229]		C_3F_5H			14.2			
	3461 (3230 3232)		C_3F_6		1,2	60.0	1,3 2,3	40.3 120.2	
1040 1044	3462 (3231 3233)		C_3F_6		1,2	57	1,3 2,3	40 120	
1061	3463		C_3F_6		1,2	57			
1046	3464		C_3F_6		1,2	57.5	1,3 2,3	39.4 118	
1045 (3234)	3465	P	C_3F_6ClN			86.0 (-35°)			

Table B.1.f. (contd.)

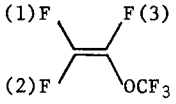
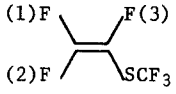
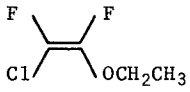
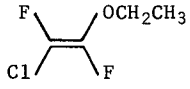
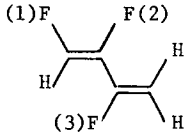
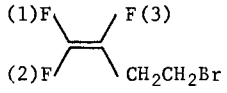
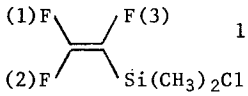
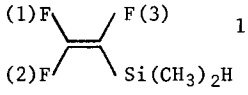
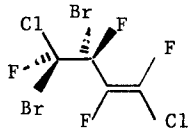
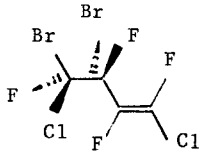
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1001	3466		$C_3F_6N_2$	$CF_2{=}NCF_2N{=}CF_2$		82.0				
1046	3467		C_3F_6O		1,2	87.5	1,3 2,3	65.1 111.0		
	(3236)									
1046	3468		C_3F_6S		1, 2	30.4	1,3 2,3	41.7 122.3		
	(3237)									
1047	3469		$C_4F_2H_5ClO$					35		
1047	3470		$C_4F_2H_5ClO$					115		
245	3471		$C_4F_3H_3$				1,2 2,3	10.9 35.9	1,3	10.9
	(1020)									
1046	3472		$C_4F_3H_4Br$		1,2	84.8	1,3 2,3	32.9 113.7		
1046	3473		$C_4F_3H_6ClSi$		1,2	60.5	1,3 2,3	25.5 117.8		
1046	3474		$C_4F_3H_7Si$		1,2	68.3	1,3 2,3	25.6 117.5		
954	3475	*	$C_4F_4Br_2Cl_2$					-132.35		
	(2787 3238)		erythro							
			threo					-132.36		

Table B.1.f. (contd.)

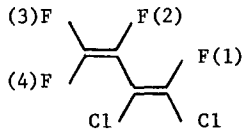
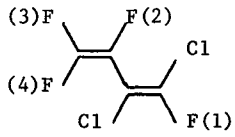
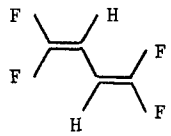
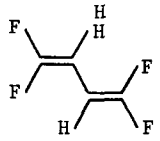
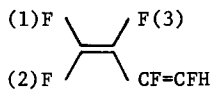
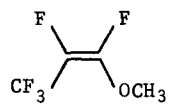
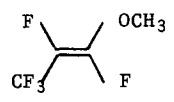
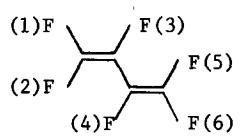
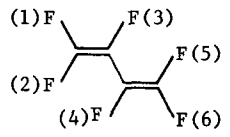
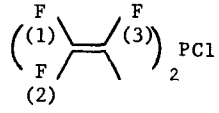
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1150	3476		$C_4F_4Cl_2$		3,4	±54.3	2,3 2,4	+32.9 ∓115.9	1,2 1,3 1,4	+10.9 +4.4 +18.5
1150	3477		$C_4F_4Cl_2$		3,4	+52.1	2,3 2,4	+32.2 ∓115.5	1,2 1,3 1,4	+3.3 +2.5 +3.3
1064	3478 (1021)		$C_4F_4H_2$			+35.7				
1061	3479		$C_4F_4H_2$			36.6				
1046	3480		C_4F_5H		1,2	49	1,3 2,3	30 111		
1047	3481 (3239)		$C_4F_5H_3O$					16.5		
1047	3482 (3240)		$C_4F_5H_3O$					120.0		
1065 1066	3483	B*	C_4F_6		1,2	+50.74	1,3 2,3 3,4	+31.91 -118.58 -30.30	1,4 2,4 1,5 1,6 2,5	+2.41 +14.19 +2.45 +4.80 +11.31
1067	3484	B*	C_4F_6		1,2	+52.4	1,3 2,3 3,4	+32.4 -118.8 -30.0	1,4 2,4 1,5 1,6 2,5	+2.5 +14.3 +2.4 +4.9 +11.2
227	3485 (6029)		C_4F_6ClP		1,2	36	2,3	121		

Table B.1.f. (contd.)

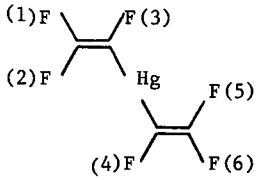
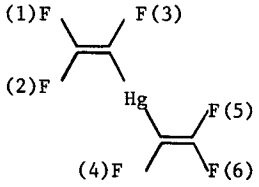
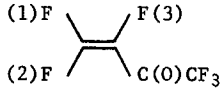
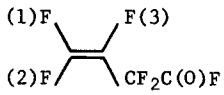
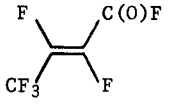
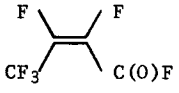
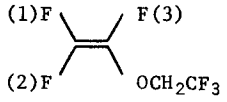
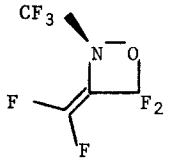
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1063	3486		C_4F_6Hg		1,2	75	1,3 2,3	37 109		
243	3487 (5564)		C_4F_6Hg		1,2	+74.7	1,3	+36.72 -108.80	3,4 2,4 1,4 2,5 2,6 1,6	+3.35 +0.10 +2.47 -0.09 +0.45 +0.47
1048	3488 (3241)		C_4F_6O		1,2	6-7	1,3 2,3	34-35 110		
1049	3489 (3242 3649)		C_4F_6O		1,2	56.9	1,3 2,3	40.2 118.4		
1049	3490 (3243 3650)		C_4F_6O					138.2		
1049	3491 (3244 3651)		C_4F_6O					9.1		
1046	3492 (917 3245)		$C_4F_6H_2O$		1,2	101.6	1,3 2,3	57.8 106.8		
1001	3493		$C_4F_7ClN_2$	$CF_2{=}NCF_2CFClN{=}CF_2$		84.0				
988	3494 [3249 2805 4098 4099]		C_4F_7NO			45.0				

Table B.1.f. (contd.)

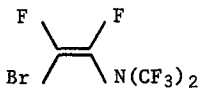
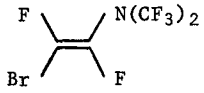
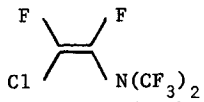
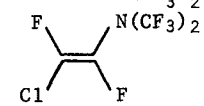
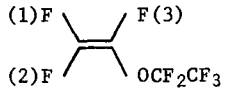
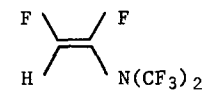
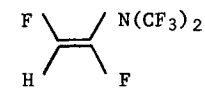
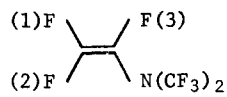
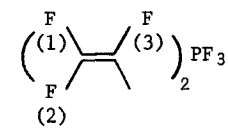
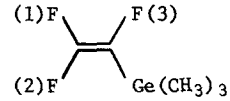
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
1060	3495		C_4F_8BrN					37.9
1060	3496		C_4F_8BrN					133.7
1060	3497		C_4F_8ClN					38.0
1060	3498		C_4F_8ClN					126.6
1001	3499		$C_4F_8N_2$	$CF_2{=}NCF_2CF_2N{=}CF_2$				83.0
1046	3500 (3256)		C_4F_8O		1,2	88.0	1,3 2,3	65.8 111.1
1060	3501		C_4F_8HN					10.1
1060	3502		C_4F_8HN					130.8
1060	3503		C_4F_9N				1,3 2,3	53.9 115.3
826	3503a		C_4F_9N	$CF_3C\ {}_2CF_2N{=}CF_2$		80		
994	3504 (2821 3257)		C_4F_9N	$(CF_3)_2CFN{=}CF_2$ -63°		84.7		
763	3505 [4776 6057 4964]		C_4F_9P		1,2	5	1,3 2,3	39 111
478	3506		$C_5F_3H_9Ge$		1,2	79.4	1,3 2,3	30.9 117.4

Table B.1.f. (contd.)

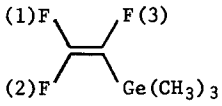
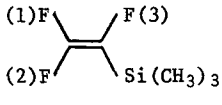
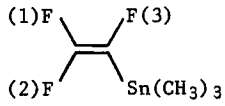
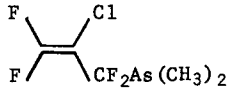
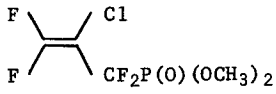
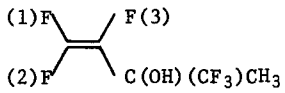
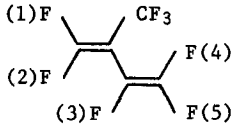
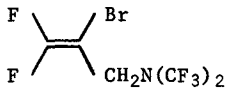
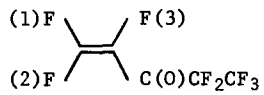
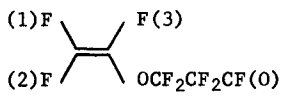
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ	
1046	3507		$C_5F_3H_9Ge$		1,2	72	1,3 2,3	32 118		
1046	3508		$C_5F_3H_9Si$		1,2	71.6	1,3 2,3	25.9 116.8		
1046	3509		$C_5F_3H_9Sn$		1,2	75	1,3 2,3	34 116		
768	3510 (3259)		$C_5F_4H_6AsCl$			24.6				
565	3511 (3262 6098)		$C_5F_4H_6ClO_3P$			19.0				
1046	3512		$C_5F_6H_4O$		1,2	73.3	1,3 2,3	37.8 114		
208	3513 (2865 3270)	P	C_5F_8	$CF_3CF_2CF{=}C{=}CF_2$ (-80°)				37.9		
118	3514		C_5F_8		4,5	61.6	3,4 3,5	120.2 36.6	1,4 2,4 1,5 2,5	7.3 2.7 2.7
119	3515		C_5F_8BrN			29.9				
1048	3516 (3271)		C_5F_8O		1,2	12	1,3 2,3	36 113		
991	3517 (3655 2868)		$C_5F_8O_2$		1,2	109.9	1,3 2,3	64.5 83.6		

Table B.1.f. (contd.)

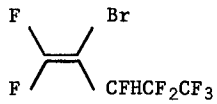
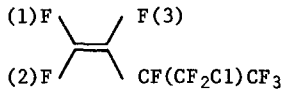
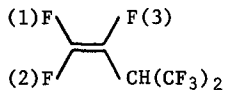
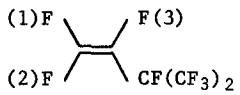
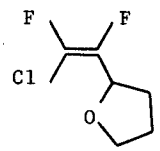
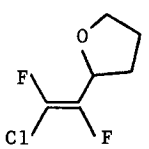
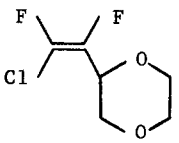
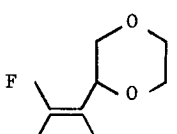
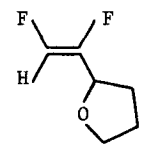
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
190	3518 [371 2869 3272]	P	C_5F_8HBr		16		
1000	3519 (2876 3276)	B*	C_5F_9Cl		1,2 ±57.4	1,3 ±39.1 2,3 ∓116.1	
118	3520 (374 3278)	G	C_5F_9H		1,2 63.8	1,3 37.8 2,3 119.0	
1000	3521 (2886 3281)	B*	C_5F_{10}		1,2 ±57.7	1,3 ±39.3 2,3 ∓117.5	
1001	3522 (2887 3282)		$C_5F_{10}N_2$	$CF_2{=}NCF_2CF(CF_3)N{=}CF_2$	81.0		
1002	3523 (2891)		$C_5F_{11}N$	$CF_2{=}N(CF_2)_3CF_3$	86		
230	3524 (937)	G	$C_6F_2H_7ClO$				14
230	3525 (938)	G	$C_6F_2H_7ClO$				138
230	3526 (939)	G	$C_6F_2H_7ClO_2$				16
230	3527 (940)	G	$C_6F_2H_7ClO_2$				139
230	3528 (941 1067)	G	$C_6F_2H_8O$				10

Table B.1.f. (contd.)

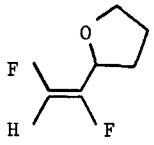
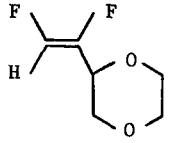
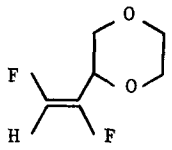
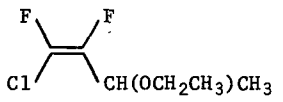
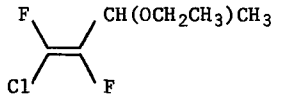
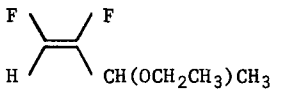
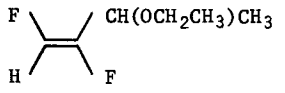
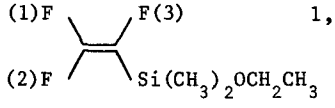
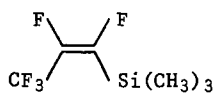
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
230	3529 (942 1068)	G	$C_6F_2H_8O$			135	
230	3530 (943 1070)	G	$C_6F_2H_8O_2$			11	
230	3531 (944 1069)	G	$C_6F_2H_8O_2$			137	
230	3532 (945)	G	$C_6F_2H_9ClO$			14	
230	3533 (946)	G	$C_6F_2H_9ClO$			138	
230	3534 (947 1074)	G	$C_6F_2H_{10}O$			9	
230	3535 (948 1073)	G	$C_6F_2H_{10}O$			135	
1046	3536		$C_6F_3H_{11}OSi$		1,2 67.2	1,3 25.6 2,3 117	
1051	3537 (3285)		$C_6F_5H_9Si$			10.7	

Table B.1.f. (contd.)

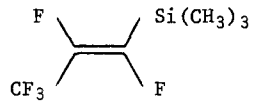
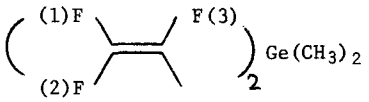
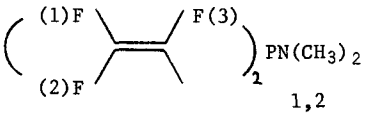
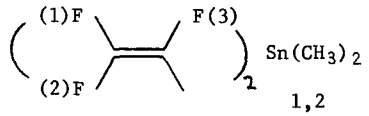
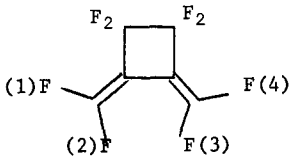
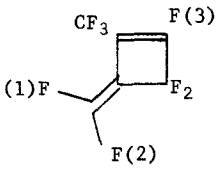
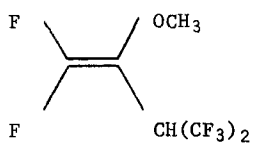
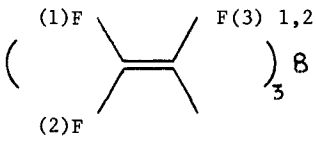
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1051	3538 (3286)		$C_6F_5H_9Si$			138	
1063 805	3539		$C_6F_6H_6Ge$		1,2 72	1,3 32 2,3 118	
227	3540 (950 6172)		$C_6F_6H_6NP$		1,2 53	1,3 32 2,3 119	
1063 805	3541		$C_6F_6H_6Sn$		1,2 75	1,3 34 2,3 116	
1064	3542		C_6F_8		1,2 +14.7		1,4 +23.2 1,3 6.7 2,3 7.6
1052	3543 [2920 3287 3754]		C_6F_8		1,2 55.2		1,3 22.6 2,3 25.1
118	3543 (425 951)	B	$C_6F_8H_4O$		64.0		
1046	3544		C_6F_9B		1,2 5	1,3 24 2,4 110	

Table B.1.f. (contd.)

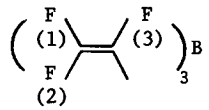
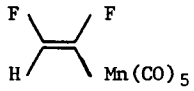
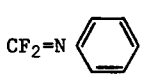
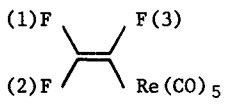
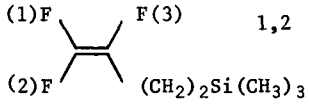
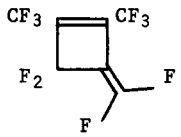
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1063	3545		C_6F_9B		1,2	<5	1,3 2,3	24 110	
634	3546 (3293 5568)		$C_6F_{10}Hg$	$[CF_2=C(CF_3)]_2Hg$		15.6			
634	3547 [431 3295 5569]		$C_6F_{11}HHg$	$CF_2=C(CF_3)HgCH(CF_3)_2$		15.6			
247	3548		$C_7F_2HMnO_5$					2.4	
561	3549		$C_7F_2H_5N$			50			
248	3550 (1089)	G	$C_7F_2H_{12}$	$CF_2=CH(CH_2)_4CH_3$		49			
805 1044	3551		$C_7F_3O_5Re$		1,2	98.0	1,3 2,3	36.6 120.0	
1046	3552		$C_7F_3H_{13}Si$		1,2	92.5	1,3 2,3	31.9 113.9	
1023	3553 (2973 3301)		C_7F_{10}			28.8			
248	3554 (1094)	G	$C_8F_2H_5Cl$	$CF_2=CH(oClC_6H_4)$		28			
248	3555 (1095)	G	$C_8F_2H_5Cl$	$CF_2=CH(pClC_6H_4)$		31			
248	3556 (1098)	G	$C_8F_2H_6$	$CF_2=CHC_6H_5$		33			
248	3557 (1099)	G	$C_8F_2H_{14}$	$CF_2=CH(CH_2)_5CH_3$		50			

Table B.1.f. (contd.)

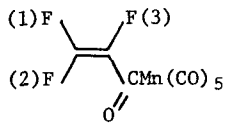
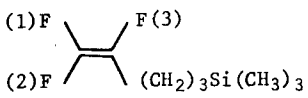
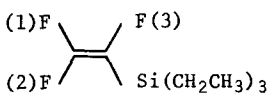
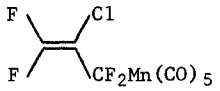
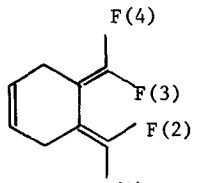
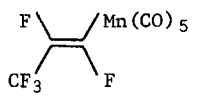
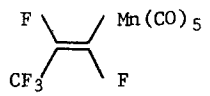
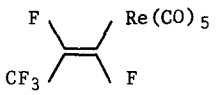
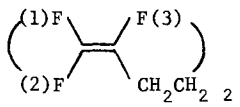
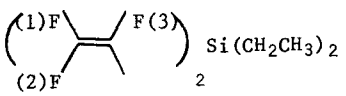
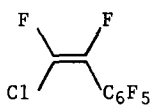
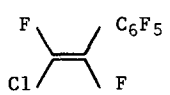
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
247	3558		$C_8F_3MnO_6$		1,2	92.5	1,3 40.6 2,3 111.5	
1046	3559		$C_8F_3H_{15}Si$		1,2	90.9	1,3 32.3 2,4 114.0	
1072	3560		$C_8F_3H_{15}Si$		1,2	71	1,3 27 2,3 115	
768	3561 (3304)		$C_8F_4ClMnO_5$			35.8		
1064	3562	*	$C_8F_4H_6$		1,2	39.0		1,4 +31.4 1,3 4.8 2,3 3.3
1040 1043 1044	3563 (3307)		$C_8F_5MnO_5$				127	
166	3564		$C_8F_5MnO_5$				135	
1044	3565 (3308)		$C_8F_5O_5Re$				141	
1046	3566		$C_8F_6H_8$		1,2	91.4	1,3 32.5 2,3 113.8	
1063	3567		$C_8F_6H_{10}Si$		1,2	62	1,3 26 2,3 117	
896	3568 (3365)		C_8F_7Cl				13.8	
896	3569 (3366)		C_8F_7Cl				134.5	

Table B.1.f. (contd.)

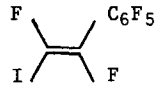
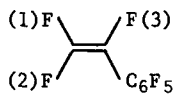
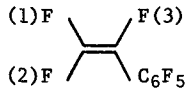
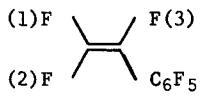
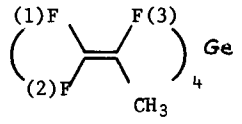
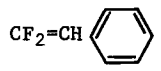
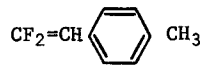
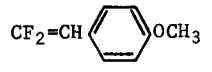
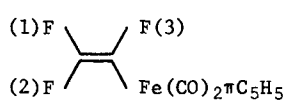
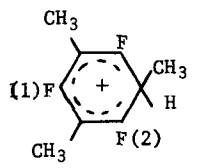
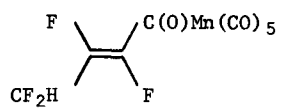
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
1073	3570		C_8F_7I					152	
896	3571 (3369)		C_8F_8		1,2	61.6	1,3 2,3	35.5 118.8	
1073	3572 (3370, 4418)	B	C_8F_8		1,2	63	1,3 2,3	36 117	
929	3573 (3371, 4417)	*	C_8F_8		1,2	+62.5	1,3 2,3	+35.4 -118.3	
1063	3574		$C_8F_{12}Ge$		1,2	71	1,3 2,3	32 118	
248	3575 (1109)	G	$C_9F_2H_8$			32			
248	3576 (1110)	G	$C_9F_2H_8$			34			
248	3577 (1111)	G	$C_9F_2H_8O$			38			
1044	3578		$C_9F_3H_5FeO_2$		1,2	107.1	1,3 2,3	46.8 122.4	
450	3579	F^2	$C_9F_3H_{10}^+$				1,2	70.0	
199	3580 [604, 964, 3314]	A	$C_9F_4HMnO_6$					129.0	

Table B.1.f. (contd.)

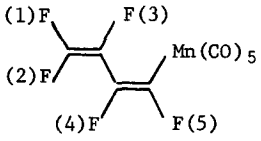
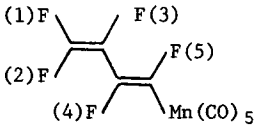
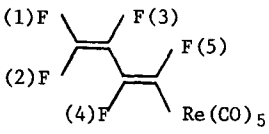
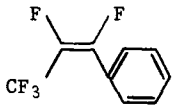
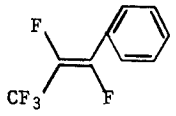
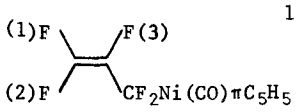
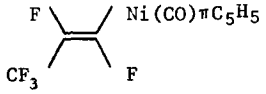
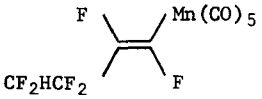
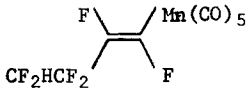
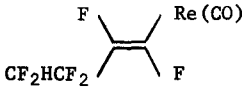
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1057	3581	A	C_9F_5MnO		1,2	76	1,3 2,3 4,5	27 128 34	2,4	16
1057	3582	A	$C_9F_5MnO_5$		1,2	56	1,3 2,3 4,5 3,4	28 114 130 35	1,4 2,4 3,5 1,5 2,5	3 13 9 5 16
1057	3583	R	$C_9F_5O_5Re$		1,2	60	1,3 2,3 4,5 3,4	28 117 137 36	1,4 2,4 3,5 1,5 2,5	4 12 9 6 17
1055	3584 (3318)		$C_9F_5H_5$					9		
1055	3585 (3319)		$C_9F_5H_5$					131		
1056	3586 (3321)		$C_9F_5H_5NiO$		1,2	72	1,3 2,3	32 113		
1056	3587 (3320)		$C_9F_5H_5NiO$					130		
1057	3588 (608 3322)	A	$C_9F_6HMnO_5$					124		
199	3589 (608)	A	$C_9F_6HMnO_5$					126.5		
199	3590 (610)	A	$C_9F_6HO_5Re$					129.5		

Table B.1.f. (contd.)

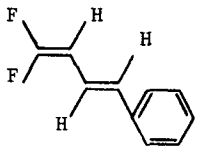
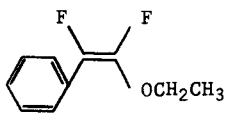
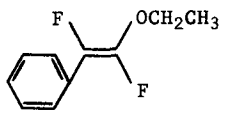
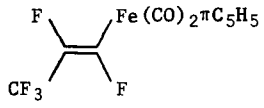
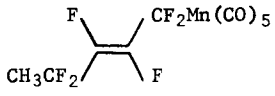
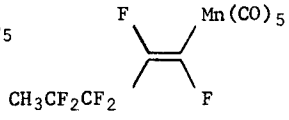
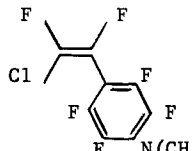
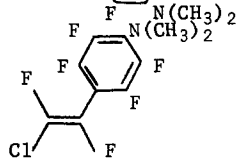
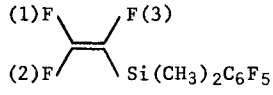
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
248	3591 (1116)	G	$C_{10}F_2H_8$		28		
1058	3592		$C_{10}F_2H_{10}O$			11	
1058	3593		$C_{10}F_2H_{10}O$			112	
1056 1040	3954 (3330)		$C_{10}F_5H_5FeO_2$			131	
164	3595 [652 971 3082 3331]		$C_{10}F_6H_3MnO_5$			132.2	
164	3596 [653 972 3332]		$C_{10}F_6H_3MnO_5$			129.0	
896	3597 (2104 3378)		$C_{10}F_6H_6ClN$			11.6	
896	3598 (2105 3379)		$C_{10}F_6H_6ClN$			129.5	
1046	3599		$C_{10}F_8H_6Si$		1,2 64.2	1,3 24.6 2,3 117.6	

Table B.1.f. (contd.)

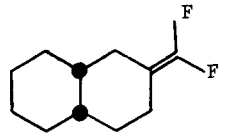
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ	
1070	3600	P	$C_{11}F_2H_{10}$	 (Room temp.)		63.5				
1046	3601		$C_{11}F_3H_9O_2$	(1)F, F(3), (2)F, $C_6H_4CO_2CH_2CH_3$	1,2	65.0	1,3 2,3	33.3 108		
1057	3602	R	$C_{11}F_5H_5FeO_2$	(1)F, F(3), $Fe(CO)_2\pi C_5H_5$, (2)F, (4)F, F(5)	1,2	79	1,3 2,3 3,4 4,5	25 114 14 41	1,4 2,4 3,5 1,5 2,5	4 13 7 3 3
813	3603	R	$C_{12}F_3H_{18}BrN_2Pd$	(1)F, F(3), (2)F, D, Pd, D, Br; D = $CNC(CH_3)_3$	1,2	97.5	1,3 2,3	48.0 107.0		
813	3604	R	$C_{12}F_3H_{18}ClN_2Pd$	(1)F, F(3), (2)F, D, Pd, D, Cl	1,2	95.0	1,3 2,3	45.0 108.0		
1000	3605 (3341)	B*	$C_{12}F_5H_7N_2O$	(1)F, F(3), (2)F, CF_2, O, N, N, R; R = CH_2; or R = CH_3; or R = CH_3	1,2	±55.9	1,3 2,3	±37.9 ∓117.2	same couplings to within ± 0.2 Hz	
805	3606 (6354 6565)		$C_{13}F_2H_{20}BrClNPPt$	$(CH_3CH_2)_3PPtL(Br)(CCl{=}CF_2)$ 66; L = 						

Table B.1.f. (contd.)

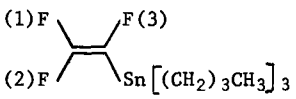
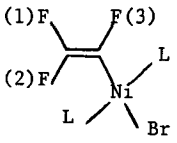
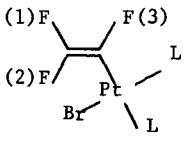
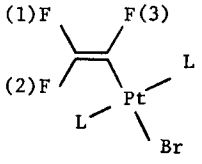
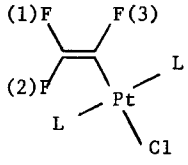
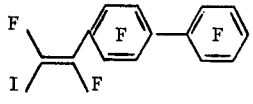
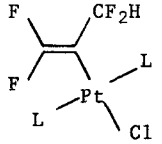
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
1063	3607		$C_{14}F_3H_{27}Sn$		1,2	79	1,3 2,3	34 115	
805	3608 (6361)		$C_{14}F_3H_{30}BrNiP_2$	 L = $P(CH_2CH_3)_3$	1,2	107	1,3 2,3	36 107	
805 807	3609 (6362 6569)	A	$C_{14}F_3H_{30}BrP_2Pt$	 L = $P(CH_2CH_3)_3$	1,2	104	1,3 2,3	34 104	
80	3610	A	$C_{14}F_3H_{30}BrP_2Pt$	 L = $P(CH_2CH_3)_3$	1,2	107	1,3 2,3	34 107	
807 173	3611 (6364 6570)	A	$C_{14}F_3H_{30}ClP_2Pt$		1,2	120	1,3 2,3	35.6 120	
1073	3612	U^2	$C_{14}F_{11}I$					152	
565	3613 (3347 6370)		$C_{15}F_4H_{10}ClOP$	$CF_2=CClCF_2P(O)(C_6H_5)_2$		14.8			
173	3614 (732 6574)		$C_{15}F_4H_{31}ClP_2Pt$	 L = $P(CH_2CH_3)_3$		26.5			

Table B.1.f. (contd.)

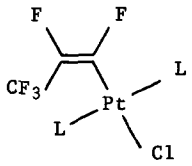
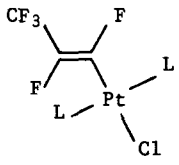
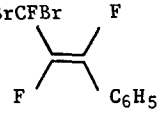
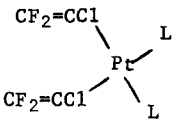
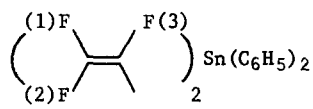
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
173	3615 [3350 6373 6575]		$C_{15}F_5H_{30}ClP_2Pt$	 L = $P(CH_2CH_3)_3$		12.8	
173	3616 [3351 6374 6576]		$C_{15}F_5H_{30}ClP_2Pt$	 L = $P(CH_2CH_3)_3$		124	
1137	3617 (3161 3352)		$C_{16}F_4H_{10}Br_2$	$C_6H_5CFBrCFBr$ 		130	
805	3618 (6381)		$C_{16}F_4H_{30}Br_2Cl_2P_2Pd_2$	trans$[(CH_3CH_2)_3P]_2Pd_2(CCl{=}CF_2)_2Br_2$	69		
805	3619 (6382 6578)		$C_{16}F_4H_{30}Br_2Cl_2P_2Pt_2$	trans$[(CH_3CH_2)_3P]_2Pt_2(CCl{=}CF_2)_2Br_2$	64		
805	3620 (6579)		$C_{16}F_4H_{30}Cl_2P_2Pt$	 L = $P(CH_2CH_3)_3$	65		
1063	3621		$C_{16}F_6H_{10}Sn$		1,2	68	1,3 34 2,3 118

Table B.1.f. (contd.)

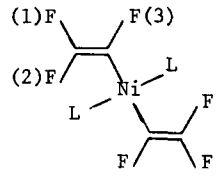
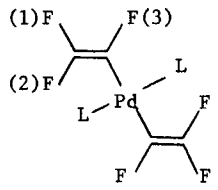
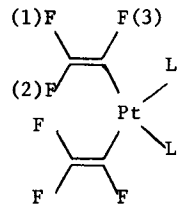
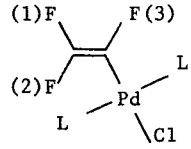
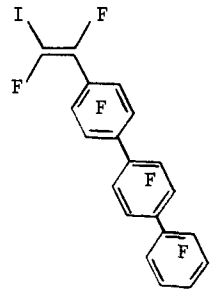
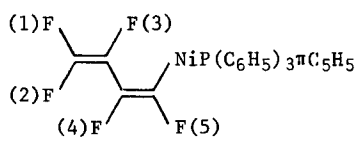
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
805	3622		$C_{16}F_6H_{30}NiP_2$	 L = $P(CH_2CH_3)_3$	1,2 112	1,3 32 2,3 112	
805	3623 (6387)		$C_{16}F_6H_{30}P_2Pd$		1,2 109	1,3 40 2,3 104	
805 807	3624 (6388, 6577)	A	$C_{16}F_6H_{30}P_2Pt$	 L = $P(CH_2CH_3)_3$	1,2 104	1,3 33 2,3 104	
813	3625	R	$C_{18}F_6H_{22}As_2ClPd$	 L = $As(CH_3)_2C_6H_5$	1,2 105.0	1,3 43.0 2,3 108.0	
1073	3626	E	$C_{20}F_{15}I$			151	
1056	3627		$C_{27}F_5H_{20}NiP$		1,2 82	1,3 23 2,3 113 3,4 15 4,5 42	1,4 6 2,4 20 3,5 5 1,5 6 2,5 7

Table B.1.f. (contd.)

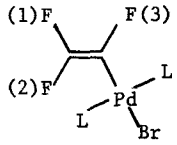
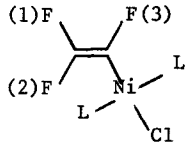
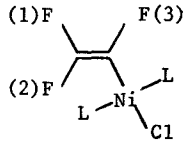
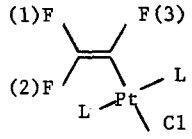
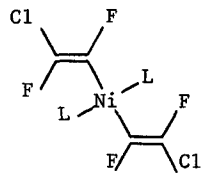
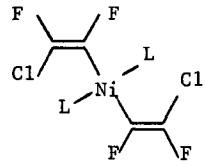
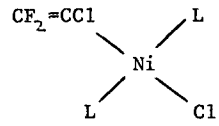
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	3	^3J	^nJ
823	3630 (6508)	A	$C_{28}F_3H_{26}BrP_2Pd$	 L = $P(C_6H_5)_2CH_3$	1,2	102.0	1,3 2,3	42.0 105.0	
822	3629 (6509)	J	$C_{28}F_3H_{26}ClNiP_2$		1,2	105	1,3 2,3	40 110	
823	3630 (6510)	A	$C_{28}F_3H_{26}ClP_2Pd$		1,2	95.5	1,3 2,3	43.0 104.0	
807	3631 (6511 / 6610)	A	$C_{28}F_3H_{26}ClP_2Pt$		1,2	101	1,3 2,3	31.1 106	
822	3632	J	$C_{30}F_4H_{26}Cl_2NiP_2$	 L = $P(C_6H_5)_2CH_3$				121.5	
822	3633 (6516)	J	$C_{30}F_4H_{26}Cl_2NiP_2$	 L = $PCH_3(C_6H_5)_2$				12.0	
822	3634 (6531)	J	$C_{38}F_2H_{30}Cl_2NiP_2$	 L = $P(C_6H_5)_3$		72			

Table B.1.f. (contd.)

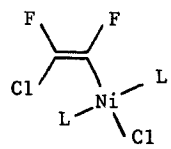
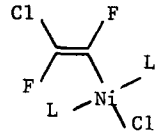
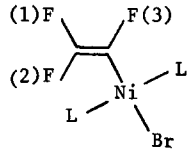
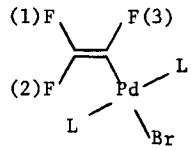
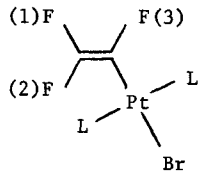
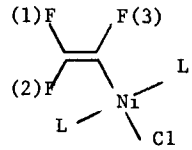
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
822	3635 (6532)	J	$C_{38}F_2H_{30}Cl_2NiP_2$	 L = $P(C_6H_5)_3$		13.0	
822	3636 (6533)	J	$C_{38}F_2H_{30}Cl_2NiP_2$	 L = $P(C_6H_5)_3$		122	
822	3637 (6534)	J	$C_{38}F_3H_{30}BrNiP_2$	 L = $P(C_6H_5)_3$	1,2 114	1,3 36.0 2,3 110	
823	3638 (6535)	A	$C_{38}F_3H_{30}BrP_2Pd$		1,2 97.0	1,3 46.0 2,3 106.0	
807	3639 (6536 6614)	A	$C_{38}F_3H_{30}BrP_2Pt$		1,2 101	1,3 32.0 2,3 105	
822	3640 (6537)	J	$C_{38}F_3H_{30}ClNiP_2$		1,2 105	1,3 40.0 2,3 110.0	

Table B.1.f. (contd.)

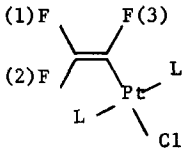
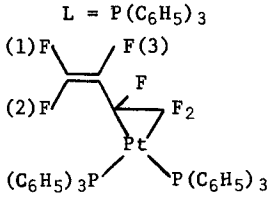
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
807	3641 (6538 6615)	A	$C_{38}F_3H_{30}ClP_2Pt$		1,2	98	1,3 2,3	31.0 105	
807	3642 (3353 6625)	A	$C_{40}F_6H_{30}P_2Pt$	L = $P(C_6H_5)_3$ 	1,2	67.3	1,3 2,3	27.2 110.0	

Table B.1.g. One fluorine bonded to sp^2 carbon of a carbonyl group, the other to sp^3 or sp^2 carbon.

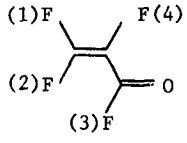
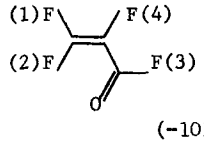
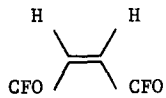
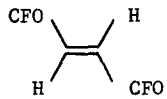
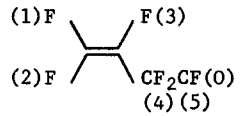
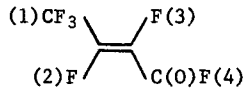
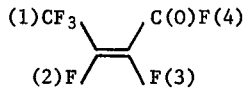
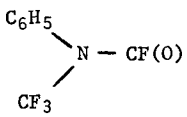
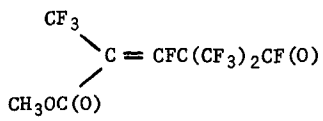
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J		^nJ
1082	3643		C_2F_4O	$CF_3C(O)F$		6.1			
869	3644	P	$C_2F_4O_3$	$CF_3OOC(O)F$					2
20	3645 [159 983 2685]	B	$C_3F_3HBr_2O$	$CF_2BrCHBrC(O)F$			12.3		
1042 857	3646 (3443)		C_3F_4O		3,4	34.4	1,3 2,3	<2 84.5	
				 (-105°)	3,4	31.1	1,3 2,3	41.6 <2	
256	3647 (1130 5454)		$C_4F_2H_2O_2$						4.78
256	3648 (1131 5455)		$C_4F_2H_2O_2$						±0.22

Table B.1.g. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
1049	3649 (3242 3489)	B	C_4F_6O		4,5	8.4	3,5	4.4	1,5 2,5	∿0 3.6
1049	3650 (3243 3490)	B	C_4F_6O		3,4	21.5	2,4	55.6	1,4	⩽0.3
1049	3651 (3244 3491)	B	C_4F_6O		3,4	26.3	2,4	22.3	1,4	12.5
961	3652 (4845)		$C_4F_8O_4S$	$(CF_3)_2C(OSO_2F)CFO$ (1) (2)			1,2	8		
961	3653		C_4F_9NO	$(CF_3)_2C(NF_2)CF(O)$ (1) (2)			1,2	9		
569	3654 (4720)		C_4F_9NO	$(CF_3)_2C(NF_2)CF(O)$ (1) (2)			1,2	8.9		
991	3655 (2868 3517)		$C_5F_8O_2$	$CF_2{=}CFOCF_2CF_2CF(O)$		5.9		8.0		
952	3656 (2930)	P	$C_6F_{10}O_4$	$CF_3OOC(O)CF_2CF_2CF_2CF(O)$		7		7		2
117	3657 (2972)	B	$C_7F_9H_3O_2$	$(CF_3)_2C{=}C(OCH_3)CF_2CF(O)$		10.9				
113	3658		$C_7F_{10}O$	$(CF_3)_2C{=}C{=}C(CF_3)CF(O)$				10		
561	3659		$C_8F_4H_5NO$					15.0		
634	3660 (5575)		$C_8F_{14}HgO_2$	$[(CF_3)_2C(CFO)]_2Hg$				14.8		
113	3661 (3323)		$C_9F_{11}H_3O_3$					10		

B.2. Fluorine bonded to carbon in alicyclic, non-aromatic ring systems.

Table B.2.a. Three membered rings.

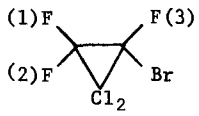
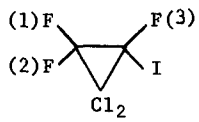
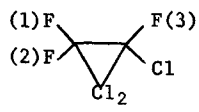
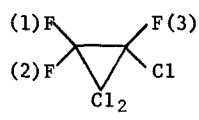
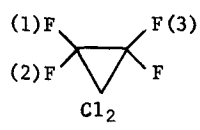
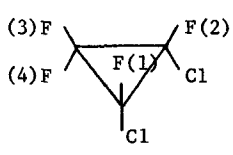
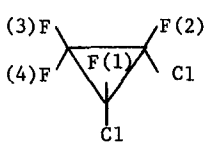
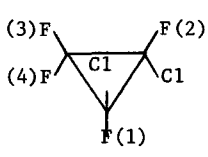
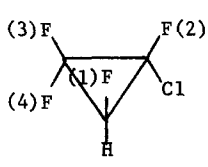
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
1084	3662	Q	C_3F_3BrCl		1,2	153.0	1,3 2,3	-5.4 -5.4	
1084	3663	Q	$C_3F_3Cl_2I$		1,2	150.5	1,3 2,3	-6.8 -10.0	
1084	3664	Q	$C_3F_3Cl_3$		1,2	155.0	1,3 2,3	-4.1 -1.3	
1085	3665	B	$C_3F_3Cl_3$				1,3 2,3	-4.1 -1.3	
1085	3666	B	$C_3F_4Cl_2$				1,3 2,3	1.44 4.10	
1085	3667	B	$C_3F_4Cl_2$		3,4	173.1	1,2 2,3 2,4	5.5 5.62 -5.23	
261	3668	B	$C_3F_4Cl_2$		3,4	174	2,3 2,4	5.6 5.3	
1085	3669	B	$C_3F_4Cl_2$				1,2 2,3 2,4	-12.2 ∿0 ∿-5	
261	3670 (1142)	B	C_3F_4HCl		3,4	184	1,2 1,3 1,4 2,3 2,4	7.5 7.5 4.9 4.8 2.1	

Table B.2.a. (contd.)

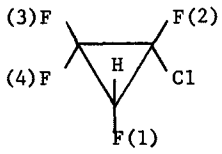
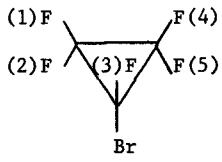
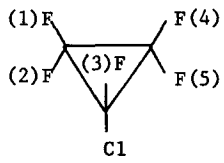
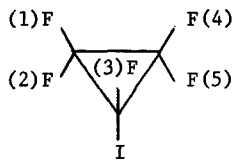
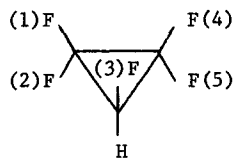
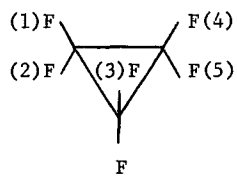
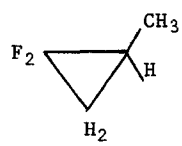
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
261	3671 (1141)	B	C_3F_4HCl		3,4	190	1,2 1,3 1,4 2,3 2,4	11.1 2.8 - 5.7 -	
1086	3672	B	C_3F_5Br		1,2	185.72	1,4 1,5 2,5 1,3 2,3	10.41 2.42 1.91 6.59 -10.13	
1085 1086	3673	B	C_3F_5Cl		1,2	189.04	1,4 1,5 2,5 1,3 2,3	10.73 0.88 4.87 8.27 -5.82	
1086	3674	B	C_3F_5I		1,2	181.44	1,4 1,5 2,5 1,3 2,3	9.78 4.34 -1.29 4.72 -15.44	
261	3675 (1143)	B	C_3F_5H		1,2	208	1,3 2,3	9.8 4.9	
1087	3676		C_3F_6		1,2	160			
1087	3677		$C_4F_2H_6$			157			

Table B.2.a. (contd.)

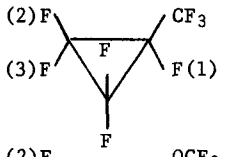
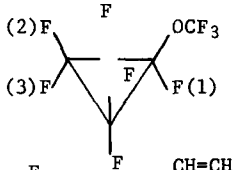
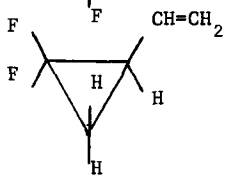
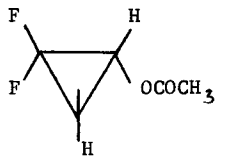
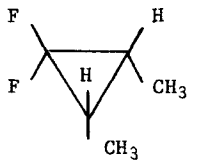
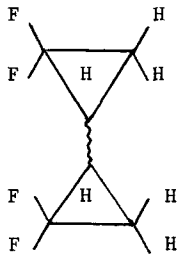
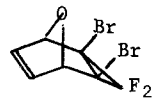
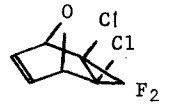
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
261	3678 (2809)	B	C_4F_8				1,2 1,3	2.7 4.3	
261	3679 (2814)	B	C_4F_8O		2,3	201	1,2 1,3	3.2 9.2	
256	3680 (1148)		$C_5F_2H_6$			158.9			
266	3681 (1149)	A*	$C_5F_2H_6O_2$			171.4			
265	3682 (1150 1186)		$C_5F_2H_8$			157.6			
265	3683		$C_6F_4H_6$			161.2			
269	3684 (1196)		$C_7F_2H_4Br_2O$			144			
269	3685 (1193c)		$C_7F_2H_4Cl_2O$			147.5			

Table B.2.a. (contd.)

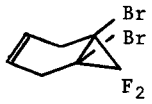
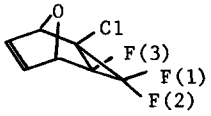
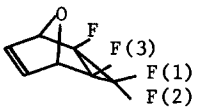
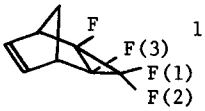
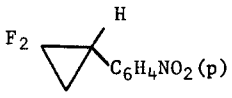
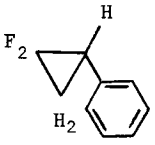
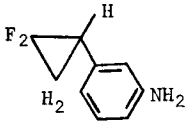
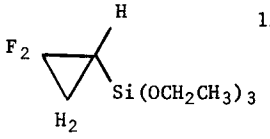
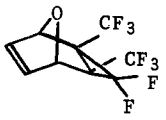
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
269	3686 (1193d)		$C_7F_2H_6Br_2$			152			
269	3687 (1194)		$C_7F_2H_6Cl_2$			156			
269	3688		$C_7F_3H_4ClO$		1,2	160	1,3 2,3	7 23	
269	3689		$C_7F_3H_6Cl$		1,2	170	1,3 2,3	<3 4	
274	3690 (1199)	B	$C_7F_4H_4O$		1,2	175	1,3 2,3	0 23.4	
274	3691 [1202 1275 1344]	B	$C_8F_4H_6$		1,2	177	1,3 2,3	1.4 24.3	
266	3692 (1174)	A*	$C_9F_2H_7NO_2$			155.2			
266	3693 (1175)	A*	$C_9F_2H_8$			154.4			
266	3694 (1176)	A*	$C_9F_2H_9N$			154.5			
266	3695 (1177)	A*	$C_9F_2H_{18}O_3Si$			150.2			
274	3696 (1203 3067)	B	$C_9F_8H_4O$			166			

Table B.2.a. (contd.)

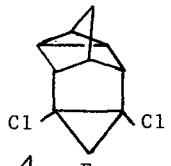
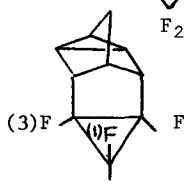
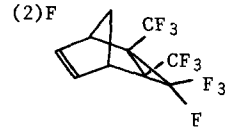
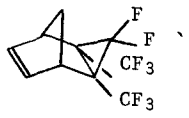
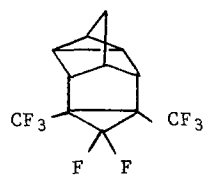
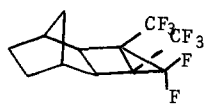
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
269	3697		$C_{10}F_2H_8Cl_2$			158			
274	3698	B	$C_{10}F_4H_8$		1,2	179	1,3 2,3	22.7 0	
274	3699 (1205 3095)	B	$C_{10}F_8H_6$			178			
274	3700 (1206 3096)	B	$C_{10}F_8H_6$			177			
274	3701 (3129)	B	$C_{12}F_8H_8$			176			
274	3702 (3130)	B	$C_{12}F_8H_{10}$			172			

Table B.2.b. Four membered rings.

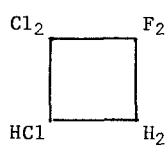
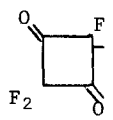
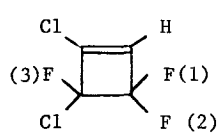
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
1088	3703		$C_4F_2H_3Cl_3$			187			
1089	3704		$C_4F_3O_2^-$						20
278	3705 (1212)	P	$C_4F_3HCl_2$		1,2	+190.2	1,3 2,3	-12.2 +26.0	
					(Angle between F(3) and F(1) approx 0^o)				

Table B.2.b. (contd.)

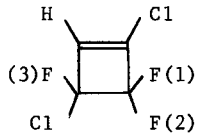
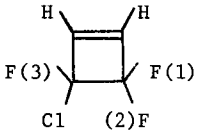
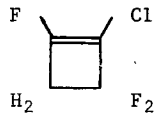
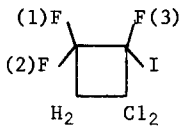
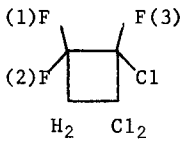
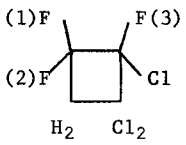
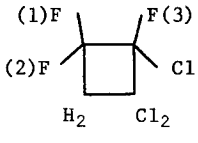
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
278	3706 (1213)	P	$C_4F_3HCl_2$		1,2 +183.4	1,3 -12.6 2,3 -25.6	
278 279	3707 (1214)	P	$C_4F_3H_2Cl$		1,2 +192.24 (60% by volume in P) 1,2 +192.33 (30% by volume in P) 1,2 +192.55 (15% by volume in P)	1,3 -12.43 2,3 +28.66 1,3 -12.21 2,3 +28.62 1,3 -12.00 2,3 +28.77	
278	3708	P	$C_4F_3H_2Cl$				4.9
279	3709 (1215)	P (30%)	$C_4F_3H_2Cl_2I$		1,2 +200.07	1,3 -8.76 2,3 -5.05	
280	3710 (1217)	B	$C_4F_3H_2Cl_3$		1,2 +202.65	1,3 -9.46 2,3 +2.84	
1090	3711	P-A[3]	$C_4F_3H_2Cl_3$		1,2 202.7	1,3 -8.88 2,3 +2.73	
279	3712 (1216)	P	$C_4F_3H_2Cl_3$		1,2 202.89 (50% in P) 1,2 203.12 (10% in P)	1,3 -9.46 2,3 +2.82 1,3 -9.34 2,3 +2.80	

Table B.2.b. (contd.)

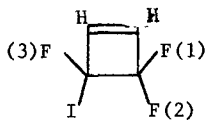
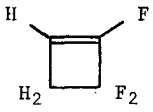
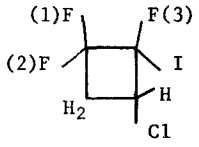
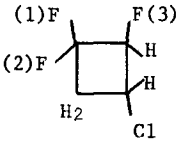
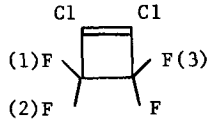
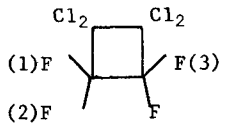
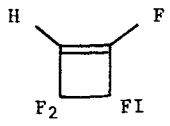
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
279	3713	P	$C_4F_3H_2I$		1,2	+190.08	1,3	-11.74	
278	(1218)						2,3	+21.78	
278	3714	P	$C_4F_3H_3$					3.8	
	(1219)								
279	3715	P	$C_4F_3H_3ClI$		1,2	+197.62	1,3	-8.92	
	(1220)						2,3	-5.56	
281	3716		$C_4F_3H_4Cl$		1,2	210.19	1,3	-3.69	
	(1221)						2,3	0.93	
280	3717	B*	$C_4F_4Cl_2$		1,2	+200.0	1,3	-12.77	
1091							2,3	+25.13	
		C			1,2	190.0			
280	3718	G	$C_4F_4Cl_4$		1,2	+200.0	1,3	-11.93	
1091							2,3	+5.86	
		C			1,2	191.3			
1092	3719		C_4F_4HI			182			

Table B.2.b. (contd.)

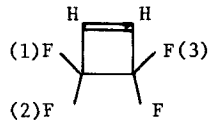
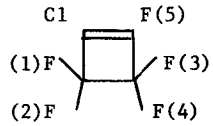
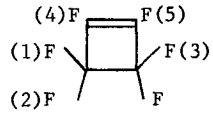
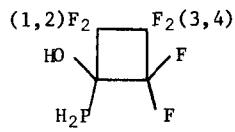
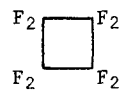
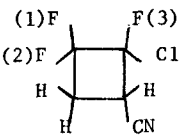
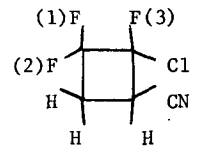
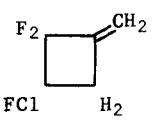
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
280	3720 (1223)	B*	$C_4F_4H_2$		1,2	+199.37	1,3 2,3	-12.92 +30.45		
278	3721	P*	C_4F_5Cl		1,2 3,4	+188.22 +197.13	1,3 2,3	-12.71 +25.61	1,5 3,5	+16.96 +5.76
1093	3722	B*	C_4F_6		1,2	+198.92	1,3 2,3 4,5 1,4 or	-12.27 +26.50 -8.84 ±6.77 ±16.36	1,5 cr	±16.36 ± 6.77
759	3723 (6038)		$C_4F_6H_3OP$		1,2 3,4	216 229				
1087	3724		C_4F_8			220				
1090	3725	P-A[3]	$C_5F_3H_3ClN$		1,2	197.8	1,3 2,3	-6.75 +6.46		
1090	3726	P-A[3]	$C_5F_3H_3ClN$		1,2	199.6	1,3 2,3	-6.37 +0.76		
283	3727 (1225)		$C_5F_3H_4Cl$			210				

Table B.2.b. (contd.)

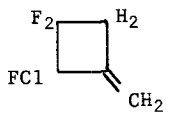
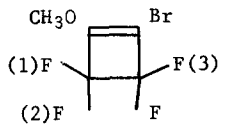
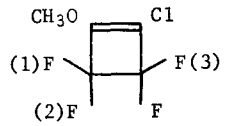
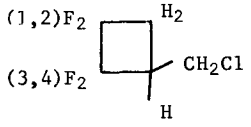
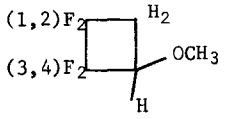
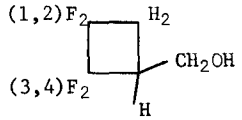
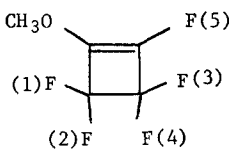
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
283	3728		$C_5F_3H_4Cl$		195		
278	3729	P*	$C_5F_4H_3BrO$			1,3 -16.5 2,3 +25.1	
278	3730	P*	$C_5F_4H_3ClO$			1,3 -16.4 2,3 +25.5	
1087	3731		$C_5F_4H_5Cl$		1,2 224 3,4 230		
1087	3732		$C_5F_4H_6O$		1,2 210 3,4 213		
1087	3733		$C_5F_4H_6O$		1,2 219 3,4 218		
284	3734 (1228)	P*	$C_5F_5H_3O$		1,2 +200.72 3,4 +199.28	1,3 ±26.56 2,3 ∓16.85 3,5 ±20.03	1,5 ±7.39

Table B.2.b. (contd.)

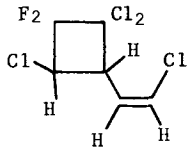
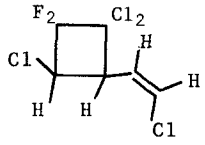
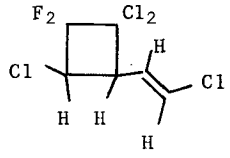
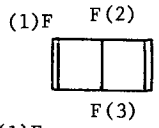
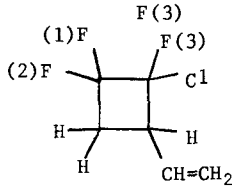
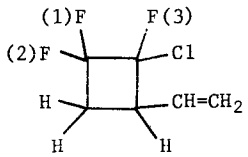
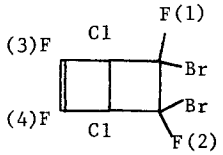
Ref. No.	Serial S No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ	
1094	3735	G	$C_6F_2H_4Cl_4$			179.2				
1094	3736	G	$C_6F_2H_4Cl_4$			182.7				
1094	3737	G	$C_6F_2H_4Cl_4$			187.5				
284	3738 (1231)	P	$C_6F_3H_3$				1,2 2,3	3.5 4.3		
1090	3739	P-A[3]	$C_6F_3H_6Cl$		1,2	196.0	1,3 2,3	-7.81 +5.94		
1090	3740	P-A[3]	$C_6F_3H_6Cl$		1,2	199.6	1,3 2,3	-6.53 -1.25		
284	3741	P	$C_6F_4Br_2Cl_2$				1,2 3,4	11.6 10.6	1,3 1,4 2,3 2,4	0.8 1.1 4.8 1.8

Table B.2.b. (contd.)

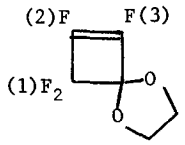
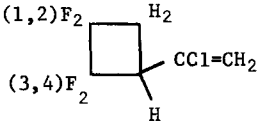
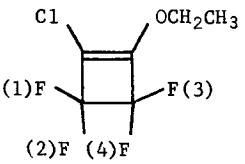
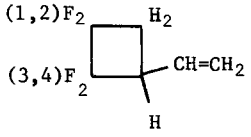
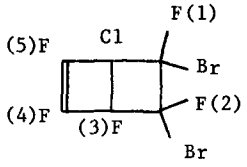
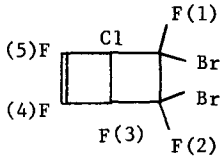
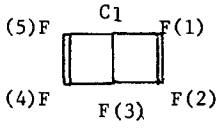
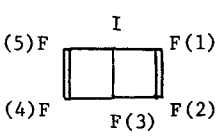
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
278	3742	P	$C_6F_4H_4O_2$			1,2 +6.1 2,3 -8.3	1,3 +19.1
1087	3743		$C_6F_4H_5Cl$		1,2 {211 3,4 {202		
278 1095	3744 (1247)	P*	$C_6F_4H_5ClO$		1,2 {200.21 3,4 {191.0	1,3 {+25.2 2,3 {-16.7	
1087	3745	P	$C_6F_4H_6$		1,2 220 3,4 220		
284	3746	P	$C_6F_5Br_2Cl$			1,2 8.5 2,3 5.0 3,4 13.9 4,5 10.5	1,3 6.7 3,5 5.0 1,4 ⩽0.5 2,4 ⩽0.5 2,5 1.7 1,5 < 0.5
284	3747	P	$C_6F_5Br_2Cl$			1,2 10.0 2,3 4.4 3,4 13.4 4,5 11.6	1,3 2.5 3,5 5.5 1,4 5.2 1,5 2.0 2,4 0.8 2,5 1.0
284	3748	P	C_6F_5Cl			1,2 2.25 2,3 ±8.00	1,3 ±8.40 1,5 ±0.23 2,4 ∓0.63 1,4 ∓13.75
284	3749	P	C_6F_5I			1,2 ±1.4 2,3 7.6	1,3 8.4 1,4 ∓13.3

Table B.2.b. (contd.)

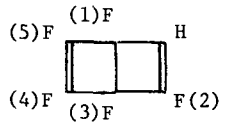
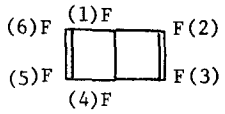
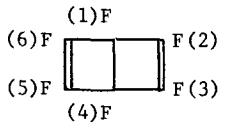
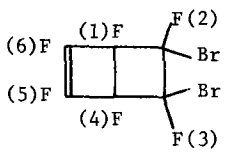
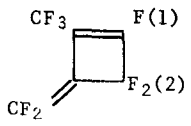
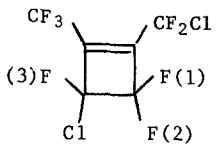
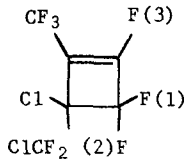
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
284	3750 (1233)	P	C_6F_5H			2,3	3.9	1,4	9.4
						3,4	7.2	3,5	9.3
						4,5	3.8	1,2	6.6
						1,5	7.9	2,4	0.9
						1,3	7.9	2,5	13.7
1096	3751	B-P*	C_6F_6			1,2	∓7.12	1,3	±9.92
						2,3	∓3.01	2,6	±0.10
						1,4	∓9.36	2,5	±14.03
1097	3752	B-A^3*	C_6F_6			1,2	∓7.09	1,3	10.02
						2,3	-3.02	2,6	0.06
						1,4	-9.40	2,5	14.08
284	3753	P	$C_6F_6Br_2$			1,2	3.0	1,3	5.6
						2,3	11.0	1,5	5.6
						3,4	4.0	4,6	7.4
						4,5	19.0	2,6	5.6
						5,6	12.0	2,5	1.8
						1,6	17.0	3,5	1.0
						1,4	1.4	3,6	2.0
1052	3754 [2920 3543 3287]		C_6F_8			1,2	8.5		
1052	3755		$C_6F_8Cl_2$		1,2	+194.5	1,3	-29.1	
278	(2923)						2,3	-5.0	
1052	3756 (2924 3288)		$C_6F_8Cl_2$		1,2	200.3	1,3	4.1	
							2,3	5.3	

Table B.2.b. (contd.)

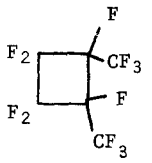
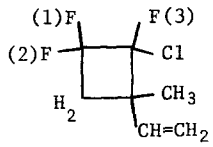
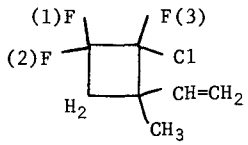
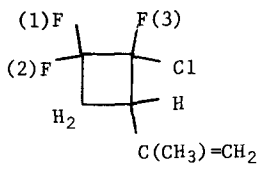
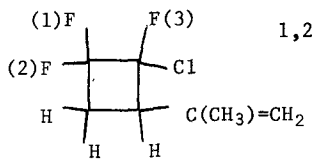
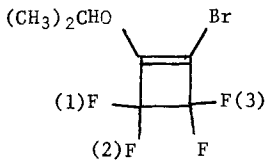
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
1024	3757		C_6F_{12}			240			
1090	3758	P-A[3]	$C_7F_3H_8Cl$		1,2	199.8	1,3 2,3	-8.60 +3.78	
1090	3759	P-A[3]	$C_7F_3H_8Cl$		1,2	202.2	1,3 2,3	-8.61 -0.82	
1090	3760	P-A[3]	$C_7F_3H_8Cl$		1,2	192.8	1,3 2,3	-7.54 +7.23	
1090	3761	P-A[3]	$C_7F_3H_8Cl$		1,2	∿200	1,3 2,3	-8.07 -0.42	
278	3762	P*	$C_7F_4H_7BrO$				1,3 2,3	+24.5 -16.9	

Table B.2.b. (contd.)

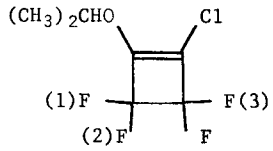
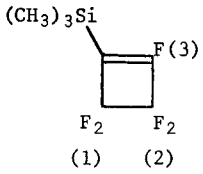
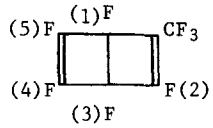
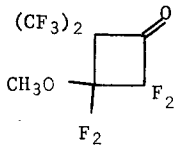
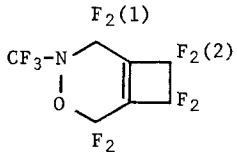
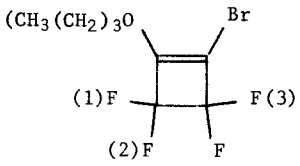
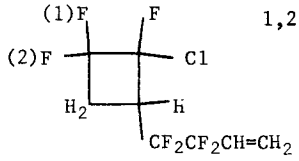
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
278	3763	P*	$C_7F_4H_7ClO$			1,3 +25.0 2,3 -16.9	
1051	3764		$C_7F_5H_9Si$			1,2 -15.05 2,3 4.5	1,3 22.9
284	3765 (2967, 3297)	P	C_7F_8			2,3 7 3,4 7.4 1,3 7 4,5 3.1 1,5 7.2	1,2 7 1,4 10.3 3,5 10.2 2,4 ⩽0.5 2,5 13.4
117	3766	B	$C_7F_9H_3O_2$		260		
1022	3767 (2975, 4104)		$C_7F_{11}NO$			1,2 1.95	
278	3768	P*	$C_8F_4H_9BrO$			1,3 +25.0 2,3 -17.0	
196	3769	P	$C_8F_7H_6Cl$		1,2 195		

Table B.2.b. (contd.)

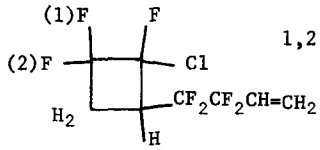
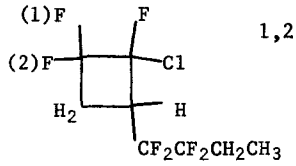
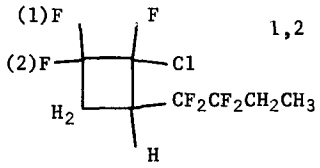
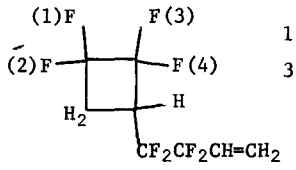
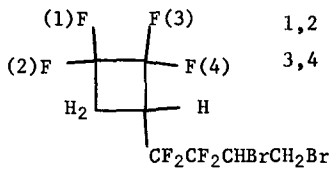
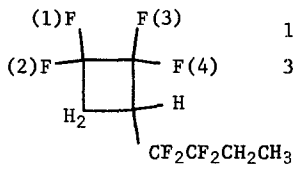
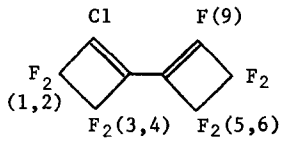
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
196	3770 (3013)	P	$C_8F_7H_6Cl$		1,2	196		
196	3771 (563 3014)	P	$C_8F_7H_8Cl$		1,2	195		
196	3772	P	$C_8F_7H_8Cl$		1,2	196		
196	3773	P	$C_8F_8H_6$		1,2 3,4	210 218		
196	3774 (3018 567)	P	$C_8F_8H_6Br_2$		1,2 3,4	210 214		
196	3775 (568)	P	$C_8F_8H_8$		1,2 3,4	212 215		
1098	3776	P*	C_8F_9Cl		1,2 3,4 5,6 7,8	+202.6 +200.0 +195.0 +207.3	1,3 2,3 5,7 6,7	{+26.2(1,2)(7,8) 2.8 -11.8 +26.5 -11.8

Table B.2.b. (contd.)

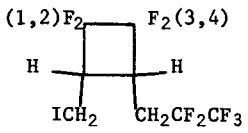
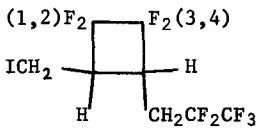
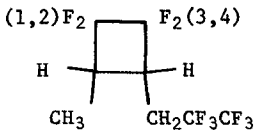
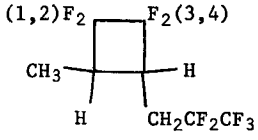
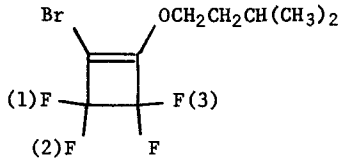
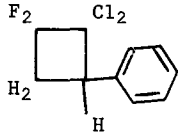
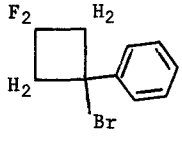
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
198	3777	P	$C_8F_9H_6I$		1,2 3,4	213 212		
198	3778 (3026)	P	$C_8F_9H_6I$		1,2 3,4	216 216		
198	3779	P	$C_8F_9H_7$		1,2 3,4	210 212		
190	3780	P	$C_8F_9H_7$		1,2 3,4	211 211		
278	3781	P*	$C_9F_4H_{11}BrO$				1,3 +25.0 2,3 -17.0	
1088	3782		$C_{10}F_2H_8Cl_2$			183		
1088	3783		$C_{10}F_2H_9Br$			196		

Table B.2.b. (contd.)

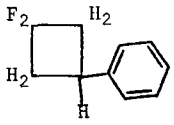
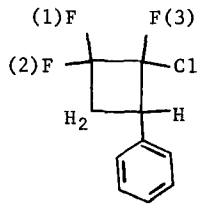
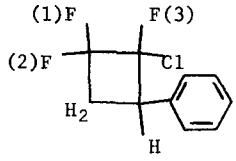
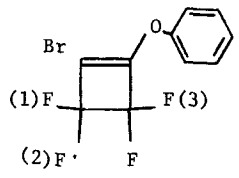
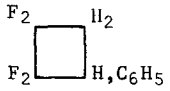
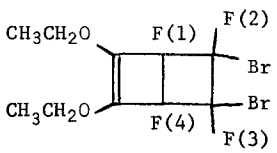
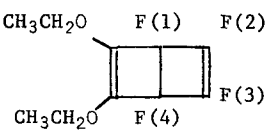
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ	
108	3784		$C_{10}F_2H_{10}$			192				
1090	3785	P-A[3]	$C_{10}F_3H_8Cl$		1,2	195.0	1,3 2,3	-7.81 +6.97		
1090	3786	P-A[3]	$C_{10}F_3H_8Cl$		1,2	199.6	1,3 2,3	-9.15 -0.20		
278	3787	P*	$C_{10}F_4H_5BrO$				1,3 2,3	+24.9 -16.0		
1087	3788		$C_{10}F_4H_8$			206 206				
284	3789	P	$C_{10}F_4H_{10}Br_2O_2$				1,2 2,3 3,4 1,4	4-5 13.0 4-5 8.5	1,3 2,4	4-5 18.6
290	3790 (1248)		$C_{10}F_4H_{10}O_2$				1,4 2,3	14.6 4.2		

Table B.2.b. (contd.)

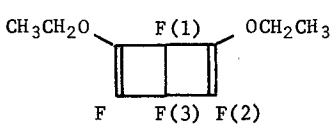
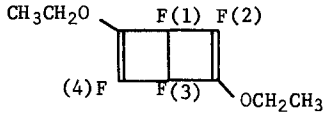
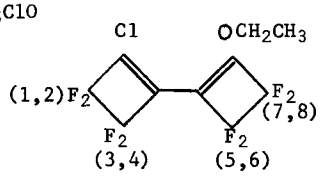
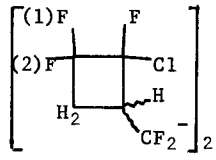
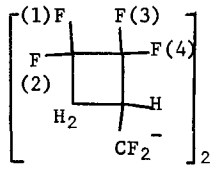
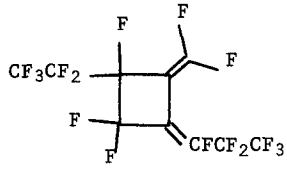
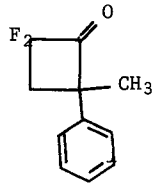
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
290	3791 (1249)		$C_{10}F_4H_{10}O_2$			1,3	14.4	1,2	11.6
290	3792 (1250)		$C_{10}F_4H_{10}O_2$			1,2 1,3	±4.0 14.5	2,3 2,4	±11.1 14.5
1098	3793	P*	$C_{10}F_8H_5ClO$		1,2 3,4 5,6 7,8	+200.0 +200.0 +195.0 +208.9	1,3 2,3 5,7 6,7	+25.8(1,2(1,8) -13.2 +25.4 -15.7	3.6
196	3794	P	$C_{10}F_{10}H_6Cl_2$		1,2	195			
				Mixture of isomers					
196	3795	P	$C_{10}F_{12}H_6$		1,2 3,4	210 215			
208	3796		$C_{10}F_{16}$			216			
1088	3797		$C_{11}F_2H_{10}O$			248			

Table B.2.b. (contd.)

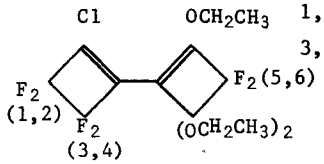
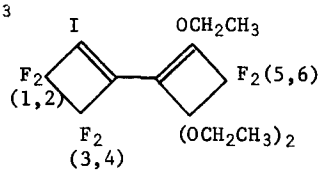
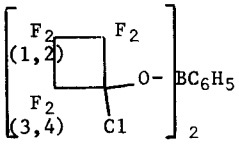
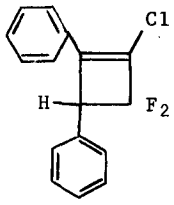
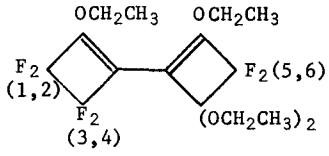
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
1098	3798	P*	$C_{14}F_6H_{15}ClO_3$		1,2 3,4	+190.5 +190.0	1,3 2,3	+25.7(1,2)(5,6) -13.9	3.6
1098	3799	P*	$C_{14}F_6H_{15}IO_3$		1,2 3,4	+181.1 +180.0	1,3 2,3	+25.2(1,2)(5,6) -14.6	3.4
759	3800		$C_{14}F_{12}H_5BCl_2O$		1,2 3,4	230 210			
1088	3801		$C_{16}F_2H_{11}Cl$			192			
1098	3802	P*	$C_{16}F_6H_{20}O_4$		1,2 3,4	+199.2 +190.0	1,3 2,3	+26.3(1,2)(5,6) -18.0	4.3

Table B.2.c. Five membered rings.

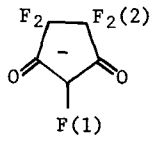
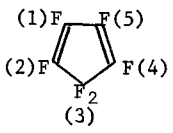
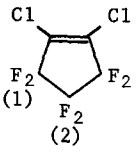
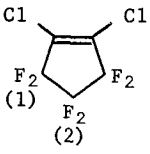
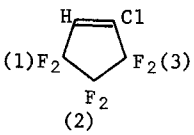
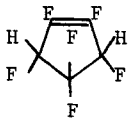
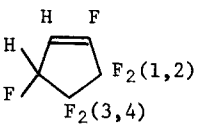
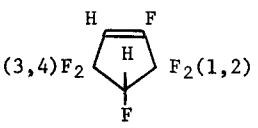
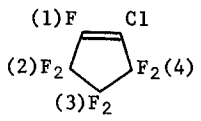
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ
1089	3803		$C_5F_5O_2^-$					1,2	9.1
1100	3804		C_5F_6			1,2	±16.0 or ∓ 8.4	1,3	7.3
								2,4	13.7 or 16.1
						1,5	16.1 or 13.7	1,4	∓ 8.4 or ±16.0
						2,3	6.7		
1101	3805		$C_5F_6Cl_2$			1,2	3.1		
1102	3806		$C_5F_6Cl_2$			1,2	3.2		
627	3807 (1256)		C_5F_6HCl			2,3 1,2	2.7 3.2	1,3	2.9
292	3808		$C_5F_6H_2$		1,2	267			
292	3809 (1258)		$C_5F_6H_2$		1,2 3,4	265 255			
292	3810 (1259)		$C_5F_6H_2$		1,2 3,4	269 263			
627	3811		C_5F_7Cl			1,2 2,3 3,4	13.9 1.9 1.4	1,3 2,4 1,4	4.8 2.1 10.0

Table B.2.c. (contd.)

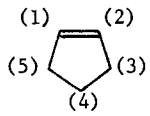
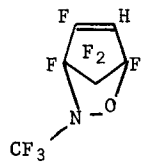
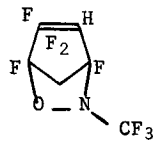
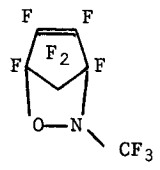
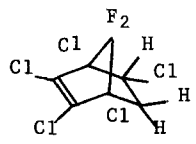
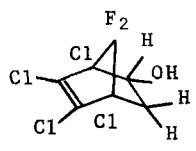
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J		^nJ	
627	3812		C_5F_8			1,2	3	1,3	±12
						2,3	±15	3,5	1
						3,4	2	1,4	3
292	3813	B	C_6F_8HNO		174				
292	3814	B	C_6F_8HNO		174				
1100	3815		C_6F_9NO		172				
294	3816 (1266)	P*	$C_7F_3H_2Cl_5$		+178				
294	3817 (1267)	P*	$C_7F_2H_4Cl_4O$		+182				

Table B.2.c. (contd.)

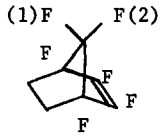
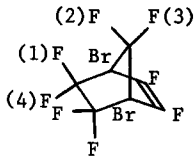
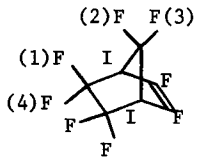
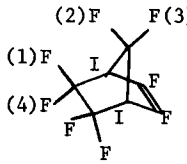
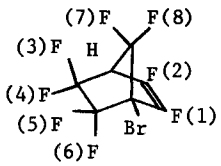
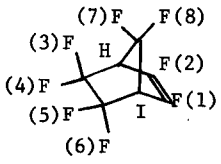
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
1103	3818 (3932)	J	$C_7F_2H_{10}$			222				
1100	3819		$C_7F_6H_4$		1,2	177				
1151	3820		$C_7F_8Br_2$		2,3	191.0			1,2	23.6
1151	3821		$C_7F_8I_2$		2,3	191.5			1,2	20.2
1104	3822 (3934)		$C_7F_8I_2$		1,4 2,3	218 193				
1151	3823 (3935)		C_7F_8HBr		3,4 5,6 7,8	228.5 220.0 200.0			1,3 2,5 3,7 5,7	7.1 5.9 22.7 23.2
1151	3824 (3936)		C_7F_8HI		3,4 5,6 7,8	226.5 217.5 203.5			1,3 2,5 3,7 5,7	5.8 4.9 21.6 22.0

Table B.2.c.(contd.)

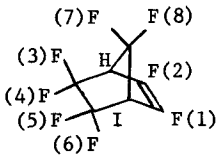
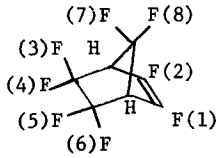
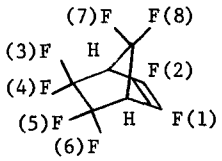
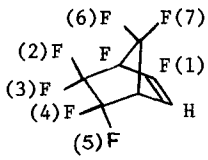
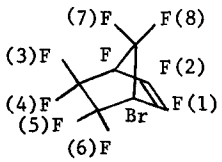
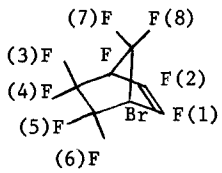
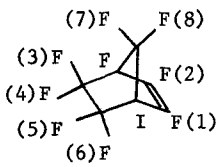
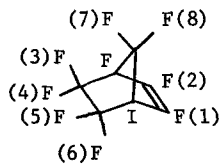
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	
1104	3825		C_7F_8HI		3,4	226		
	(3937)				5,6	218		
					7,8	196		
1151	3826		$C_7F_8H_2$		7,8	206.0	3,7	18.8
1104	3827		$C_7F_8H_2$		3,4	233		
	(3938)				7,8	207		
1151	3828		$C_7F_8H_2$		2,3	224.5	1,4	6.0
	(3939)				4,5	227.5	2,6	19.0
					6,7	203.5	4,6	20.5
1151	3829		C_7F_9Br		3,4	223.5	1,3	6.2
	(3941)				5,6	220.0	2,6	6.6
					7,8	197.0	3,7	19.1
							5,7	23.2
1104	3830		C_7F_9Br		3,4	218		
	(3942)				7,8	188		
1151	3831		C_7F_9I		3,4	220.0	2,5	7.2
	(3943)				5,6	218.0	5,7	21.6
					7,8	192.0		
1104	3832		C_7F_9I		3,4	220		
	(3944)				7,8	195		

Table B.2.c. (contd.)

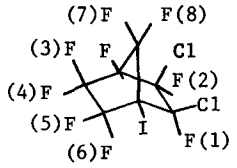
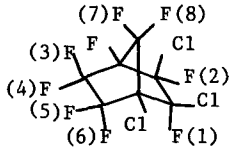
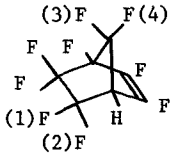
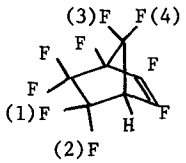
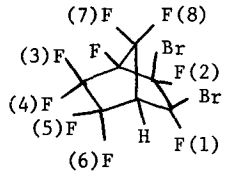
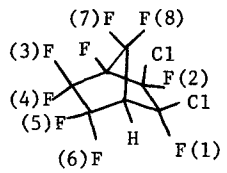
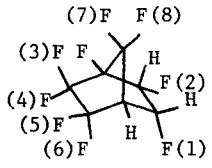
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ	
1151	3833		$C_7F_9Cl_2I$		3,4	238	1,6	81	
	(3945)				5,6	223	2,4	81	
					7,8	231	3,7	33	
							5,7	27	
1151	3834		$C_9F_9Cl_3$		3,4	239	1,6	81	
	(3946)				5,6	237	2,4	78	
					7,8	232	3,7	28	
							5,7	26	
1151	3835		C_7F_9H		1,2	230.0	1,3	22.1	
	(3947)				3,4	203.0			
1104	3836		C_7F_9H		1,2	229			
	(3948)				3,4	205			
1151	3837		$C_7F_9HBr_2$		3,4	240	1,6	73	
	(3951)				5,6	246	2,4	76	
					7,8	244	3,7	30	
							5,7	31	
1151	3838		$C_7F_9HCl_2$		3,4	239	1,6	74	
	(3952)				5,6	237	2,4	75	
					7,8	239	3,7	29	
							5,7	25	
1151	3839		$C_7F_9H_3$		3,4	244	1,6	55	
	[1269 3955 1355]				5,6	249	2,4	54	
							3,7	17	

Table B.2.c. (contd.)

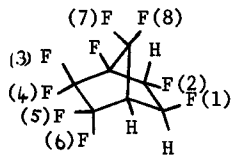
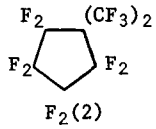
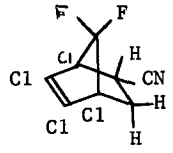
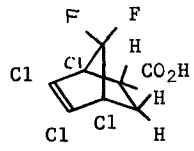
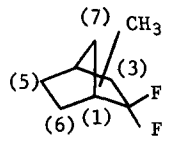
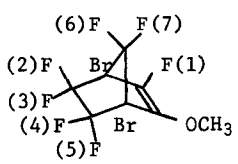
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ	
1151	3840		$C_7F_9H_3$		3,4	247			1,8	16
	[1270				5,6	245			2,4	47
	3956				7,8	237			3,7	20
	1366]								5,7	17
1071	3841	G	C_7F_{14}				1,2	2.3		
	(2986)									
294	3842	P*	$C_8F_2H_3Cl_4N$			+174				
	(1273)									
294	3843	P*	$C_8F_2H_4Cl_4O_2$			+174				
	(1274)									
1103	3844	J	$C_8F_2H_{12}$							
				(1)-CH_3		222				
				exo (3)-CH_3		223				
				endo (3)-CH_3		226				
				endo (5)-CH_3		221				
				endo (6)-CH_3		228				
				anti (7)-CH_3		222				
1151	3845		$C_8F_7H_3Br_2O$		2,3	219.5			1,4	6.8
	[1297				4,5	213.0			2,6	21.2
	3966				6,7	192.0			4,6	22.6
	1384]									

Table B.2.c. (contd.)

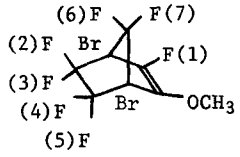
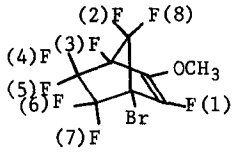
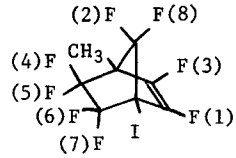
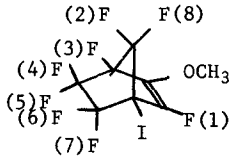
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J		^nJ
1151	3846		$C_8F_7H_3I_2O$		2,3	216.0			1,4	5.0
	[1298				4,5	216.0			2,6	20.0
	3967				6,7	193.0			4,6	22.5
	1385]									
1151	3847	*	$C_8F_8H_3BrO$		4,5	221.5	3,4	8.4	1,4	4.9
	[1300				6,7	217.6	3,5	3.0	1,2	3.8
	3968				2,8	193.2	3,8	8.4	4,8	0.0
	1387]						3,2	3.3	4,2	20.9
							4,6	1.8	5,8	2.4
							4,7	2.7	5,2	4.5
							5,6	1.5	6,8	0.0
							5,7	2.8	6,2	23.5
									7,8	1.0
									7,2	5.0
1151	3848	*	$C_8F_8H_3I$		4,5	225.1	1,3	5.0	1,4	5.3
	(3969)				6,7	222.1	4,6	1.4	1,2	1.9
					2,8	198.4	4,7	2.9	3,6	6.0
							5,6	1.4	3,2	5.0
							5,7	2.1	4,8	0.1
									4,2	22.8
									5,8	4.5
									5,2	4.3
									6,8	0.1
									6,2	21.8
									7,8	2.0
									7,2	4.5
1151	3849	*	$C_8F_8H_3IO$		4,5	219.9	3,4	8.8	1,4	6.3
	[1301				6,7	217.6	3,5	3.9	1,2	2.1
	3970				2,8	199.1	3,8	8.6	4,8	0.0
	1388]						3,2	3.8	4,2	19.3
							4,6	2.2	5,8	4.2
							4,7	1.0	5,2	6.5
							5,6	1.3	6,8	0.1
							5,7	1.5	6,2	21.9
									7,8	2.3
									7,2	4.2

Table B.2.c. (contd.)

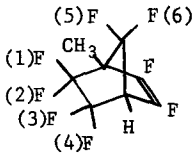
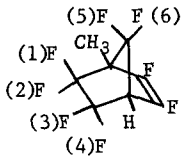
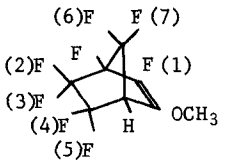
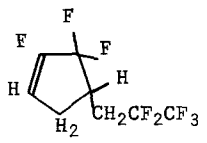
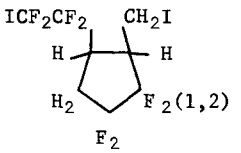
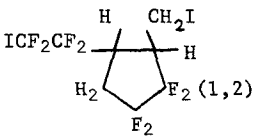
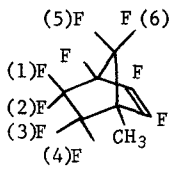
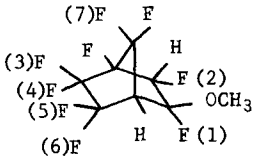
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1151	3850 (3971)		$C_8F_8H_4$		1,2 3,4 5,6	214.0 232.0 204.5		3,5	21.0
1104	3851 (3972)		$C_8F_8H_4$		3,4 5,6	231 205			
1151	3852 [1302 3973 1389]		$C_8F_8H_4O$		2,3 4,5 6,7	213.0 219.5 193.5		1,2 2,6 4,6	6.5 22.6 21.6
198	3853 (3017)	P	$C_8F_8H_6$			252			
1076	3854 (3019)		$C_8F_8H_6I_2$		1,2 3,4	241 242			
1076	3855 (3020)		$C_8F_8H_6I_2$		1,2	243			
1151	3856 (3974)		$C_8F_9H_3$		1,2 3,4 5,6	229.0 228.5 201.0		3,5	17.9
1151	3857 [1276 3975 1345]		$C_8F_9H_5O$		3,4 5,6	247 245		1,6 2,4 5,7	73 46 19

Table B.2.c. (contd.)

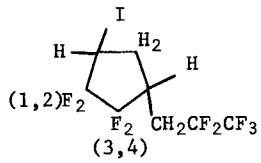
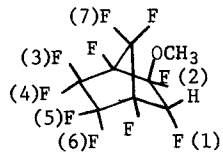
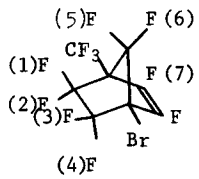
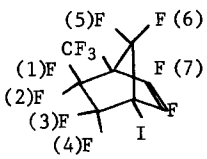
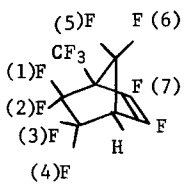
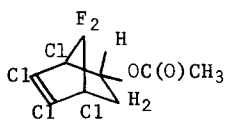
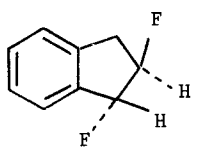
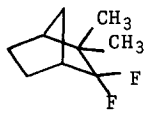
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
198	3858 (3025)	P	$C_8F_9H_6I$		1,2 3,4	239 232			
1151	3859 [1278 3976 1347]		$C_8F_{10}H_4O$		3,4 5,6	241 243		1,6 2,4 3,7 5,7	45 72 19 17
1151	3860 (3977)		$C_8F_{11}Br$		3,4 5,6	224.0 197.0		3,5	22.2
1151	3861 (3978)		$C_8F_{11}I$		1,2 3,4 5,6	219.5 221.5 196.0		1,7 3,5	6.8 22.6
1151	3862 (3979		$C_8F_{11}H$		1,2 3,4 5,6	230.0 226.0 205.0		3,5	22.0
298	3863 (1279)	P*	$C_9F_2H_6Cl_4O_2$			+179			
295	3864 (1280 3981)		$C_9F_2H_8$				4		
1103	3865	J	$C_9F_2H_{14}$			224			

Table B.2.c. (contd.)

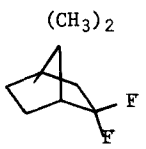
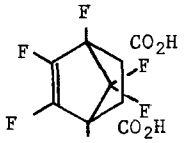
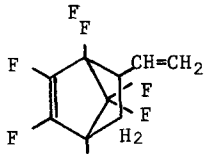
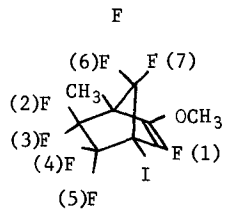
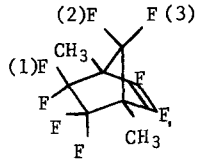
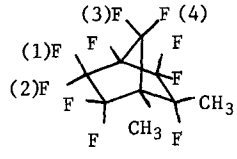
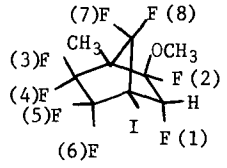
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1103	3866	J	$C_9F_2H_{14}$		228					
1100	3867		$C_9F_6H_2O_4$		175					
1100	3868		$C_9F_6H_5$		180					
1151	3869		$C_9F_7H_6IO$		2,3	215.3	2,4	1.5	1,2	5.6
	[1303				4,5	218.4	2,5	2.2	1,6	3.2
	3986				6,7	198.0	3,4	1.8	2,7	0.8
	1393]						3,5	2.4	2,6	22.2
									3,7	6.2
									3,6	5.0
									4,7	0.2
									4,6	21.2
									5,7	2.2
									5,6	4.4
1151	3870		$C_9F_8H_6$		2,3	206.0			1,2	17.9
	(3987)									
1151	3871		$C_9F_8H_6$		1,2	226.0				
	(3988)				3,4	196.0				
1151	3872		$C_9F_8H_7IO$		3,4	220			1,6	49
	[1281				5,6	246			2,4	84
	3989				7,8	243			3,7	20
	1352]								5,7	20

Table B.2.c. (contd.)

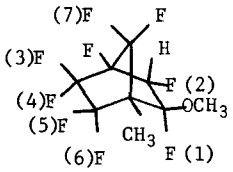
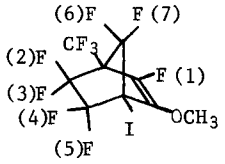
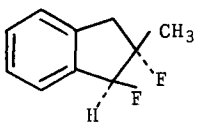
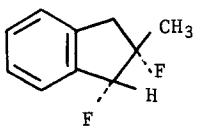
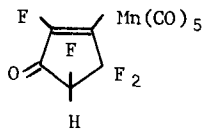
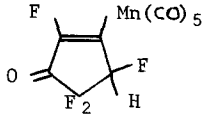
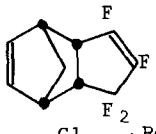
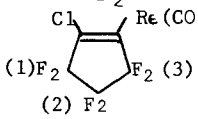
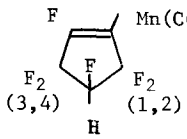
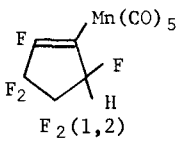
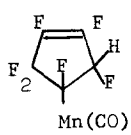
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1151	3873 (1353, 3990)		$C_9F_9H_7O$		3,4 5,6	241 248		1,6 2,4 5,7	81 48 21
1151	3874 [1304, 3991, 1394]		$C_9F_{10}H_3IO$		4,5 6,7	218.5 198.0		1,4 2,6 4,6	6.6 17.1 21.2
295	3875 (1283, 1305)		$C_{10}F_2H_{10}$				0		
295	3876 (1284, 1306)		$C_{10}F_2H_{10}$				8		
292	3877 (1285)		$C_{10}F_4HMnO_6$			259			
292	3878 (1286)		$C_{10}F_4HMnO_6$			280			
274	3879	B	$C_{10}F_4H_8$			251			
1102	3880		$C_{10}F_6ClO_5Re$				1,2 2,3	6.7 6.7	1,3	3.74
292	3881 (1288)		$C_{10}F_6HMnO_5$		1,2 3,4	257 258			
292	3882 (1287)		$C_{10}F_6HMnO_5$		1,2	243			
292	3883 (1289)		$C_{10}F_5H_2MnO_5$			253			

Table B.2.c. (contd.)

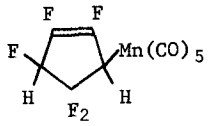
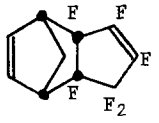
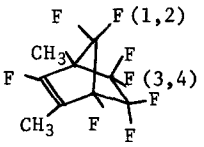
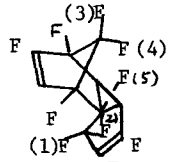
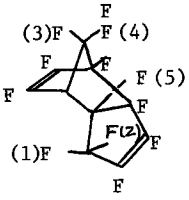
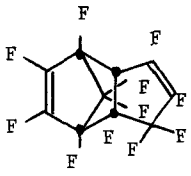
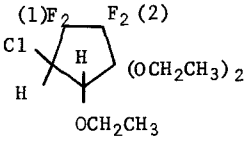
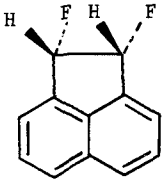
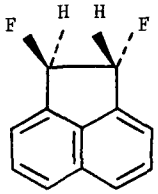
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
292	3884 (1290)		$C_{10}F_5H_2MnO_5$		237					
1100	3885		$C_{10}F_6H_6$		260					
110	3886		$C_{10}F_8H_6$		1,2 3,4	209 225				
1105	3887		$C_{10}F_{10}H_2$		1,2 3,4	260 183			4,5	34
1105	3888		$C_{10}F_{12}$		1,2 3,4	266 185			4,5 4,6 1,7	24 37 43.8
1100	3889		$C_{10}F_{12}$		1,2	179				
1102	3890		$C_{11}F_4H_{15}ClO_3$				1,2	5.15		
295	3891 (1291)		$C_{12}F_2H_8$					16.4		
295	3892 (1292)		$C_{12}F_2H_8$					0.1		

Table B.2.c. (contd.)

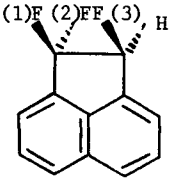
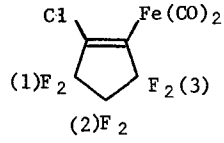
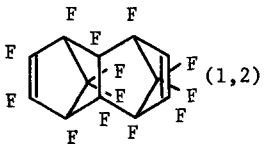
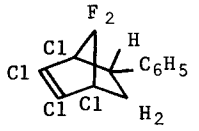
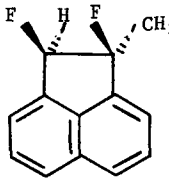
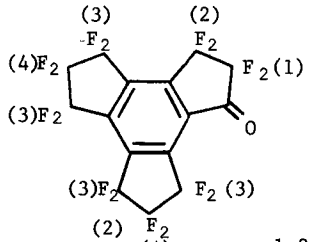
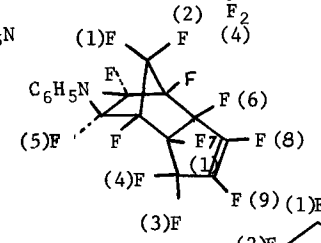
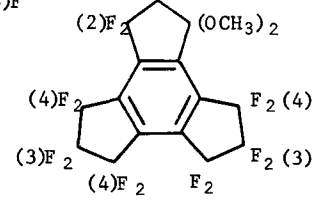
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
295	3893 (1293)		$C_{12}F_3H_7$		1,2	265.3	1,3 2,3	9.8 1.2		
1102	3894		$C_{12}F_6H_5ClFeO_2$				1,2 2,3	6.82 6.82	1,3	3.65
1100	3895		$C_{12}F_{14}$		1,2	175				
294	3896 (1294)	P*	$C_{13}F_2H_8Cl_4$			+169				
295	3897 (1295, 1307)		$C_{13}F_2H_{10}$					16		
1092	3898		$C_{15}F_{16}O$				1,2 3,4	2.2 4.5		
1106	3899	A	$C_{16}F_{12}H_5N$		1,2 3,4	220 260	8,9	20	3,5 2,6 2,7	105 73 22
1092	3900		$C_{17}F_{16}H_6O_2$				1,2 3,4	4 4-4.5		

Table B.2.c. (contd.)

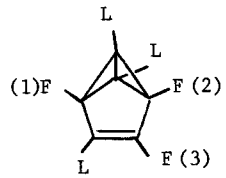
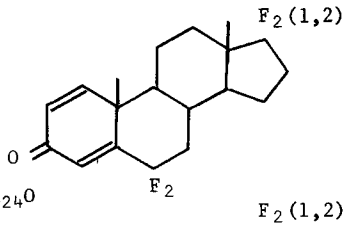
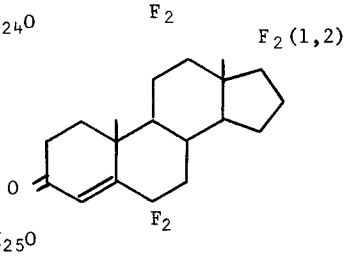
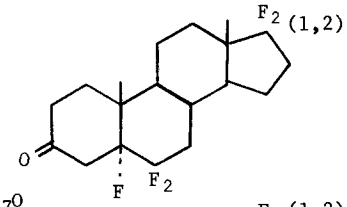
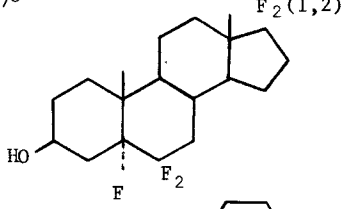
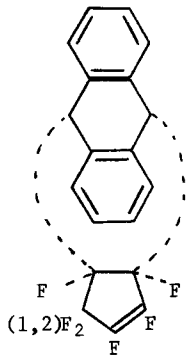
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
890	3901		$C_{18}F_3H_{29}$	 L = $C(CH_3)_3$		2,3 4	1,2 10 1,3 <2
320	3902 (1416 4012)		$C_{19}F_4H_{22}O$		1,2	220	
320	3903 (1417 4013)		$C_{19}F_4H_{24}O$		1,2	218	
320	3904 (1418)		$C_{19}F_5H_{25}O$		1,2	219	
320	3905 (1419)		$C_{19}F_5H_{27}O$		1,2	220	
1100	3906		$C_{19}F_6H_8$		1,2	248	

Table B.2.c. (contd.)

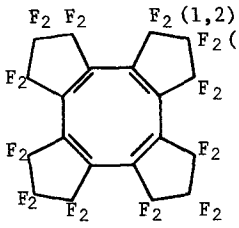
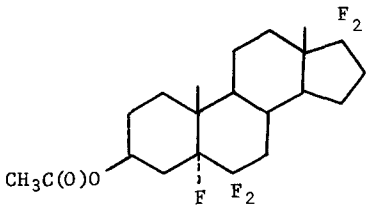
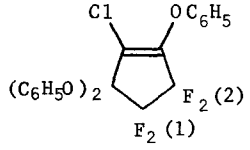
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1092	3907		$C_{20}F_{24}$		1,2 280 3,4 244		
320	3908 (1450)		$C_{21}F_5H_{29}O_2$		220		
1101	3909		$C_{23}F_4H_{15}ClO_3$			1,2	4.6

Table B.2.d. Six membered rings.

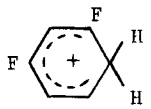
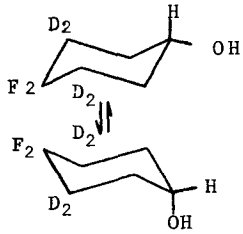
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	2	3	^nJ
398 392	3910 (1315)	F^2	$C_6F_2H_5^+$				80 82
1107	3911	E^2	$C_6F_2H_6D_4O$		237 236		

Table B.2.d. (contd.)

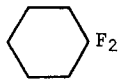
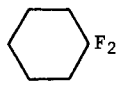
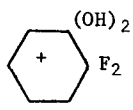
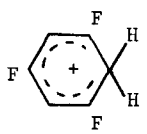
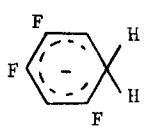
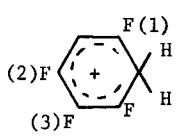
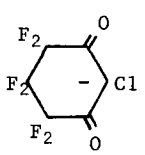
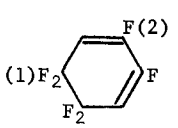
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
297	3912 (1318)		$C_6F_2H_{10}$		235.3		
1108	3913		$C_6F_2H_{10}$	 (-70^o)	228		
1108	3914		$C_6F_2H_{10}O_2$	 (-70^o)	236		
392	3915 (1320)	F^2	$C_6F_3H_4^+$				70
392	3916	F^2	$C_6F_3H_4^+$			20	80
392	3917	F^2	$C_6F_4H_3^+$		2,3	20	1,2 70
1089	3918		$C_6F_6ClO_2^-$			11.3	
213	3919 (1321)		$C_6F_6H_2$				1,2 3.7

Table B.2.d. (contd.)

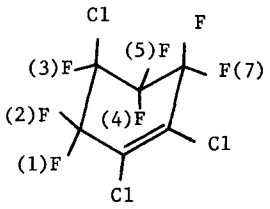
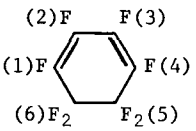
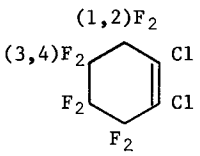
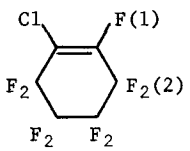
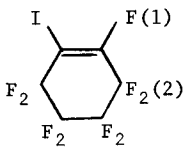
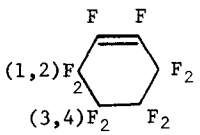
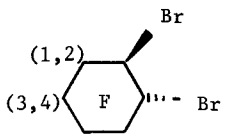
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1109	3920		$C_6F_7Cl_3$		1,2	286.8	4,6	11.7	1,4	8.9
					4,5	276.4	1,3	13.5	1,5	2.1
					6,7	287.7	3,4	18.3	2,4	1.8
							4,7	13.1	3,6	1.9
							5,6	13.2	2,5	17.8
							2,3	7.1	3,7	18.7
							3,5	7.8	1,6	1.5
							5,7	1.6	1,7	1.4
									2,6	1.7
									2,7	4.7
627	3921		C_6F_8				1,2	2	1,3	10
							2,3	1	1,4	1
							1,6	15	2,6	10
							5,6	1	1,5	5
									2,5	6
1110	3922	T^3	$C_6F_8Cl_2$		1,2	280				
					3,4	277				
213	3923		C_6F_9Cl				1,2	23.5		
213	3924		C_6F_9I				1,2	25.4		
1110	3925	T^3	C_6F_{10}		1,2	287				
					3,4	277				
1111	3926		$C_6F_{10}Br_2$		1,2	286				
					3,4	275				

Table B.2.d. (contd.)

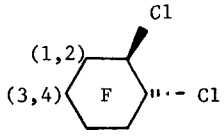
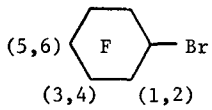
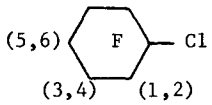
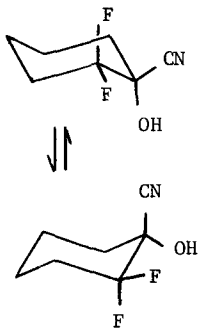
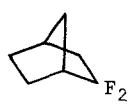
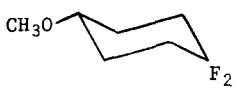
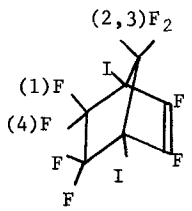
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
1111	3927		$C_6F_{10}Cl_2$		1,2 3,4	289 274		
1111	3928		$C_6F_{11}Br$		1,2 3,4 5,6	289 282 280		
1111	3929		$C_6F_{11}Cl$		1,2 3,4 5,6	285 285 285		
1112	3930	P	C_6F_{12}	 (-66^{o})		284		
108	3931	G	$C_7F_2H_9NO$			236$^+$ 239$^+$		
1103	3932 (3818)	J	$C_7F_2H_{10}$			222		
291	3933	A	$C_7F_2H_{12}O$			236		
1104	3934 (3822)		$C_7F_8I_2$		1,4 2,3	218 193		

Table B.2.d. (contd.)

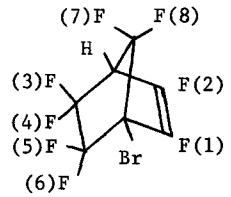
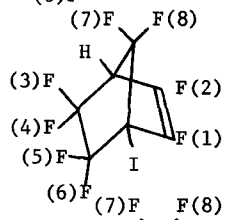
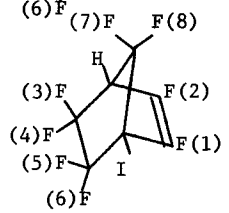
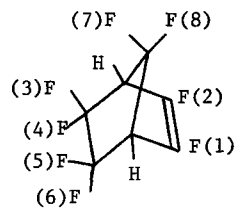
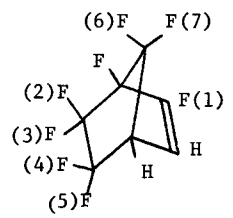
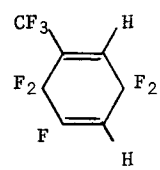
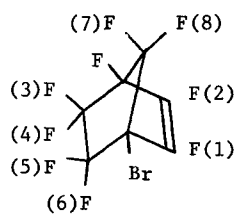
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1151	3935		C_7F_8HBr		3,4	228.5		1,3	7.1
	(3823)				5,6	220.0		2,5	5.9
								3,7	22.7
								5,7	23.2
1151	3936		C_7F_8HI		3,4	226.5		1,3	5.8
	(3824)				5,6	217.5		2,5	4.9
								3,7	21.6
								5,7	22.0
1104	3937		C_7F_8HI		3,4	226			
	(3825)				5,6	218			
1104	3938		$C_7F_8H_2$		3,4	233			
	(3827)								
1151	3939		$C_7F_8H_2$		2,3	224.5		1,4	6.0
	(3828)				4,5	227.5		2,6	19.0
					6,7	203.5		4,6	20.5
213	3940		$C_7F_8H_2$				22.7		
	[852 1333 2969 3299]								
1151	3941		C_7F_9Br		3,4	223.5		1,3	6.2
	(3829)				5,6	220.0		2,6	6.6
								3,7	19.1
								5,7	23.2

Table B.2.d. (contd.)

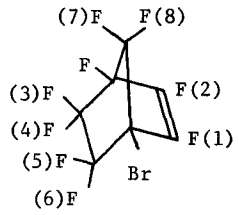
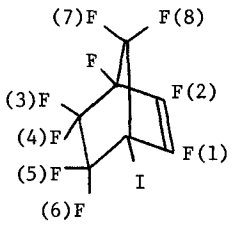
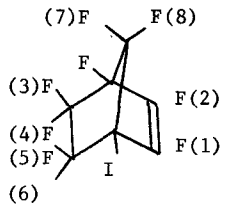
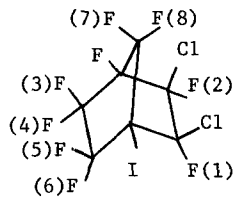
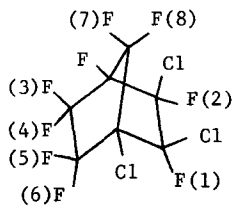
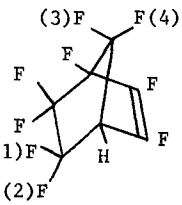
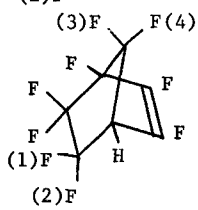
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ	
1104	3942 (3830)		C_7F_9Br		3,4	218			
1151	3943 (3831)		C_7F_9I		3,4 5,6	220.0 218.0		2,5 5,7	7.2 21.6
1104	3944 (3832)		C_7F_9I		3,4	220			
1151	3945 (3833)		$C_7F_9Cl_2I$		3,4 5,6	238 223		1,6 2,4 3,7 5,7	81 81 33 26
1151	3946 (3834)		$C_7F_9Cl_3$		3,4 5,6	239 237		1,6 2,4 3,7 5,7	81 78 28 26
1151	3947 (3835)		C_7F_9H		1,2 3,4	230.0 203.0		1,3	22.1
1104	3948		C_7F_9H		1,2 3,4	229 205			

Table B.2.d. (contd.)

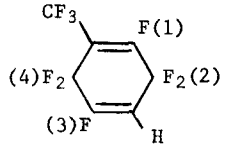
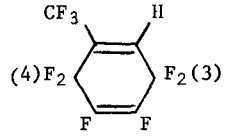
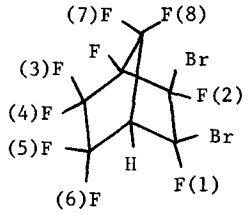
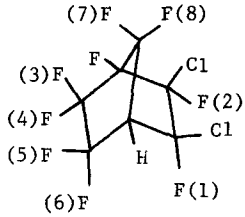
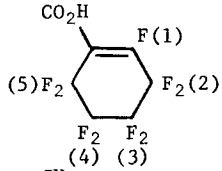
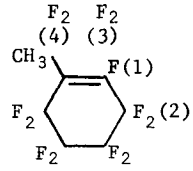
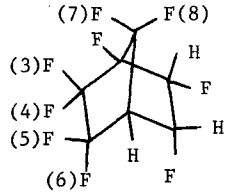
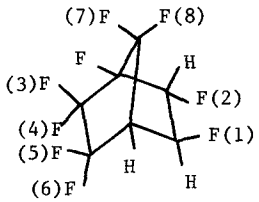
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
213	3949 [1334 2970 3300]		C_7F_9H				1,2 or 1,4	21.6		
213	3950		C_7F_9H				1,2	8.45		
							1,4 or 2,3	2.8		
1151	3951 (3837)		$C_7F_9HBr_2$		3,4	240			1,6	73
					5,6	246			2,4	76
									3,7	30
									5,7	31
1151	3952 (3838)		$C_7F_9HCl_2$		3,4	239			1,6	74
					5,6	237			2,4	75
									3,7	29
									5,7	25
213	3953		$C_7F_9HO_2$				1,2	22.5	1,5	10.3
									1,3	2.8
									1,4	2.8
213	3954 (1382)		$C_7F_9H_3$				1,2	20.7		
1151	3955 [1269 3839 1335]		$C_7F_9H_3$		3,4	244			1,6	55
					5,6	249			2,4	54
									3,7	17
1151	3956 [1270 3840 1336]		$C_7F_9H_3$		3,4	247			1,8	16
					5,6	245			2,4	47
									3,7	20
									5,7	17

Table B.2.d. (contd.)

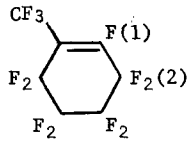
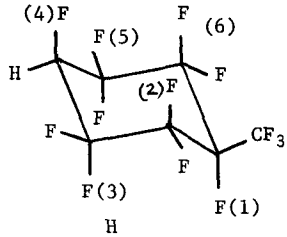
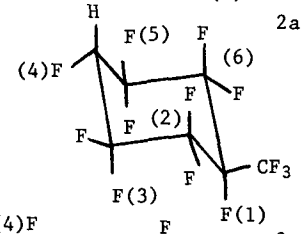
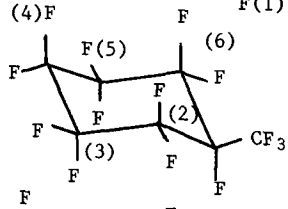
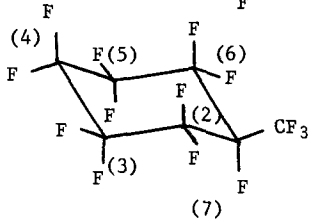
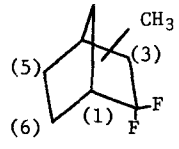
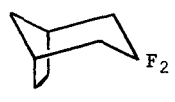
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
213	3957		C_7F_{12}			1,2	15.1			
	(2977 3303)									
301	3958	P*	$C_7F_{13}H$		2a,2e	305	1,2a	2.8	1,3a	28.3
	(1339 2981)				3a,3e	300	1,2e	16.6	1,3e	∿0
							4,3a	3.2		
							4,3e	14.9		
301	3959	P*	$C_7F_{13}H$		2a,2e	302	1,2a	1.0	1,3a	27
	1340						1,2e	14.2	1,3e	∿0
	2980						4,3a	12.5		
							4,3e	12.5		
301	3960	P*	C_7F_{14}		2a,2e	302	1,2a	2.2	1,3a	25.1
	(2983)				3a,3e	297	1,2e	14.7	1,3e	∿0
					4a,4e	289				
1069	3961	B-R	C_7F_{14}		2a,2e	291	3a,4e	13.5	3a,5e	25
	(2984)				3a,3e	286	3e,4e	13.5	3e,5e	6
					4a,4e	284	3a,4a	0	3a,5e	2
							3e,4a	13	4a,2a	20
									4a,2e	3
				(7)						
1103	3962	J	$C_8F_2H_{12}$							
	(3844)									
				(1)-CH_3		222				
				exo (3)-CH_3		223				
				endo (3)-CH_3		226				
				endo (5)-CH_3		221				
				endo (6)-CH_3		228				
				anti (7)-CH_3		222				
1113	3963	P	$C_8F_2H_{12}$			251				
				(30^o)						

Table B.2.d. (contd.)

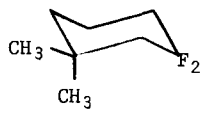
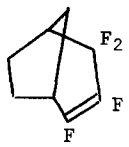
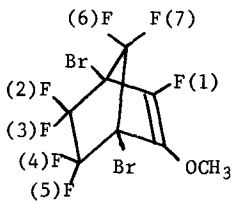
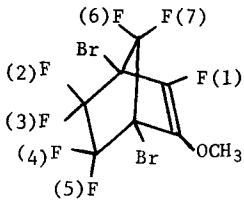
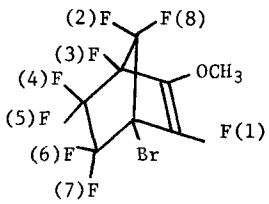
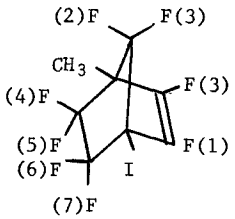
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1113	3964	P	$C_8F_2H_{14}$	 (-55°)		240			
274	3965	B	$C_8F_4H_8$			263			
1151	3966 [1297 3845 1384]		$C_8F_7H_3Br_2O$		2,3 4,5	219.5 213.0		1,4 2,6 4,6	6.8 21.2 22.6
1151	3967 [1298 3846 1385]		$C_8F_7H_3I_2O$		2,3 4,5	216.0 216.0		1,4 2,6 4,6	5.0 20.0 22.5
1151	3968 [1300 3847 1387]	*	$C_8F_8H_3BrO$		4,5 6,7	221.5 217.6	3,4 3,5 3,8 3,2 4,6 4,7 5,6 5,7	8.4 3.0 8.4 3.3 1.8 2.7 1.5 2.8	1,4 1,2 4,8 4,2 5,8 5,2 6,8 6,2 7,8 7,2	4.9 3.8 0.0 20.9 2.4 4.5 0.0 23.5 1.0 5.0
1151	3969 (3848)	*	$C_8F_8H_3I$		4,5 6,7	225.1 222.1	1,3 4,6 4,7 5,6 5,7	5.0 1.4 2.9 1.4 2.1	1,4 1,2 3,6 3,2 4,8 4,2 5,8 5,2 6,8 6,2 7,8 7,2	5.3 1.9 6.0 5.0 0.1 22.8 4.5 4.3 0.1 21.8 2.0 4.5

Table B.2.d. (contd.)

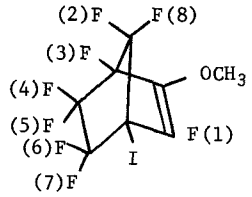
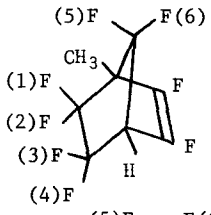
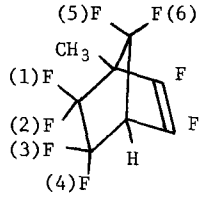
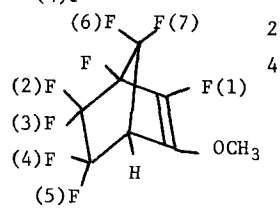
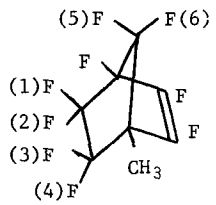
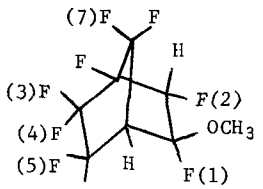
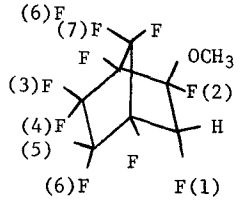
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1151	3970	*	$C_8F_8H_3IO$		4,5	219.9	3,4	8.8	1,4	6.3
	[1301				6,7	217.6	3,5	3.9	1,2	2.1
	3849						3,8	8.6	4,8	0.0
	1388]						3,2	3.8	4,2	19.3
							4,6	2.2	5,8	4.2
							4,7	1.0	5,2	6.5
							5,6	1.3	6,8	0.1
							5,7	1.5	6,2	21.9
									7,8	2.3
									7,2	4.2
1151	3971		$C_8F_8H_4$		1,2	214.0			3,5	21.0
	(3850)				3,4	232.0				
1104	3972		$C_8F_8H_4$		3,4	231				
	(3851)									
1151	3973		$C_8F_8H_4O$		2,3	213.0			1,2	6.5
	[1302				4,5	219.5			2,6	22.6
	3852								4,6	21.6
	1389]									
1151	3974		$C_8F_9H_3$		1,2	229.0			3,5	17.9
	(3856)				3,4	228.5				
					5,6	201.0				
1151	3975		$C_8F_9H_5O$		3,4	247			1,6	73
	[1276				5,6	245			2,4	46
	3857								5,7	19
	1345]									
1151	3976		$C_8F_{10}H_4O$		3,4	241			1,6	4.5
	[1278				5,6	243			2,4	72
	3859									
	1347]									

Table B.2.d. (contd.)

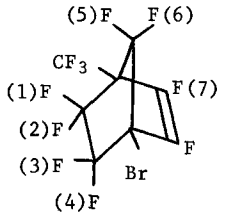
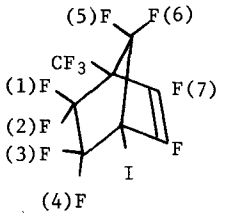
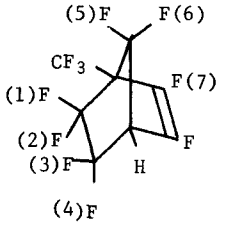
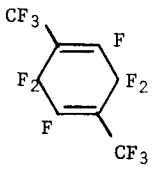
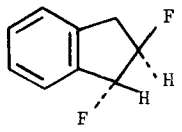
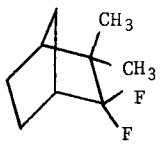
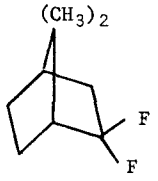
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1151	3977 (3860)		$C_8F_{11}Br$		3,4	224.0		3,5	22.2
1151	3978 (3861)		$C_8F_{11}I$		1,2 3,4	219.5 221.5		1,7 3,5	4.8 22.6
1151	3979 (3862)		$C_8F_{11}H$		1,2 3,4	230.0 226.0		3,5	22.0
213	3980 (3029 3310)		C_8F_{12}				9.4		
295	3981 (1280 3864)		$C_9F_2H_8$				4		
1103	3982	J	$C_9F_2H_{14}$			224			
1103	3983	J	$C_9F_2H_{14}$			228			

Table B.2.d. (contd.)

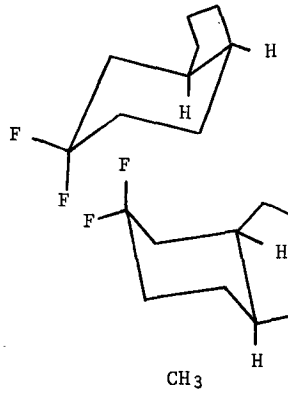
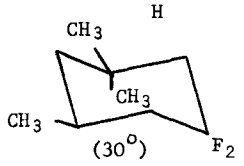
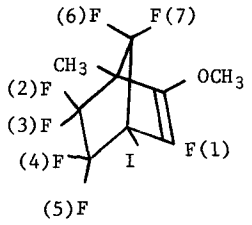
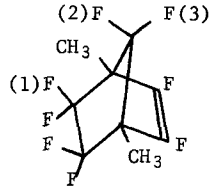
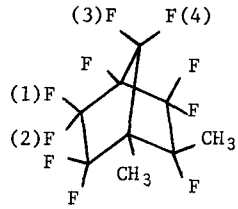
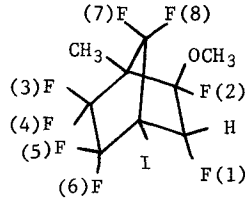
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
1114	3984	E	$C_9F_2H_{14}$		223					
					223					
1113	3985	P	$C_9F_2H_{16}$		251					
1151	3986		$C_9F_7H_6IO$		2,3	215.3	2,4	1.5	1,2	5.0
	[1303 3869 1393]				4,5	218.4	2,5	2.2	1,6	3.2
							3,4	1.8	2,7	0.8
							3,5	2.4	2,6	22.2
									3,7	6.2
									3,6	5.0
									4,7	0.2
									4,6	21.2
									5,7	2.2
									5,6	4.4
1151	3987 (3870)		$C_9F_8H_6$		2,3	206.0			1,2	17.9
1151	3988 (3871)		$C_9F_8H_6$		1,2	226.0				
1151	3989		$C_9F_8H_7IO$		3,4	220			1,6	49
	[1281 3872 1352]				5,6	246			2,4	84
									3,7	20
									5,7	20

Table B.2.d. (contd.)

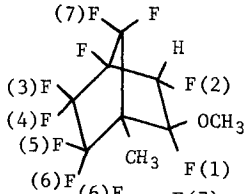
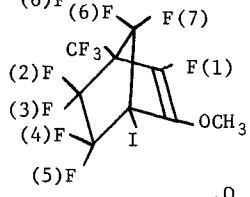
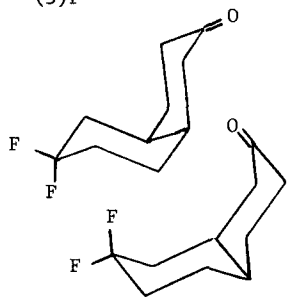
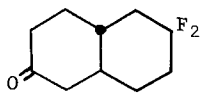
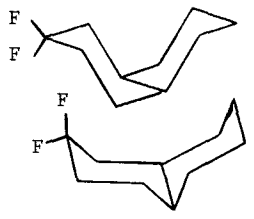
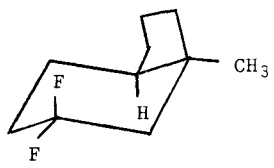
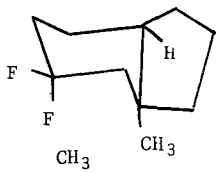
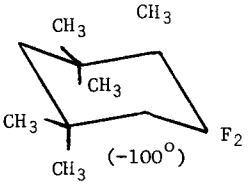
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1151	3990		$C_9F_9H_7O$		3,4	241		1,6	81
	(1353 3873)				5,6	248		2,4	48
								5,7	21
1151	3991		$C_9F_{10}H_3IO$		4,5	218.5		1,4	6.6
	[1304 3874 1394]							2,6	17.1
								4,6	21.2
1114	3992	R	$C_{10}F_2H_{14}O$			241			
1115						241			
1115	3993	R	$C_{10}F_2H_{14}O$			241			
1114	3994	E	$C_{10}F_2H_{16}$			234			
						236			
1114	3995	E	$C_{10}F_2H_{16}$			237			
						237			
1113	3996	P	$C_{10}F_2H_{18}$			243			

Table B.2.d. (contd.)

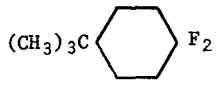
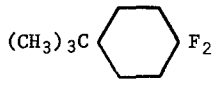
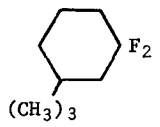
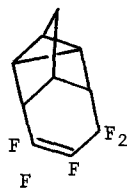
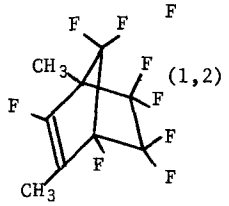
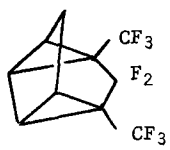
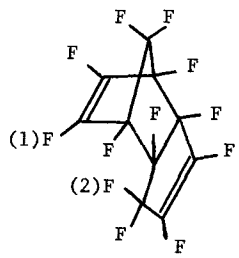
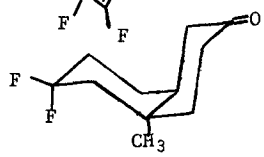
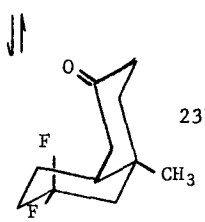
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
306	3997 (1361)	B	$C_{10}F_2H_{18}$		236		
1108	3998		$C_{10}F_2H_{18}$		228		
306	3999	B	$C_{10}F_2H_{18}$		236		
274	4000	B	$C_{10}F_4H_8$		266		
1104	4001 (3886)		$C_{10}F_8H_6$		1,2 225		
274	4002 (1204 3907)	B	$C_{10}F_8H_6$		242		
1105	4003		$C_{10}F_{10}H_2$			1,2	43.8
1114	4004	E	$C_{11}F_2H_{16}O$		237		
					237		

Table B.2.d. (contd.)

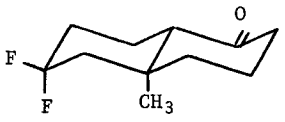
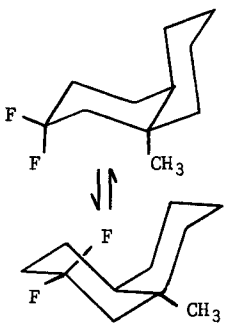
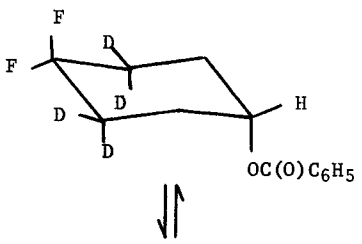
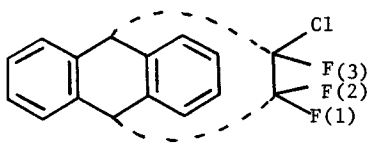
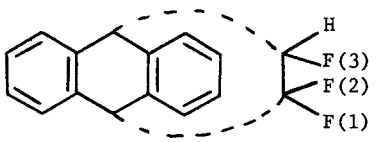
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1115	4005		$C_{11}F_2H_{16}O$		237		
1114	4006	Z^4	$C_{11}F_2H_{18}$		239 242		
1107	4007	E	$C_{13}F_2H_{10}D_4O_2$		236 237		
1119	4008	A	$C_{16}F_3H_{10}Cl$			1,3 2,3	-2.2 +11.4
1119	4009	H	$C_{16}F_3H_{11}$			1,3 2,3	-1.2 +9.4

Table B.2.d. (contd.)

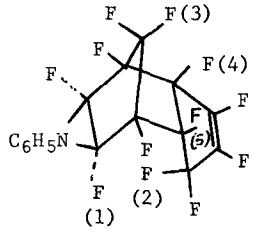
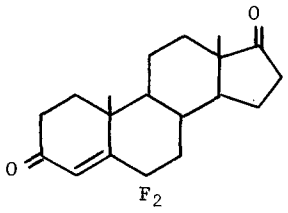
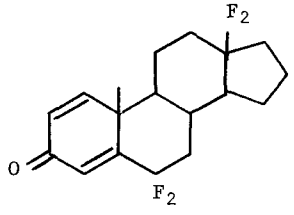
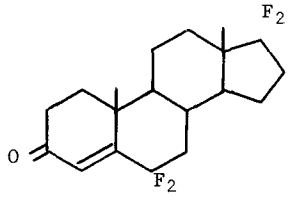
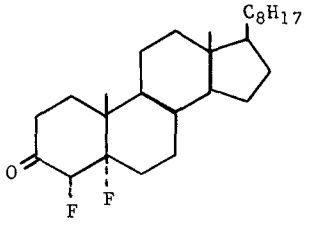
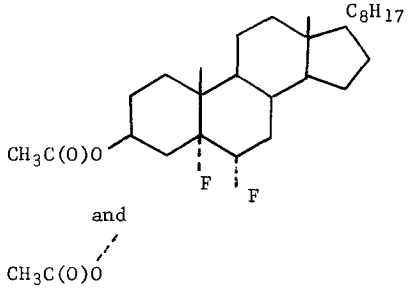
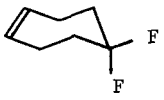
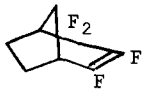
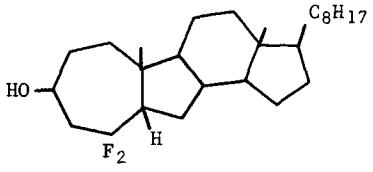
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1106	4010	A	$C_{16}F_{12}H_5N$				1,2 105 3,4 73 3,5 22
320	4011 (1414)		$C_{19}F_2H_{24}O_2$		252		
320	4012 (1416 3902)		$C_{19}F_4H_{22}O$		248		
320	4013 (1417 3903)		$C_{19}F_4H_{24}O$		254		
343	4014 (1533)		$C_{27}F_2H_{44}O$			12	
242	4015	A	$C_{29}F_2H_{48}O_2$			15	

Table B.2.e. Seven membered rings.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1117	4016		$C_7F_2H_{10}$		248		
274	4017	B	$C_8F_4H_8$		263		
242	4018	A	$C_{27}F_2H_{40}O$		245		

B.3. Fluorine bonded to carbon in heterocyclic, non-aromatic ring system.

Table B.3.a. Heterocycles containing one nitrogen atom.

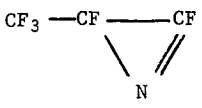
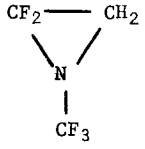
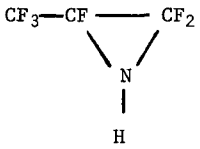
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
904	4019 (2697, 3227)		C_3F_5N			49.1	
1015	4020		$C_3F_5H_2N$		100		
904	4021		C_3F_6HN		102		

Table B.3.a. (contd.)

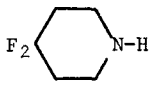
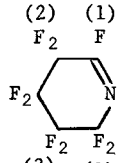
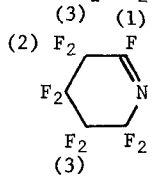
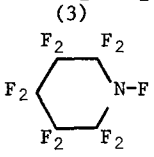
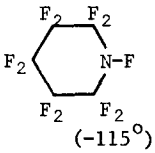
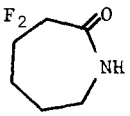
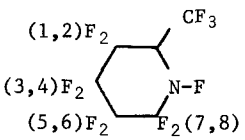
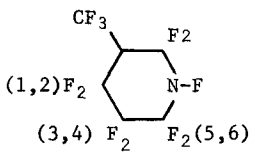
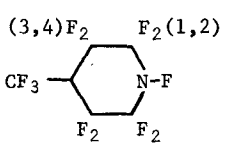
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1120	4022	A	$C_5F_2H_9N$		234		
993	4023		C_5F_9N		1,2	∿25	
1121	4024		C_5F_9N		1,2	24	2,3 7.6
1122	4025		$C_5F_{11}N$		1,2 185 3,4 282 5,6 285		
1123	4026		$C_5F_{11}N$	 (-115°)	1,2 185 3,4 278 5,6 284		
349	4027 (1571)	E	$C_6F_2H_9NO$		241		
1122	4028		$C_6F_{13}N$		1,2 293 3,4 289 5,6 289 7,8 199		
1122	4029 (2935)		$C_6F_{13}N$		1,2 289 3,4 284 5,6 198		
1122	4030 (2936)		$C_6F_{13}N$		1,2 196 3,4 286		

Table B.3.d. Heterocycles containing one oxygen atom (excluding carbohydrates).

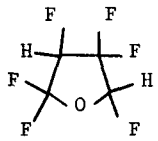
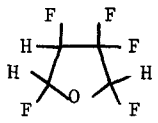
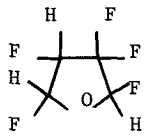
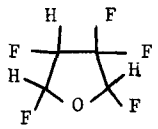
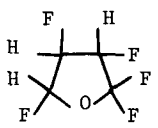
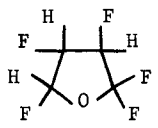
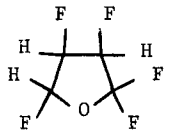
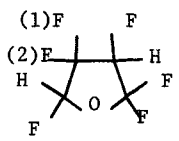
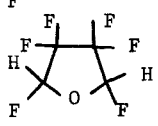
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
1118	4031 (2726)		C_3F_6O		2,3	43.5	1,2 1,3	16.5 16.5	
188	4032 (1587)		$C_4F_5H_3O$			264.4			
188	4033 (1588)		$C_4F_5H_3O$			282.4			
188	4034 (1589)		$C_4F_5H_3O$			251.8			
188	4035 (1590)		$C_4F_5H_3O$			267.0			
188	4036 (1591)		$C_4F_5H_3O$			150.0			
188	4037 (1592)		$C_4F_5H_3O$			140.0			
188	4038 (1593)		$C_4F_5H_3O$			144.5			
188	4039 (1594)		$C_4F_6H_2O$		1,2 3,4	260 141.2			
188	4040 (1595)		$C_4F_6H_2O$		A B	264.2 264.1			

Table B.3.b. (contd.)

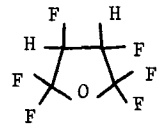
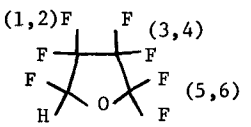
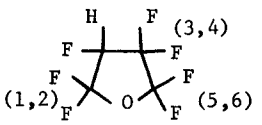
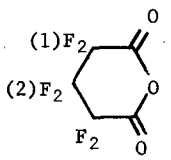
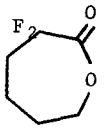
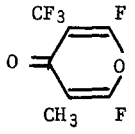
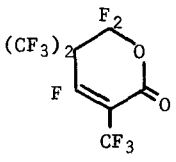
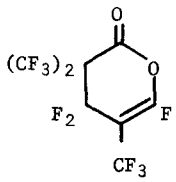
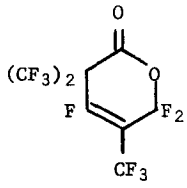
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
188	4041		$C_4F_6H_2O$			144.8		
188	4042 (1596)		C_4F_7HO		1,2 3,4 5,6	256.6 264.4 137.7		
188	4043 (1597)		C_4F_7HO		1,2 3,4 5,6	142.7 259.4 136.6		
1049	4044	B	$C_5F_6O_3$				1,2 9.0	
349	4045 (1608)	E	$C_6F_2H_8O_2$			240		
125	4046 (1629)	A	$C_7F_5H_3O_2$					7
113	4047 (3033 3313)		$C_8F_{12}O_2$					7
113	4048 (3032 3312)		$C_8F_{12}O_2$					14
113	4049 (3031 3311)		$C_8F_{12}O_2$					14

Table B.3.c. Carbohydrates

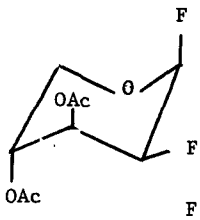
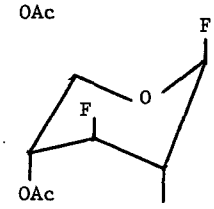
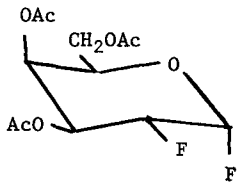
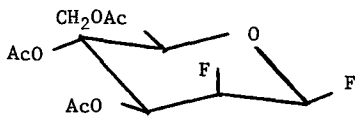
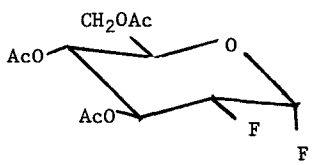
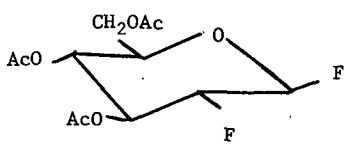
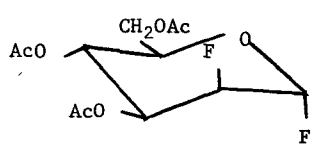
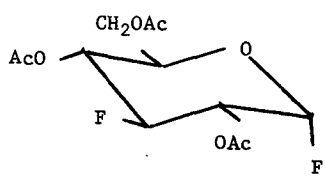
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^{2}J	^{3}J	^{n}J
358	4050 (1665)	A	$C_9F_2H_{12}O_5$			19	
365	4051 (1667)	A	$C_9F_2H_{12}O_5$				+10.4
358	4052 (1708)	A	$C_{12}F_2H_{16}O_7$			20	
381 1119	4053 (1709)	A	$C_{12}F_2H_{16}O_7$			-13.5	
381 1119	4054 (1710)	A	$C_{12}F_2H_{16}O_7$			-18.8	
381 1119	4055 (1711)	A	$C_{12}F_2H_{16}O_7$			-15.8	
381 1119	4056 (1712)	A	$C_{12}F_2H_{16}O_7$			-20	
365	4057 (1713)	A	$C_{12}F_2H_{16}O_7$				+1.0

Table B.3.c. (contd.)

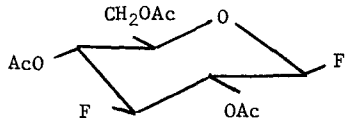
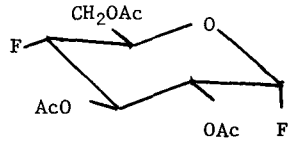
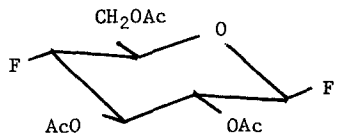
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
365	4058 (1714)	A	$C_{12}F_2H_{16}O_7$				-3.0
372	4059 (1717)	A	$C_{12}F_2H_{16}O_7$				-0.6
372	4060 (1718)	A	$C_{12}F_2H_{16}O_7$				+3.1

Table B.3.d. Heterocycles containing one metal atom.

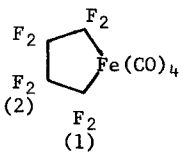
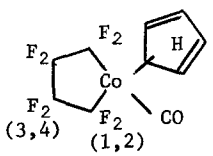
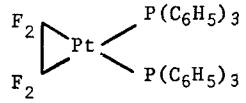
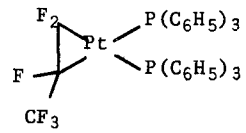
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J	^nJ
I124	4061		$C_8F_8FeO_4$			1,2	2.4	
1124	4062		$C_{10}F_8CoO$		1,2	218	1,3	4.3
807	4063	A	$C_{38}F_4H_{30}P_2Pt$					3.0
826	(6540 6617)							1.0
807	4064	A	$C_{39}F_6H_{30}P_2Pt$			188		
826	(6623)							

Table B.3.e. Heterocycles containing two nitrogen atoms.

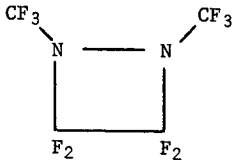
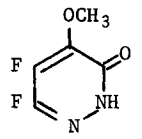
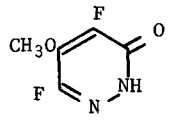
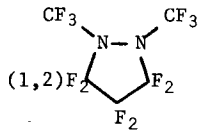
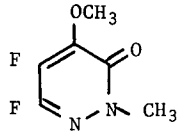
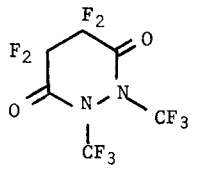
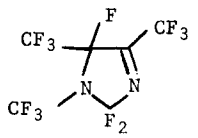
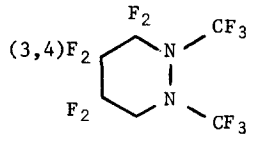
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
997 991	4065 (2832)		$C_4F_{10}N_2$	 (-86°)	135		
944	4066	E	$C_5F_2H_4N_2O_2$			28	
944	4067	E	$C_5F_2H_4N_2O_2$			22	
991 997	4068		$C_5F_{12}N_2$	 (84°)	1,2 190		
944	4069	E	$C_6F_2H_6N_2O_2$			29	
991	4070		$C_6F_{10}N_2O_2$		282		
1050	4071		$C_6F_{12}N_2$		166		
997 991	4072		$C_6F_{14}N_2$	(1,2) 	1,2 215 3,4 265		

Table B.3.e. (contd.)

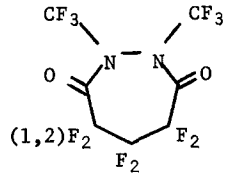
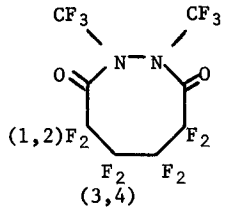
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
991	4073		$C_7F_{12}N_2O_2$		1,2 282		
991	4074		$C_8F_{14}N_2O_2$		1,2 or 3,4 294		

Table B.3.f. Heterocycles containing two oxygen atoms.

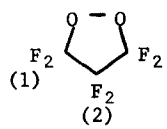
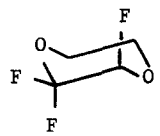
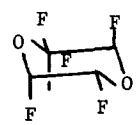
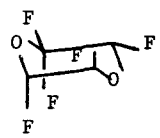
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1128	4075		$C_3F_6O_2$			1,2 33	
353	4076 (1765)	G	$C_4F_3H_5O_2$		162		
353	4077 (1772)	G	$C_4F_5H_3O_2$		166		
353	4078 (1771)	G	$C_4F_5H_3O_2$		155		

Table B.3.f. (contd.)

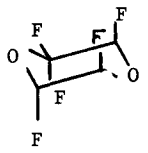
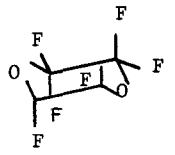
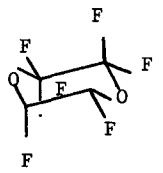
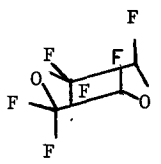
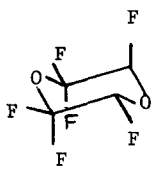
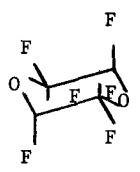
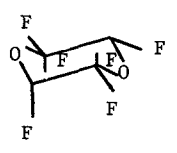
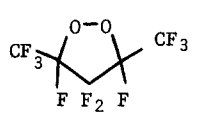
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
353	4079 (1770)	G	$C_4F_5H_3O_2$		167		
353	4080 (1773)	G	$C_4F_6H_2O_2$		139		
353	4081 (1774)	G	$C_4F_6H_2O_2$		154		
353	4082 (1775)	G	$C_4F_6H_2O_2$		168		
353	4083 (1776)	G	$C_4F_6H_2O_2$		160		
353	4084 (1777)	G	$C_4F_6H_2O_2$		168		
353	4085 (1778)	G	$C_4F_6H_2O_2$		167		
1130	4086		$C_5F_{10}O_2$		256		

Table B.3.g. Heterocycles containing two sulphur atoms.

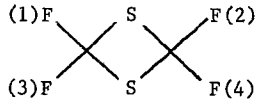
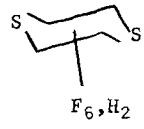
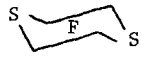
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
1127	4087 (5439)	C	$C_2F_4S_2$		1,3	137.06	1,2 1,4	5.19 31.91	
353	4088 (1793)	G	$C_4F_6H_2S_2$						
				Isomer 1		237			
				2		226			
				3		255			
				4		249			
				5		231			
1145	4089	A-E	$C_4F_8S_2$			230			
									
				(-90°)					

Table B.3.h. Heterocycles containing two phosphorus atoms.

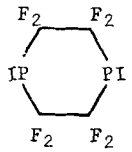
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
761	4090 (6053)		$C_4F_8I_2P_2$		280		

Table B.3.i. Heterocycles containing both oxygen and nitrogen.

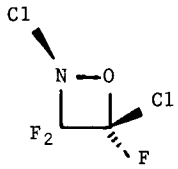
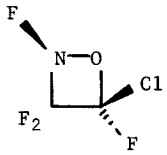
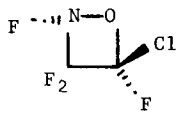
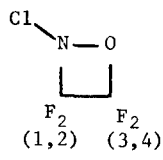
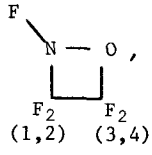
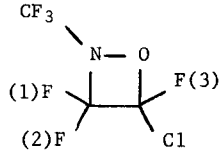
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
1125	4091	P	$C_2F_3Cl_2NO$			116		
1125	4092	P	C_2F_4ClNO			128		
						128		
1126	4093	P	C_2F_4ClNO		1,2 3,4	122 89		
1126	4094	P	C_2F_5NO		1,2 3,4	140 89		
988	4095 (2723)		C_3F_6ClNO					
					Isomer I 1,2	133	1,3	8.2
							2,3	8.3
					II 1,2	132	1,3	11.8
							2,3	3.5
					(-79°)			

Table B.3.i. (contd.)

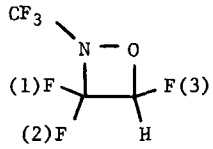
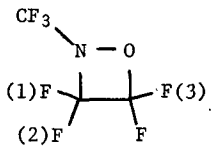
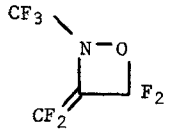
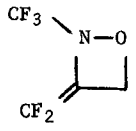
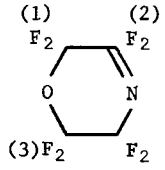
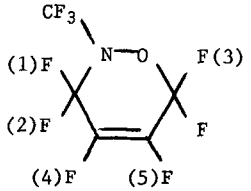
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J		^3J		^nJ	
988	4096 [229, 1780, 2732]		C_3F_6HNO							
				Isomer I	1,2	152	1,3	<1		
							2,3	16.0		
				II	1,2	149	1,3	<1		
							2,3	12.6		
				(-79^o)						
988	4097 (2749)		C_3F_7NO							
				Isomer I	1,2	143	1,3	6.7		
				II	1,2	143	2,3	6.7		
				(-75^o)						
988	4098 [2805, 3249, 3494]		C_4F_7NO							
				Isomer I + II		99				
989	4099 [2805, 3249, 3494]		C_4F_7NO			98.9				
1121	4100		C_4F_7NO				1,2	21.4	1,3	4.6
988	4101 (3277)		C_5F_9NO				4,5	2.0	1,3	1.6
							1,4	18.4	2,3	1.6

Table B.3.i. (contd.)

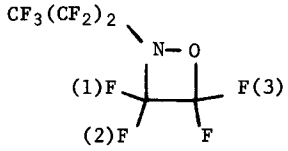
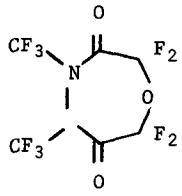
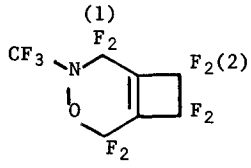
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
988	4102 (2892)		$C_5F_{11}NO$	 Isomers I and II		1,3 <1 <1	
991	4103		$C_6F_{10}N_2O_3$		158		
1022	4104 (2975 3767)		$C_7F_{11}NO$			1,2	1.95

Table B.3.j. Heterocycles containing both oxygen and sulphur.

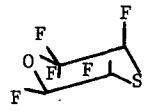
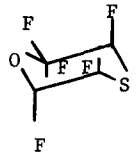
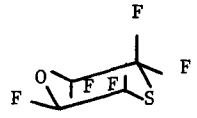
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
353	4105 (1781)	G	$C_4F_5H_3OS$		165		
353	4106 (1782)	G	$C_4F_5H_3OS$		166		
353	4107 (1783)	G	$C_4F_5H_3OS$		251		

Table B.3.j. (contd.)

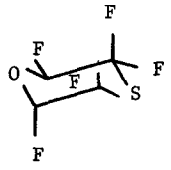
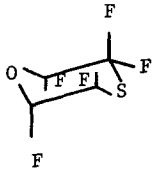
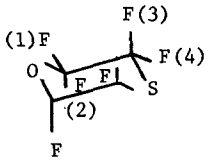
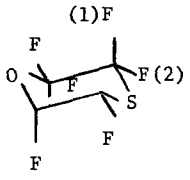
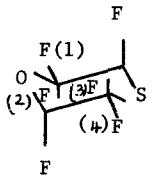
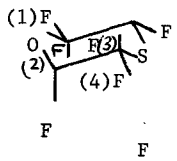
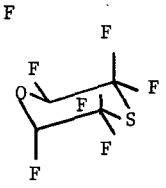
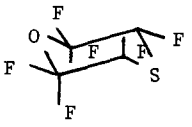
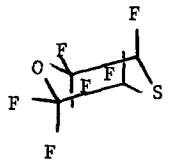
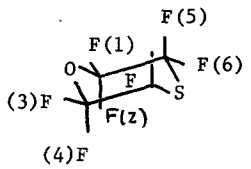
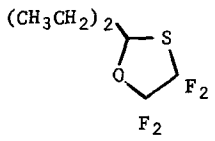
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
353	4108 (1784)	G	$C_4F_5H_3OS$		227		
353	4109 (1785)	G	$C_4F_5H_3OS$		254		
353	4110 (1786)	G	$C_4F_6H_2OS$		1,2 3,4	156 242	
353	4111 (1787)	G	$C_4F_6H_2OS$		1,2	245	
353	4112 (1788)	G	$C_4F_6H_2OS$		1,2 3,4	170 260	
353	4113 (1789)	G	$C_4F_6H_2OS$		1,2 3,4	160 222	
353	4114 (1790)	G	$C_4F_6H_2OS$			238	
353	4115 (1791)	G	$C_4F_6H_2OS$			140	

Table B.3.j. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
353	4116 (1792)	G	$C_4F_6H_2OS$		169		
353	4117 (1795)	G	C_4F_7HOS		1,2 154 3,4 166 5,6 241		
152	4118		$C_7F_4H_{10}OS$			6	

B.4. Fluorine bonded to carbon in alicyclic aromatic systems.

Table B.4.a. Substituted difluorobenzenes.

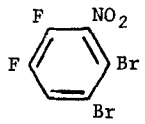
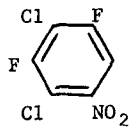
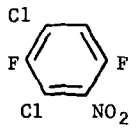
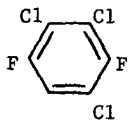
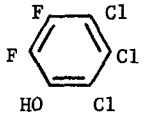
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
383	4119 (1879)		$C_6F_2HBr_2NO_2$		20.2		
383	4120 (1880)		$C_6F_2HCl_2NO_2$			4.2	
383	4121 (1881)		$C_6F_2HCl_2NO_2$				14.4
383	4122 (1882)		$C_6F_2HCl_3$				12.0
420	4123		$C_6F_2HCl_3O$		21.1		

Table B.4.a. (contd.)

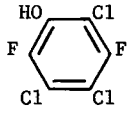
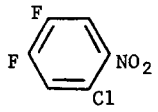
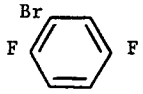
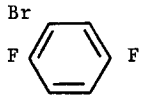
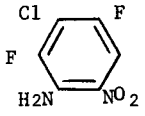
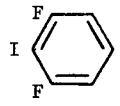
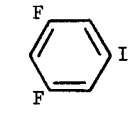
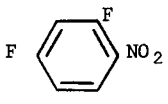
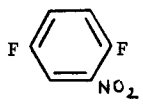
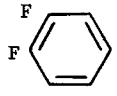
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
420	4124		$C_6F_2HCl_3O$				9.8
383	4125 (1884)		$C_6F_2H_2ClNO_2$		20.8		
384	4126 (1887)	E*	$C_6F_2H_3Br$				15.62
411	4127 (1888)	G*	$C_6F_2H_3Br$				15.33
383	4128 (1889)		$C_6F_2H_3ClN_2O_2$			3.1	
412 413	4129 (1890)	A*	$C_6F_2H_3I$			2.30	
411	4130 (1891)	G*	$C_6F_2H_3I$			6.24	
384	4131 (1893)	E*	$C_6F_2H_3NO_2$			13.36	
384	4131a (1892)	E*	$C_6F_2H_3NO_2$				17.19
384	4132	E*	$C_6F_2H_4$		-20.53		
414	[1894 1895 5507]	B*			-20.43		

Table B.4.a. (contd.)

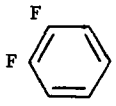
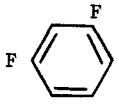
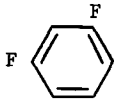
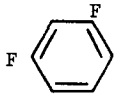
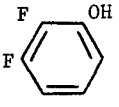
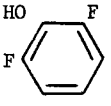
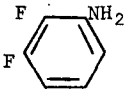
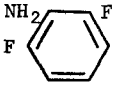
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
415 877	4133 (1896)	G* (15% v/v)	$C_6F_2H_4$		-21.16		
		G* E* * (50% v/v)			20.9 20.6 20.5		
416	4134 (1899 5509)	B*	$C_6F_2H_4$			3.0	
417	4135 (1900)	G*	$C_6F_2H_4$			6.57	
877	4136	G* E* (50% v/v)	$C_6F_2H_4$			6.64 6.56	
418	4137 (1902 5513)	*	$C_6F_2H_4$				17.79
877	4138	G*	$C_6F_2H_4$ (50% v/v)				17.64
415	4139 (1904)	G*	$C_6F_2H_4O$		-19.91		
412 413	4140 (1903)	*	$C_6F_2H_4O$			10.3	
415	4141 (1906)	G*	$C_6F_2H_5N$		-19.78		
412 413	4142 (1905)	A*	$C_6F_2H_5N$			12.1	

Table B.4.a. (contd.)

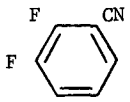
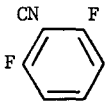
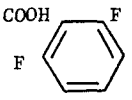
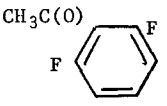
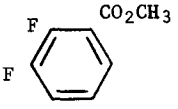
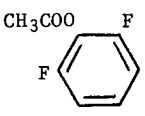
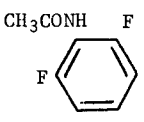
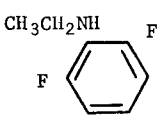
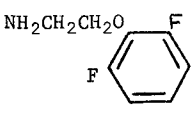
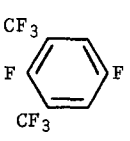
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
415	4143 (1908)	G*	$C_7F_2H_3N$		-19.94		
412 413	4144 (1907)	F*	$C_7F_2H_3N$			0.0	
412 413	4145 (1909)	F*	$C_7F_2H_4O_2$			3.0	
412 413	4146 (1911)	G*	$C_8F_2H_6O$			3.9	
415	4147 (1913)	G*	$C_8F_2H_6O_2$		-20.0		
412 413	4148 (1912)	G*	$C_8F_2H_6O_2$			2.7	
412 413	4149 (1914)	A*	$C_8F_2H_7NO$			4.5	
412 413	4150 (1915)	A*	$C_8F_2H_9N$			11.0	
412 413	4151 (1916)	A*	$C_8F_2H_9NO$			8.0	
876	4152 (1917 3372)	B	$C_8F_8H_2$				19.0

Table B.4.a. (contd.)

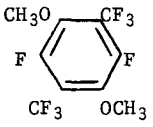
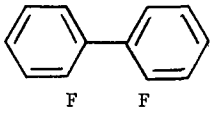
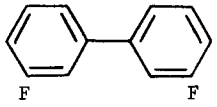
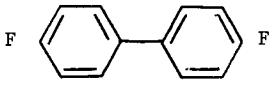
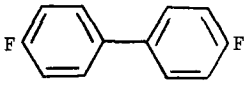
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
419	4153 (2027 3380)		$C_{10}F_8H_6O_2$				13.2
877	4154	B-HH	$C_{12}F_2H_8$			18.2	
877	4155 (1857)	B-G	$C_{12}F_2H_8$				< 0.2
877	4156	B-HH	$C_{12}F_2H_8$				< 0.3
454	4157 (1856)	G* H* J*	$C_{12}F_2H_8$				0.21 0.16 0.21

Table B.4.b. Substituted trifluorobenzenes.

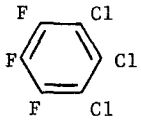
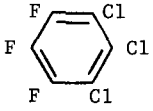
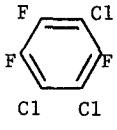
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
420	4158		$C_6F_3Cl_3$		20.9		
880	4159		$C_6F_3Cl_3$		20.1		
420	4160		$C_6F_3Cl_3$		20.9	0.7	9.0

Table B.4.b. (contd.)

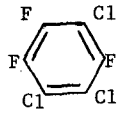
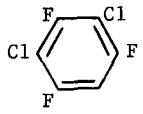
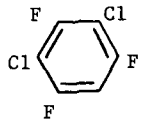
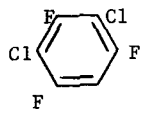
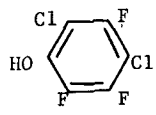
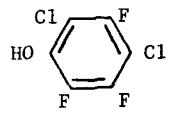
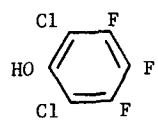
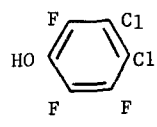
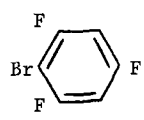
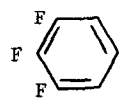
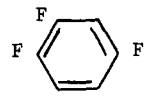
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
880	4161		$C_6F_3Cl_3$		20.6	0.75	9.0
383	4162 (1919)		$C_6F_3HCl_2$			1.9	
420	4163 (1920)		$C_6F_3HCl_2$			1.9	
421	4164 (1921)	B	$C_6F_3HCl_2$			1.7	
420	4165		$C_6F_3HCl_2O$		21.1	1.9	8.5
892	4166	B	$C_6F_3HCl_2O$		21.0		8.0
892	4167	B	$C_6F_3HCl_2O$		21.0		
892	4168	B	$C_6F_3HCl_2O$		22.0		8.2
422	4169	B	$C_6F_3H_2Br$			5.94	
413	4170 (1923)	G*	$C_6F_3H_3$		-20.0	6.4	
424 877	4171 (1926)	G*	$C_6F_3H_3$		-20.34	3.14	14.57

Table B.4.b. (contd.)

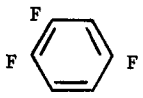
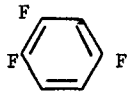
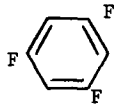
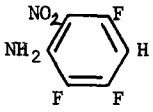
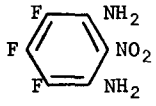
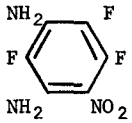
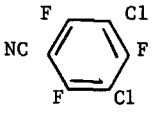
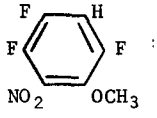
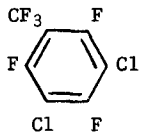
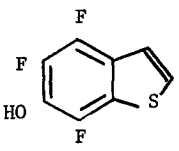
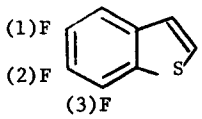
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
423	4172 (1925)	B*	$C_6F_3H_3$		-20.01	3.14	15.04
384	4173 (1924)	E*	$C_6F_3H_3$		-20.46	3.24	15.15
425	4174 (1927)		$C_6F_3H_3$			5.83	
878	4175		$C_6F_3H_3N_2O_2$			8.6	
879	4176		$C_6F_3H_4N_3O_2$		22.3		
878	4177		$C_6F_3H_4N_3O_2$		20.8	3.7	8.2
421	4178	B	$C_7F_3Cl_2N$			5.9	
427	4179		$C_7F_3H_4NO_3$		22.0		12.2
881	4180		$C_7F_6Cl_2$			5.8	
451	4181 (2046)	G	$C_8F_3H_3OS$		19.2	4.8	16.3
451	4182 (1941 2047)	G	$C_8F_3H_3S$		1,2 19.9 2,3 19.4	1,3 4.7	

Table B.4.b. (contd.)

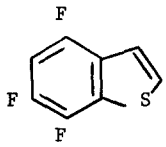
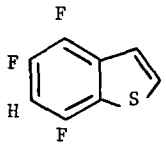
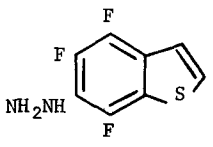
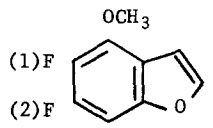
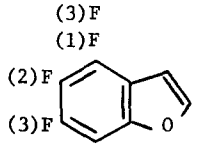
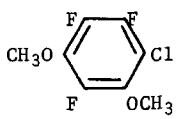
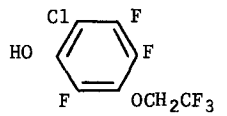
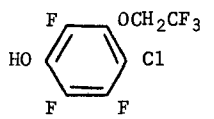
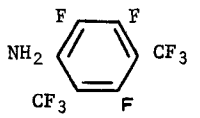
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
451	4183 (1942, 2048)	G	$C_8F_3H_3S$		20.0	1.55	18.2
451	4184 (1943, 2049)	G	$C_8F_3H_3S$		19.15	1.45	18.85
451	4185 (2050)	G	$C_8F_3H_5N_2S$		19.8	4.55	16.9
882	4186	G	$C_8F_3H_5O_2$		1,2 18 2,3 19.5	1,3 2.8	
882	4187	G	$C_8F_3H_5O_2$		1,2 20.3 2,3 18.5	1,3 2.4	
197	4188	B	$C_8F_3H_6ClO_2$		21.2		8.2
892	4189 (555)	B	$C_8F_6H_3ClO_2$		22.2		7.9
892	4190 (556)	B	$C_8F_6H_3ClO_2$		23.0		8.0
419	4191 (3373)		$C_8F_9H_2N$		19.3		10.8

Table B.4.b. (contd.)

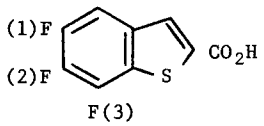
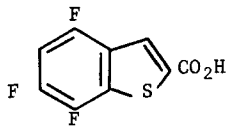
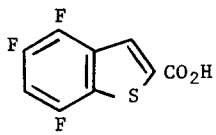
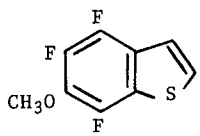
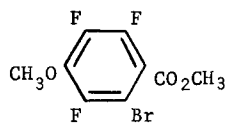
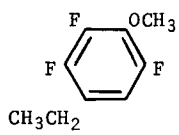
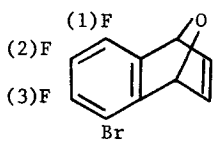
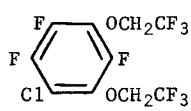
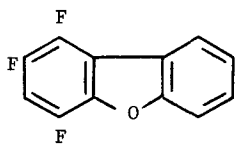
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
451	4192 (1956, 2065)	E	$C_9F_3H_3O_2S$		1,2 2,3	19.2 19.15	1,3	4.62	
451	4193 (1957, 2066)	E	$C_9F_3H_3O_2S$			19.71		3.23	18.82
451	4194 (1958, 2067)	E	$C_9F_3H_3O_2S$			19.1		1.99	19.0
451	4195 (2068)	G	$C_9F_3H_5OS$			19.0		3.2	14.65
883	4196		$C_9F_3H_6BrO_3$			20.2		7.1 or 9.6	9.6 or 7.1
430	4197 (1959, 2069)		$C_9F_3H_9O$			20.0		4.0	13.3
432	4198	J^2	$C_{10}F_3H_4BrO$		1,2 2,3	16.5 21	1,3	4.5	
197	4199 (662)	B	$C_{10}F_9H_4ClO_2$			21.8			7.7
455	4200 (1960)	G	$C_{12}F_3H_5O$			20.5		0.0	19.4

Table B.4.b. (contd.)

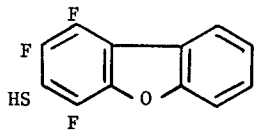
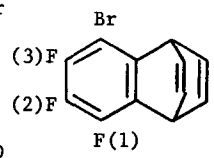
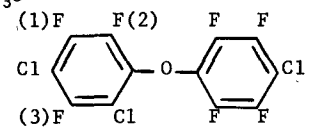
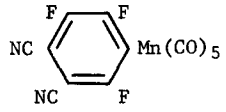
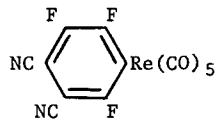
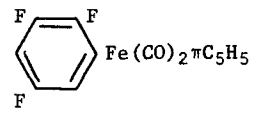
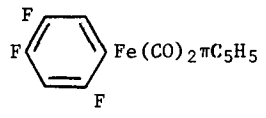
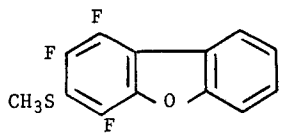
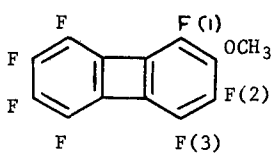
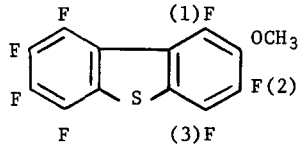
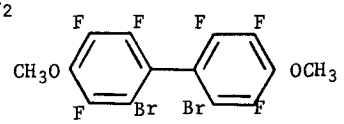
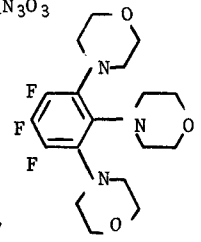
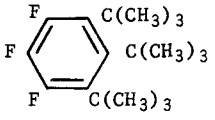
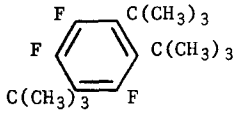
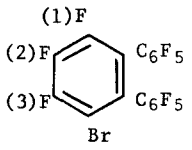
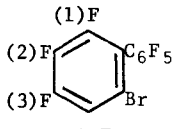
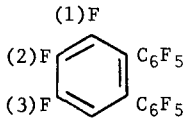
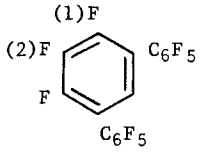
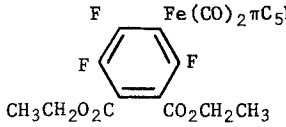
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
455	4201	A	$C_{12}F_3H_5S$			21.4		2.2		17.9
448	4202		$C_{12}F_3H_6Br$		1,2 2,3	21.2 18.4	1,3	3.8		
885	4203 (4278)		$C_{12}F_7Cl_3O$		1,2	21.2			2,3	7.9
434	4204	U^{2}*	$C_{13}F_3MnN_2O_5$			26.43		12.6		3.95
434	4205	U^{2}*	$C_{13}F_3N_2O_5Re$			26.75		12.65		4.35
434	4206 (1961)	U^{2}*	$C_{13}F_3H_7FeO_2$			16.1		1.67		28.7
434	4207 (1962)	U^{2}*	$C_{13}F_3H_7FeO_2$			20.4		15.2		3.33
455	4208 (2076)	G	$C_{13}F_3H_7S$			22.4		1.4		18.4
457	4209 (2078 / 4289)	A^{3}*	$C_{13}F_7H_3O$		2,3	-16.1	1,2	+7.2	1,3	+18.6

Table B.4.b. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
887	4210 (4290)		$C_{13}F_7H_3OS$		2,3	19.4	1,2	7.5	1,3	13.5
887	4211		$C_{14}F_6H_6Br_2$			20.3		6.8		9.6
888	4212		$C_{18}F_3H_{24}N_3O_3$			20.5				
889	4213		$C_{18}F_3H_{27}$			19.5		4		
890	4214		$C_{18}F_3H_{27}$			16				
891	4215 (4495)		$C_{18}F_{13}Br$		1,2 2,3	20.8 20.8	1,3	10.4	1,1'	4.2
891	4216 (4496)		$C_{18}F_{13}Br$		1,2 2,3	21.0			1,1'	1.8*
891	4217 (4497)		$C_{18}F_{13}H$		1,2 2,3	20.4 20.4	1,3	10.3	1,1'	5.0*
891	4218 (4498)		$C_{18}F_{13}H$		1,2	19.8			1,1'	3.5*
434	4219	U^{2}*	$C_{19}F_3H_{15}FeO_6$			27.65		14.5		3.15

*Inter-ring J

Table B.4.b. (contd.)

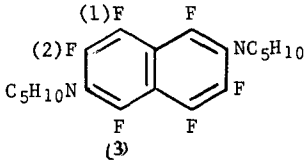
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
940	4220 (4599)	A	$C_{20}F_6H_{20}N_2$				1,3 15

Table B.4.c. Substituted tetrafluorobenzenes.

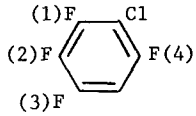
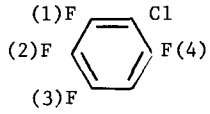
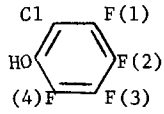
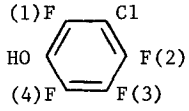
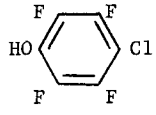
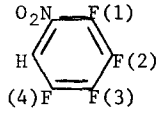
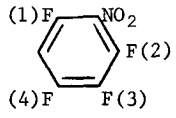
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
420	4221 (1969)		C_6F_4HCl		1,2 2,3	19.9 20.7	1,4 3,4 1,3	1.5 0.9 4.9	2,4	9.8
421	4222 (1970)	G	C_6F_4HCl		1,2 2,3	19.9 21.1	1,4 3,4 1,3	1.5 0.6 5.0	2,4	9.7
892	4223	B	C_6F_4ClO		1,2 3,4 2,3	21.0 21.0 21.0				
892	4224	B	C_6F_4ClO		2,3 3,4	19.0 19.0			1,3	8.7
892	4225	B	C_6F_4ClO			19.5				
878	4226		$C_6F_4HNO_2$				1,3 2,4	10.5 3.6		
878	4227		$C_6F_4HNO_2$				1,2 2,4 1,4	-6.2 10.0 4.9		

Table B.4.c. (contd.)

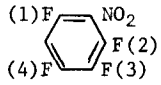
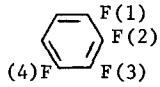
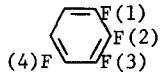
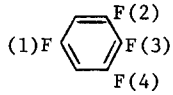
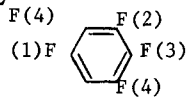
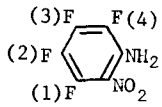
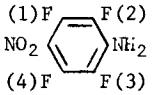
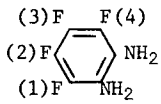
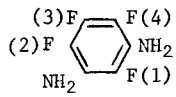
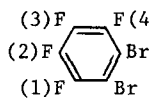
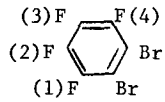
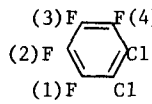
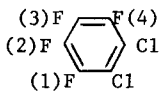
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
881	4228		$C_6F_4HNO_2$						1,3	10.4
436	4229 (1973)	B*	$C_6F_4H_2$		1,2 2,3	-19.00 -19.02	1,3	+2.72	1,4	+12.60
877	4230	G*	$C_6F_4H_2$		1,2 2,3	19.72 19.00	1,3	2.70	1,4	12.70
893	4231 (1974)	*	$C_6F_4H_2$		2,3	19.7	1,2 2,4	1.7 5.8	1,3	11.02
877	4232	G*	$C_6F_4H_2$		2,3	20.36	1,2	1.64	1,3	10.94
878 879	4233	*	$C_6F_4H_2N_2O_2$		1,2 2,3 3,4	22.5 21.1 19.9	1,3 2,4	7.7 6.4	1,4	8.8
878 879	4234	*	$C_6F_4H_2N_2O_2$		1,2	±21.5	1,4 2,3	8.8 9.5	1,3	±5.3
878 879	4235	*	$C_6F_4H_4N_2$		1,2 2,3	21.6 21.4	1,3	6.6	1,4	6.2
878	4236	*	$C_6F_4H_4N_2$			21.2		0		6.6
411	4237	G*	$C_6F_4Br_2$		1,2 2,3	-21.53 -19.63	1,3	2.80	1,4	8.18
894	4238	*	$C_6F_4Br_2$		1,2 2,3	-21.6 -19.6	1,3	2.9	1,4	8.2
420	4239		$C_6F_4Cl_2$		1,2 2,3	20.5 19.1	1,3	2.5	1,4	7.4
880	4240		$C_6F_4Cl_2$		1,2 2,3	±20.8 19.9	1,3	±1.7	1,4	7.8

Table B.4.c. (contd.)

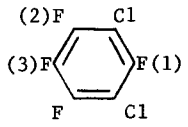
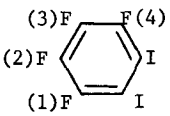
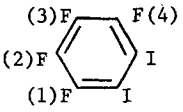
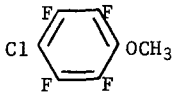
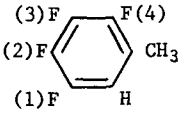
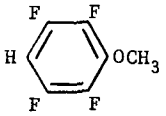
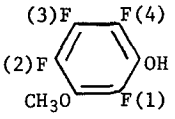
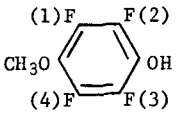
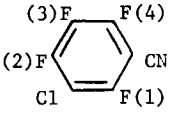
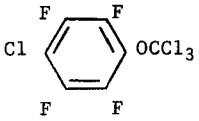
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
420	4241		$C_6F_4Cl_2$		2,3	20.1	1,2	2,3	1,3	7.9
434	4242	A*	$C_6F_4I_2$		1,2 2,3	22.2 19.5	1,3	4.1	1,4	6.4
411	4243	G*	$C_6F_4I_2$		1,2	-22.23	1,3 2,3	4.36 -18.83	1,4	9.50
197	4244	B	$C_7F_4H_3ClO$			19.5				
440	4245 (1977)	B	$C_7F_4H_4$		1,2 2,3 3,4	19.8 19.8 19.8	1,3 2,4	2.0 8.2	1,4	13.0
434	4246		$C_7F_4H_4O$			20.4		1.75		9.6
892	4247	B	$C_7F_4H_2O_2$		2,3 3,4	22.4 22.4			1,3	7.2
892	4248	B	$C_7F_4H_2O_2$			23.0	1,4 2,3	6.4 6.4		
421	4249	B	C_7F_4ClN		2,3 3,4	19.8 19.8	1,2 1,4 2,4	2.5 5.1 9.6	1,3	9.0
197	4250	B	$C_7F_4Cl_4O$			17.8				

Table B.4.b. (contd.)

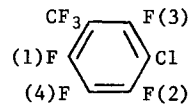
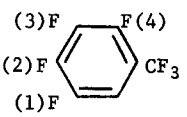
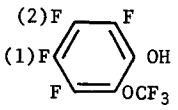
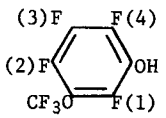
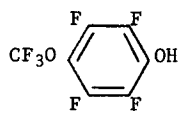
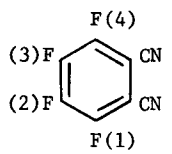
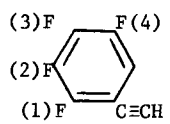
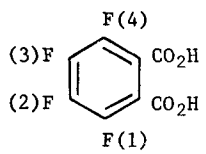
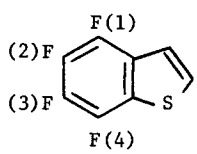
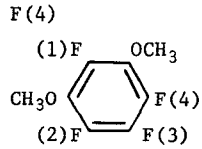
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
881	4251		C_7F_7Cl				1,2 1,3 2,3	9.5 4.3 2.3	3,4	9.8
440	4252	B	C_7F_7H		1,2 2,3 3,4	18.6 19.2 18.5	1,3 2,4	3.8 7.7	1,4	13.3
892	4253 (3356)	B	$C_7F_7HO_2$		1,2	20.6				
892	4254	B	$C_7F_7HO_2$		2,3 3,4	19.2 19.2	1,4	6.7		
892	4255 (3357)	B	$C_7F_7HO_2$			21.4				
434	4256	A*	$C_8F_4N_2$		1,2 2,3	20.5 19.5	1,3	10.4	1,4	9.9
440	4257 (1979)	B	$C_8F_4H_2$		1,2 2,3 3,4	19.3 19.5 20.0	1,3 2,4	4.5 2.9	1,4	11.9
434	4258	J^2*	$C_8F_4H_2O_4$		1,2 2,3	21.2 19.0	1,3	5.6	1,4	12.3
451	4259 (2064)	G	$C_8F_4H_2S$		1,2 2,3 3,4	20.6 19.1 19.1	1,3 2,4	1.25 0.33	1,4	16.2
443	4260		$C_8F_4H_6O_2$		2,3	21	1,2	∿0	1,3	6

Table B.4.c. (contd.)

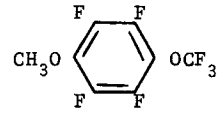
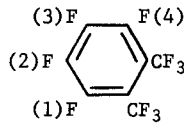
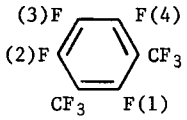
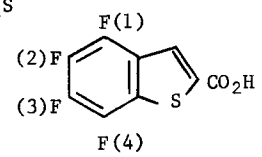
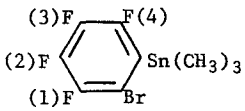
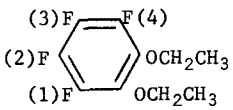
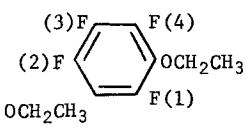
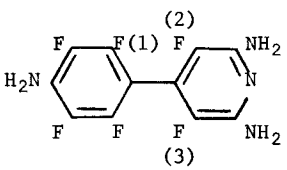
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
197	4262	B	$C_8F_7H_3O_2$			17.3				
419	4263		C_8F_{10}		1,2	±18.2	1,3	∓9.2	1,4	6.8
	(3374)				2,3	17.6				
419	4264		C_8F_{10}			19.6		14.6		11.3
876	(3375)									
419	4265		C_8F_{10}			18.6				13.2
	(3376)									
451	4266	E	$C_9F_4H_2O_2S$		1,2	18.8	1,3	-0.4	1,4	16.1
	(2070, 2096)				2,3	18.39	2,4	0.70		
					3,4	18.68				
895	4267		$C_9F_4H_9BrSn$		1,2	19.3	1,3	3.3	1,4	12.8
					2,3	18.9	2,4	3.5		
					3,4	26.2				
290	4268		$C_{10}F_4H_{10}O_2$		1,2	±21.2	1,3	±2.9	1,4	6.1
					2,3	21.2				
290	4269		$C_{10}F_4H_{10}O_2$		2,3	21.5	1,3	~0	1,3	6.0
897	4270	E	$C_{11}F_6H_6N_4$				1,2	7.8		
							1,3	7.8		

Table B.4.c. (contd.)

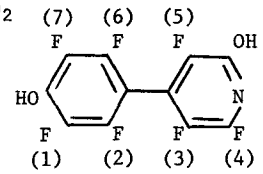
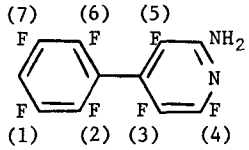
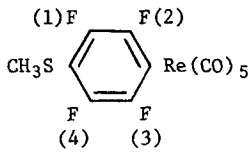
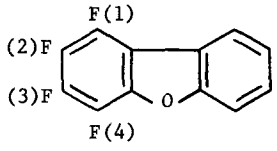
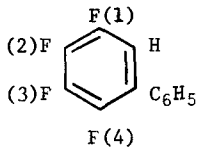
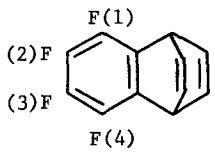
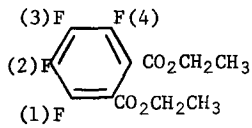
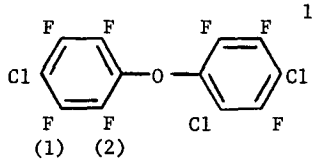
Ref. No	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
897	4271 (4659)	E	$C_{11}F_7H_2NO_2$		6,7	21.6	1,7 2,6	4.9 5.7	1,6 5,6	8.9 9.7 9.4
897	4272	E	$C_{11}F_7H_4N_3$		6,7	20.7	1,7 1,4	8.6 4.1	5,6 3,6 1,6	9.7 9.3 8.2
910	4273	A	$C_{12}F_4H_3O_5SRe$		1,2	29.6	1,4 2,3	4.7 3.8	1,3	14.6
455	4274	G	$C_{12}F_4H_4$		1,2 2,3 3,4	20.2 18.5 19.2	1,3 2,4	0.0 2.0	1,4	15.3
440	4275 (1981)	G	$C_{12}F_4H_6$		1,2 2,3 3,4	20.4 19.8 19.8	1,3 2,4	2.4 2.8	1,4	12.4
448	4276		$C_{12}F_4H_6$		1,2 2,3	21.9 17.9	1,3	0.5	1,4	15.7
434	4277	J^2	$C_{12}F_4H_{10}O_4$		1,2 2,3	±18.3 18.7	1,3	∓4.4	1,4	12.1
885	4278 (4203)		$C_{12}F_7Cl_3O$		1,2	19.8				

Table B.4.c. (contd.)

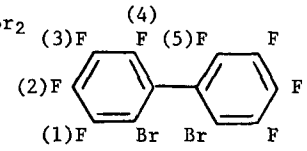
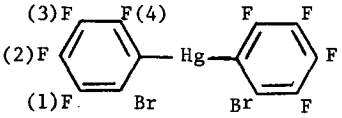
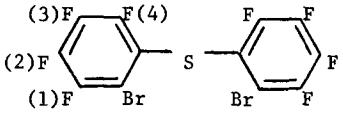
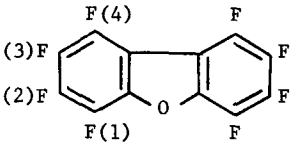
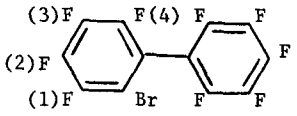
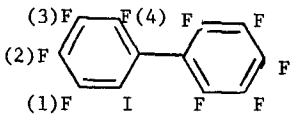
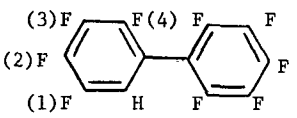
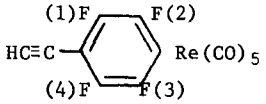
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
887	4279		$C_{12}F_8Br_2$		1,2 2,3 3,4	20.6 19.2 21.2	1,3 2,4	3.7 4.4	1,4 4,5	9.6 1.6
898	4280		$C_{12}F_8Br_2Hg$		1,2 2,3 3,4	20.15 18.85 26.4	1,3 2,4	2.65 2.55	1,4	11.55
898	4281		$C_{12}F_8Br_2S$		1,2 2,3 3,4	21.3 19.55 22.15	1,3 2,4	3.1 5.0	1,4	9.3
899	4282		$C_{12}F_8O$		1,2 2,3 3,4	19.1 18.5 18.6			1,4	12.5
900	4283 (4448)		$C_{12}F_9Br$		1,2 2,3 3,4	21.5 19.6 21.3	1,3 2,4	3.9 4.7	1,4	9.8
900	4284 (4449)		$C_{12}F_9I$		1,2 2,3 3,4	22.4 19.1 20.8	1,3 2,4	4.6 5.0	1,4	10.7
900	4285		$C_{12}F_9H$		1,2	22.4	1,3	2.7	1,4	12.4
434	4286	U[2]	$C_{13}F_4HO_5Re$		1,2	33.4	1,4 2,3	4.2 6.4	1,3	17.6

Table B.4.c. (contd.)

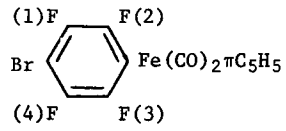
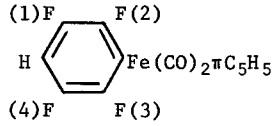
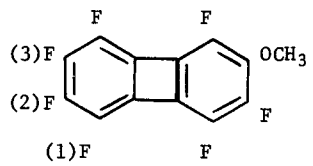
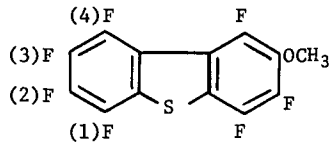
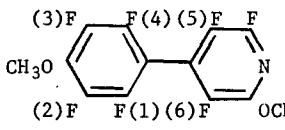
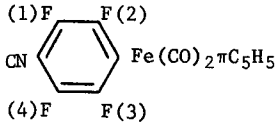
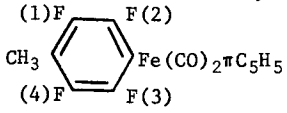
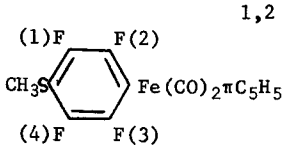
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
902	4287	U[2]	$C_{13}F_4H_5BrFeO_2$		1,2	32.2	1,4 2,3	6.4 6.4	1,3	14.8
434	4288 (1985)	A	$C_{13}F_4H_6FeO_2$		1,2	29.0	1,4 2,3	1.2 3.45	1,3	13.2
457	4289 (2078 4209)	A[3]	$C_{13}F_7H_3O$		$J_{13} + J_{13} - 11.6$					
887	4290 (4210)		$C_{13}F_7H_3OS$		1,2 3,4	18.9 18.0			1,4	13.0
897	4291 (2110 4667)	E	$C_{13}F_7H_6NO_2$		1,2	20.6	1,4 2,3	4.7 2.1	1,3 4,5 1,6	8.2 9.2 8.8
434	4292	U[2]	$C_{14}F_4H_5FeNO_2$		1,2	28.5	2,3 1,4	7.3 1.55	1,3	12.8
902	4293	U[2]	$C_{14}F_4H_8FeO_{22}$		1,2	28.65	2,3 1,4	4.1 0	1,3	11.9
901	4294	A	$C_{14}F_4H_8FeO_2S$		1,2	30.8	1,4 2,3	4.2 3.3	1,3	12.65

Table B.4.c. (contd.)

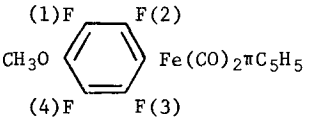
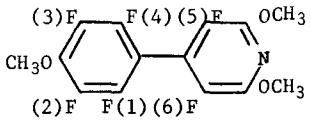
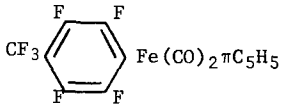
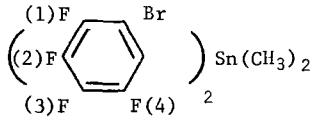
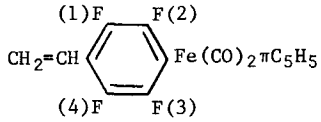
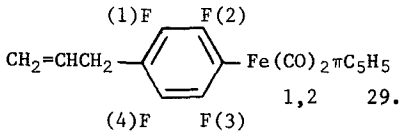
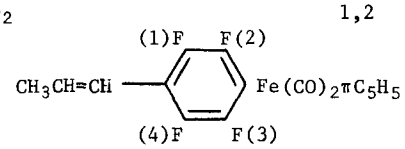
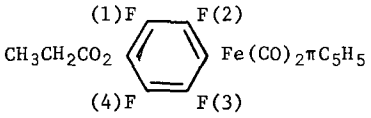
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}			J_{para}
902	4295	U[2]	$C_{14}F_4H_8FeO_3$		1,2	29.35	1,4 2,3	5.9 1.0	1,3	9.55
897	4296	E	$C_{14}F_6H_9NO_3$		1,2	20.7	1,4 2,3	4.8 2.1	1,3 4,5 1,6	8.5 8.2 8.2
434	4297 (3382)	U[2]	$C_{14}F_7H_5FeO_2$			29.0		7.7 1.8		13.2
895	4298		$C_{14}F_8H_6Br_2Sn$		1,2 2,3 3,4	20.15 18.7 25.15	1,3 2,4	3.85 4.25	1,4	12.0
434 902	4299	U[2]	$C_{15}F_4H_8FeO_2$		1,2	27.35	1,4 2,3	3.25 3.25	1,3	12.6
902	4300	U[2]	$C_{16}F_4H_{10}FeO_2$		1,2	29.0	1,4 2,3	1.6 4.2	1,3	13.6
902	4301	U[2]	$C_{16}F_4H_{10}FeO_2$		1,2	27.35	1,4 2,3	2.35 4.3	1,3	11.8
434	4302	U[2]	$C_{16}F_4H_{10}FeO_4$		1,2	29.7	1,4 2,3	5.4 2.95	1,3	13.8

Table B.4.c. (contd.)

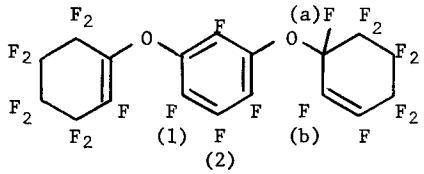
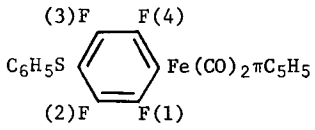
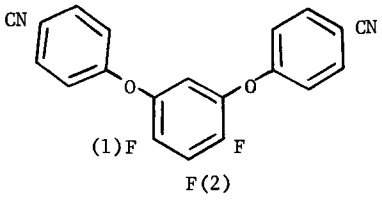
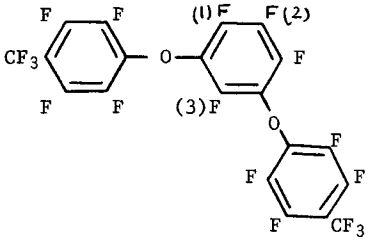
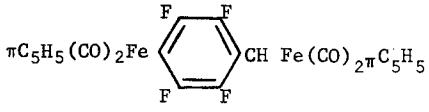
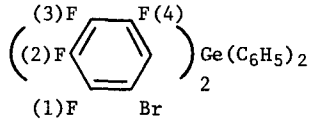
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
903	4303	E	$C_{18}F_{22}O_2$		1,2	21				
						(or double bond between (a) and (b))				
901	4304	A	$C_{19}F_4H_{10}O_2SFe$		1,2	31.2	1,4 2,3	3.8 4.7	1,3	12.5
903	4305	E	$C_{20}F_{12}N_2O_2$		1,2	22			2,3	6
903	4306 (3386)	E	$C_{20}F_{18}O_2$		1,2	21			2,3	6
434	4307	U^2	$C_{21}F_4H_{12}Fe_2O_4$			28.1		4.4 2.1		10.9
898	4308		$C_{24}F_8H_{10}Br_2Ge$		1,2 2,3 3,4	20.70 19.2 23.35	1,3 2,4	3.65 5.05	1,4	10.7

Table B.4.c. (contd.)

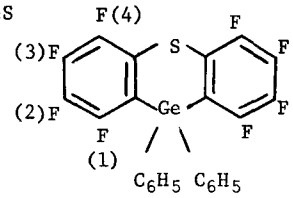
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
898	4309		$C_{24}F_8H_{10}GeS$		1,2 2,3 3,4	23.6 19.6 20.5	1,3 2,4	5.35 3.4	1,4	12.3

Table B.4.d. Substituted pentafluorobenzenes.

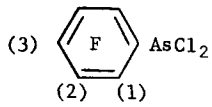
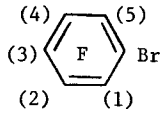
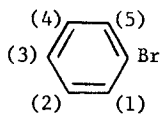
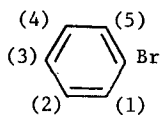
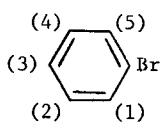
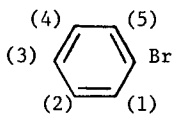
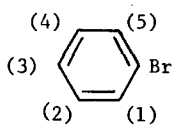
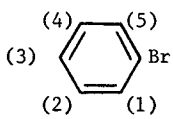
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
908	4310	A	$C_6F_5AsCl_2$		1,2 2,3	21.0 21.1	1,3	6.0		
880	4311		C_6F_5Br		1,2 2,3	±21.8 ±19.9	1,3 2,4 1,5	1.1 5.4 1.7	1,4	6.4
438	4312		C_6F_5Br		1,2 2,3	21.0 19.3	1,3 2,4 1,5	1.1 1.8 5.6	1,4	6.3
910	4313	G	C_6F_5Br		1,2 2,3	-21.8 -19.6	1,3 2,4 1,5	1.4 1.6 5.4	1,4	+6.3
434	4314	A-B	C_6F_5Br		1,2 2,3	21.6 19.7	1,3 2,4 1,5	1.1 4.7 1.4	1,4	6.4
778	4315	H	C_6F_5Br		1,2 2,3	21.6 19.9	1,3 2,4 1,5	1.1 5.5 1.6	1,4	6.3
411	4316	G*	C_6F_5Br		1,2 2,3	-21.77 -20.05	1,3 2,4 1,5	1.14 -1.73 -5.48	1,4	6.39
912	4317	N^4*	C_6F_5Br		1,2 2,3	-21.32 -19.46	1,3 2,4 1,5	1.21 -1.63 -5.43	1,4	6.36

Table B.4.d. (contd.)

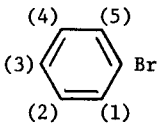
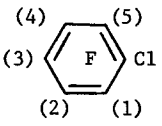
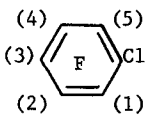
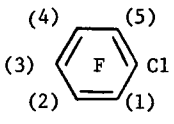
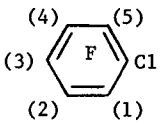
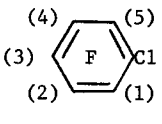
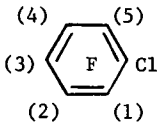
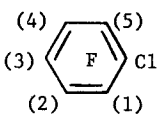
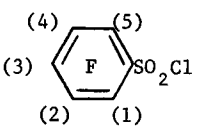
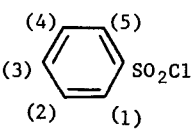
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
914	4318	O^4*	C_6F_5Br		1,2 2,3	-21.37 -19.57	1,3 2,4 1,5	1.18 -1.71 -5.42	1,4 6.43
880	4319		C_6F_5Cl		1,2 2,3	±20.4 ±19.5	1,3 2,4 1,5	<0.5 5.2 2.0	1,4 6.1
438	4320		C_6F_5Cl		1,2 2,3	20.8 19.5	1,3 2,4 1,5	1.0 2.0 5.4	1,4 6.3
420	4321		C_6F_5Cl		1,2 2,3	±20.7 19.6	1,3 2,4 1,5	∿1 5.3 2.0	1,4 ∓6.4
910	4322	G	C_6F_5Cl		1,2 2,3	-21.3 19.9	1,3 2,4 1,5	<1 2.1 5.2	1,4 +6.3
434	4323	A-B	C_6F_5Cl		1,2 2,3	21.8 20.4	1,3 2,4 1,5	∿0.8 5.6 2.1	1,4 5.8
912	4324	N^4	C_6F_5Cl		1,2 2,3	-20.58 -19.68	1,3 2,4 1,5	0.47 -1.95 -5.33	1,4 6.08
914	4325	O^4	C_6F_5Cl		1,2 2,3	-20.68 -19.86	1,3 2,4 1,5	0.41 -2.07 -5.40	1,4 6.17
912	4326	N^4	$C_6F_5ClO_2S$		1,2 2,3	-21.90 -19.97	1,3 2,4 1,5	9.59 0.32 -11.19	1,4 7.75
434	4327	A-B	$C_6F_5ClO_2S$		1,2 2,3	23.0 20.1	1,3 2,4 1,5	9.1 0 11.2	1,4 8.4

Table B.4.d. (contd.)

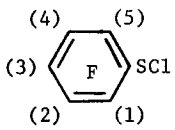
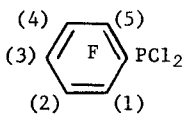
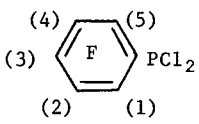
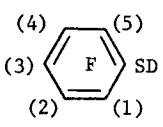
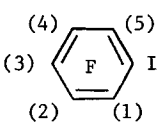
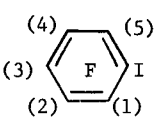
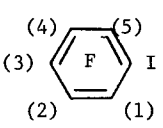
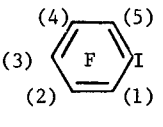
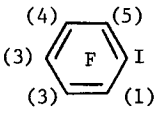
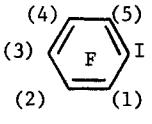
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
921	4328	G	C_6F_5ClS		2,3	±20.0	1,3	±5.9		
777	4329 (6166)		$C_6F_5Cl_2P$		1,2 2,3	±22.0 19.4	1,3 2,4 1,5	6.2 6.8 0.4	1,4	∓9.7
778	4330 (6167)		$C_6F_5Cl_2P$		1,2 2,3	∓22.3 ∓19.6	1,3 2,4 1,5	±6.2 ∓0.4 ∓6.8	1,4	±9.7
922	4331	B*	C_6F_5DS		1,2 2,3	-21.36 -19.57	1,3 2,4 1,5	-0.54 -1.34 -3.18	1,4	+7.47
438	4332		C_6F_5I		1,2 2,3	22.9 19.8	1,3 2,4 1,5	2.1 1.4 5.2	1,4	7.3
880	4333		C_6F_5I		1,2 2,3	±23.0 ±19.9	1,3 2,4 1,5	1.9 5.0 1.2	1,4	7.1
923	4334	*	C_6F_5I		1,2 2,3	∓22.7 ∓19.4	1,3 2,4 1,5	±2.1 ∓1.2 ∓4.9	1,4	±7.1
910	4335		C_6F_5I		1,2 2,3	-23.0 19.7	1,3 2,4 1,5	2.1 1.0 4.9	1,4	+7.5
434	4336	A-B	C_6F_5I		1,2 2,3	±22.8 ±19.9	1,3 2,4 1,5	2.1 1.3 5.0	1,4	∓7.2
411	4337	G*	C_6F_5I		1,2 2,3	-22.87 -19.73	1,3 2,4 1,5	2.05 -1.26 -5.12	1,4	7.24

Table B.4.d. (contd.)

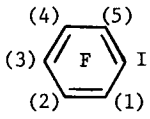
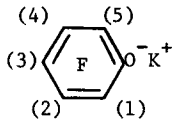
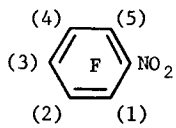
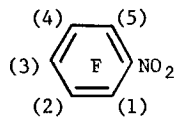
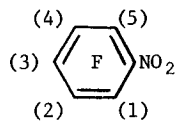
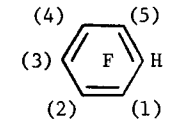
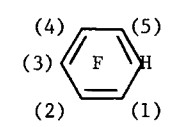
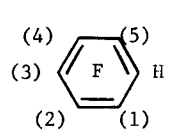
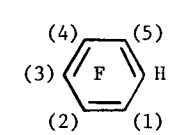
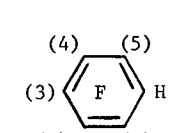
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
914	4338	O^4*	C_6F_5I		1,2 2,3	-22.25 -19.07	1,3 2,4 1,5	2.10 -1.20 -5.03	1,4	7.26
914	4339	E*	C_6F_5KO		1,2 2,3	-23.04 -22.68	1,3 2,4 1,5	-12.67 -4.84 14.17	1,4	2.43
878	4340		$C_6F_5NO_2$				1,3 1,5 2,4	6.0 -10.0 0		
910	4341	G	$C_6F_5NO_2$		1,2 2,3	-21.1 -19.3	1,3 1,5 2,4	+5.4 -10.1 0.0	1,4	+6.8
434	4342	A-B	$C_6F_5NO_2$		1,2 2,3	21.6 20.4	1,3 1,5 2,4	5.1 10.3 ≈0	1,4	7.5
880	4343 (5517)		C_6F_5H		1,2 2,3	±21.0 ±18.7	1,3 1,5 2,4	1.3 1.2 2.2	1,4	∓8.9
438	4344 (1987 5517)		C_6F_5H		1,2 2,3	20.6 18.8	1,3 1,5 2,4	1.3 1.2 2.4	1,4	8.8
439	4345 (1988 5517)	G*	C_6F_5H		1,2 2,3 2,4	+21.19 19.51	1,3 1,5 2,4	+1.29 -1.15 -2.28	1,4	-8.85
434	4346 (1986 5517)	A-B	C_6F_5H		1,2 2,3	±21.2 ±19.2	1,3 1,5 2,4	1.45 1.15 2.45	1,4	∓8.4
778	4347 (5517)	H	C_6F_5H		1,2 2,3	20.0 18.4	1,3 1,5 2,4	1.3 1.1 2.2	1,4	8.6

Table B.4.d. (contd.)

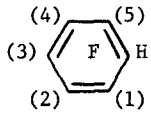
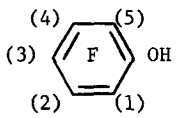
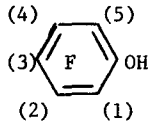
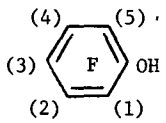
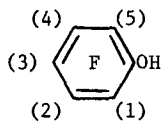
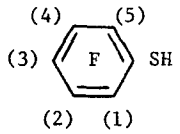
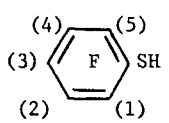
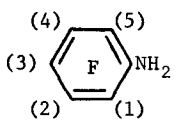
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
905	4348 (1989 5517)	G	C_6F_5H		1,2 2,3	-21.0 -19.0	1,3 1,5 2,4	+1.3 ±2.2 ±1.2	1,4	+9.0
880	4349		C_6F_5HO		1,2 2,3	±21.0 ±21.1	1,3 1,5 2,4	6.1 2.8 3.4	1,4	4.4
914	4350	G*	C_6F_5HO		1,2 2,3	-21.54 -21.51	1,3 1,5 2,4	-5.37 1.05 -2.71	1,4	4.83
912	4351	N^4*	C_6F_5HO		1,2 2,3	-20.56 -20.57	1,3 1,5 2,4	-5.09 1.29 -2.57	1,4	4.54
924	4352		C_6F_5HO		$-J_{1,3}$	$-J_{2,3}$	$-J_{1,3}$	$J_{1,5}$	$-J_{2,4}$	$J_{1,4}$
		F*			22.48	22.47	6.70	3.74	3.79	3.92
		G*			21.22	21.27	5.28	1.14	3.29	4.81
		H*			22.07	21.76	5.34	1.59	2.67	4.56
		M*			21.12	21.08	5.90	2.84	3.20	4.11
		N*			20.90	21.02	5.68	2.19	2.95	4.14
		E^2*			21.00	21.19	6.48	3.45	3.54	4.10
		K^2*			20.58	20.23	4.89	1.89	1.51	4.53
		V^2*			21.87	21.90	6.91	4.00	3.86	3.91
		P^4*			21.95	21.59	5.63	1.50	2.89	4.57
		Q^4				21.55	6.55			
		A*			21.53	21.57	5.28	1.74	3.29	4.57
		E*			21.18	21.35	6.24	3.01	3.43	4.21
434	4353	A-B	C_6F_5HS		1,2 2,3	±23.1 ±20.1	1,3 1,5 2,4	1.4 1.4 3.2	1,4	∓8.0
778	4354	H*	C_6F_5HS		1,2 2,3	∓22.2 ∓20.2	1,3 1,5 2,4	±0 ∓3.0 ∓0	1,4	±7.6
438	4355	N^4*	$C_6F_5H_2N$		1,2 2,3	20.4 20.8	1,3 1,5 2,4	6.9 4.6 2.6	1,4	4.9

Table B.4.d. (contd.)

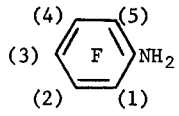
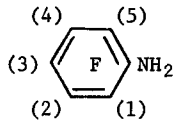
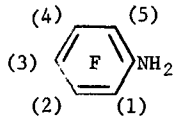
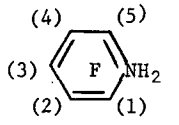
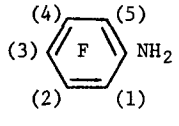
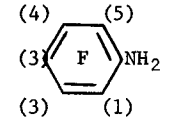
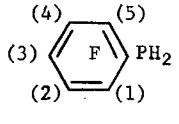
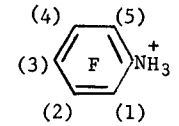
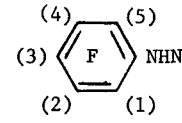
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
878 879	4356		$C_6F_5H_2N$		1,2 2,3	±20 21.6	1,3 1,5 2,4	8.2 6 3	1,4 ∓4
970	4357	G	$C_6F_5H_2N$		1,2 2,3	-20.8 -20.8	1,3 1,5 2,4	-7.1 +4.1 -2.2	1,4 +5.3
434	4358	A–B	$C_6F_5H_2N$		1,2 2,3	±20.1 ±21.1	1,3 1,5 2,4	7.3 2.5 4.6	1,4 ∓4.9
778	4359	H*	$C_6F_5H_2N$		1,2 2,3	20.2 20.4	1,3 1,5 2,4	-7.0 -4.6 2.3	1,4 5.1
912	4360	N^4*	$C_6F_5H_2N$		1,2 2,3	-20.55 -20.71	1,3 1,5 2,4	-7.05 4.18 -2.25	1,4 5.26
914	4361	Q^4*	$C_6F_5H_2N$		1,2 2,3	-21.15 -21.33	1,3 1,5 2,4	-7.82 4.98 -2.60	1,4 5.15
777	4362 (4168)		$C_6F_5H_2P$		1,2 2,3	±23.2 19.4	1,3 1,5 2,4	2.3 1.5 3.6	1,4 ∓9.4
914	4363	A^2*	$C_6F_5H_3N^+$	 (sat. soltn. in 12 M HCl)	1,2 2,3	-22.71 -22.27	1,3 1,5 2,4	1.83 -7.40 -0.60	1,4 6.22
434	4364	A	$C_6F_5H_3N_2$		1,2 2,3	±20.25 ±21.3	1,3 1,5 2,4	4.6 1.55 3.65	1,4 ∓4.8

Table B.4.d. (contd.)

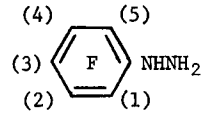
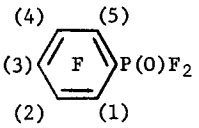
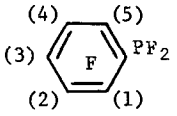
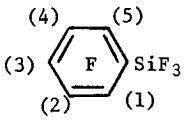
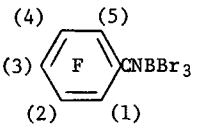
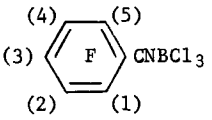
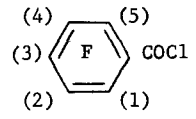
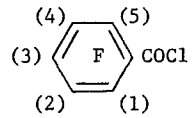
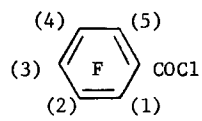
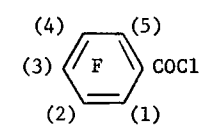
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
910	4365	G	$C_6F_5H_3N_2$		1,2 2,3	-22.7 22.7	1,3 1,5 2,4	4.8 2.3 2.3	1,4	+5.1
778	4366 (6176)	H*	C_6F_7OP		1,2 2,3	∓21.5 ∓19.9	1,3 1,5 2,4	±8.6 ∓9.4 ∓0	1,4	±9.0
777	4367 (4778 6177)		C_6F_7P		1,2 2,3	±21.6 18.6	1,3 1,5 2,4	5.9 ∿0 4.8	1,4	∓9.9
926	4368 (4856 6718)		C_6F_8Si		2,3	17.7	1,3	6.6		
778	4369	H*	$C_7F_5BBr_3N$		1,2 2,3	∓22.6 ∓21.0	1,3 1,5 2,4	±4.6 ∓8.5 ∓0	1,4	±8.0
778	4370	H*	$C_7F_5BCl_3N$		1,2 2,3	∓18.4 ∓20.4	1,3 1,5 2,4	±8.5 ∓10.1 ∓ 1.0	1,4	±7.2
434	4371	A-B	C_7F_5ClO		1,2 2,3	±23.0 ±20.1	1,3 1,5 2,4	5.7 0.9 7.5	1,4	∓8.9
910	4372	G	C_7F_5ClO		1,2 2,3	-21.0 19.8	1,3 1,5 2,4	6.1 7.5 0.0	1,4	+8.3
986	4373	H*	C_7F_5ClO		1,2 2,3	∓20.6 ∓19.1	1,3 1,5 2,4	±6.0 ∓7.6 ∓0	1,4	±8.5
912	4374	N^4*	C_7F_5ClO		1,2 2,3	-21.10 -19.63	1,3 1,5 2,4	6.04 -7.63 -0.32	1,4	8.56

Table B.4.d. (contd.)

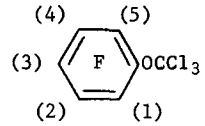
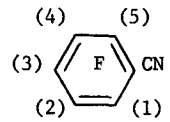
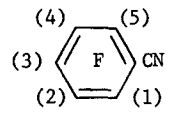
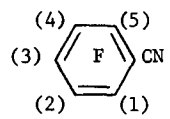
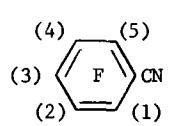
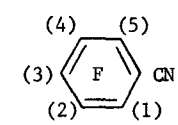
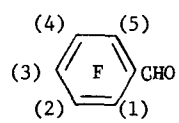
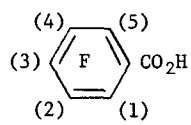
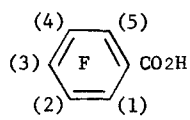
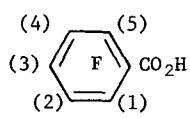
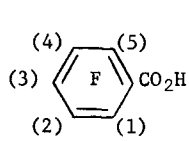
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
197	4375	B	$C_7F_5Cl_3O$		1,2 2,3	18.7 21.3				
579	4376		C_7F_5N		1,2 2,3	19.9 19.0	1,3 1,5 2,4	5.9 7.8 ≤1	1,4	8.2
910	4377	G	C_7F_5N		1,2 2,3	-20.1 19.2	1,3 1,5 2,4	6.0 7.9 0.0	1,4	+8.3
912	4378	N^4*	C_7F_5N		1,2 2,3	-19.92 -19.29	1,3 1,5 2,4	5.91 -7.95 0.32	1,4	8.19
778	4379	H*	C_7F_5N		1,2 2,3	∓19.5 ∓18.7	1,3 1,5 2,4	5.8 ∓7.9 ∓0	1,4	±8.3
914	4380	B	C_7F_5N		1,2 2,3	-19.72 -19.06	1,3 1,5 2,4	5.93 0.28 -7.97	1,4	8.18
905	4331 (2126)	G	C_7F_5HO		1,2 2,3	-20.5 -19.5	1,3 1,5 2,4	+6.5 -4.9 -1.2	1,4	+9.7
910	4382	G	$C_7F_5HO_2$		1,2 2,3	-21.1 19.4	1,3 1,5 2,4	4.1 5.1 0.0	1,4	+8.2
434	4383	J^2	$C_7F_5HO_2$		1,2 2,3	±22.5 ±19.4	1,3 1,5 2,4	3.8 {1.2 {4.8	1,4	∓8.9
912	4384	N^4*	$C_7F_5HO_2$		1,2 2,3	-21.48 -19.77	1,3 1,5 2,4	4.59 -5.45 -1.05	1,4	8.64
778	4385	H*	$C_7F_5HO_2$		1,2 2,3	∓21.5 ∓20.1	1,3 1,5 2,4	±4.0 ∓5.1 ∓1.2	1,4	±8.6

Table B.4.d. (contd.)

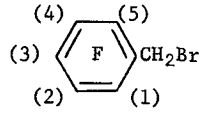
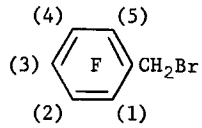
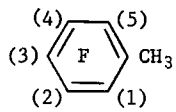
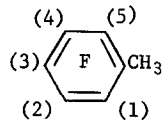
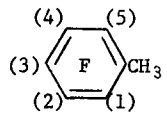
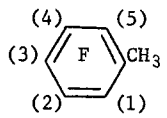
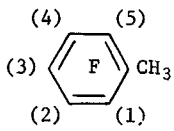
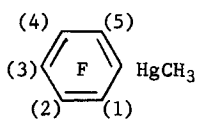
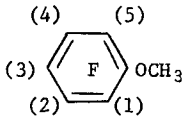
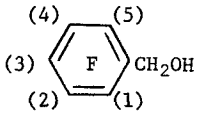
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
434	4386	A-B	$C_7F_5H_2Br$		1,2 2,3	±21.2 ±19.7	1,3 1,5 2,4	2.0 1.6 4.2	1,4	∓8.8
445	4387	H	$C_7F_5H_2Br$		1,2 2,3	∓22.4 ∓20.8	1,3 1,5 2,4	±2.1 ∓3.9 ∓0.7	1,4	±8.9
438	4388 (2128)		$C_7F_5H_3$		1,2 2,3	20.3 18.9	1,3 1,5 2,4	∿0 1.8 0.6	1,4	8.5
910	4389	G	$C_7F_5H_3$		1,2 2,3	-20.3 19.5	1,3 1,5 2,4	<1 0.0 1.9	1,4	+8.8
778	4390	H*	$C_7F_5H_3$		1,2 2,3	∓20.4 ∓18.9	1,3 1,5 2,4	±0 ∓1.9 ∓0.4	1,4	±8.6
434	4391 (2127)	A-B	$C_7F_5H_3$		1,2 2,3	22.0 19.7	1,3 1,5 2,4	∿0 1.0 5.0	1,4	8.8
905	4392 (2128)	G	$C_7F_5H_3$		1,2 2,3	-21.1 -19.7	1,3 1,5 2,4	0 0.7 2.1	1,4	+8.5
880	4393		$C_7F_5H_3Hg$		1,2 2,3	±28.0 ±19.5	1,3 1,5 2,4	1.1 1.6 6.6	1,4	11.6
927	4394	*	$C_7F_5H_3O$		1,2 2,3	-21.5 -21.9	1,3 1,5 2,4	-3.3 0.8 -3.4	1,4	+4.6
445	4395	H	$C_7F_5H_3O$		1,2 2,3	∓26.1 ∓20.3	1,3 1,5 2,4	±1.5 ±5.3 ∓2.0	1,4	∓2.0

Table B.4.d. (contd.)

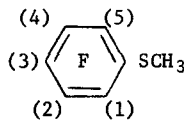
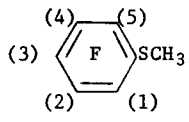
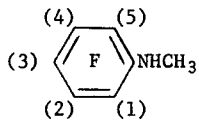
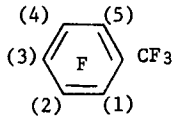
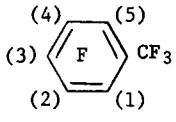
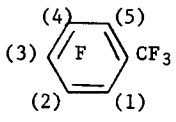
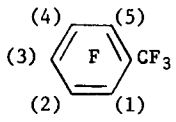
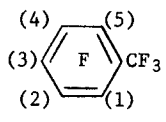
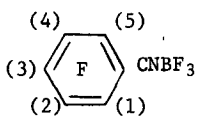
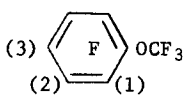
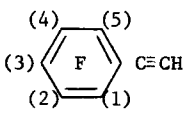
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
434	4396	A-B	$C_7F_5H_3S$		1,2 2,3	±26.5 ±22.8	1,3 1,5 2,4	1.7 2.0 3.5	1,4 ∓9.0
901	4397	A	$C_7F_5H_3S$		1,2 2,3	26.5 22.8	1,3 1,5 2,4	1.7 2.0 3.5	1,4 9.0
880	4398		$C_7F_5H_4N$		1,2 2,3	±21.1 ±21.6	1,3 1,5 2,4	6.9 2.3 3.9	1,4 4.5
438	4399 (3359)		C_7F_8		1,2 2,3	20.2 18.9	1,3 1,5 2,4	5.7 7.6 ≤1	1,4 8.4
910	4400	G	C_7F_8		1,2 2,3	-20.5 19.1	1,3 1,5 2,4	5.9 7.9 0.0	1,4 +8.3
778	4401	H*	C_7F_8		1,2 2,3	∓20.0 ∓20.2	1,3 1,5 2,4	5.8 ∓7.6 ∓0	1,4 ±8.4
905	4402	G	C_7F_8		1,2 2,3	-19.7 -18.9	1,3 1,5 2,4	+5.6 7.7 ±0	1,4 +8.2
434	4403	A-B	C_7F_8		1,2 2,3	±20.3 ±20.0	1,3 1,5 2,4	5.6 0 7.65	1,4 ∓7.9
778	4404	H*	C_7F_8BN		1,2 2,3	∓19.4 ∓20.2	1,3 1,5 2,4	6.3 ∓8.5 ∓0.1	1,4 ±7.8
197	4405 (3361)	B	C_7F_8O		1,2 2,3	17.0 20.8			
434	4406 (2131)		C_8F_5H		1,2 2,3	±20.8 ±19.8	1,3 1,5 2,4	2.15 1.4 4.2	1,4 ∓8.4

Table B.4.d. (contd.)

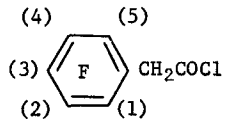
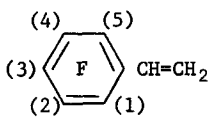
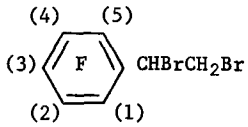
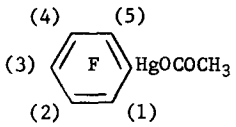
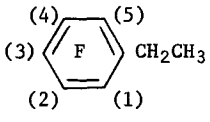
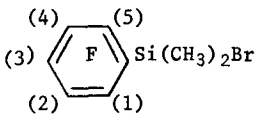
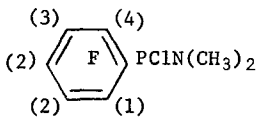
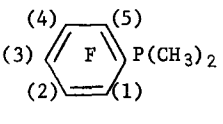
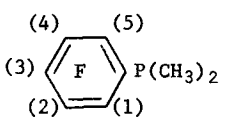
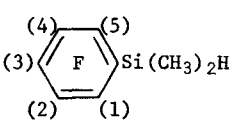
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
445	4407	H	$C_8F_5H_2ClO$		1,2	∓22.2	1,3	±1.8	1,4	±8.5
					2,3	∓20.9	1,5	∓3.9		
							2,4	∓1.3		
434	4408	A-B	$C_8F_5H_3$		1,2	±20.6	1,3	~0.8	1,4	∓8.8
					2,3	±19.4	1,5	1.5		
							2,4	2.5		
434	4409	A-B	$C_8F_5H_3Br_2$		1,2	±22.1	1,3	2.95	1,4	∓8.1
					2,3	±21.15	1,5	1.3		
							2,4	5.2		
636	4410	E	$C_8F_5H_3HgO_2$		1,2	-25.9	1,3	+1.0	1,4	+9.7
	(5574)				2,3	-19.5	1,5	-7.3		
							2,4	-1.7		
910	4411	G	$C_8F_5H_5$		1,2	-21.3	1,3	<1	1,4	+8.8
					2,3	19.7	1,5	1.0		
							2,4	2.5		
445	4412	H	$C_8F_5H_6BrSi$		1,2	∓23.6	1,3	±4.8	1,4	±10.5
					2,3	∓19.7	1,5	∓5.2		
							2,4	∓0.7		
777	4413		$C_8F_5H_6ClNP$		1,2	±22.2	1,3	5.4	1,4	∓8.7
	(6255)				2,3	±19.8	1,5	1.2		
							2,4	6.1		
777	4414		$C_8F_5H_6P$		1,2	±23.2	1,3	2.8	1,4	∓9.5
	(6256)				2,3	19.8	1,5	1.8		
							2,4	3.6		
778	4415	H*	$C_8F_5H_6P$		1,2	∓23.2	1,3	±2.9	1,4	±9.4
928	(6256)				2,3	∓19.8	1,5	∓3.6		
							2,4	∓1.8		
445	4416	H	$C_8F_5H_7Si$		1,2	∓24.8	1,3	±3.4	1,4	±10.9
	(2133)				2,3	∓19.1	1,5	∓0.9		
							2,4	∓4.3		

Table B.4.d. (contd.)

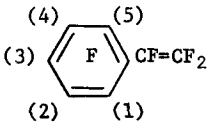
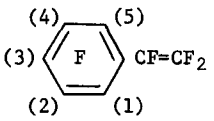
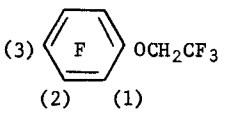
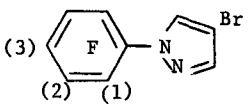
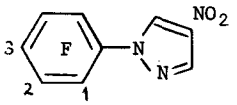
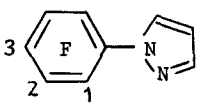
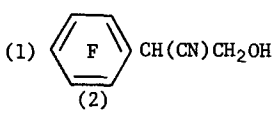
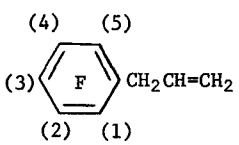
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
929	4417 (3371, 3573)		C_8F_8		1,2 2,3	-20.0 -19.0	1,3 1,5 2,4	+4.0 -6.1 -0.7	1,4	+8.5
1073	4418 (3370, 3572)		C_8F_8		2,3	20				
197	4419 (566)	B	$C_8F_8H_2O$		1,2 2,3	20.0 21.6				
930	4420	A	$C_9F_5H_2BrN_2$		1,2 2,3	15.8 21.5				
930	4421	A	$C_9F_5H_2N_3O_2$		1,2 2,3	15.4 21.5				
930	4422	A	$C_9F_5H_3N_2$		1,2 2,3	16.4 21.2				
931	4423		$C_9F_5H_4NO$		1,2	20				
434	4424	A-B	$C_9F_5H_5$		1,2 2,3	±22.2 ±20.35	1,3 1,5 2,4	~0 1.95 1.95	1,4	∓8.4

Table B.4.d. (contd.)

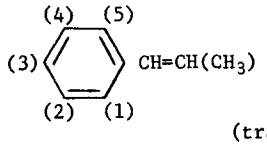
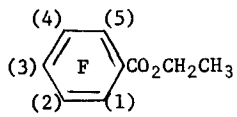
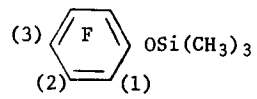
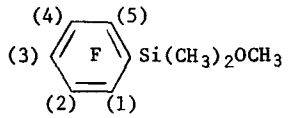
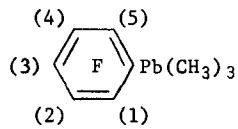
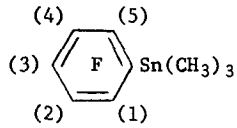
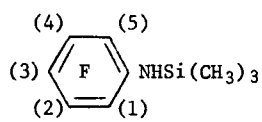
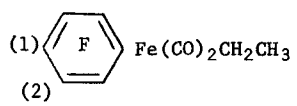
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
910	4425	G	$C_9F_5H_5$		(cis)	1,2	-22.5	1,3	<1	1,4 +8.5
						2,3	20.4	1,5	2.0	
								2,4	2.0	
					(trans)	1,2	-20.6	1,3	<1	1,4 +8.4
						2,3	19.4	1,5	1.9	
								2,4	1.9	
434	4426	J^2	$C_9F_5H_5O_2$			1,2	±20.4	1,3	4.4	1,4 ∓ 8.0
						2,3	±19.1	1,5	1.1	
								2,4	5.8	
778	4427	H*	$C_9F_5H_9OSi$			2,3	∓21.0	1,3	±4.4	
445	4428 (2136)	H	$C_9F_5H_9OSi$			1,2	∓24.0	1,3	± 3.8	1,4 ±10.9
						2,3	∓19.1	1,5	∓4.5	
								2,4	∓1.1	
932	4429	G	$C_9F_5H_9Pb$			1,2	∓29.3	1,3	±1.1	1,4 ±12.5
						2,3	∓19.0	1,5	∓7.9	
								2,4	∓1.9	
880 932	4430	G	$C_9F_5H_9Sn$			1,2	∓26.7	1,3	∓6.5	1,4 ±12.0
						2,3	∓19.1	1,5	±1.9	
								2,4	∓1.4	
778	4431	H*	$C_9F_5H_{10}NSi$			1,2	∓21.5	1,3	-7.0	1,4 ±4.6
						2,3	∓21.4	1,5	-3.3	
								2,4	∓2.7	
447	4432		$C_{10}F_5H_5FeO_2$			1,2	21			

Table B.4.d. (contd.)

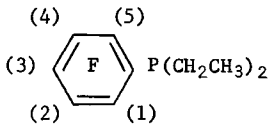
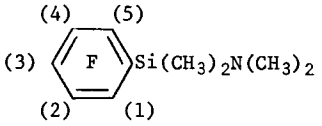
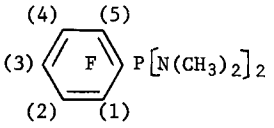
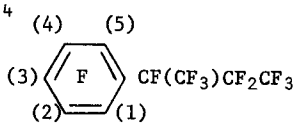
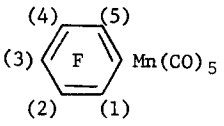
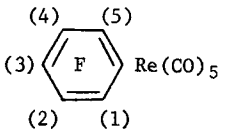
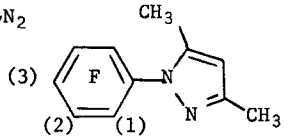
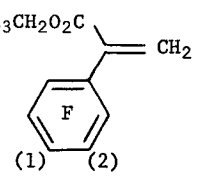
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
777	4433 (6290)		$C_{10}F_5H_{10}P$		1,2 2,3	±23.7 20.2	1,3 1,5 2,4	3.3 1.7 4.0	1,4	∓9.8
445	4434 (2143)		$C_{10}F_5H_{12}NSi$		1,2 2,3	∓25.3 ∓19.4	1,3 1,5 2,4	±3.1 ∓1.5 ∓4.4	1,4	±10.9
777	4435 (6291)		$C_{10}F_5H_{12}N_2P$		1,2 2,3	±26.0 20.2	1,3 1,5 2,4	2.6 2.8 3.3	1,4	∓9.6
933	4436 (3100 3381)		$C_{10}F_{14}$		1,2 2,3	-19.8 -19.9	1,3 1,5 2,4	+6.4 6.0 0	1,4	+7.9
816	4437	E	$C_{11}F_5MnO_5$		1,2 2,3	∓28.1 ∓19.1	1,3 1,5 2,4	0 ∓8.3 ∓2.8	1,4	±9.2
		H			2,3	∓19.5	1,3	±0		
434	4438	U[2]	$C_{11}F_5O_5Re$		1,2 2,3	±28.55 ±19.35	1,3 1,5 2,4	0 2.68 7.75	1,4	∓10.5
930	4439	A	$C_{11}F_5H_7N_2$		1,2 2,3	15.6 21.2				
934	4440		$C_{11}F_5H_7O_2$		1,2	15.5				

Table B.4.d. (contd.)

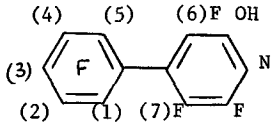
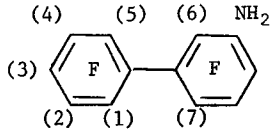
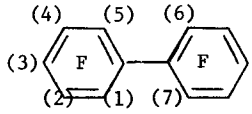
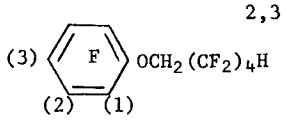
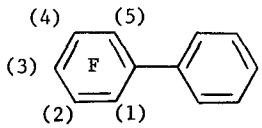
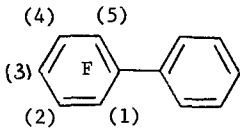
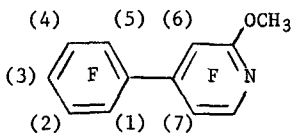
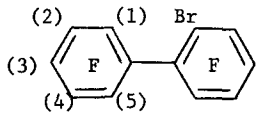
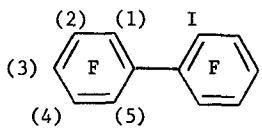
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
897	4441	E	$C_{11}F_8HNO$		1,2	21.2	1,3	3.2	1,4	7.7
	(4661)				2,3	20.4	1,5	5.4	5,6	9.1
							2,4	<0.5	5,7	8.8
897	4442	E	$C_{11}F_8H_2N_2$		1,2	22.0	1,3	3.1	1,4	8.2
	(4662)				2,3	20.1	1,5	5.3	5,6	8.5
							2,4	0.8	5,7	8.3
897	4443	E	$C_{11}F_9N$		1,2	21.2	1,3	3.9	1,4	8.0
	(4663)				2,3	19.9	1,5	6.1	5,6	9.9
							2,4	0.4	5,7	9.9
197	4444	B	$C_{11}F_{13}H_3O$		1,2	21.8				
	(692)				2,3	21.7				
881	4445		$C_{12}F_5H_5$				1,3	1.5	1,4	8.2
							2,4	0		
							1,5	1.5		
910	4446	G	$C_{12}F_5H_5$		1,2	-22.7	1,3	<1	1,4	+8.0
					2,3	20.8	2,4	1.6		
							1,5	1.6		
897	4447		$C_{12}F_8H_3NO$		1,2	21.4	1,3	3.3	1,4	7.8
	(4666)				2,3	20.1	1,5	5.5	5,6	8.9
							2,4	0.3	5,7	8.6
900	4448		$C_{12}F_9Br$		1,2	±21.5	1,3	2.5	1,4	∓9.2
	(4283)				2,3	20.4	1,5	5.2		
							2,4	1.0		
900	4449		$C_{12}F_9I$		1,2	±21.5	1,3	2.7	1,4	∓8.3
	(4284)				2,3	20.0	1,5	5.1		
							2,4	1.0		

Table B.4.d. (contd.)

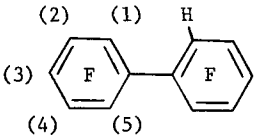
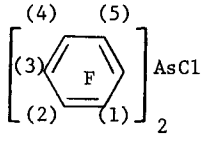
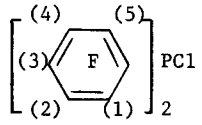
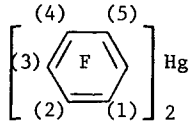
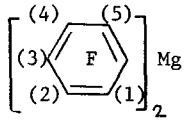
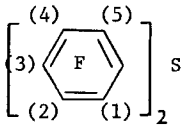
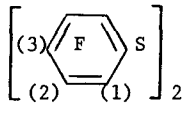
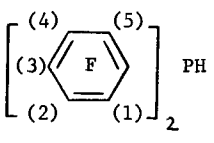
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
900	4450 (2144 4285)		$C_{12}F_9H$		1,2 2,3	±22.6 19.9	1,3 1,5 2,4	2.7 3.7 1.5	1,4	∓8.6
908	4451	A	$C_{12}F_{10}AsCl$		1,2 2,3	22.2 21.0	1,3	5.0		
777	4452 (6341)		$C_{12}F_{10}ClP$		1,2 2,3	±22.7 19.6	1,3 1,5 2,4	5.5 0.2 5.5	1,4	∓9.3
636	4453 (5577)	E	$C_{12}F_{10}Hg$		1,2 2,3	-26.0 -18.9	1,3 1,5 2,4	+1.4 -7.2 -1.7	1,4	+10.3
936	4454		$C_{12}F_{10}Mg$		2,3	19.2				
921	4455	G	$C_{12}F_{10}S$		2,3	20.6	1,3	3.5		
921	4456	E	$C_{12}F_{10}S_2$		2,3	19.8	1,3	4.0		
777	4457 (6342)		$C_{12}F_{10}HP$		1,2 2,3	±20.3 19.4	1,3 1,5 2,4	3.8 2.4 6.5	1,4	∓7.1

Table B.4.d. (contd.)

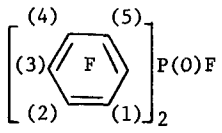
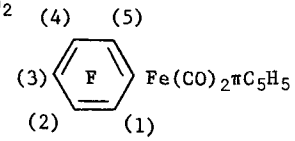
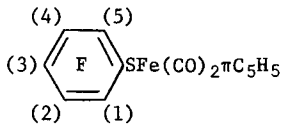
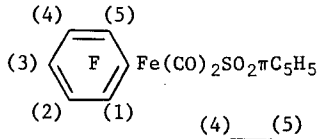
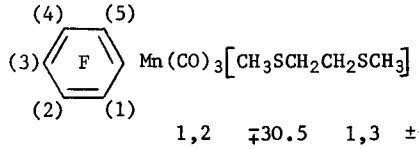
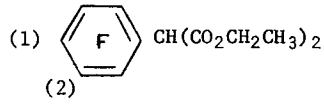
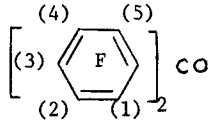
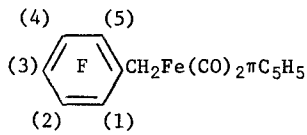
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
778	4458 (6343)	H*	$C_{12}F_{11}OP$		1,2 2,3	∓22.3 ∓20.9	1,3 1,5 2,4	±7.9 ∓7.4 ∓0	1,4	±8.8
434	4459	U[2]	$C_{13}F_5H_5FeO_2$		1,2 2,3	±30.15 ±19.6	1,3 1,5 2,4	∿1.0 3.45 5.7	1,4	∓8.8
901	4460	A	$C_{13}F_5H_5FeO_2S$		1,2 2,3	25.0 21.2	1,3 1,5 2,4	<1 1.4 1.4	1,4	8.2
434	4461	U[2]	$C_{13}F_5H_5FeO_4S$		1,2 2,3	±28.05 ±25.2	1,3 1,5 2,4	1.7 0 3.0	1,4	∓9.25
816	4462	E	$C_{13}F_5H_{10}MnO_3S_2$		1,2 2,3	∓30.5 ∓19.4	1,3 1,5 2,4	±<0.7 ∓7.1 ∓4.5	1,4	±10.5
934	4463		$C_{13}F_5H_{11}O_4$		1,2	20				
434	4464	A	$C_{13}F_{10}O$		1,2 2,3	±22.4 ±20.1	1,3 1,5 2,4	5.25 0.4 5.35	1,4	∓8.85
434	4465	U[2]	$C_{14}F_5H_7FeO_2$		1,2 2,3	±21.4 ±19.9	1,3 1,5 2,4	0 1.8 1.8	1,4	∓8.1

Table B.4.d. (contd.)

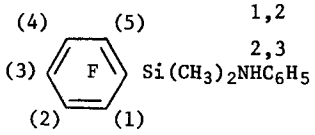
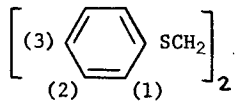
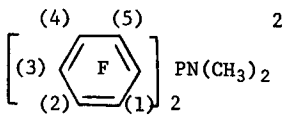
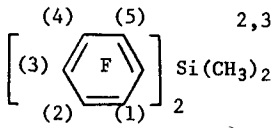
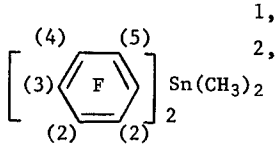
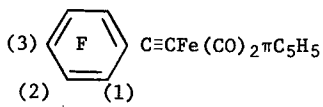
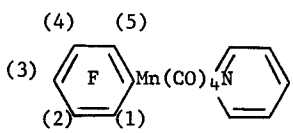
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
445	4466 (2145)		$C_{12}F_5H_{12}NSi$		1,2 2,3	∓24.4 ∓19.5	1,3 1,5 2,4	±3.9 ∓4.3 ∓1.0	1,4 ±10.7
921	4467	G	$C_{14}F_{10}H_4S_2$		2,3	20.0	1,3	2.0	
777	4468 (6365)		$C_{14}F_{10}H_6NP$		1,2 2,3	±23.9 19.8	1,3 1,5 2,4	3.3 1.2 4.4	1,4 ∓9.2
445	4469 (2146)	H	$C_{14}F_{10}H_6Si$		1,2 2,3	∓24.1 ∓19.6	1,3 1,5 2,4	±4.2 ∓4.9 ∓0.7	1,4 ±10.6
932	4470	B-G	$C_{14}F_{10}H_6Sn$		1,2 2,3	∓27.0 ∓19.0	1,3 1,5 2,4	±1.8 ∓6.5 ∓1.4	1,4 ±12.0
434	4471	U[2]	$C_{15}F_5H_5FeO_2$		2,3	20.45	1,3	4.4	
816	4472	E	$C_{15}F_5H_5MnNO_4$		1,2 2,3	∓29.6 ∓19.2	1,3 1,5 2,4	±0 ∓7.6 ∓3.7	1,4 ±10.2

Table B.4.d. (contd.)

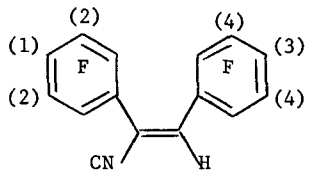
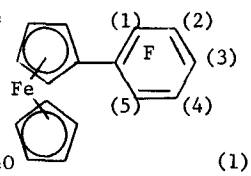
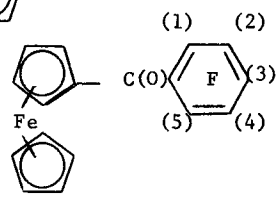
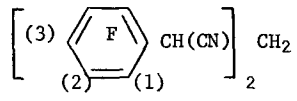
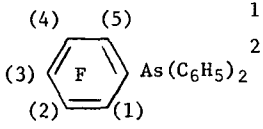
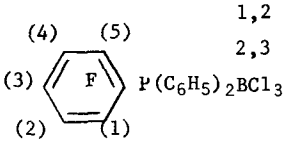
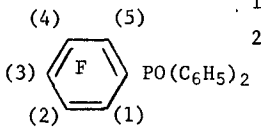
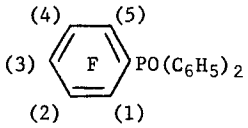
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
931	4473		$C_{15}F_{10}HN$		1,2 3,4	19.5 19.5				
937	4474		$C_{16}F_{5}H_{9}Fe$		1,2 2,3	±21.67 ±20.3	1,3 1,5 2,4	0 2.25 2.25	1,4	∓7.07
937	4475	U[2]	$C_{17}F_{5}H_{9}FeO$		1,2 2,3	±21.96 ±20.4	1,3 1,5 2,4	0 0 4.2	1,4	∓8.36
931	4476		$C_{17}F_{10}H_{4}N_{2}$		2,3	20	1,3	2.5		
812	4477	A	$C_{18}F_{5}H_{10}As$		1,2 2,3	-25.4 -19.8	1,3 1,5 2,4	+3.2 -1.5 -4.8	1,4	+9.8
778 928	4478 (6410)	H*	$C_{18}F_{5}H_{10}BCl_{3}P$		1,2 2,3	∓23.4 ∓20.3	1,3 1,5 2,4	±7.3 ∓9.2 ∓0	1,4	±9.0
778	4479 (6411)	H*	$C_{18}F_{5}H_{10}OP$		1,2 2,3	∓23.4 ∓20.6	1,3 1,5 2,4	±5.9 ∓5.1 ∓0	1,4	±9.2
812	4480 (6412)	A	$C_{18}F_{5}H_{10}OP$		1,2 2,3	-23.5 -20.8	1,3 1,5 2,4	+6.3 - -5.5	1,4	+9.5

Table B.4.d. (contd.)

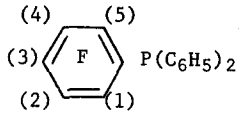
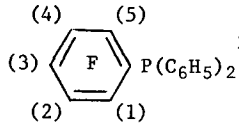
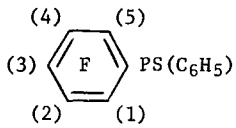
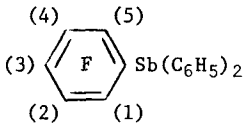
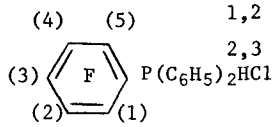
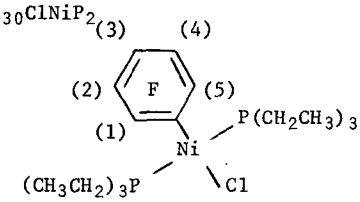
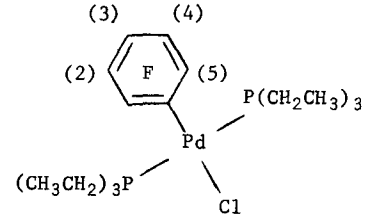
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
778 928	4481 (6414)	H*	$C_{18}F_5H_{10}P$		1,2 2,3	∓24.1 ∓20.9	1,3 1,5 2,4	±4.0 ∓4.5 ∓1.5	1,4	±9.4
812	4482 (6413)	A	$C_{18}F_5H_{10}P$		1,2 2,3	-24.2 -20.4	1,3 1,5 2,4	+4.0 -1.6 -4.4	1,4	+10.0
778	4483 (6415)	H*	$C_{18}F_5H_{10}PS$		1,2 2,3	∓23.4 ∓20.8	1,3 1,5 2,4	±5.8 ∓5.9 ∓0.6	1,4	±8.7
812	4484	A	$C_{18}F_5H_{10}Sb$		1,2 2,3	-26.9 -20.2	1,3 1,5 2,4	+2.9 -1.5 -5.8	1,4	+10.8
778 928	4485 (6416)	H*	$C_{18}F_5H_{11}ClP$		1,2 2,3	∓22.6 ∓20.1	1,3 1,5 2,4	±7.5 ∓8.5 ∓0	1,4	±8.2
830	4486		$C_{18}F_5H_{30}ClNiP_2$		1,2 2,3	-35.2 -20.2	1,3 1,5 2,4	-2.4 -7.9 -3.4	1,4	+11.8
830	44 87		$C_{18}F_5H_{30}ClP_2Pd$		1,2 2,3	-31.5 -19.7	1,3 1,5 2,4	-2.7 -7.4 -3.8	1,4	+10.1

Table B.4.f. (contd.)

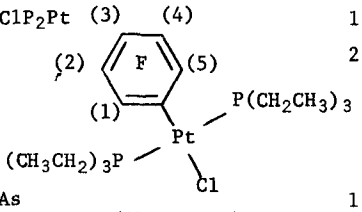
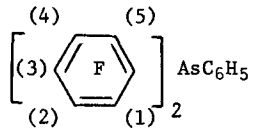
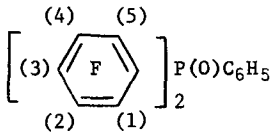
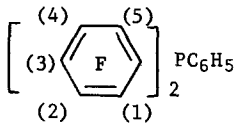
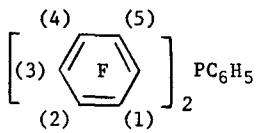
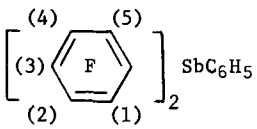
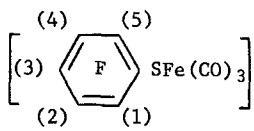
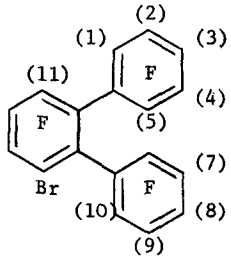
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
830	4488		$C_{18}F_5H_{30}ClP_2Pt$		1,2 2,3	-33.1 -19.7	1,3 1,5 2,4	-2.8 -8.9 -3.2	1,4 +11.3
812	4489	A	$C_{18}F_{10}H_5As$		1,2 2,3	-27.3 -18.9	1,3 1,5 2,4	+3.1 - -5.2	1,4 +10.3
812	4490 (6423)	A	$C_{18}F_{10}H_5OP$		1,2 2,3	-23.9 -19.9	1,3 1,5 2,4	+6.6 - -7.2	1,4 +8.6
778 928	4491 (6425)	H*	$C_{18}F_{10}H_5P$		1,2 2,3	∓23.5 ∓20.1	1,3 1,5 2,4	±4.2 ∓4.6 ∓0	1,4 ±9.3
812	4492 (6424)	A	$C_{18}F_{10}H_5P$		1,2 2,3	-23.3 -20.0	1,3 1,5 2,4	+4.0 — -3.6	1,4 +8.9
812	4493	A	$C_{18}F_{10}H_5Sb$		1,2 2,3	-25.0 -19.7	1,3 1,5 2,4	+3.1 — -5.5	1,4 +9.2
778	4494	A	$C_{18}F_{10}FeO_6S_2$		1,2 2,3	24.1 21.2	1,3 1,5 2,4	2.4 3.6 3.6	1,4 8.2
891	4495 (4215)		$C_{18}F_{13}Br$		2,3 4,5	20.1 20.4	1,3 6,8	2.5 2.7	1,11 4.2

Table B.4.d. (contd.)

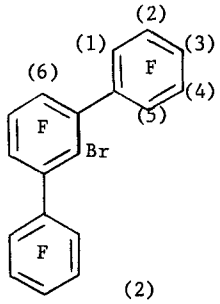
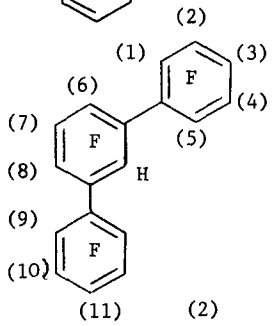
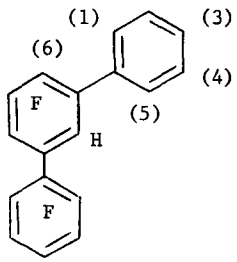
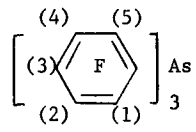
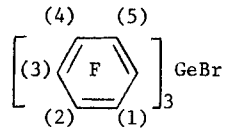
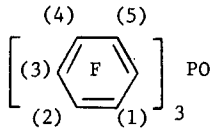
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
891	4496 (4216)		$C_{18}F_{13}Br$		1,2 2,3	21.9 20.0	1,3 1,5 2,4	2.9 5.6 1.6	1,4 1,6	8.2 1.8
891	4497 (4217)		$C_{18}F_{13}H$		2,3 7,8 1,2 6,7	20.0 20.2 22.0 21.8	1,3 6,8 1,5 6,10 2,4 7,9	1.2 1.5 4.0 3.9 0.9 0.8	1,4 6,9 1,11	8.5 8.2 5.0
891	4498 (4218)		$C_{18}F_{13}H$		1,2 2,3	22.0 20.0	1,3 1,5 2,4	2.4 3.7 0.9	1,4 1,6	8.5 3.5
812	4499	A	$C_{18}F_{15}As$		1,2 2,3	-24.8 -19.6	1,3 1,5 2,4	+3.9 - -4.5	1,4	+9.8
932	4500	G	$C_{18}F_{15}BrGe$		1,2 2,3	∓22.9 ∓19.3	1,3 1,5 2,4	±4.4 ∓6.5 ∓0.9	1,4	±9.7
778	4501 (6427)	H	$C_{18}F_{15}OP$		2,3	∓20.8	1,3	±7.2		

Table B.4.d. (contd.)

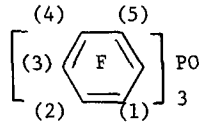
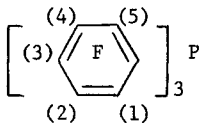
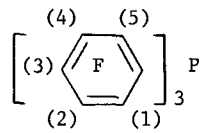
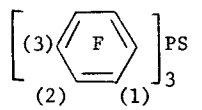
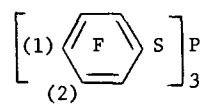
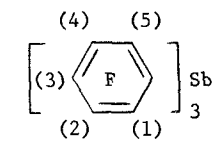
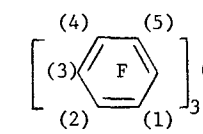
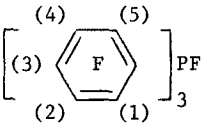
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
812	4502 (6428)	A	$C_{18}F_{15}OP$		1,2 2,3	-26.3 -20.5	1,3 1,5 2,4	+4.4 — -3.6	1,4	+11.5
778	4503	H	$C_{18}F_{15}P$		2,3	$\mp$20.5	1,3	±4.5		
812	4504 (6430)	A	$C_{18}F_{15}P$		1,2 2,3	-24.2 -20.0	1,3 1,5 2,4	+4.3 — -4.6	1,4	+8.8
778	4505 (6431)	H	$C_{18}F_{15}PS$		2,3	$\mp$20.8	1,3	±7.2		
921	4506	G	$C_{18}F_{15}PS_3$		1,2	∿20				
812	4507	A	$C_{18}F_{15}Sb$		1,2 2,3	-25.2 -19.5	1,3 1,5 2,4	+3.4 - -5.7	1,4	+9.7
932	4508	G	$C_{18}F_{15}HGeO$		1,2 2,3	$\mp$24.2 $\mp$19.5	1,3 1,5 2,4	±4.2 $\mp$5.6 $\mp$0.9	1,4	±9.6
778	4509 (6433)	H	$C_{18}F_{17}P$		1,2 2,3	$\mp$21.9 $\mp$19.7	1,3 1,5 2,4	±6.0 $\mp$7.7 $\mp$0	1,4	±7.5

Table B.4.d. (contd.)

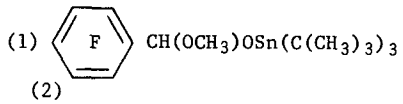
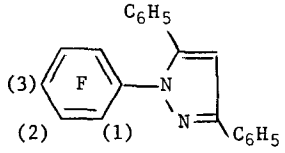
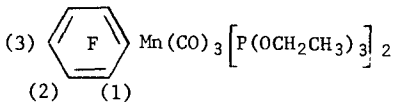
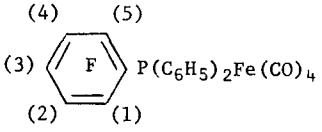
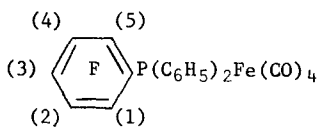
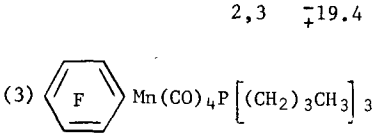
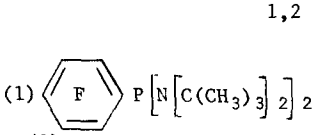
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
938	4510		$C_{20}F_5H_{31}O_2Sn$		1,2	21				
930	4511		$C_{21}F_5H_{11}N_2$		1,2 2,3	15.8 21.5				
816	4512	E	$C_{21}F_5H_{30}MnO_9P_2$		2,3	19.3	1,3	0		
928	4513 (6456)		$C_{22}F_5H_{10}FeO_4P$				1,3	5.0		
778	4514 (6455)	H	$C_{22}F_5H_{10}FeO_4P$		1,2 2,3	∓23.4 ∓20.9	1,3 1,5 2,4	±5.0 ∓6.8 ∓0	1,4	±8.7
816	4515		$C_{22}F_5H_{27}MnO_4P$		2,3	∓19.4	1,3	±0		
777	4516		$C_{22}F_5H_{36}N_2P$		1,2	20.4				

Table B.4.d. (contd.)

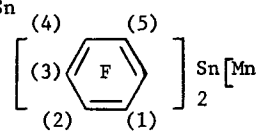
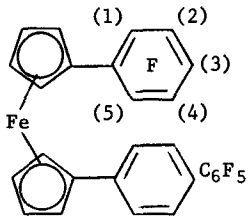
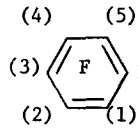
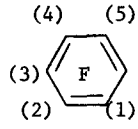
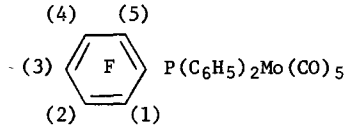
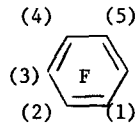
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
778	4517	H	$C_{22}F_{10}Mn_2O_{10}Sn$		1,2 2,3	$\mp$29.2 $\mp$19.6	1,3 1,5 2,4	$\pm$2.7 $\mp$7.6 $\mp$0	1,4	$\pm$8.6
937	4518		$C_{22}F_{10}H_8Fe$		1,2 2,3	$\pm$21.8 $\pm$24.0	1,3 1,5 2,4	0 2.6 2.6	1,4	$\mp$7.5
778	4519 (6465)	H	$C_{23}F_5H_{10}CrO_5P$		1,2 2,3	$\mp$23.7 $\mp$20.8	1,3 1,5 2,4	$\pm$5.0 $\mp$6.3 $\mp$0	1,4	$\pm$8.9
778	4520	H	$C_{23}F_5H_{10}MnO_5Sn$		1,2 2,3	$\mp$21.3 $\mp$19.2	1,3 1,5 2,4	$\pm$2.6 $\mp$7.3 $\mp$1.1	1,4	$\pm$8.3
928	4521 (6466)		$C_{23}F_5H_{10}MoO_5P$				1,3	4.8		
778	4522 (6467)	H	$C_{23}F_5H_{10}MoO_5P$		1,2 2,3	$\mp$23.0 $\mp$20.4	1,3 1,5 2,4	$\pm$4.8 $\mp$6.2 $\mp$1.0	1,4	$\pm$8.6

Table B.4.d. (contd.)

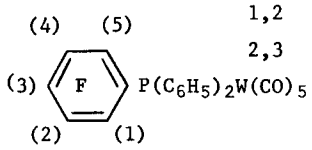
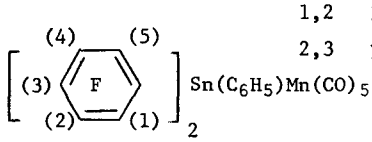
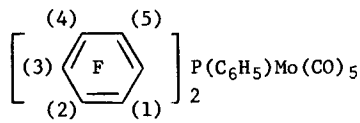
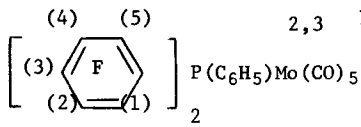
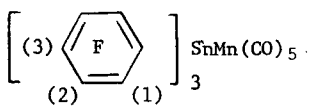
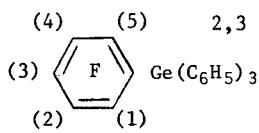
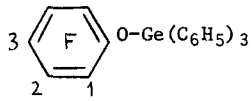
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
778	4523 (6468)	H	$C_{23}F_5H_{10}O_5PW$		1,2 2,3	∓23.7 ∓20.6	1,3 1,5 2,4	±5.2 ∓3.3 ∓0	1,4 ±9.2
778	4524	H	$C_{23}F_{10}H_5MnO_5Sn$		1,2 2,3	∓26.3 ∓19.4	1,3 1,5 2,4	±2.8 ∓7.0 ∓0	1,4 ±10.6
928	4525 (6470)		$C_{23}F_{10}H_5MoO_5P$				1,3	5.2	
778	4526 (6469)	H	$C_{23}F_{10}H_5MoO_5P$		1,2 2,3	∓22.3 ∓20.4	1,3 1,5 2,4	±5.2 ∓6.6 ∓0	1,4 ±7.2
778	4527	H	$C_{23}F_{15}MnO_5Sn$		2,3	∓19.5	1,3	±3.4	
932	4528	G	$C_{24}F_5H_{15}Ge$		1,2 2,3	∓25.1 ∓19.6	1,3 1,5 2,4	±3.3 ∓5.7 ∓1.5	1,4 ±10.7
778	4529	H	$C_{24}F_5H_{15}GeO$		2,3	∓21.6	1,3	-5.0	

Table B.4.d. (contd.)

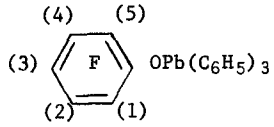
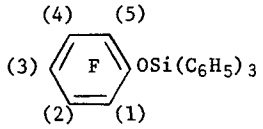
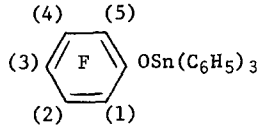
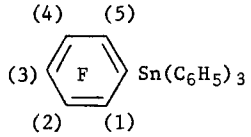
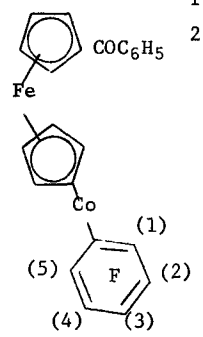
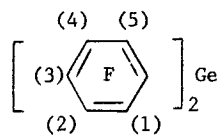
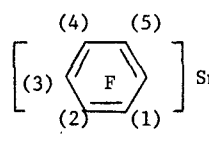
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}	
778	4530	H	$C_{24}F_5H_{15}OPb$		1,2 2,3	∓25.2 ∓22.2	1,3 1,5 2,4	-8.0 -5.5 ∓0	1,4	±6.0
778	4531	H	$C_{24}F_5H_{15}OSi$		2,3	∓21.6	1,3	-4.3		
778	4532	H	$C_{24}F_5H_{15}OSn$		2,3	∓21.9	1,3	-6.4		
778	4533	H	$C_{24}F_5H_{15}Sn$		1,2 2,3	∓22.6 ∓19.2	1,3 1,5 2,4	±2.6 ∓6.9 ∓1.1	1,4	±9.8
937	4534		$C_{24}F_{10}H_8FeO_2$		1,2 2,3	±22.63 ±19.85	1,3 1,5 2,4	2.75 0 4.8	1,4	∓8.54
932	4535	G	$C_{24}F_{10}H_{10}Ge$		1,2 2,3	∓24.4 ∓19.9	1,3 1,5 2,4	±3.7 ∓5.5 ∓0.7	1,4	±10.5
778	4536	H	$C_{24}F_{10}H_{10}Sn$		1,2 2,3	∓24.7 ∓19.2	1,3 1,5 2,4	±3.0 ∓6.8 ∓0	1,4	±10.3

Table B.4.d. (contd.)

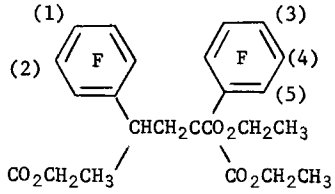
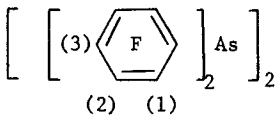
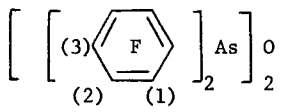
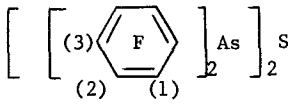
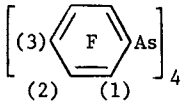
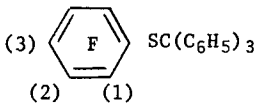
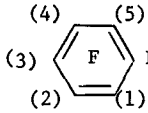
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}	J_{para}
934	4537	A	$C_{24}F_{10}H_{18}O_6$		1,2 3,4	20 20	3,5	3.4	
908	4538	A	$C_{24}F_{20}As_2$						
				Isomer 1	1,2 2,3	23.1 23.0	1,3	∿5.0	
				Isomer 2	1,2 2,3	20.0 20.5	1,3	∿5.0	
908	4539	A	$C_{24}F_{20}As_2O$		1,2 2,3	20.3 21.1	1,3	5.0	
908	4540	A	$C_{24}F_{20}As_2S$		1,2 2,3	22.0 21.0	1,3	6.1	
908	4541	A	$C_{24}F_{20}As_4$		1,2 2,3	21.8 21.0	1,3	5.0	
921	4542	G	$C_{22}F_5H_{15}S$		2,3	±20.5	1,3	±3.7	
816	4543	E	$C_{28}F_5H_{15}AsMnO_4$		1,2 2,3	∓29.4 ∓19.4	1,3 1,5 2,4	±0 ∓8.5 ∓3.4	1,4 ±9.6

Table B.4.d. (contd.)

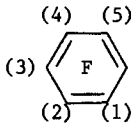
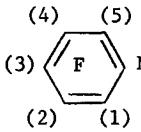
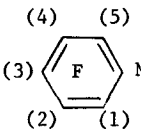
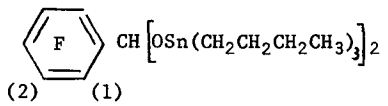
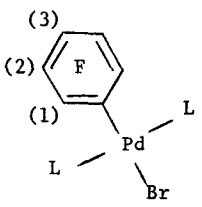
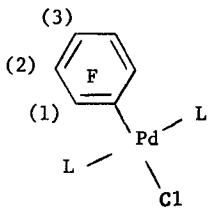
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}		J_{meta}		J_{para}
816	4544 (6512)	E	$C_{28}F_5H_{15}MnO_4P$	 $Mn(CO)_4P(C_6H_5)_3$	1,2 2,3	∓29.3 ∓19.3	1,3 1,5 2,4	±0 ∓8.7 ∓3.6	1,4 ±9.4
816	4545	E	$C_{28}F_5H_{15}MnO_4Sb$	 $Mn(CO)_4Sb(C_6H_5)_3$	1,2 2,3	∓29.5 ∓19.3	1,3 1,5 2,4	±0 ∓8.5 ∓3.2	1,4 ±9.5
816	4546 (6513)	E	$C_{28}F_5H_{15}MnO_7P$	 $Mn(CO)_4P(OC_6H_5)_3$	1,2 2,3	∓29.3 ∓19.5	1,3 1,5 2,4	0 ∓8.4 ∓3.4	1,4 ±9.5
938	4547		$C_{31}F_5H_{55}O_2Sn_2$	 $CH\left[OSn(CH_2CH_2CH_2CH_3)_3\right]_2$	1,2	23			
823	4548 (6519)	A	$C_{32}F_5H_{26}BrP_2Pd$	 $L = P(C_6H_5)_2CH_3$	1,2 2,3	28.0 20.0			
823	4549 (6520)	A	$C_{32}F_5H_{26}ClP_2Pd$	 $L = P(C_6H_5)_2CH_3$	1,2 2,3	26.0 22.0			

Table B.4.d. (contd.)

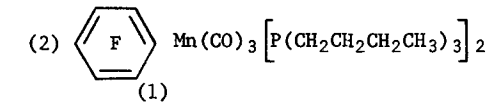
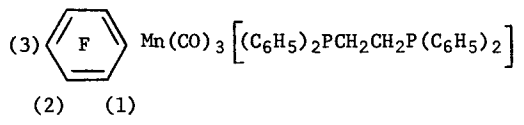
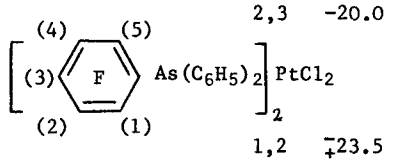
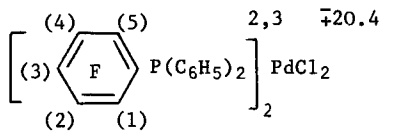
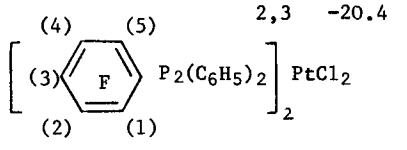
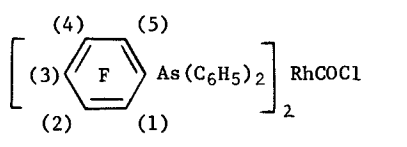
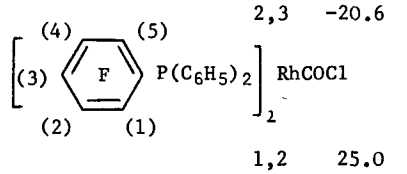
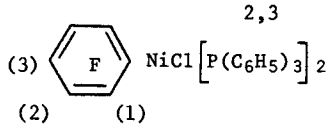
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
816	4550	E	$C_{33}F_5H_{54}MnO_3P_2$			1,2 0	
816	4551 (6524)	E	$C_{33}F_5H_{24}MnO_3P_2$		2,3 19.5	1,3 0	
812	4552	A	$C_{36}F_{10}H_{20}As_2Cl_2Pt$		1,2 -24.9 2,3 -20.0	1,3 +4.6 1,5 0.8 2,4 -6.5	1,4 +9.2
778	4553 (6527)	H	$C_{36}F_{10}H_{20}Cl_2P_2Pd$		1,2 ∓23.5 2,3 ∓20.4	1,3 ±5.1 1,6 ∓6.7 2,4 ∓0	1,4 ±8.5
812	4554 (6528)	A	$C_{36}F_{10}H_{20}Cl_2P_2Pt$		1,2 -24.0 2,3 -20.4	1,3 +4.8 1,5 - 2,4 -6.3	1,4 +8.6
812	4555	A	$C_{37}F_{10}H_{20}As_2ClORh$		1,2 -24.7 2,3 -20.5	1,3 +4.2 1,5 - 2,4 -7.7	1,4 +9.2
812	4556 (6530)	A	$C_{37}F_{10}H_{20}ClOP_2Rh$		1,2 -23.0 2,3 -20.6	1,3 +4.6 1,5 - 2,4 -5.8	1,4 +7.7
822	4557		$C_{42}F_5H_{30}ClNiP_2$		1,2 25.0 2,3 18.5		

Table B.4.e. Condensed-ring systems.

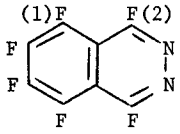
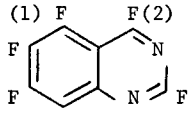
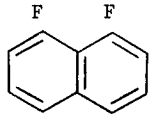
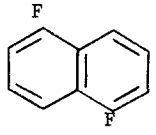
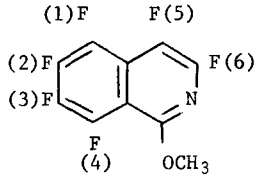
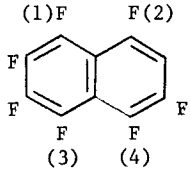
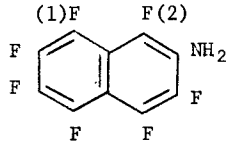
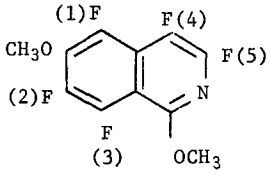
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
946	4558	E	$C_8F_6N_2$				1,2	57		
948	4559	H	$C_8F_6N_2$				1,2	50		
877	4560	B-E	$C_{10}F_2H_6$					58.8		
877	4561	B-E	$C_{10}F_2H_6$							4.1
951	4562		$C_{10}F_6H_3NO$		1,2	17.3	1,3	4.0	1,4	15.8
					2,3	19.0	2,4	8.0	1,6	0.7
					3,4	17.8	1,5	49.7	2,5	3.7
					5,6	17.7			3,6	7.9
									3,5	7.9
									3,5	3.7
									4,6	4.7
									4,5	1.5
939	4563		$C_{10}F_7H$				1,2	65.7		
							3,4	59.4		
940	4564	A	$C_{10}F_7H_2N$				3,4	60		
951	4565		$C_{11}F_5H_6NO_2$		2,3	14.3	1,2	2.0	1,3	14.3
					4,5	16.3	1,4	50.7	1,5	2.0
									3,4	1.5
									2,4	3.8
									2,5	3.8
									3,5	4.3

Table B.4.e. (contd.)

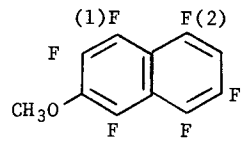
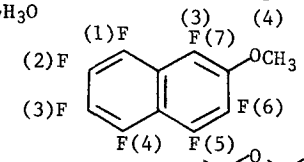
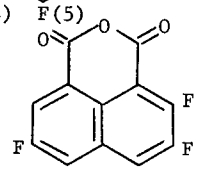
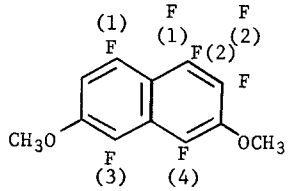
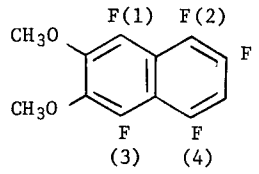
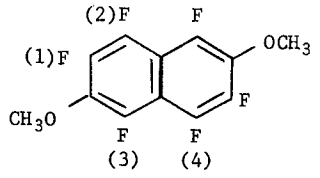
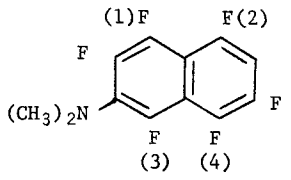
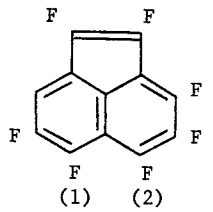
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
939	4566		$C_{11}F_6H_4O$				1,2 3,4	63.7 65.2		
940	4567	A	$C_{11}F_7H_3O$		1,2 3,4 5,6	15 15 14	1,7 4,5	68 60	1,4 5,7	15 14
939	4568		$C_{12}F_5HO_3$				1,2	53.9		
939	4569		$C_{12}F_5H_7O_2$				1,2 3,4	61.8 68.2		
939	4570		$C_{12}F_5H_7O_2$				1,2 3,4	63.4 69.3		
940	4571	A	$C_{12}F_6H_6O_2$		1,2	16	3,4	67	2,3	16
939	4572		$C_{12}F_6H_7N$				1,2 3,4	62.6 69.7		
939	4573		$C_{12}F_7H$				1,2	32.7		

Table B.4.e. (contd.)

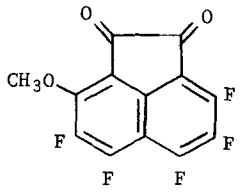
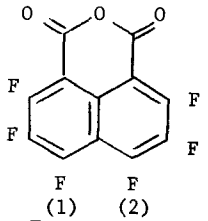
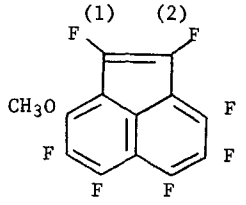
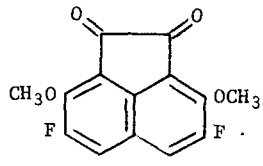
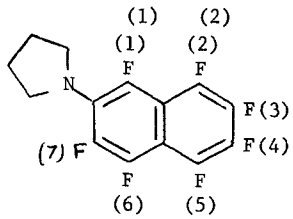
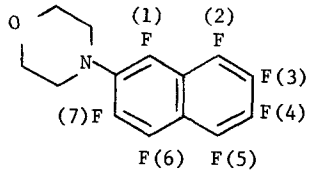
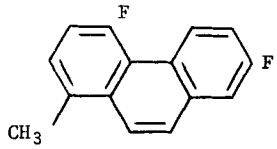
Ref. No.	Serial No.	Solventq	Molecular formula	Structure	^3J		^4J		^nJ	
939	4574		$C_{13}F_5H_3O_3$				1,2	29.4		
939	4575		$C_{13}F_5H_3O_4$				1,2	58.2		
939	4576 (2031)		$C_{13}F_7H_3O$				1,2	35.7		
939	4577 (2032)		$C_{14}F_4H_6O_4$				1,2	30.7		
940	4578	A	$C_{14}F_7H_8N$		2,3 3,4 4,5	16 16 16	1,2 5,6	74 58	1,6	16
940	4579	A	$C_{14}F_7H_8NO$		2,3 3,4 4,5	18 16 18	1,2 5,6	73 58	2,5 1,6	16 16
877	4580	A	$C_{15}F_2H_{10}$							0.8

Table B.4.e. (contd.)

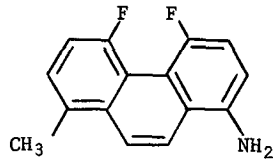
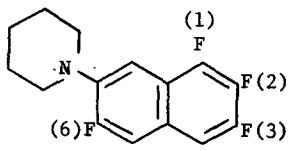
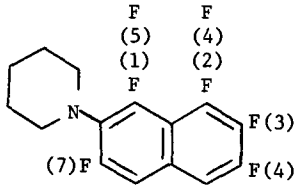
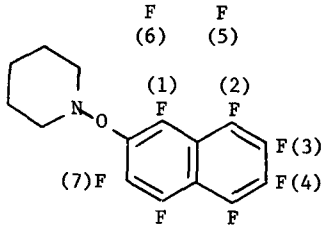
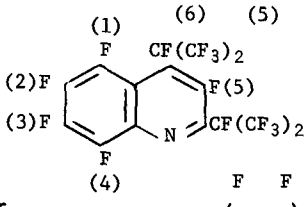
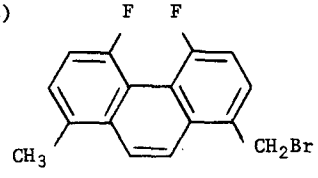
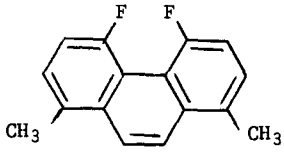
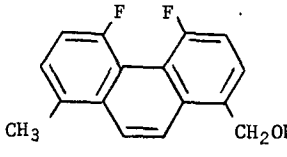
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
461	4581	E	$C_{15}F_2H_{11}N$							167
940	4582	A	$C_{15}F_6H_{11}N$		1,2 2,3 3,4 5,6	16 16 16 16	4,5	50	1,4	16
940	4583	A	$C_{15}F_7H_{10}N$		2,3 3,4 6,7	16 18 16	1,2 5,6	68 55	1,6 2,5	16 16
940	4584	A	$C_{15}F_7H_{10}NO$		2,3 3,4 4,5	16 16 16	1,2 5,6	81 59	2,5 1,6	16 18
933	4585 [3384 3400 3159]	B-P	$C_{15}F_{19}N$		1,2 2,3 3,4	-14.6 -19.2 -18.0	1,3 2,4	+5.4 +5.2	1,4 2,5 3,5 4,5	+15.1 ±1.9 ∓7.2 ±4.1
461	4586	E H	$C_{16}F_2H_{11}Br$							170 170
460 461	4587	E	$C_{16}F_2H_{12}$							170
461	4588	E	$C_{16}F_2H_{12}O$							170
460	4589		$C_{16}F_2H_{14}O_2$							98

Table B.4.e. (contd.)

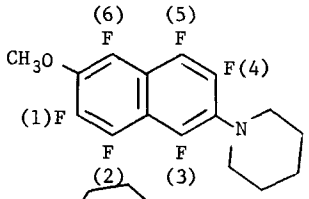
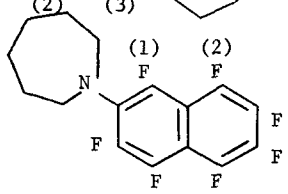
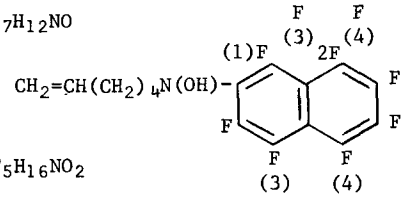
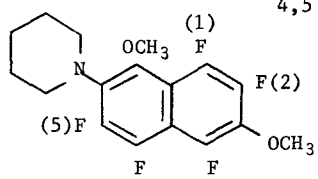
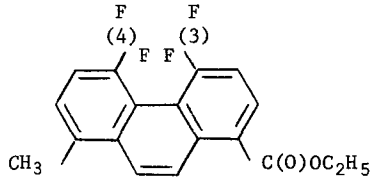
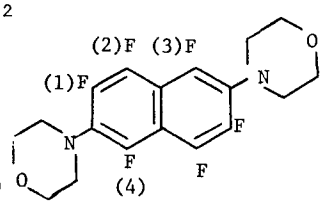
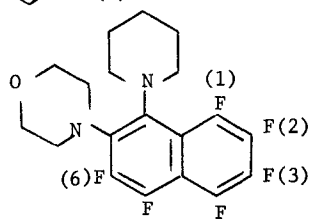
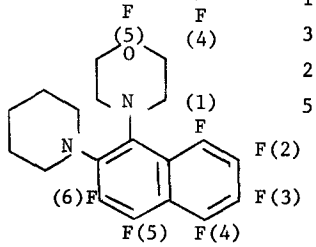
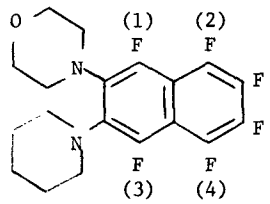
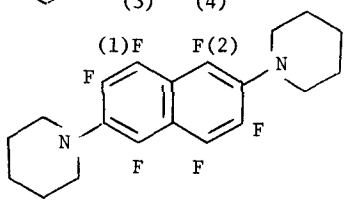
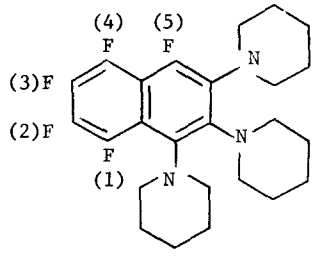
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
940	4590	A	$C_{16}F_6H_{13}NO$		1,2 4,5	16 15	5,6 2,3	62 69	3,5 2,6	15 15
940	4591	A	$C_{16}F_7H_{12}N$				1,2 3,4	70 58		
940	4592	A	$C_{16}F_7H_{12}NO$				1,2 3,4	68 58	1,4 1,3	16 16
940	4593	A	$C_{17}F_5H_{16}NO_2$		1,2 4,5	16 18	3,4	67	1,3	17
461	4594 [1869 2026]	E* H	$C_{18}F_2H_{14}O_2$							170 167
740	4595	A	$C_{18}F_6H_{16}N_2O_2$		1,2	15	2,3	66	2,4	15
940	4596	A	$C_{19}F_6H_{18}N_2O$		1,2 2,3 3,4 5,6	17 17 17 16	4,5	68	1,4	17
940	4597	A	$C_{19}F_6H_{18}N_2O$		1,2 3,4 2,3 5,6	18.5 17.5 17.5 16.5	4,5	67	1,4	16

Table B.4.e. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ	
940	4598	A	$C_{19}F_6H_{18}N_2O$				1,2 3,4	65 65		
940	4599 (4220)	A	$C_{20}F_6H_{20}N_2$				1,2	67		
940	4600	A	$C_{25}F_5H_{30}N_3$		1,2 2,3 3,4	17 19.5 17	4,5	82	1,4	17

B.5. Fluorine bonded to carbon in heterocyclic aromatic systems.

Table B.5.a. Heterocycles containing nitrogen.

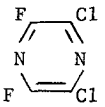
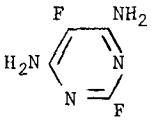
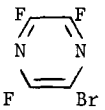
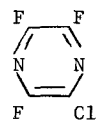
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
941	4601	E	$C_4F_2Cl_2N_2$			<8	
228	4602	L	$C_4F_2H_4N_4$				27.1
941	4603	R	$C_4F_3BrN_2$		17.5	6.9	39.9
941	4604	R	$C_4F_3ClN_2$		17.2	5.6	44.6

Table B.5.a. (contd.)

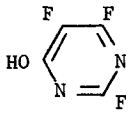
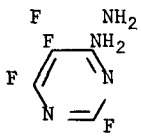
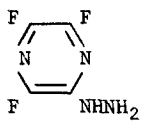
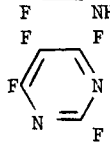
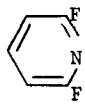
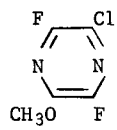
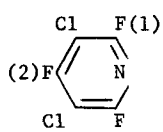
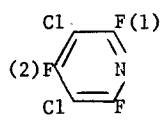
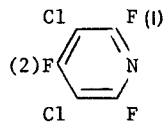
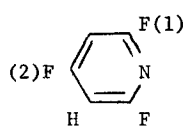
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
941	4605	R	$C_4F_3HN_2O$		16.5	12.0	51.0
228	4606	B	$C_4F_3HN_2O$		16.4	4.6	24.8
941	4607	R	$C_4F_3H_2N_3$		16.2	10.8	49.8
228	4608	E	$C_4F_3H_2N_3$		17.5		25.7
941	4609	R	$C_4F_3H_3N_4$		15.0	13.2	50.1
228 945	4610	B	$C_4F_4N_2$		17.9		26.0
462	4611 (2156)	A*	$C_5F_2H_3N$			12.23	
941	4612	R	$C_5F_2H_3ClN_2O$				47.0
649	4613 (5596)	B	$C_5F_3Cl_2N$			1,2 14.10	
468	4614	B	$C_5F_3Cl_2N$			1,2 14.0	
465	4615		$C_5F_3Cl_2N$			1,2 14.3	
466	4616		$C_5F_3H_2N$			1,2 19.7	

Table B.5.a. (contd.)

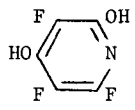
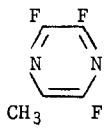
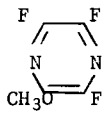
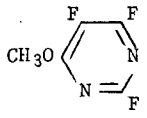
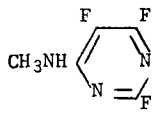
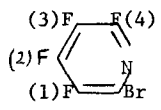
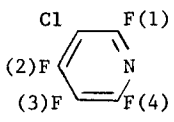
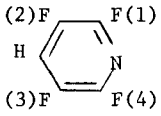
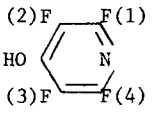
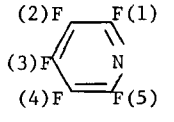
Ref. No.	Serial	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
942	4617	A[2]	$C_5F_3H_2NO_2$		24.4	2.5	24.4
941	4618	R	$C_5F_3H_3N_2$		19.7	7.9	43.9
941	4619	R	$C_5F_3H_3N_2O$		15.1	12.3	51.2
228	4620 (2176)	A	$C_5F_3H_3N_2O$		16.9		25.9
228	4621 (2497)	E	$C_5F_3H_4N_3$		17.5		26.5
943	4622	B	C_5F_4BrN		1,2 17.2 3,4 25.6 2,3 18.2	1,3 4.6 2,4 17.0	1,4 22
649	4623	B	C_5F_4ClN		2,3 17.60 3,4 20.35	1,2 10.55 2,4 17.60 1,4 14.5	1,3 24.85
942	4624 (2159)		C_5F_4HN		1,2 21.0	1,4 13.3 2,3 1.4	1,3 30.4
942	4625		C_5F_4HNO		1,2 20.6	1,4 15.5 2,3 7.9	1,3 22.2
942	4626		C_5F_5N		1,2 19.8 2,3 16.9	1,3 13.9 2,4 1.0 1,5 15.6	1,4 25.4

Table B.5.a. (contd.)

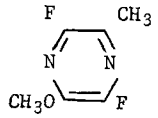
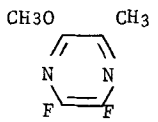
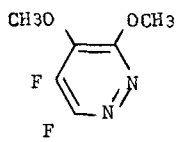
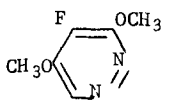
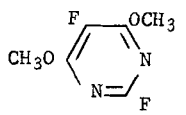
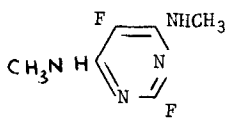
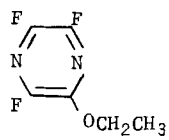
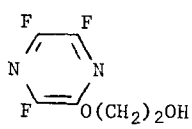
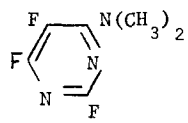
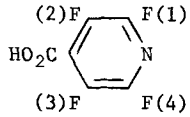
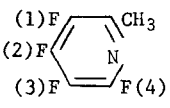
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	J_{ortho}	J_{meta}	J_{para}
941	4627	B	$C_6F_2H_6N_2O$				49.3
941	4628	B	$C_6F_2H_6N_2O$		22.5		
944	4629	G	$C_6F_2H_6N_2O_2$		29		
944	4630	G	$C_6F_2H_6N_2O_2$			26	
228	4631 (2180)	A	$C_6F_2H_6N_2O_2$				26.7
228	4632 (2498)	E	$C_6F_2H_8N_4$				27.4
941	4633	R	$C_6F_3H_5N_2O$		13.8	12.0	50.7
941	4634	E	$C_6F_3H_5N_2O_2$		14.8	11.7	50.6
228	4635 (2181)	A	$C_6F_3H_6N_3$		17.5		26.1
942	4636	K^2	$C_6F_4HNO_2$		1,2 19.2 2,3	1,4 13.4 2,3 4.1	1,3 31.2
942	4637 (2182)		$C_6F_4H_3N$		1,2 16.8 2,3 16.2 3,4 22.7	1,3 9.7 2,4 18.2	1,4 26.6

Table B.5.a. (contd.)

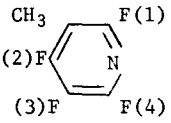
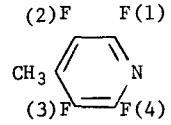
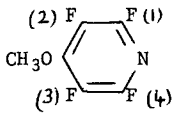
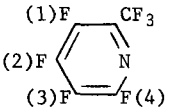
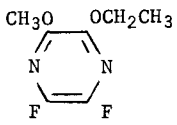
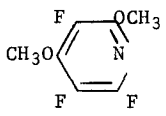
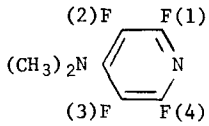
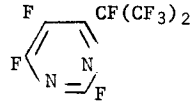
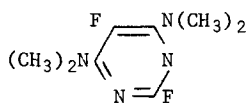
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
942	4638 (2183)		$C_6F_4H_3N$		2,3 3,4	16.7 20.3	1,2 2,4	8.1 25.2	1,3	24.3
942	4639 (2184)		$C_6F_4H_3N$		1,2	19.9	1,4 2,3	15.5 9.6	1,3	31.9
942	4640 (2185)		$C_6F_4H_3NO$		1,2	20.0	1,4 2,3	15.5 4.7	1,3	22.6
943	4641	B	C_6F_7N		1,2 2,3 3,4	17.7 17.0 24.1	1,3 2,4	10.1 19.8	1,4	28.1
941	4642	R	$C_7F_2H_8N_2O_2$			16.0				
942	4643 (2188)		$C_7F_3H_6NO_2$			22.4		1		25.5
468	4644 (2187)	B	$C_7F_3H_6NO_2$			25.20		0		21.55
942	4645 (2189)		$C_7F_4H_6N_2$		1,2	22.1	1,4 2,3	15.5 9.6	1,3	22.1
945	4646 [2974 3387]	B	$C_7F_{10}N_2$			20.0				29.0
228	4647 (2191)	A	$C_8F_2H_{12}N_4$							27.0

Table B.5.a. (contd.)

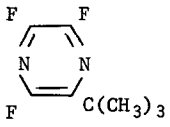
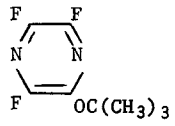
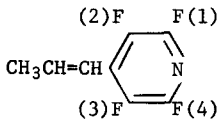
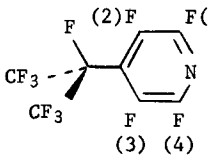
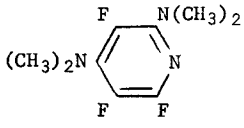
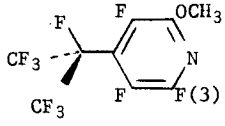
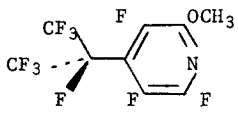
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
941	4648	R	$C_8F_3H_9N_2$			20.7		6.9		43.9
941	4649	R	$C_8F_3H_9N_2O$			16.1		12.0		50.1
942	4650		$C_8F_4H_5N$		1,2	20.9	1,4 2,3	14.4 1.0	1,3	29.5
				(Most abundant isomer)						
949 933	4651 (3388)	B-E	$C_8F_{11}N$		1,2 3,4	-21.0 -22.0	1,4 2,3	14.0 8	1,3 2,4	+29.0 +30.2
				(-40^{o})						
942	4652 (2192)	G	$C_9F_3H_{12}N_3$			25.6		1		25.6
949 933	4653 [3071 3072 3389]	B	$C_9F_{10}H_3NO$			-23.0		-10		+29.5
						-22.0		-10		+28.5
				(-40^{o})						

Table B.5.a. (contd.)

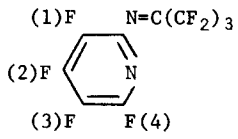
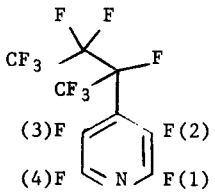
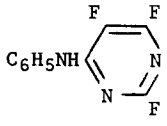
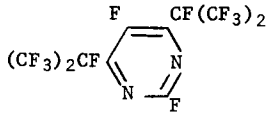
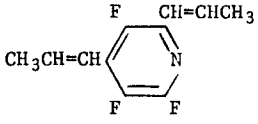
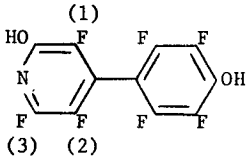
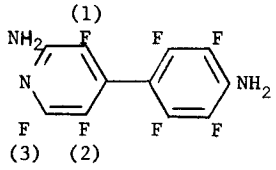
Ref. No.	Serial No.	Solvent	Structure		J_{ortho}		J_{meta}		J_{para}
943	4654	B-G	$C_9F_{10}N_2$ 	1,2	17.8	2,4	18.8	1,4	26.4
				2,3	17.8				
				3,4	24.3				
933	4655 (3390)	P	$C_9F_{13}N$ 	1,2	-19.5	1,4	6	1,3	+31.0
				3,4	-20.5	2,3	14.0	2,4	+29.5
228	4656 (2501)	E	$C_{10}F_3H_6N_3$ 		16.9		2.8		26.6
945	4657 [3105 3393]		$C_{10}F_{16}N_2$ 						32.0
942	4658		$C_{11}F_3H_{10}N$ 						
			Most abundant isomer		27.8		1		30.2
			Intermediate abundant isomer		27.2		1		29.9
			Least abundant isomer		28.1		1		30.8
897	4659 (4271)	E	$C_{11}F_7H_2NO_2$ 	2,3	22.9	1,2	4.7	1,3	29.5
897	4660 (2502)	E	$C_{11}F_7H_4N_3$ 	2,3	24.6	1,2	6.4	1,3	30.4

Table B.5.a. (contd.)

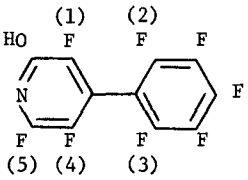
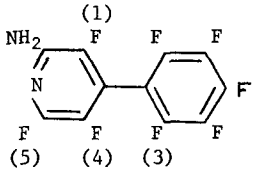
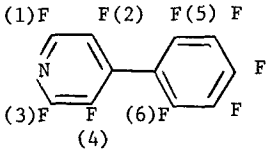
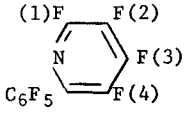
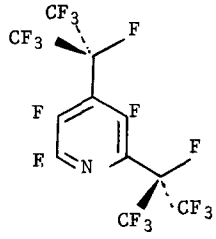
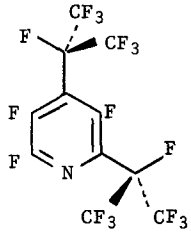
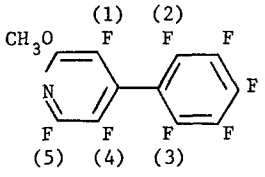
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
897	4661	E	$C_{11}F_8HNO$		4,5	22.7	1,4	5.8	1,5	30.2
	(4441)						1,2/3	9.1	4,2/3	8.8
897	4662	E	$C_{11}F_8H_2N_2$		4,5	24.3	1,4	8.4	1,5	30.9
	(4442)						1,2/3	8.5	4,2/3	8.3
897	4663	E	$C_{11}F_9N$		1,2	20.4	1,3	14.4	1,4	29.0
	(4443)						2,4	1.3		
						*	2,4/5,6	9.9		
943	4664	G	$C_{11}F_9N$		1,2	25.4	1,3	17.8	1,4	24.9
					2,3	17.4	2,4	4.7		
					3,4	17.2				
949	4665	B-E	$C_{11}F_{17}N$			25		0		30
	[3117 3396]									
						24		0		29
				(-40°)						
897	4666	E	$C_{12}F_8H_3NO$		4,5	21.7	1,4	4.9	1,5	30.2
	(4447)						1,2/3	8.9	4,2/3	8.6

Table B.5.a. (contd.)

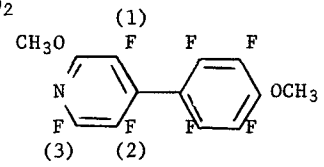
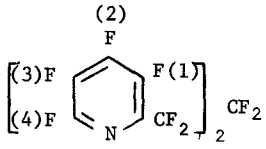
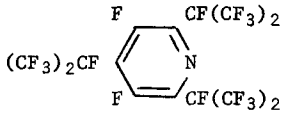
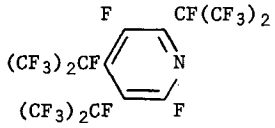
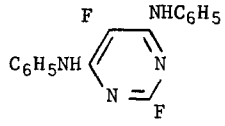
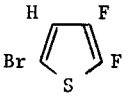
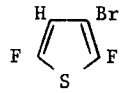
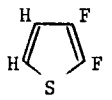
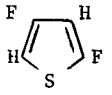
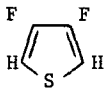
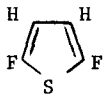
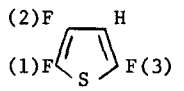
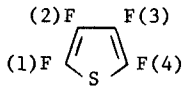
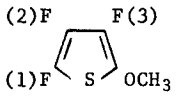
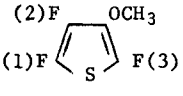
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		J_{ortho}		J_{meta}		J_{para}
897	4667 [2110 4291]	E	$C_{13}F_7H_6NO_2$		2,3	21.9	1,2	4.4	1,3	30.0
943	4668	G	$C_{13}F_{14}N_2$		1,2 2,3 3,4	18.2 18.2 24.2	2,4	18.6	1,4	27.4
949	4669 [3152 3399]	E	$C_{14}F_{23}N$					10		
949	4670 [3151 3398]	P	$C_{14}F_{23}N$							32
228	4671	E	$C_{16}F_2H_{12}N_4$							28.2

Table B.5.b. Heterocycles containing sulphur.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^4J		^5J	^nJ
473	4672 (2167)	B-D	C_4F_2HBrS			3.46		
473	4673 (2168)	B-D H	C_4F_2HBrS				25.06 25.09	
473	4674 (2169)	D H	$C_4F_2H_2S$				0.22 0.77	
473	4675 (2170)	B-D B-H	$C_4F_2H_2S$				9.28 9.23	
473	4676 (2172)	D H	$C_4F_2H_2S$			-12.88 -13.19		
473	4677 (2171)	H	$C_4F_2H_2S$				22.91	
473	4678 (2173)	B G	C_4F_3HS		1,2 1,2	4.78 4.85	1,3 2,3 1,3 2,3	27.70 15.22 27.76 15.26
229	4679		C_4F_4S		1,2 2,3	7 7	1,3 1,4	17 31
229	4680 (2194)		$C_5F_3H_3OS$		1,2 2,3	5.4 10.0	1,3	17.8
229	4681 (2195)		$C_5F_3H_3OS$		1,2	5.4	1,3 2,3	30.6 15.4

B.6. Fluorine bonded to elements other than carbon.

Table B.6.a. One fluorine bonded to carbon, the other bonded to nitrogen.

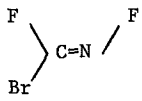
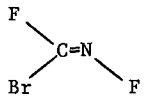
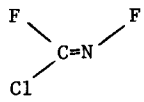
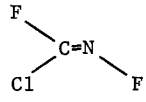
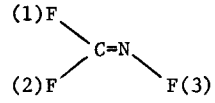
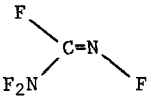
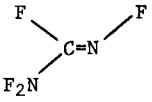
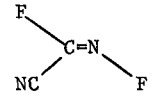
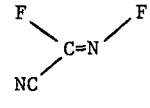
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
958	4682		CF_2BrN		17.6		
958	4683		CF_2BrN		21.8		
958	4684		CF_2ClN		10.6		
958	4685		CF_2ClN		20.9		
920	4686	B	CF_2Cl_3N	$FCCl_2NFCl$	28		
920	4687 (2583)	B	CF_3Cl_2N	$ClCF_2NFCl$	24 13		
958	4688 (3402)		CF_3N		1,3 184 2,3 22.1		
959	4689		CF_4N_2	 or 	12		
645	4690 (5590)		CF_5NO	CF_3ONF_2			3.2
499	4691		$C_2F_2N_2$		265		
499	4692		$C_2F_2N_2$		52		
993	4693		$C_2F_3Cl_2N$	$CFCl_2CF{=}NF$	31.9		
569	4694		$C_2F_5H_2N_3$	$F_2NCF_2\underset{\underset{NF}{\|}}{C}NH_2$			4.3

Table B.6.a. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J	^nJ
913	4695		C_2F_5NO	$CF_3C(O)NF_2$				7.9	
960	4696		$C_2F_5N_3$	$F_2NCF_2NFC{\equiv}N$ (1)(2)	1,2	22.8			
959	4697		$C_2F_7N_3O$	$(F_2N)_2CF\text{-}NFCF(O)$ (2)(1)	1,2	60			
960	4698		$C_2F_8N_4$	$F_2NC(=NF)NFCF_2NF_2$ (2)(1)	1,2	22.8			
971	4699		$C_2F_{10}NS$	$CF_3CF_2NFSF_5$				10	
64	4700 (2213 148)		$C_3F_2H_2N_2$	CH_2FCCN ‖ N, N–F				10	
64	4701 (2214 149)		$C_3F_2H_2N_2$	CH_2FCCN ‖ N, N–F				6.0	
485	4702 (2218)		$C_3F_2H_5NO$	CH_3CH_2NFCFO		44			
64	4703 (202 2223)		$C_3F_4H_4N_2$	$CH_2FCCH_2NF_2$ ‖ N, N–F				10	
64	4704 (203 2293)		$C_3F_4H_4N_2$	$CH_2FCCH_2NF_2$ ‖ N, N–F				2.4	
569	4705		$C_3F_5N_3$	F_2NCF_2CCN ‖ NF				6.3	
993	4706		$C_3F_6N_2$	$FN{=}CFCF_2CF{=}NF$		38.5			
569	4707 (2748)		C_3F_7N	(1)CF_3, F(3), C=N, (2)CF_3			1,3 2,3	26.5 9.7	
913	4708 (2750)		C_3F_7NO	$CF_3CF_2C(O)NF_2$				9.6	2
64	4708a (256 2751)		$C_3F_7HN_2$	$CF_3C(=NF)CHFNF_2$ (1) (2)			1,2	25	
920	4709 (2760)	B	C_3F_8ClN	$(CF_3)_2CFNFCl$ (1,2) (3)			1,3 2,3	24.1 9.7	
569	4710		$C_3F_8N_2$	(1)$CF_3CCF_2NF_2$ ‖ N(3), F(2)			1,2 2,3	28.6 9.6	
				$CF_3CCF_2NF_2$ ‖ N(1), (2)F			1,2	9.6	

Table B.6.a. (contd.)

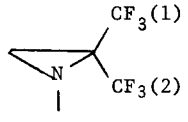
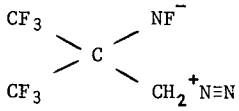
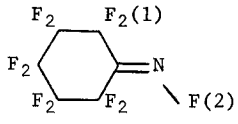
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J	^nJ
907	4711 (2770)		C_3F_9N	$CF_3CF_2CF_2NF_2$	≤1		10.5	2.2
485	4712 (2232)		$C_4F_2H_7NO$	$CH_3CH_2CH_2NFCF(O)$	44			
64	4713		$C_4F_4N_4$	$CF(NF_2)(CN)C(CN)=NF$	14			
569	4714		$C_4F_4H_6N_2$	$CF_3C(=NF)NHCH_2CH_3$			5.6	
569	4715		$C_4F_5H_5N_2O$	$F_2NCF_2C(=NF(2))OCH_2CH_3$ (1)		1,2	4.8	
569	4716 (2522)		$C_4F_7HN_2$	$(CF_3)_2C(CN)NHF$			10.5	
114	4717 [311 2867 2241]	K	$C_4F_7H_2N$			1,3 2,3	<6 46	
569	4718		$C_4F_7H_2N_3$				11.3	
993	4719		C_4F_9N	$CF_3(CF_2)_2CF=NF$	36.3			
569	4720 (3654)		C_4F_9NO	$(CF_3)_2C(NF_2)CF(O)$ (1) (2)		1,2	12.9	
961	4721		$C_4F_9O_4S$	$(CF_3)_2C(NF_2)C(O)OSO_2F$			16	
913	4722		$C_4F_{10}N_2O_2$	$CF_3CO_2C(NF_2)_2CF_3$			10.9	
485	4723 (2246)		$C_5F_2H_9NO$	$CH_3(CH_2)_3NFCF(O)$	56			
569	4724 (2524)		$C_5F_4H_6N_2O$	$CF_3C(CN)(NFH)OCH_2CH_3$			12.2	
569	4725 (2525)		$C_5F_7H_6NO$	$(CF_3)_2C(NHF)OCH_2CH_3$			11.6	
993	4726		$C_6F_{11}N$			1,2	57	
985	4727 (4908)		$C_7F_3H_5ClN$	$C_6H_5CClFNF_2$	8			
495	4728 (4916)	B	$C_8F_5H_5Cl_2N_2$	$C_6H_5CF(NF_2)CCl_2NF_2$	12			
64	4729 (4919)		$C_9F_5H_5N_2O$	$C_6H_5CF(NF_2)C(=NF)CFO$ (2)(1)	1,2	30		
234	4730 (2265)		$C_{10}F_3H_{12}N$	$C_6H_5CF_2NFCH(CH_3)_2$ (1,2)(3)	1,3 2,3	8 8		
234	4731		$C_{11}F_3H_{14}N$	$C_6H_5CF_2NFC(CH_3)_3$		23		

Table B.6.a. (contd.)

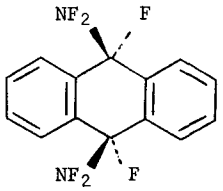
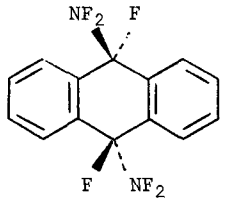
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J	^nJ
234	4732		$C_{11}F_3H_{14}N$	$C_6H_5CF_2NFCH(CH_3)CH_2CH_3$				
	(2266 3107)			(1,2)(3)	1,3	19		
					2,3	<1		
234	4733		$C_{11}F_3H_{14}N$	$C_6H_5CF_2NFCH_2CH(CH_3)_2$	1,3	13		
	(2267)			(1,2)(3)	2,3	13		
234	4734		$C_{12}F_3H_{16}N$	$C_6H_5CF_2NFCH(CH_3)CH_2CH_2CH_3$				
	(2268 3120)			(1,2)(3)	1,3	18		
					2,3	<1		
497	4735		$C_{14}F_6H_8N_2$			7		
497	4736		$C_{14}F_6H_8N_2$			15		
234	4737		$C_{15}F_3H_{14}N$	$C_6H_5CF_2NFCH(CH_3)C_6H_5$	1,3	20		
	(2275)			(1,2)(3)	2,3	10		

Table B.6.b. One fluorine bonded to carbon, the other bonded to oxygen.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
1079	4738	B	CF_2O_2	FC(O)OF	141		
863	4739		CF_4O	CF_3OF	33.8		
1035	4740		CF_4O	CF_3OF	33.2		
1080	4741		CF_4O_2	$FOCF_2OF$	39.0		
1081	4742		CF_4O_2	$FOCF_2OF$	38.6		
863	4743		$C_2F_3Cl_3O$	$FOCF_2CCl_3$	2.2		
863	4744		$C_2F_4Cl_2O$	$FOCF_2CFCl_2$	3.8	3.8	
863	4745		C_2F_5ClO	$FOCF_2CF_2Cl$	5.6	6.2	
863	4746		$C_2F_5NO_3$	$FOCF_2CF_2NO_2$	11.3	5.8	
	(2648)						
863	4747		C_2F_6O	$FOCF_2CF_3$	8.5	8.5	
	(2660)						

Table B.6.b. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
868	4748 (2663)		$C_2F_6O_2$	$CF_3CF(OF)_2$	26.2	10.3	
869	4749 (2664)	P	$C_2F_6O_3$	CF_3OOCF_2OF	35.1		1.4
863	4750 (2762)		C_3F_8O	$FOCF(CF_3)_2$	23.1	16.8	
868	4751		$C_3F_8O_2$	$(FO)_2C(CF_3)_2$		14.5	
952	4752 (2765)		$C_3F_8O_3$	$CF_3OOCF(OF)CF_3$	37.0	12.5	1.7
869	4753 (2767)	P	$C_3F_8O_5$	$FOCF(OOCF_3)_2$	25		<3
863	4754		$C_4F_{10}O$	$FOC(CF_3)_3$		15.5	
961	4755 (2834)		$C_4F_{10}O$	$(CF_3)_2CFCF_2OF$	~3		

Table B.6.c. One fluorine bonded to carbon, the other bonded to phosphorus.

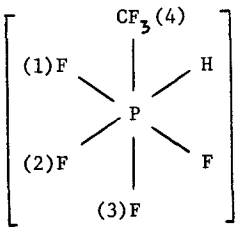
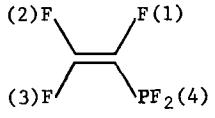
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J	^nJ
962	4756 (5799)	B	CF_5OP	$CF_3P(O)F_2$		11		
712	4757 (5300, 5801)		CF_5P	CF_3PF_2		5.8		
507	4758		CF_7P	CF_3PF_4		12		
562	4759	M	CF_7HKP	trans $K^+[CF_3PF_4H]^-$		15.3		
583	2505, 2552, 4938, 5805			cis $K^+[CF_3PF_4H]^-$	1,4	14		
					2,4	14		
					3,4	4.5		
								
722	4760 (4939, 5307)	M	CF_8CsP	$Cs^+[CF\ PF_5]^-$ (1) (2)	1,2e	12		
227	4761		C_2F_5P		1,4	±11.1	2,4	±13.2
726	(3435, 4701)						3,4	±2.9

Table B.6.c. (contd.)

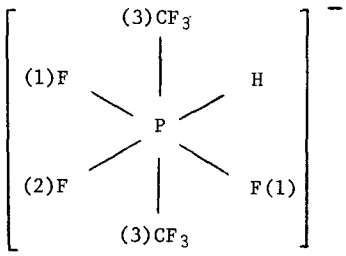
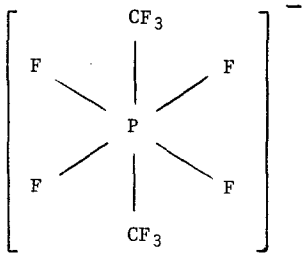
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
729	4762 (5891)	P	C_2F_7OP	$(CF_3)_2P(O)F$	7.8		
712	4763 (2670 5893)		C_2F_7P	$(CF_3)_2PF$	3.5		
736	4764 (5895)		$C_2F_8Cl_2NP$	$(CF_3)_2NPF_2Cl_2$		14.1	
736	4765 (5896)		C_2F_8NOP	$(CF_3)_2NP(O)F_2$		8.6	
736	4766 (5897)		C_2F_9ClNP	$(CF_3)_2NPF_3Cl$		10.8	
562	4767 (2509 2556 4950 5899)		C_2F_9HKP	$K^+[(CF_3)_2PF_3H]^-$			
					1,3 2,3	12.5 15.5	
737 578	4768 (5901)	M*	$C_2F_{10}SP$	$Cs^+[(CF_3)_2PF_4]^-$	14.3		
							
75	4769 (2333 5933)		$C_3F_4H_6NP$	$CF_3PFN(CH_3)_2$	2.3		
76	4770 (206)	P	$C_3F_4H_6NPS$	$CF_3PF(S)N(CH_3)_2$	5.8		
745	4771 (5958)	B	C_3F_8BrOP	$(CF_3)_2C(OPF_2)Br$			1.6
745	4772 (5959)	B	C_3F_8IOP	$(CF_3)_2C(OPF_2)I$			0.9
755	4773 (6030)		$C_4F_6CoO_3P$	$CF_3Co(CO)_3PF_3$ (25^o)		6	

Table B.6.c. (contd.)

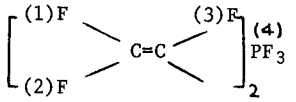
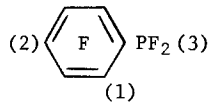
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
	4774			trans $CF_3Co(CO)_3PF_3$				9		
	(6030)			(-70^o)						
	4775			cis $CF_3Co(CO)_3PF_3$				3		
	(6030)			(-70^o)						
763	4776		C_4F_9P		3,4e	0	1,4e	0		
	[3505				3,4a	2.5	1,4a	12		
	6057						2,4e	5		
	4964]						2,4a	58		
				(-60^o)						
766	4777		$C_4F_{13}OP$	$(CF_3)_3COPF_4$						5.3
	(6065)									
777	4778		C_6F_7P				1,3	13.6	2,3	2.1
	(4367									
	6177)									
758	4779		$C_6F_{10}MoO_4P_2$	cis $(CF_3PF_2)_2Mo(CO)_4$		3.0				
	(6178)									
758	4780		$C_8F_{14}MoO_4P_2$	cis $[(CF_3)_2PF]_2Mo(CO)_4$		2				
	(6263)									
766	4781		$C_8F_{22}O_2P$	$[(CF_3)_3CO]_2PF_4$						6.6
	(6265)									
820	4782	J	$C_{25}F_8H_{20}AsP$	$[(C_6H_5)_4As]^+[PF_5CF_3]^-$		13.4				
	(6488)									
820	4783	J	$C_{26}F_{10}H_{20}AsP$	$[(C_6H_5)_4As]^+[PF_4(CF_3)_2]^-$		13.8				
	(6502)									

Table B.6.d. One fluorine bonded to carbon, the other bonded to sulphur.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J	^nJ
963	4784		CF_2Cl_2S	$FCCl_2SF$	4.85		
916	4785		CF_3ClO_3S	$ClCF_2OSO_2F$		7.8	
963	4786		CF_3ClS	$ClCF_2SF$	6.85		
964	4787		CF_3NOS	$FC(O)N{=}SF_2$		4	
				(-80^o)			
49	4788		$CF_4AgNO_4S_2$	$Ag^+(CF_3SO_2NSO_2F)^-$			3.4
965	4789		CF_4ClNO_2S	$CF_3N(Cl)SO_2F$		6.5	
935	4790		CF_4OS	$CF_3S(O)F$	8		

Table B.6.d. (contd.)

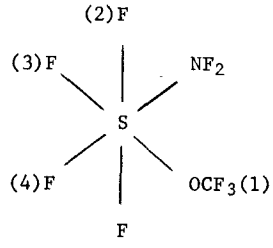
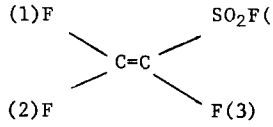
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
966	4791		CF_4O_3S	CF_3OSO_2F				8		
966	4792		$CF_4O_6S_2$	$CF_2(OSO_2F)_2$				8		
966	4793		$CF_4O_9S_3$	$CF(OSO_2F)_3$				8		
963	4794		CF_4S	CF_3SF		27				
559	4795 (2565)		CF_4HNO_2S	CF_3NHSO_2F				6		
49	4796		$CF_4HNO_4S_2$	$CF_3SO_2NHSO_2F$						2.9
967	4798 (5036)		CF_6OS	$FC(O)SF_5$ (1) (AB_4)	1,A 1,B	+7.7 +35.0				
967	4799 (5037)		CF_6O_2S	$FC(O)OSF_5$ (1) (AB_4)			1,A 1,B	+0.4 +9.75		
967	4800 (5038)		CF_6O_3S	$FC(O)OOSF_5$ (1) (AB_4)					1,A 1,B	~0 3
12	4801 (18 5041a)		CF_6H_2S	CFH_2FSF_4 (1) (2)	1,2	10.6				
969	4802		CF_8OS	CF_3OSF_5 (1) (AB_4)			1,A 1,B	1.5 9.9		
969	4803		CF_8S	CF_3SF_5	1,A 1,B	6.4 22.4				
970	4804 (5044 5280)		CF_9NOS				1,2 1,3 1,4	12.8 1 12.8		
968	4805		CF_9NS	trans $CF_3SF_4NF_2$		22				
41	4806 (98)		$C_2F_3H_3O_3S$	$CH_3CF_2SO_3F$				9		
20	4807 (2361)	B	$C_2F_4Br_2O_2S$	$CF_2BrCFBrSO_2F$		2.4		19.4 6.8		
20	4808 (2634)	B	$C_2F_4Cl_2O_2S$	$CF_2ClCFClSO_2F$		0.0		14.9 7.6		
186	4809 (3432)		$C_2F_4O_2S$		3,4	5.1	1,4 2,4	3.7 13.5		

Table B.6.d. (contd.)

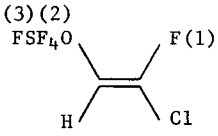
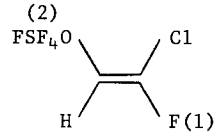
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
20	4810	B	$C_2F_4HBrO_2S$	$CF_2BrCHFSO_2F$	3,4	6.0	1,4	7.6		
	(101 2635)			(1,2) (3) (4)			2,4	10.7		
540	4811	A	$C_2F_4H_2O_3S$	$CF_3CH_2OSO_2F$						2.5
	(109)									
49	4812		$C_2F_4H_3NO_4S_2$	$CF_3SO_2N(CH_3)SO_2F$						2.4
	(110)									
20	4813	B	$C_2F_5HO_2S$	CF_3CHFSO_2F		6.7		9.3		
186	[117 2427 2650]									
865	4814		C_2F_6ClNOS	$ClCF_2CF_2NS(O)F_2$				9.3		1.5
	(2654)									
935	4815		C_2F_6OS	$CF_3CF_2S(O)F$				12		
53	4816		C_2F_6HClOS						1,2	4.5
	(1008 5050)									
187	4817		C_2F_6HClOS						1,2	2.4
	[1007 2430 5051]									
54	4818	B	C_2F_8BrClS	$CF_2BrCFClFSF_4$	3,5	11	1,5	11		
	(2674 5058)			(1,2)(3)(4)(5)	3,4	4.9	2,5	14		
							1,4 2,4	1		
54	4819	B	C_2F_8BrClS	$CF_2ClCFBrFSF_4$	3,5	8	1,5	13		
	(2673 5057)			(1,2) (3)(4)(5)	3,4	4.9	2,5	13		
							1,4 2,4	1		
54	4820	B	$C_2F_8Br_2S$	$CF_2BrCFBrFSF_4$	2,4	9	1,4	13		
	(2675 5059)			(1) (2)(3)(4)	2,3	5	1,3	1.5		
54	4821	B	$C_2F_8Cl_2S$	$CF_2ClCFClFSF_4$	3,5	11.0	1,5	12.1		
	(2676 5060)			(1,2)(3)(4)(5)	3,4	5.2	2,5			
							1,4	1.0		
							2,4	1.0		
54	4822	B	$C_2F_8Cl_2S$	$CFCl_2CF_2FSF_4$	2,4	15.7	1,4	7.6		
	(2677 5061)			(1)(2)(3)(4)	2,3	5.5				
971	4823		$C_2F_8N_2S$	$CF_3N{=}SF_2{=}NCF_3$				8		

Table B.6.d. (contd.)

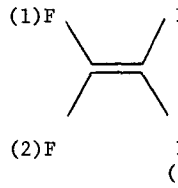
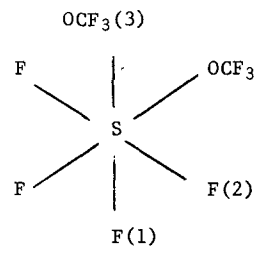
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J	^nJ
972	4824	*	C_2F_8S		3,4	3.0	1,4	±0.9	
	(3436				3,5	6.1	1,5	±11.1	
	5063)						2,4	±1.8	
							2,5	±15.3	
54	4825	B	C_2F_8HBrS	$CF_2BrCFHFSF_4$	3,5	~0.0	1,5	12.2	
	[123			(1,2)(3)(4)(5)	3,4	2.5	2,5	11.5	
	2678						1,4	0.9	
	5068]						2,4	1.5	
187	4826		C_2F_8HClOS	$CF_2ClCFHOFSF_4$			1,2	2.0	
	[124			(1)(2)(3)			1,3	5.0	
	2679								
	5065]								
54	4827	B	C_2F_8HClS	$CF_2ClCFHFSF_4$	3,5	0.0	1,5	11.9	
	[126			(1,2)(3)(4)(5)	3,4	2.4	2,5	11.6	
	2680						1,4	1.1	
	5066]						2,4	1.6	
54	4828	B	C_2F_8HClS	$CFHClCF_2FSF_4$	2,5	15.0	1,5	11.2	
	[125			(1) (2,3)(4)(5)	3,5	15.2	1,4	1.3	
	2681				2,4	4.9			
	5067]				3,4	5.0			
970	4829		$C_2F_{10}O_2S$				1,3	7	
	(5069)						2,3	9	
870	4830		$C_2F_{10}S$	$CF_3CF_2FSF_4$	2,4	14.36	1,3	4.82	
	(2683			(1)(2)(3)(4)			1,4	8.56	
	5070)								

Table B.6.d. (contd.)

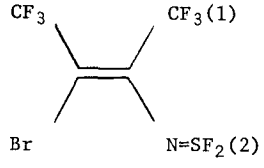
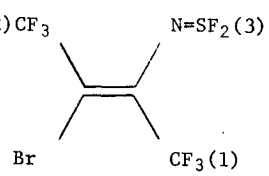
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
974	4831		$C_2F_{11}NS$	$FSF_4N(CF_3)_2$			1,3	16.8		
	(5071)			(2)(1) (3)			2,3	2.1		
870	4832		$C_2F_{14}S_2$	$CF_3SF_4CF_2SF_5$	1,3	22.92			1,A	5.28
	(5072)				2,3	21.42				
					2,B	21.42				
20	4833	B	$C_3F_4H_4O_3S$	$CH_3OCF_2CHFSO_2F$		5.6		9.1		
186	[204							9.8		
	2695									
	2431]									
916	4834		$C_3F_6O_7S$	$FO_2SOCF_2CF_2C(O)OSO_2F$			1,2	8.1		
	(2728)			(1) (2)						
935	4835		C_3F_8OS	$(CF_3)_2CFS(O)F$		5		9.2		
	(2764)									
925	4836		C_3F_8S	$(CF_3)_2CFSF$		22		10		
	(2768)									
54	4837	R	$C_3F_8H_4OS$	$CH_3OCF_2CFHFSF_4$	3,5	∿0.0	1,5	9.6		
	[257			(1,2)(3)(4)(5)	3,4	2.3	2,5	10.6		
	2769						1,4	∿1.1		
	2433						2,5	∿0.5		
	5074]									
925	4838		$C_3F_{10}S$	$(CF_3)_2CFSF_2F$	1,4	0.4	2,4	0.7		
	(2778)			(2) (1)(3)(4)	1,3	2.8	2,3	1		
54	4839	P	$C_3F_{11}IS$	$CF_3CF_2CFIFSF_4$			1,3	12		
	(5075)			(1,2) (3)			2,3	19		
870	4840		$C_3F_{12}S$	$CF_3SF_4CF_2CF_3$	1,4	24.00	3,4	9.40		
				(1)(4)(2)(3)	2,4	15.10				
925	4841		$C_4F_5H_7S$	$(CH_3)_2CHSF_2CF_3$		12				
975	4842		C_4F_8BrNS						1,2	6
975	4843		C_4F_8BrNS						1,3	6.4
	(2811)								2,3	6.4
975	4844		$C_4F_8Br_3NS$	$CF_3CBr_2CBr(CF_3)NSF_2$			1,2	9.7		
	(2812)									

Table B.6.d. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J		^4J		^nJ
961	4845		$C_4F_8O_4S$	$(CF_3)_2C(OSO_2F)CF(O)$					1,2	3.2
	(3652)			(1) (2) (3)					3,2	5.4
961	4846		$C_4F_8O_7S_2$	$(CF_3)_2C(OSO_2F)(C(O)OSO_2F$					1,2	3.6
				(1) (2)						
870	4847		$C_4F_9H_3O_2S$	$CF_3SF_4CF_2CO_2CH_3$	1,3	23.50				
				(1) (3) (2)	2,3	13.60				
971	4848		$C_4F_{12}N_2S$	$CF_3CF_2N{=}SF_2{=}NCF_2CF_3$				8		
925	4849		$C_4F_{12}S$	$(CF_3)_2CFSF_2CF_3$	1,3	19				
	(2845)			(2) (3) (1)	2,3	28				
870	4850		$C_4F_{14}S$	$(CF_3CF_2)_2SF_4$		15.70		9.33		
	(2847)									
870	4851		$C_4F_{14}S$	$CF_3CF_2CF_2CF_2SF_5$	1,A	2.47	2,B	∿8.9	3,A	4.93
	2846			(3) (2) (1) (AB_4)	1,B	17.0				
	5079									
925	4852		$C_6F_{16}S$	$[(CF_3)_2CF]_2SF_2$		4.0		10		
	(2950)									

Table B.6.e. One fluorine bonded to carbon, the other bonded to silicon

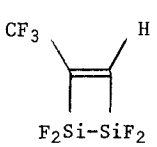
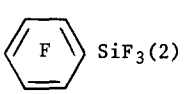
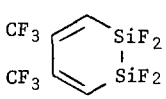
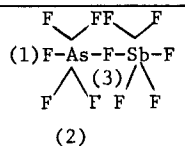
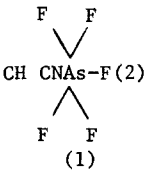
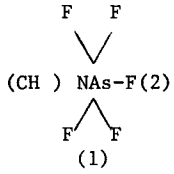
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J		^4J		^nJ
14	4853	B	$C_2F_6H_2Si$	$CFH_2CF_2SiF_3$	5.8		5.5		
	[122 2460 2669]								
14	4854	B	C_2F_7HSi	$CF_2HCF_2SiF_3$	4.9		2.5		
	[122a 2461 6696 2672]								
203	4855		C_3F_7HSi				2.4		0.8
	(785 2469)								
926	4856		C_6F_8Si			1,2	10.3		
	(4368 6718)								
203	4857		$C_6F_{10}H_2Si_2$						0.6
	(836)								

Table B.6.f. Both fluorines bonded to the same element, M (other than carbon).

i) M = arsenic (As).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J
976	4858 (5093)	J	$F_{11}AsSb$	 (1)F-As-F-Sb-F (3) F F F F (2)	1,2 2,3	126 47
728	4859		$C_2F_5H_3AsN$	 CH CNAs-F(2) F F (1)	1,2	115
474	4860 (5292)		$C_3F_5H_9AsN$	 (CH) NAs-F(2) F F (1)	1,2	120
530	4861		$C_{12}F_3H_{10}As$	$(C_6H_5)_2AsF_2F$		67
977	4862	R^4	$C_{16}F_{11}H_{36}As_2N$	$CH_3(CH_2)_3{}_4N^+As_2F_{11}^-$ (-140°)	1,2 2,3 1,3	127 51 ∿0

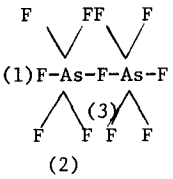


Table B.6.f. (contd.)

ii) M = boron (B).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J
978	4863		$C_4F_2H_9B$	$(CH_3)_2CHCH_2BF_2$	∿88

iii) M = chlorine (Cl).

980	4864	B	F_3Cl	ClF_3 (gas)	441
				(liquid -63^o)	422.2
		G		(-30^o)	420
		P			426.3
981	4865	B	F_3Cl	ClF_3 (gas)	403
982	4866	B-P	F_5Cl	ClF_5	130

iv) M = germanium (Ge).

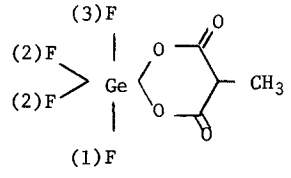
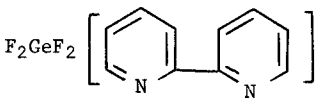
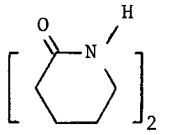
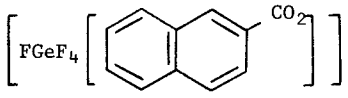
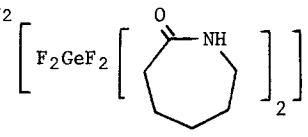
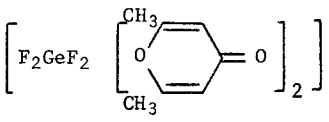
853	4867	E^2	$CF_5H_3GeO^{2-}$	$[FGeF_4(OCH_3)]^{2-}$	35.2
853	4868	E^2	$C_2F_4GeO_4^{2-}$	$[F_2GeF_2(O_2CCO_2)]^{2-}$	49.2
853	4869	A	$C_2F_5H_3GeO_2^{2-}$	$[FGeF_4(O_2CCH_3)]^{2-}$	45
853	4870	J^2	$C_2F_5H_5GeO^{2-}$	$[FGeF_4(OCH_2CH_3)]^{2-}$	36.3
853	4871	E^2	$C_3F_4H_2GeO_4^{2-}$	$[F_2GeF_2(O_2CCH_2CO_2)]^{2-}$	46.7
853	4872	A	$C_3F_5H_5GeO_2^{2-}$	$[FGeF_4(O_2CCH_2CH_3)]^{2-}$	46
853	4873	E^2	$C_4F_4H_4GeO_4^{2-}$		
				1,2	44.0
				1,3	<3
				2,3	48.9
983	4874	S^4	$C_4F_4H_{12}GeN_2$	$[F_2GeF_2NH_2(CH_2)_4NH_2]$	57.6
853	4875	A	$C_4F_5H_7GeO_2^{2-}$	$[FGeF_4(O_2CCH(CH_3)_2)]^{2-}$	46
853	4876	E^2	$C_5F_4H_6GeO_4^{2-}$	$[F_2GeF_2(O_2CC(CH_3)_2CO_2)]^{2-}$	44.5
853	4877	A	$C_5F_5H_9GeO_2^{2-}$	$[FGeF_4(O_2CC(CH_3)_3)]^{2-}$	45
853	4878	A	$C_7F_5H_4GeNO_4^{2-}$	$[FGeF_4(pNO_2C_6H_4CO_2)]^{2-}$	47
853	4879	A	$C_7F_5H_5GeO_2^{2-}$	$[FGeF_4(C_6H_5CO_2^-)]^{2-}$	48

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J
983 G	4880	S^4	$C_{10}F_4H_8GeN_2$		54
983	4881	S^4	$C_{10}F_4H_{18}GeN_2O_2$	 (-4.5° to -15.5°)	61
983	4882	S^4	$C_{10}F_4H_{24}GeN_2O_2$	$F_2GeF_2[CO(N(CH_3)_2)_2]_2$ (-59°)	62.3
853	4883		$C_{11}F_5H_7GeO_2^{2-}$		45
983	4884		$C_{12}F_4H_{22}GeN_2O_2$		61.9
983	4885		$C_{14}F_4H_{16}GeO_4$		63.5

v) M = iodine (I)

981	4886	F_5I	IF_5	81
872	4887	F_5I	IF_5	85.0
812	4888	F_5IO	IOF_5	280

vi) M = nitrogen (N)

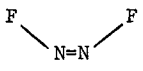
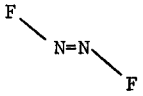
638	4889	F_2N_2		99
	5582			
	5583			322

Table B.6.f. (contd.)

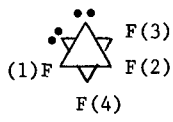
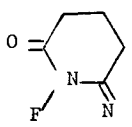
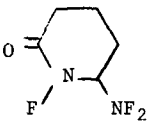
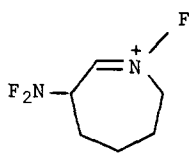
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
986 987	4890	*	F_4N_2		1,2	±489.6	1,4 ∓13.4 1,3 ∓ 8.8 ±109.0	
480	4891 (2206)	A	$C_2F_2H_5NO$	$CH_3CH(OH)NF_2$		570		
495	4892	B	$C_2F_4Br_3N$	$F_2NCFBrCBr_2N{=}F$		446		
487	4893 (2224)	B	$C_3F_4H_6N_2$	$F_2NCH_2CH(NF_2)CH_3$ (1,2) (3,4) (-86^o)	1,2 3,4	589 600		
479	4894 (2225)		$C_3F_4H_6N_2O$	$F_2NCH_2CH_2CH(OH)NF_2$ (1,2)	1,2	602		
64	4895		$C_3F_7N_2$	$CF_3C(=NF)CHFNF_2$		600		
984	4896	G	$C_4F_3H_6BrN_2$	$CH_3CBr(NF_2)C(CH_3){=}NF$		568		
984	4897	G	$C_4F_3H_6ClN_2$	$CH_3CCl(NF_2)C(CH_3){=}NF$		580		
492	4898 (2235)		$C_4F_3H_8N_3O$	$CH_3CHCH(NF_2)CH_3$ O→N=NF		595		
493	4899	P	$C_4F_4H_4N_2$	$CH_3C(NF_2)_2C{\equiv}CH$		615		
487	4900 (2239)	B	$C_4F_4H_8N_2$	$NF_2CH_2CH(NF_2)CH_2CH_3$ (1,2) (3,4) (-78^o)	1,2 3,4	591 578		
487	4901 (2238)	K	$C_4F_4H_8N_2$	$CH_3CH(NF_2)CH(NF_2)CH_3$		595		
351	4902		$C_5F_2H_6N_2O$					96
351	4903 (2247)		$C_5F_3H_7N_2O$					~25
479	4904 (2248)		$C_5F_4H_8N_2O_2$	$CH_3C(NF_2)_2CO_2CH_2CH_3$		630		
487	4905 (2249)	K	$C_5F_4H_{10}N_2$	$CH_3CH(NF_2)C(CH_3)_2NF_2$	1,2 3,4	570 566		
494	4906 (2255)	Z[2]	$C_6F_3H_{10}N_2^+$			611		
984	4907	G	$C_6F_4H_8ClN_3$	$CCl(NF_2)_2(CH_2)_4CN$		605		

Table B.6.f. (contd.)

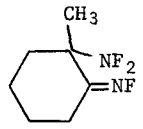
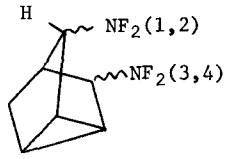
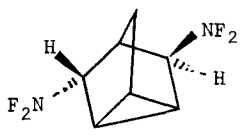
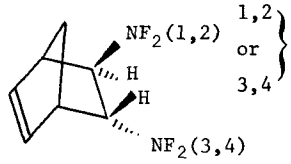
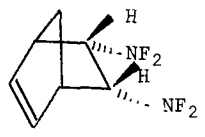
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
985	4908 (4727)		$C_7F_3H_5ClN$	$C_6H_5CFCl(NF_2)$		588	
984	4909	G	$C_7F_3H_{11}N$			582	
495	4910 (2263)	B	$C_7F_4H_8N_2$		1,2 or 3,4	580	
495	4911 (2260)	B	$C_7F_4H_8N_2$			585	
495	4912 (2261)	B	$C_7F_4H_8N_2$			585 590	
495	4913 (2262)	B	$C_7F_4H_8N_2$		1,2 or 3,4	595	
495	4914 (2264)	B	$C_7F_4H_8N_2$			590	
495	4915	B	$C_8F_4H_5ClN_2$	$C_6H_5CF(NF_2)CCl{=}NF$		514	
495	4916 (4728)	B	$C_8F_5H_5Cl_2N_2$	$C_6H_5CF(NF_2)CCl_2NF_2$ (1,2) (3,4)	1,2 3,4	585 580	
984	4917	G	$C_9F_3H_7BrClN_2$	p $BrC_6H_4C(Cl)NF_2CCH_3{=}NF$		563	
64	4918		$C_9F_4H_8N_2$	$C_6H_5CF(NF_2)C(CH_3){=}NF$		572	
64	4919 (4729)		$C_9F_5H_5N_2O$	$C_6H_5CF(NF_2)C(=NF)CF(O)$ (1)(2) (4)(3)	1,2	596	
984	4920		$C_{10}F_3H_{11}N_2$	$C_6H_5C(CH_3)NF_2CCH_3{=}NF$		580	
64	4921		$C_{14}F_4H_{10}N_2$	$C_6H_5CF(NF_2)C(C_6H_5){=}NF$		575	
498	4922 (2274)		$C_{14}F_4H_{12}N_2$	$[C_6H_5CH(NF_2)]_2$ (d1)		587	

Table B.6.f. (contd.)

vii) M = phosphorus (P).

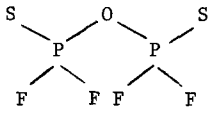
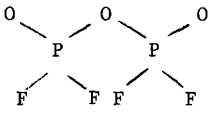
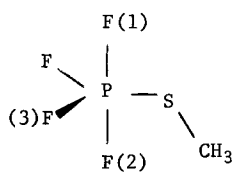
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
990	4923 (5666)		F_3Br_2P	Br_2PF_3 (<-120°)	124		
530 990	4924 (5670)		F_3Cl_2P	Cl_2PF_3 (-130°)	142		
575	4925 (2535 5689)	M	$F_3H_4N_2P$	$F_3P(NH_2)_2$	40		
671	4926 (5690)		F_4ClNP_2S	S=PFClN=PF_3 (1) (2)			1,2 5.5
693	4927 (5697)	*	$F_4OP_2S_2$		300		2.3 3.7
693	4928 (5700)	*	$F_4O_3P_2$		300		2.4
671	4929 (5704)	*	F_4P_2		1,2 300 1,3 0 2,3 34.4		
694	4930 (5706)	P	$F_4P_2S_2$	$F_2P(S)SPF_2$ (-90°)			5.9
697	4931 (5711)		F_5NP_2	$F_3P{=}N{-}PF_2$			7
562 577 578	4932	M	F_5HKP	$K^+(FPF_4H)^-$ (1)(2)	1,2 -41		
506	4933 (2291 5791)	B	CF_3H_4P	CH_3PF_3H	19		
715	4934 (5795)		$CF_4H_3NP_2$	$F_2PN(CH_3)PF_2$ (1,2) (3)			1,3 11.7 2,3 1.7
716 717	4935 (5797)		CF_4H_3PS	 (-100°)	1,2 19 1,3 104 2,3 91		

Table B.6.f. (contd.)

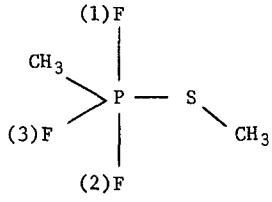
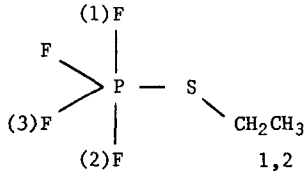
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
511	4936 (2295 5802)		$CF_5H_3P^-$	$(CH_3FPF_4)^-$		∿39		
523	4937 (2551 5803)	A	$CF_5H_5P_2$	$CH_3PH_2PF_4F$ (-75°)		-59		
562	4938 [2505 5805 4759 2552]	M	CF_7HKP	cis $K^+[CF_3PF_4H]^-$	1,2 1,3 2,3	∿28 ∿43 ∿40		
722	4939 (4760 5307)	M	CF_8PCs	$Cs^+[CF_3PF_4F]^-$		52		
507 510	4940 (2315 5835)	P	$C_2F_3H_6P$	$(CH_3)_2PF_2F$		-28.1		
506	4941 (2371 5854)	B	$C_2F_3H_6P$	$CH_3CH_2PF_2FH$		22.7		
717	4942 (5855)		$C_2F_3H_6PS$		1,3 2,3	50 65		
715	4943 (5859)		$C_2F_4H_5NP_2$	$F_2PN(CH_2CH_3)PF_2$ (1,2) (3)			1,3 2,3	11.1 2.2
716	4944 (5861)	T[2]	$C_2F_4H_5PS$		1,2 1,3 2,3	20 88 103		

Table B.6.f. (contd.)

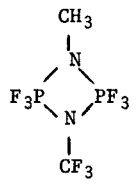
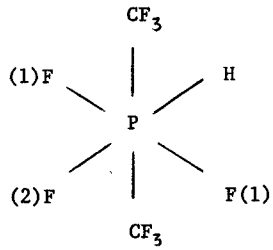
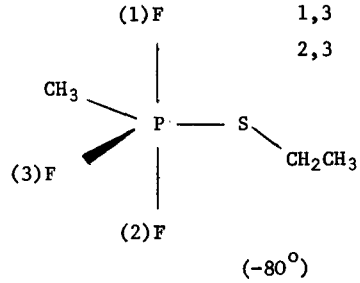
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
522	4945 (2321 5867)	M	$C_2F_5H_6CsNP$	$Cs^+[FPF_4N(CH_3)_2]^-$	35.5		
474	4946 (5866)	J	$C_2F_5H_6OP$	$F_4PFO(CH_3)_2$	5		
521	4947 (5868)		$C_2F_5H_7NP$	$F_4PFN(CH_3)_2H$	50		
523	4948 [2322 5869 2555]	J	$C_2F_5H_7P_2$	$F_4PFP(CH_3)_2H$ (-10°)	-53.2		
733	4949 (5888)		$C_2F_6H_6N_2P_2$				8.7
562	4950 [2509 2556 5899 4767]	M	C_2F_9HKP	$K^+[(CF_3)_2PF_3H]^-$	1,2 25.0		
							
725	4951 (5926)		$C_3F_3H_8OP$	$CH_3PF_3OCH_2CH_3$	62		
717	4952 (5927)	T	$C_3F_3H_8PS$	 (-80°)	(1)F 1,3 62 2,3 62		
705	4953		$C_3F_3H_9NP$	$CH_3PF_3N(CH_3)_2$	53		
515	(2332 5929)						
474	4954 (2325 5935)	J	$C_3F_5H_9NP$	$F_4PFN(CH_3)_3$	55		

Table B.6.f. (contd.)

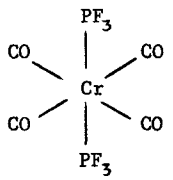
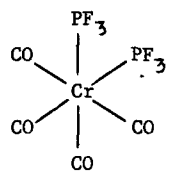
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
523	4955 (2336 5936)	M	$C_3F_5H_9P_2$	$F_4PFP(CH_3)_3$ (-37°)	-51.7		
525	4956 (2337 5937)		$C_3F_5H_{11}NP$	$[(CH_3)_2NH_2][F_4PFCH_3]$	35		
507	4957 (2353 6011)		$C_4F_3H_8P$	$(CH_2)_4PF_3$ (-100°)	50		
725	4958 (6014)		$C_4F_3H_{10}OP$	$CH_3CH_2PF_3OCH_2CH_3$	60		
507	4959 (2354 6015)		$C_4F_3H_{10}P$	$(CH_3CH_2)_2PF_3$	29		
521	4960 (6018)		$C_4F_3H_{12}N_2P$	$F_3P[N(CH_3)_2]_2$	42		
530	4961 (6024)		$C_4F_4H_{10}NP$	$F_4PN(CH_2CH_3)_2$ (-85°)	70		
521	4962 (6028)		$C_4F_5H_{11}NP$	$PF_5.N(CH_2CH_3)_2H$	50		
756	4963 (6031)		$C_4F_6CrO_4P_2$				2.6
							~0
763	4964 [3505 4776 6057]		C_4F_9P	$(CF_2{=}CF)_2PF_2F$ (-60°)	52		
507	4965 (6089)		$C_5F_3H_{10}P$	$(CH_2)_5PF_3$	42		
584	4966 (6096)		$C_5F_3H_{13}NP$	$CH_3PF_3N(CH_2CH_3)_2$	53		
584	4967 (6097)		$C_5F_3H_{13}NP$	$CH_3PF_3NHCH_2CH(CH_3)_2$	58		

Table B.6.f. (contd.)

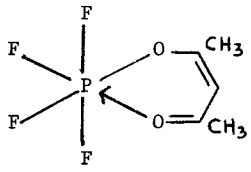
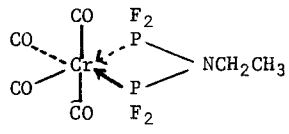
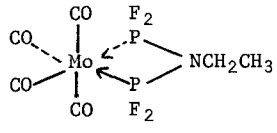
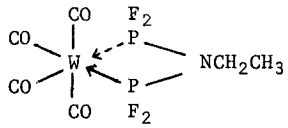
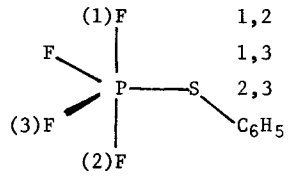
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
769	4968 (6101)		$C_5F_4H_7O_2P$		59.4		
530	4969 (6141)		$C_6F_3H_5ClP$	$C_6H_5PF_3Cl$	80		
530	4970 (2562 6142)		$C_6F_3H_6P$	$C_6H_5PF_3H$	31.5		
530 774	4971 (2369 6144)		$C_6F_3H_{15}NP$	$CH_3CH_2PF_3N(CH_2CH_3)_2$	51		
715	4972 (6149)		$C_6F_4H_4ClNP_2$	$F_2PN(\underline{m}\text{-}ClC_6H_4)PF_2$ (1,2)			1,3 {11.6 2,3 {2.6
775	4973 (6154)	B*	$C_6F_4H_5CrO_4P_2$				{9.5 {0
775	4974 (6155)	B*	$C_6F_4H_5MoO_4P_2$				{7 {0
715	4975 (6156)		$C_6F_4H_5NP_2$	$F_2PN(C_6H_5)PF_2$ (1,2) (3)			1,3 {10.0 2,3 {4.4
775	4976 (6157)	B*	$C_6F_4H_5O_4P_2W$				{5.4 {0
716 717	4977 (6159)		$C_6F_4H_5PS$		1,2 18 1,3 113 2,3 96		

Table B.6.f. (contd.)

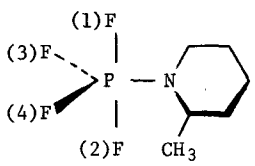
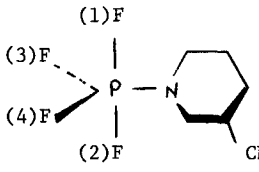
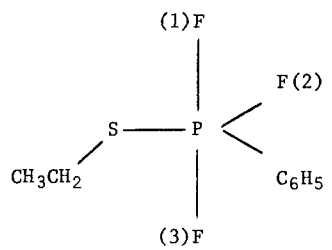
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
776	4978 (6161)	T^2	$C_6F_4H_{12}NP$	 (-100°)	1,3 1,4 3,4	74 67 51		
776	4979 (6162)	T^2	$C_6F_4H_{12}NP$	 (-100°)	1,3 1,4 3,4	77 63 50		
511	4980 (6169)		$C_6F_5H_5P^-$	$(C_6H_5PF_4F)^-$		~41		
510	4981	B-H-	$C_6F_6H_{18}N_2P_2$	$[CH_3PF(N(CH_3)_2)_2][CH_3PF_4F]$		-35.9		
515 525	(2374 6175)	M						
584	4982 (6205)		$C_7F_3H_7ClP$	$CH_3C_6H_4PClF_3$		57		
507	4983 (2382 6206)		$C_7F_3H_8P$	$CH_3(C_6H_5)PF_3$		33		
584	4984 (2563 6207)		$C_7F_3H_8P$	$CH_3C_6H_4PHF_3$		34		
717 789	4985 (6208)		$C_7F_3H_8PS$	$C_6H_5PF_3SCH_3$		60.5		
774	4986 (6209)		$C_7F_3H_9NP$	$C_6H_5PF_3NHCH_3$		52		
789 717	4987 (6242)		$C_8F_3H_{10}PS$	$C_6H_5PF_3SCH_2CH_3$		59.3		
716	4988 (6242)	T^2			1,2 1,3 2,3	62 32 62		

Table B.6.f. (contd.)

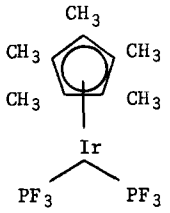
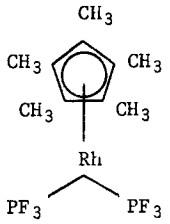
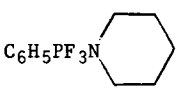
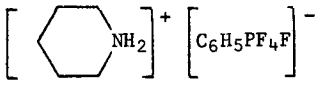
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
530	4989		$C_8F_3H_{11}NP$	$C_6H_5PF_3N(CH_3)_2$	55		
705	(6243)						
774							
507	4990		$C_8F_3H_{18}P$	$[CH_3(CH_2)_3]_2PF_3$	28		
	(6244)						
526	4991	M	$C_8F_3H_{18}P$	$[(CH_3)_3C]_2PF_3$ (-40^o)	30.0		
	(2396, 6245)						
530	4992		$C_8F_3H_{20}N_2P$	$[(CH_3CH_2)_2N]_2PF_3$	44		
774	(6246)						
521	4993		$C_8F_3H_{20}N_2P$	$[(CH_3CH_2)_2N]_2PF_3$	44		
	(6247)						
515	4994		$C_{10}F_3H_{15}NP$	$C_6H_5PF_3N(CH_2CH_3)_2$	56		
530	(6287)						
705							
774							
774	4995		$C_{10}F_5H_{17}NP$	$[(CH_3CH_2)_2NH_2]^+[C_6H_5PF_4F]^-$	40		
	(6292)						
798	4996		$C_{10}F_6H_{15}IrP_2$				0
	(6297)						
798	4997		$C_{10}F_6H_{15}P_2Rh$				≈0
	(6637, 6299)						
774	4998		$C_{11}F_3H_{15}NP$		58		
	(6304)						
774	4999		$C_{11}F_5H_{17}NP$		40		

Table B.6.f. (contd.)

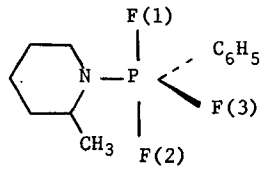
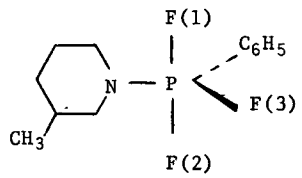
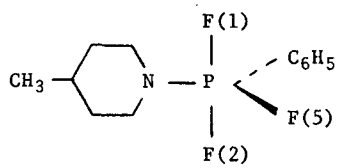
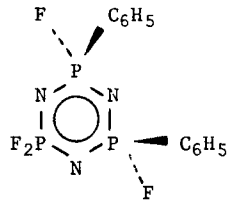
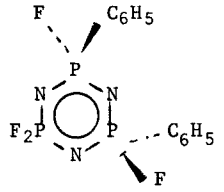
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
789	5000		$C_{12}F_3H_{10}PS$	$C_6H_5PF_3SC_6H_5$		60.0		
717	(6325)							
776	5001	T^2	$C_{12}F_3H_{17}NP$		1,2	14		
	(6326)				1,3	55		
					2,3	55		
776	5002	T^2	$C_{12}F_3H_{17}NP$		1,2	14		
	(6327)				1,3	55		
					2,3	55		
776	5003	T^2	$C_{12}F_3H_{17}NP$		1,2	0		
	(6328)				1,3	56		
					2,3	56		
744	5004	T^2	$C_{12}F_4H_{10}NP$	$F_2PF_2N(C_6H_5)_2$		81		
	(6331)			(-72°)				
803	5005	J	$C_{12}F_4H_{10}N_3P_3$			75		
	(6333)							
803	5006	J	$C_{12}F_4H_{10}N_3P_3$			70		
	(6334)							
515	5007		$C_{16}F_6H_{22}N_2P_2$	$[C_6H_5PF(N(CH_3)_2)_2]^+[C_6H_5FPF_4]^-$				
525	(6386)					41		

Table B.6.f. (contd.)

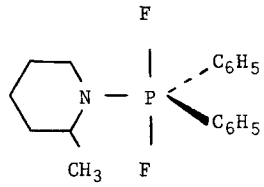
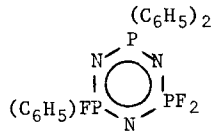
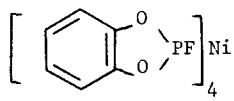
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J		^3J	^nJ
776	5008 (6402)	T	$C_{18}F_2H_{22}NP$	 (-70°)		14			
802	5009 (6408)	J	$C_{18}F_3H_{15}N_3P_3$			70			
818	5010 (6475)		$C_{24}F_4H_{16}NiO_8P_4$						5.8
viii) M = rhenium (Re).									
872	5011		F_5ORe	$ReOF_5$		68.6			
ix) M = sulphur (S).									
539	5012 (2564)		$F_2H_2N_2O_3S_2$	$FS(O)_2N{=}S(O)FNH_2$					8.5
1005	5013		F_3ClS	F_3SSCl (1,2,3)	1,2	149			
					1,3	149			
					2,3	5.1			
964 1036	5014		$F_3NO_2S_2$	$FSO_2N{=}SF_2$ (-30°)					9
1004	5015		F_4S	F_2SF_2		76.3			
1005	5016		F_4S	F_2SF_2		79.9			
1005	5017		F_4S_2	F_3SSF (1,2,3)(4)	1,2	156.0	1,4	63.5	
					1,3	86.3	2,4	32.2	
					2,3	40.2	3,4	32.8	
1006	5018		F_5BrS	FSF_4Br		143.1			

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J		^nJ
1007	5019	P*	F_5ClOS	FSF_4OCl		156			
1008	5020	B*	F_5ClOS	FSF_4OCl		161.5			
1006	5021		F_5ClS	FSF_4Cl		148.5			
675	5022	F	F_5CsOS	$Cs^+FSF_4O^-$		162			
1035	5023		F_6OS	F_4SFOF		155.0			
	(5283)								
1006	5024		$F_6O_3S_2$	FSF_4OSO_2F	1,2	153.5			
				(1)(2)(3)					
1009	5025		$F_6O_3S_2$	FSF_4OSO_2F				1,3	0.9
1010				(1)(2)(3)				2,3	7.2
1011	5026		$F_6O_6S_3$	$F_2SF_2[OS(O)_2F]_2$		156			
645	5027		F_7NOS	FSF_4ONF_2		154			
	(5278)								
1012	5028		F_7NOS	FSF_4ONF_2		157			
1013	5029		F_7NS_2	$FSF_4N{=}SF_2$	1,2	154.1		2,3	13.6
				(1)(2) (3)					
1006	5030		$F_{10}OS_2$	FSF_4OFSF_4		150			
1014	5031	B*	$F_{10}O_2S_2$	FSF_4OOFSF_4	1,2	±152.3		1,3	0.0
				(1)(2)(3)(4)				1,4	0.0
								2,4	∓4.3
1006	5032		$F_{10}O_4S_3$	$(FSF_4)_2SO_4$		153.4			
1014	5033	B*	$F_{10}S_2$	FSF_4FSF_4	1,2	±137.9		1,3	∓0.5
				(1)(2)(3)(4)				1,4	∓5.1
								2,3	∓51.5
539	5034	B	$CF_2H_4N_2O_3S_2$	$FSO_2N{=}S(O)FNHCH_3$					8.5
	(2418)								
919	5035		CF_5ClO_2S	$FSF_4OC(O)Cl$		156			
967	5036		CF_6OS	$FSF_4C(O)F$		-147.5			
	(4798)								
967	5037		CF_6O_2S	$FSF_4OC(O)F$		-157			
	(4799)								
967	5038		CF_6O_3S	$FSF_4OOC(O)F$		-156			
	(4800)								
530	5039		CF_6S	FSF_2CF_3		68			
935	5040		CF_6S	FSF_2CF_3		70			
1005	5041		CF_6S	FSF_2CF_3		63.0			
12	5041a		CF_6H_2S	CFH_2FSF_4		145.6			
	(18 4801)								
1006	5042		CF_8OS	FSF_4OCF_3		153.0			
1006	5043		CF_8S	FSF_4CF_3		145.4			

Table B.6.f. (contd.)

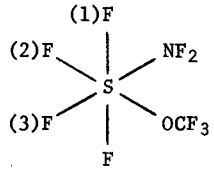
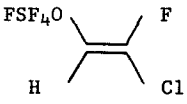
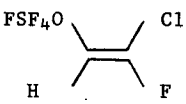
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
970	5044 (4804 5280)		CF_9NOS		1,2 1,3 2,3	150 150 149.2		
539	5045 (2425)	B	$C_2F_2H_6N_2O_3S_2$	$FSO_2N{=}S(O)FN(CH_3)_2$				8.2
541	5046 (2428)		$C_2F_5H_3S$	$FSF_4CH{=}CH_2$		147.8		
541	5047 (2429)		$C_2F_5H_4Cl$	$FSF_4CH_2CH_2Cl$		144.4		
1006	5048		$C_2F_6Cl_4OS$	$FSF_4OCCl_2CCl_2F$		154.9		
53	5049 (1006)		C_2F_6HClOS	$FSF_4OCCl{=}CHF$ (cis or trans)		153.0		
53	5050 (1008 4816)		C_2F_6HClOS			150.4		
187	5051 [1007 2430 4817]		C_2F_6HClOS			151.6		
53	5052 (119)		$C_2F_6H_2Br_2OS$	$FSF_4OCHBrCHBrF$		{150.2 150.4		
53	5053 (121)		$C_2F_6H_2Cl_2OS$	$FSF_4OCHClCHClF$		{154.1 154.2		
53	5054 (120)		$C_2F_6H_2Cl_2OS$	$FSF_4OCH_2CCl_2F$		153.2		
1006	5055		$C_2F_6H_3ClOS$	FSF_4OCH_2CFHCl		154.7		
1006	5056		$C_2F_6H_4OS$	$FSF_4OCH_2CH_2F$		153.8		
54	5057 (2673 4819)	B	C_2F_8BrClS	$FSF_4CFBrCF_2Cl$		146.5		
54	5058 (2674 4818)	B	C_2F_8BrClS	$FSF_4CFClCF_2Br$		145.6		
54	5059 (4820 2675)	B	$C_2F_8Br_2S$	$FSF_4CFBrCF_2Br$		145.9		
54	5060 (2676 4821)	B	$C_2F_8Cl_2S$	$FSF_4CFClCF_2Cl$		145.6		
54	5061 (2677 4822)	B	$C_2F_8Cl_2S$	$FSF_4CF_2CFCl_2$		145.4		

Table B.6.f. (contd.)

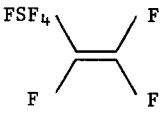
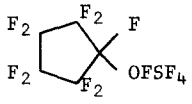
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
1015	5062		$C_2F_8N_4S$	$FSF_4N{=}C(N_3)CF_3$	11		
972	5063 (3436, 4824)		C_2F_8S		151.0		
54	5064 [123, 2678, 4825]	B	C_2F_8HBrS	FSF_4CHFCF_2Br	145.2		
187	5065 [124, 2679, 4826]		C_2F_8HClOS	$FSF_4OCHFCF_2Cl$	150.5		
54	5066 [126, 2680, 4827]	B	C_2F_8HClS	FSF_4CHFCF_2Cl	145.3		
54	5067 [125, 2681, 4828]	B	C_2F_8HClS	FSF_4CF_2CHFCl	143.4		
1006	5068		$C_2F_{10}OS$	$FSF_4OCF_2CF_3$	152.8		
973	5069 (4829)		$C_2F_{10}O_2S$	$F_2SF_2(OCF_3)_2$	146.0		
870	5070 (4830, 2683)		$C_2F_{10}S$	$CF_3CF_2FSF_4$	152.19		
974	5071 (4831)		$C_2F_{11}NS$	$FSF_4N(CF_3)_2$	156		
870	5072 (4832)		$C_2F_{14}S_2$	$CF_3SF_4CF_2FSF_4$	151.87		
541	5073 (2432)		$C_3F_5H_6ClS$	$FSF_4CH_2CHClCH_3$	144.2		
54	5074 [257, 2433, 2769, 4837]	B	$C_3F_8H_4OS$	$FSF_4CHFCF_2OCH_3$	145.5		
54	5075 (4839)	P	$C_3F_{11}IS$	$FSF_4CFICF_2CF_3$	146.2		
539	5076 (2434)		$C_4F_2H_{10}N_2O_3S_2$	$FSO_2N{=}S(O)FN(CH_2CH_3)_2$			8.0
541	5077 (2435)		$C_4F_5H_8ClS$	$FSF_4(CH_2)_4Cl$	143.8		

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
975	5078		$C_4F_8Br_3NS$	$CF_3C(Br)_2CBr(CF_3)N{=}SF_2$	11.7		
870	5079		$C_4F_{14}S$	$CF_3CF_2CF_2CF_2FSF_4$	145.96		
	(2846 4851)						
1006	5080		$C_5F_{14}OS$		154.9		

x) M = antimony (Sb)

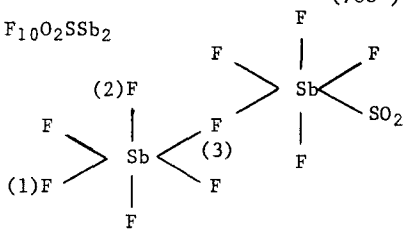
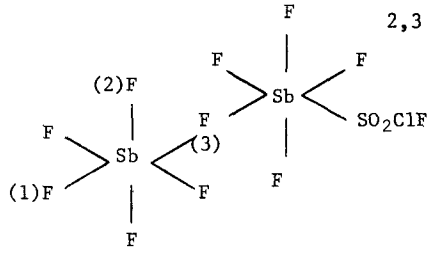
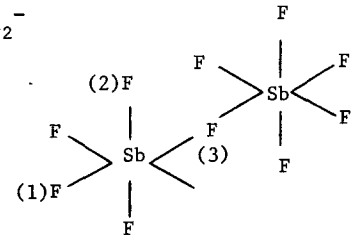
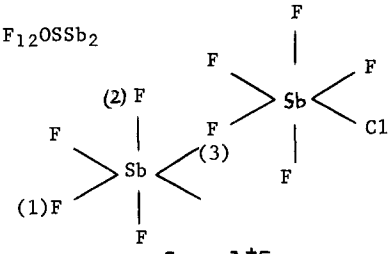
1016	5081	B^2	$F_4H_4O_2Sb$	cis $SbF_4(H_2O)_2$		130	
1016	5082	B^2	F_5H_2OSb	$SbF_5.H_2O$		~98	
1016	5083	B^2	$F_5H_2O_4SSb$	$SbF_5.H_2SO_4$		104	
1016	5084	B^2	F_5O_2SSb	$SbF_5.SO_2$		98	
		R^4				100	
1017	5085	R^4	F_6ClO_2SSb	$SbF_5.SO_2ClF$ (-115)		96	
1018	5086		$F_6O_3SSb^-$	$SbF_5.(SO_3F)^-$		100	
1018	5087		$F_6O_6S_2Sb^-$	$SbF_4.(SO_3F)_2^-$		122	
1018	5088		$F_6O_9S_3Sb^-$	$SbF_3.(SO_3F)_3^-$		126	
1017	5089	R^4	F_7OSSb	$SbF_5.SOF_2$ (-115°)		96	
		T^4		(700°)		92	
1017	5090		$F_{10}O_2SSb_2$		1,2 2,3	98 49	
1016	5091	B^2	$F_{10}H_2OSb_2$	$SbF_5.H_2O.SbF_5$		104	
1016	5092	B^2	$F_{10}H_2O_4SSb_2$	$SbF_5.H_2SO_4.SbF_5$		103	
976	5093	J	$F_{11}AsSb$	$FSbF_4FF_4AsF$	1,2	112	
	(4858)			(1)(2) (-96°)			
1017	5094		$F_{11}ClO_2SSb_2$		1,2 2,3	93 44	

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
1016	5095		$F_{11}Sb_2^-$		1,2	100		
1019					2,3	53		
1017	5096		$F_{12}OSSb_2$		1,2	95		
					2,3	49		
1020	5097		$F_{14}N_2Sb_2$	$[F_2NNF]^+[FSbF_4FF_4SbF]^-$ (1)(2)(3)	1,2	93		
					2,3	60		
1017	5098		$CF_6H_3O_2SSb$	$SbF_5.CH_3SO_2F$ (-110°)		96		

xi) M = silicon (Si)

585	5099 (2572)		$F_2H_4Si_2$	$SiFH_2SiFH_2$			5.0	
588	5100 (2577)		$F_4H_2SSi_2$	SiF_2HSiF_2SH			10.8	
585	5101 (2578)		$F_4H_2Si_2$	SiF_2HSiF_2H			8.0	
588	5102 (2579)		F_5HSi_2	SiF_3SiF_2H			12.7	
839	5103 (6667)		F_6OSi_2	SiF_3OSiF_3				0.74
839	5104 (6669)		F_6Si_2	SiF_3SiF_3			20.91	
854	5105 (6673)	B	F_8Si_3	$^*SiF_3SiF_2SiF_3$ ($Si^* = {}^{29}Si$, $Si = {}^{28}Si + {}^{30}Si$)				+3.61
1148	5106 (6674)		F_8Si_3	$SiF_3SiF_2SiF_3$			11.0	
1149	5107 (6675)		F_9BSi_3	$SiF_3SiF_2SiF_2BF_2$ (1) (2) (3)		1,2	10.0	
						2,3	9.5	
853	5108 (6693)	E^2	$C_2F_4O_4Si^{2-}$	$[SiF_4CO_2CO_2]^{2-}$	2.4			

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
xii) M = tin (Sn).								
858	5109	E^2	$F_3Br_3Sn^{2-}$	$SnF_3Br_3^{2-}$		65		
858	5110	E^2	$F_3Cl_3Sn^{2-}$	$SnF_3Cl_3^{2-}$		60		
858	5111	E^2	$F_3N_9Sn^{2-}$	$SnF_3(N_3)_3^{2-}$		52.7		
	(6733)							
858	5112	A^2	$F_3H_3O_3Sn^{2-}$	$SnF_3(OH)_3^{2-}$		37		
859	(6735)							
858	5113	E^2	$F_4BrClSn^{2-}$	$FSnF_2FBrCl^{2-}$	1,2	49.5		
	(6736)			(1)(2)(3)	2,3	42.0		
					1,3	24.6		
858	5114	A	$F_4Br_2Sn^{2-}$	$F_2SnF_2Br_2^{2-}$		48.1		
	(6737)	E^2				47.5		
858	5115	A	$F_4Cl_2Sn^{2-}$	$F_2SnF_2Cl_2^{2-}$		45.1		
	(6739)	F				48.9		
858	5116	A	$F_4I_2Sn^{2-}$	$F_2SnF_2I_2^{2-}$		52.0		
	(6740)							
858	5117	E^2	$F_4N_6Sn^{2-}$	$F_2SnF_2(N_3)_2^{2-}$		39.9		
	(6742)							
858	5118	A^2	$F_4H_2O_2Sn^{2-}$	$F_2SnF_2(OH)_2^{2-}$		32		
859	(6744)							
858	5119	A	F_5BrSn^{2-}	F_4SnFBr^{2-}		33.3		
	(6745, 6746)	E^2				31.7		
858	5120	A	F_5ClSn^{2-}	F_4SnFCl^{2-}		35.1		
	(6747, 6748)	F				38		
858	5121	A	F_5ISn^{2-}	F_4SnFI^{2-}		30.5		
	(6750)							
858	5122	E^2	$F_5N_3Sn^{2-}$	$F_4SnF(N_3)^{2-}$		32.1		
	(6751)							
858	5123	A^2	F_5HOSn^{2-}	F_4SnFOH^{2-}		29		
859	(6752)							
858	5124	A^2	$F_5H_2AsO_4Sn^{2-}$	$F_4SnF(OAsO(OH)_2)^{2-}$ (Tentative assignment)		~37		
858	5125	A^2	$F_5H_2O_4PSn^{2-}$	$F_4SnF(OPO(OH)_2)^{2-}$		38.4		
	(6754)							
858	5126	E^2	CF_5NOSn^{2-}	$F_4SnF(NCO)^{2-}$		35.5		
	(6757)							
858	5127	F	CF_5NSSn^{2-}	$F_4SnF(NCS)^{2-}$		41.8		
	(6758)							
858	5128	E^2	CF_5NSeSn^{2-}	$F_4SnF(NCSe)^{2-}$		38.2		
	(6759)							

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J	^3J	^nJ
858	5129 (6760)	A	CF_5NSn^{2-}	F_4SnFCN^{2-}		32.0		
858	5130 (6761)	J[4]	$CF_5HO_2Sn^{2-}$	$F_4SnF(O_2CH)^{2-}$		39		
858	5731 (6762)	E[2]	$CF_5H_3OSn^{2-}$	$F_4SnF(OCH_3)^{2-}$		32		
861	5132) (6763)		$CF_5H_4OSn^-$	$F_4SnF(CH_3OH)^-$		37		
854		E	$C_2F_3BrO_4Sn^{2-}$	$F_2SnFBr(CO_2CO_2)^{2-}$				
	5133			Isomer 1		~60		
	5134			Isomer 2		~37		
858		E[2]	$C_2F_3ClO_4Sn^{2-}$	$F_2SnFCl(CO_2CO_2)^{2-}$				
	5135			Isomer 1		50.4		
	5136			Isomer 2		~33		
858	5137	F	$C_2F_3H_6Cl_2OSSn^{2-}$	$F_2SnFCl_2[(CH_3)_2SO]^-$		54.6		
858	5138 (6765)	E[2]	$C_2F_4N_2O_2Sn^{2-}$	$F_2SnF_2(NCO)_2^{2-}$		34.7		
858	5139 (6767)	F	$C_2F_4N_2S_2Sn^{2-}$	$F_2SnF_2(NCS)_2^{2-}$		42.6		
858	5140 (6768)	E[2]	$C_2F_4O_4Sn^{2-}$	$F_2SnF_2(CO_2CO_2)^{2-}$		44.3		
858	5141	F	$C_2F_4H_6BrOSSn$	$FSnF_2FBr[(CH_3)_2SO]^-$	1,2	45.2		
				(1) (2) (3)	2,3	57.8		
858	5142	F	$C_2F_4H_6ClOSSn^-$	$FSnF_2FCl[(CH_3)_2SO]^-$	1,2	47.0		
				(1) (2) (3)	2,3	45.3		
858	5143	E[2]	$C_2F_4H_6O_2Sn^{2-}$	$F_2SnF_2(OCH_3)_2$		34		
858	5144 (6769)	A	$C_2F_5HCl_2O_2Sn^{2-}$	$F_4SnF(O_2CCHCl_2)^{2-}$		44		
858	5145 (6770)	A	$C_2F_5H_2ClO_2Sn^{2-}$	$F_4SnF(O_2CCH_2Cl)^{2-}$		44		
858	5146 (6771)	K[4]	$C_2F_5H_3OSSn^{2-}$	$F_4SnF(SOCCH_3)^{2-}$		28.4		
858	5147 (6772)	A	$C_2F_5H_3O_2Sn^{2-}$	$F_4SnF(OOCCH_3)^{2-}$		39		
858	5148 (6774)	J[2]	$C_2F_5H_5OSn^{2-}$	$F_4SnFOCH_2CH_3^{2-}$		33		
861	5149 (6775)		$C_2F_5H_6OSn^-$	$F_4SnF(CH_3CH_2OH)^-$		40		
858	5150 (6776)	F	$C_2F_5H_6OSSn^-$	$F_4SnF[(CH_3)_2SO]^-$		45		
861	5151		$C_2F_5H_6O_2Sn^-$	$F_4SnF(HOCH_2CH_2OH)^-$		41		
858	5152 (6777)	A	$C_2F_8O_2Sn^{2-}$	$F_4SnF(O_2CCF_3)^{2-}$		43		

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
858	5153 (6779)	E^2	$C_3F_3N_3O_3Sn^{2-}$	$F_2SnF(NCO)_3^{2-}$	35.0		
858	5154 (6780)	F	$C_3F_3N_3S_3Sn^{2-}$	$F_2SnF(NCS)_3^{2-}$	41.4		
858	5155	E^2	$C_3F_3H_2BrO_4Sn^{2-}$	$F_2SnFBr(CH_2(CO_2)_2)^{2-}$	53.3		
	5156				~33		
				(Tentative assignment)			
858	5157		$C_3F_3H_2ClO_4Sn^{2-}$	$F_2SnFCl(CH_2(CO_2)_2)^{2-}$	47.6		
	5158				~33		
858	5159 (6782)	E^2	$C_3F_4H_2O_4Sn^{2-}$	$F_2SnF_2(CH_2(CO_2)_2)^{2-}$	39.9		
858	5160 (6783)	A	$C_3F_5H_2NO_2Sn^{2-}$	$F_4SnF(O_2CCH_2CN)^{2-}$	42		
858	5161 (6784)	A	$C_3F_5H_4ClO_2Sn^{2-}$	$F_4SnF(O_2CCHClCH_3)^{2-}$	40		
858	5162 (6785)	A	$C_3F_5H_5O_2Sn^{2-}$	$F_4SnF(O_2CCH_2CH_3)^{2-}$	40		
861	5163		$C_3F_5H_7NOSn^{-}$	$F_4SnF((CH_3)_2NCHO)^{-}$	50		
858	5164 (6786)	I^4	$C_3F_5H_7OSn^{2-}$	$F_4SnF(O(CH_2)_2CH_3)^{2-}$	32		
861	5165		$C_3F_5H_8Sn^{-}$	$F_4SnF((CH_3)_2CHOH)^{-}$	42		
858	5166 (6790)	A	$C_4F_4H_2Cl_4O_4Sn^{2-}$	$F_2SnF_2(O_2CCHCl_2)_2^{2-}$	43.5		
858	5167	A	$C_4F_4H_4Cl_2O_4Sn^{2-}$	$F_2SnF_2(O_2CCH_2Cl)_2^{2-}$	44.1		
858	5168 (6791)	E^2	$C_4F_4H_4O_4Sn^{2-}$			1,2	38.1
						1,3	<2
						2,3	41.7

Table B.6.f. (contd.)

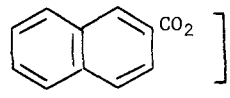
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
858	5169 (6793)	A	$C_4F_4H_6O_4Sn^{2-}$	$F_2SnF_2(O_2CCH_3)_2^{2-}$	41.2		
858	5170 (6794)	F	$C_4F_4H_{12}O_2S_2Sn^{2-}$	$F_2SnF_2((CH_3)_2SO)_2$	53		
858	5171 (6797)	A	$C_4F_5H_6ClO_2Sn^{2-}$	$F_4SnF(O_2CCH_2CHClCH_3)^{2-}$	42		
858	5172	A	$C_4F_5H_7O_2Sn^{2-}$	$F_4SnF(O_2CCH(CH_3)_2)^{2-}$	43		
858	5173 (6799)	A	$C_4F_{10}O_4Sn^{2-}$	$F_2SnF_2(O_2CCF_3)_2^{2-}$	45.9		
858	5174	E^2	$C_5F_2H_2O_8Sn^{2-}$	$F_2Sn(O_2CCO_2)(O_2CCH_2CO_2)^{2-}$	~40		
858	5175 (6800)	E^2	$C_5F_4H_6O_4Sn^{2-}$	$F_2SnF_2(O_2CC(CH_3)_2CO_2)^{2-}$	39.8		
858	5176 (6802)	A	$C_5F_5H_9O_2Sn^{2-}$	$F_4SnF(O_2CC(CH_3)_3)^{2-}$	45		
858	5177 (6803)	E^2	$C_5F_5H_{10}NS_2Sn^{2-}$	$F_4SnF(SSC.N(CH_2CH_3)_2)^{2-}$	33.6		
858	5178 (6807)	A	$C_6F_4H_4N_2O_4Sn^{2-}$	$F_2SnF_2(O_2CCH_2CN)_2^{2-}$	42.3		
858	5179 (6809)	A	$C_5F_4H_8Cl_2O_4Sn^{2-}$	$F_2SnF_2(O_2CCHClCH_3)_2^{2-}$	44.8		
858	5180 (6810)	A	$C_6F_4H_{10}O_4Sn^{2-}$	$F_2SnF_2(O_2CCH_2CH_3)_2^{2-}$	43.2		
858	5181 (6813)	A	$C_7F_5H_4NO_4Sn^{2-}$	$F_4SnF(oNO_2C_6H_4CO_2)^{2-}$	46		
858	5182 (6814)	A	$C_7F_5H_4NO_4Sn^{2-}$	$F_4SnF(pNO_2C_6H_4CO_2)^{2-}$	41		
858	5183 (6815)	A	$C_7F_5H_5O_2Sn^{2-}$	$F_4SnF(C_6H_5CO_2)^{2-}$	41		
858	5184	A	$C_8F_4H_{12}Cl_2O_4Sn^{2-}$	$F_2SnF_2(O_2CCH_2CHClCH_3)_2^{2-}$	37.8		
858	5185 (6816)	A	$C_8F_4H_{14}O_4Sn^{2-}$	$F_2SnF_2(O_2CCH(CH_3)_2)_2^{2-}$	43.4		
858	5186 (6820)	A	$C_{10}F_4H_{18}O_4Sn^{2-}$	$F_2SnF_2(O_2CC(CH_3)_3)_2^{2-}$	45.0		
858	5187 (6823)	A	$C_{11}F_5H_7O_2Sn^{2-}$	F_2SnF [ CO_2]$^{2-}$	42		
858	5188 (6827)	A	$C_{14}F_4H_8N_2O_8Sn^{2-}$	$F_2SnF_2(oNO_2C_6H_4CO_2)_2^{2-}$	45.6		
858	5189 (6828)	A	$C_{14}F_4H_8N_2O_8Sn^{2-}$	$F_2SnF_2(pNO_2C_6H_4CO_2)_2^{2-}$	42.9		
858	5190 (6829)	A	$C_{14}F_4H_{10}O_4Sn^{2-}$	$F_2SnF_2(O_2CC_6H_5)_2^{2-}$	43.2		

Table B.6.f. (contd.)

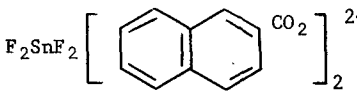
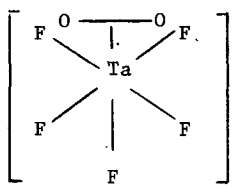
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^nJ
858	5191 (6839)	A	$C_{18}F_5H_{15}PSn^-$	$F_4SnF(P(C_6H_5)_3)^-$	45.9		
858	5192 (6840)	A	$C_{18}F_5H_{35}O_2Sn^{2-}$	$F_4SnF(O_2C(CH_2)_{16}CH_3)^{2-}$	39		
858	5193 (6842)	A	$C_{20}F_5H_{15}O_2Sn^{2-}$	$F_4SnF(O_2CC(C_6H_5)_3)^{2-}$	41		
858	5194 (6844)	A	$C_{22}F_4H_{14}O_4Sn^{2-}$		41.3		
858	5195 (6846)	A	$C_{36}F_4H_{70}O_4Sn^{2-}$	$F_2SnF_2(O_2C(CH_2)_{16}CH_3)_2^{2-}$	41.8		
858	5196	A	$C_{40}F_4H_{30}O_4Sn^{2-}$	$F_2SnF_2(O_2CC(C_6H_5)_3)_2^{2-}$	47.0		
xiii) M = tantalum (Ta).							
1033	5197		$F_5O_2Ta^{2-}$		64		
xiv) M = tellurium (Te).							
556	5198 (2483)	B	$C_2F_5H_6NTe$	$F_4TeF.N(CH_3)_2$	168		
556	5199 (2484)	B	$C_4F_4H_{12}N_2Te$	$F_2TeF_2[N(CH_3)_2]_2$	135		
556	5200	B	$C_4F_5H_8NTe$		172		
556	5201	B	$C_4F_5H_{10}NTe$	$F_4TeFN(CH_2CH_3)_2$	-165		
557	(2485 6847)						
556	5202 (2486)	B	$C_4F_5H_{12}NSiTe$	$F_4TeFNCH_3Si(CH_3)_3$	170		
556	5203	B	$C_6F_4H_{16}N_2Te$	$F_4TeFN(CH_3)_2N(CH_2CH_3)_2$	142		
556	5204	B	$C_6F_6H_{16}N_2SiTe$	$F_4TeFN(CH_3)CH_2CH_2N(CH_3)Si(CH_3)_2F$	173		

Table B.6.f. (contd.)

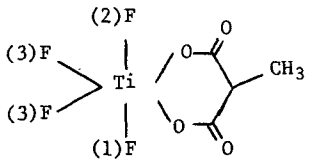
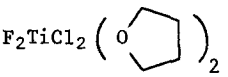
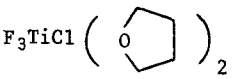
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J
xv) M = titanium (Ti).						
853	5205	E	$CF_5H_3OTi^{2-}$	$F_4TiFOCH_3^{2-}$		44.0
1026	5206		$C_2F_4H_8O_2Ti$	$F_2TiF_2(CH_3OH)_2$		36
853	5207	A	$C_2F_5H_3O_2Ti^{2-}$	$F_4TiF(O_2CCH_3)^{2-}$		36.1
853	5208	J^2	$C_2F_5H_5OTi^{2-}$	$F_4TiF(OCH_2CH_3)^{2-}$		45.1
853	5209	A	$C_3F_5H_5O_2Ti^{2-}$	$F_4TiF(O_2CCH_2CH_3)^{2-}$		42.8
853	5210	I^4	$C_3F_5H_7OTi^{2-}$	$F_4TiF(OCH_2CH_2CH_3)^{2-}$		43.4
853	5211	E	$C_4F_4H_4O_4Ti^{2-}$		1,3	~40
					2,3	~40
					1,2	<10
1026	5212		$C_4F_4H_{12}O_2S_2Ti$	$F_2TiF_2(CH_3S(O)CH_3)_2$		37
1026	5213		$C_4F_4H_{12}O_2Ti$	$F_2TiF_2(CH_3CH_2OH)_2$		36
1027	5214		$C_4F_4H_{12}O_2Ti$	$F_2TiF_2(CH_3CH_2OH)_2$		36
853	5215	A	$C_4F_5H_7O_2Ti^{2-}$	$F_4TiF(O_2CCH(CH_3)_2)^{2-}$		43.7
853	5216	U^2	$C_4F_5H_9OTi^{2-}$	$F_4TiF(O(CH_2)_3CH_3)^{2-}$		~36
853	5217	E^2	$C_5F_4H_6O_4Ti^{2-}$	$F_2TiF_2(O_2CC(CH_3)_2CO_2)^{2-}$		~40
853	5218	A	$C_5F_5H_9O_2Ti^{2-}$	$F_4TiF(O_2CC(CH_3)_3)^{2-}$		44.1
1026	5219		$C_6F_4H_{14}N_2O_2Ti$	$F_2TiF_2(HC(O)N(CH_3)_2)_2$		38
1026	5220		$C_6F_4H_{16}O_2Ti$	$F_2TiF_2((CH_3)_2CHOH)_2$		36
853	5221	A	$C_7F_5H_4NO_4Ti^{2-}$	$F_4TiF(\underline{o}NO_2C_6H_4CO_2)^{2-}$		40.4
853	5222	A	$C_7F_5H_4NO_4Ti^{2-}$	$F_4TiF(\underline{p}NO_2C_6H_4CO_2)^{2-}$		40.3
853	5223	A	$C_7F_5H_5O_2Ti^{2-}$	$F_4TiF(C_6H_5CO_2)^{2-}$		41.4
1028	5224		$C_8F_2H_{16}Cl_2O_2Ti$			45
1028	5225		$C_8F_3H_{16}ClO_2Ti$			33.1
1028	5226		$C_8F_4H_{16}O_2Ti$			37.6
1026	5227		$C_8F_4H_{18}N_2O_2Ti$	$F_2TiF_2(CH_3C(O)N(CH_3)_2)_2$		39

Table B.6.f. (contd.)

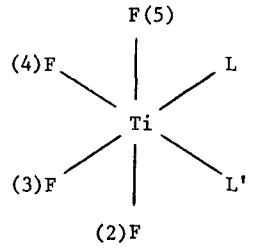
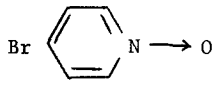
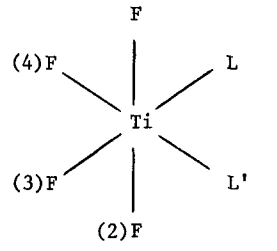
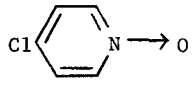
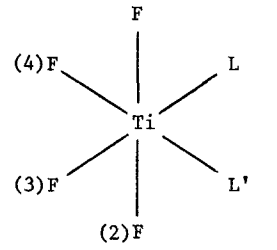
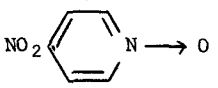
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J
1031	5228		$C_9F_4H_{13}BrN_2O_2Ti$		1,4	34
					2,3	39
					3,4	48
				$L = CH_3C(O)N(CH_3)_2$	3,4	48
				L' = 		
1031	5229		$C_9F_4H_{13}ClN_2O_2Ti$		1,4	34
1026					2,3	39
					3,4	48
				$L = CH_3C(O)N(CH_3)_2$		
				L' = 		
1031	5230		$C_9F_4H_{13}N_3O_4Ti$		1,4	34
					2,3	39
				$L = CH_3C(O)N(CH_3)_2$		
				L' = 		

Table B.6.f. (contd.)

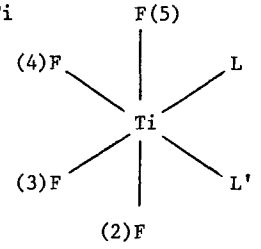
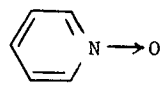
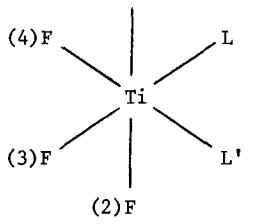
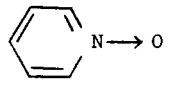
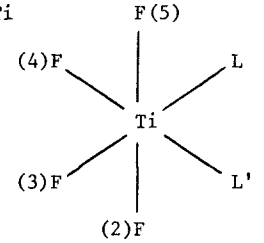
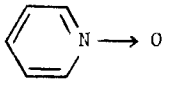
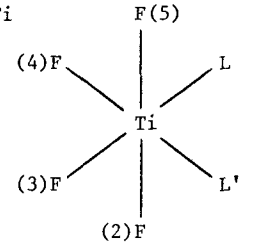
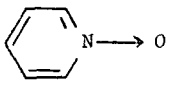
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J
1031 1026	5231		$C_9F_4H_{14}N_2O_2Ti$		1,4 2,3 3,4	35 39 48
				L = $CH_3C(O)N(CH_3)_2$ L' = 		
1026 1029 1032	5232	S^4	$C_{10}F_4H_8Cl_2N_2O_2Ti$			34
				L = L' =  (-40°)		
1026 1029 1030 1032	5233	M	$C_{10}F_4H_{10}N_2O_2Ti$			35
				L = L' = 		
1026 1031	5234		$C_{10}F_4H_{16}N_2O_2Ti$		1,4 2,3 3,4	35 39 48
				L = $CH_3C(O)N(CH_3)_2$ L' = CH_3 		

Table B.6.f. (contd.)

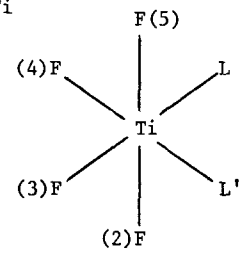
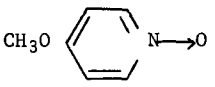
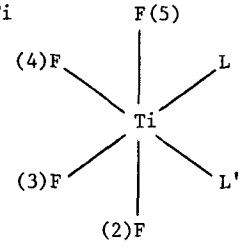
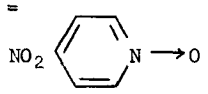
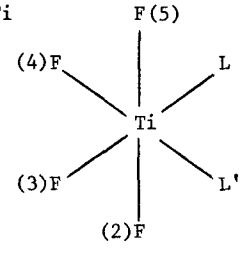
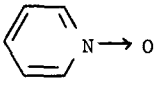
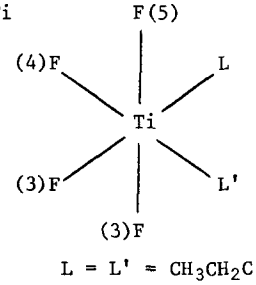
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^2J
1026	5235		$C_{10}F_4H_{16}N_2O_3Ti$		1,4	35
1031					2,3	39
					3,4	48
				L = $CH_3C(O)N(CH_3)_2$		
				L'= 		
1026	5236		$C_{10}F_4H_{16}N_4O_4Ti$		1,4	41
					2,3	34
					3,4	39
				L or L' = $OC[N(CH_3)_2]_2$		
				L' or L = 		
1026	5237		$C_{10}F_4H_{17}N_3O_2Ti$		1,4	41
					2,3	35
					3,4	49
				L or L' = $OC[N(CH_3)_2]_2$		
				L' or L = 		
1026	5238		$C_{10}F_4H_{22}N_2O_2Ti$			40
				L = L' = $CH_3CH_2C(O)N(CH_3)_2$		

Table B.6.f. (contd.

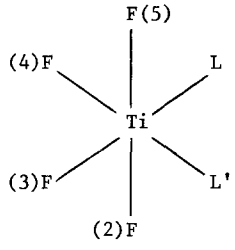
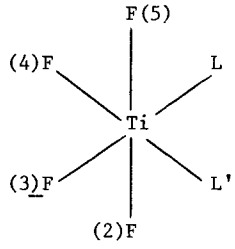
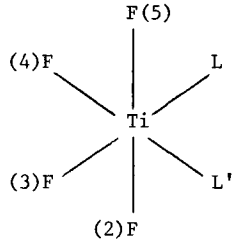
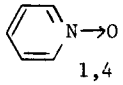
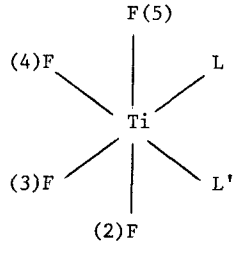
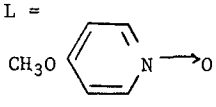
Ref. No.	Serial No	Solvent	Molecular formula	Structure		^2J
1026	5239		$C_{10}F_4H_{22}N_2O_2Ti$	 L = L' = $HC(O)N(CH_2CH_3)_2$		38
1026	5240		$C_{10}F_4H_{24}N_4O_2Ti$	 L = L' = $(CH_3)_2NC(O)N(CH_3)_2$		41
1026	5241		$C_{11}F_4H_{16}N_2O_4Ti$	 L or L' = $CH_3C(O)N(CH_3)_2$ L' or L = 	1,4 2,3 3,4	39 34 48
1026	5242		$C_{11}F_4H_{19}N_3O_3Ti$	 L or L' = OC $N(CH_3)_2$ 2 L' or L = 	1,4 2,3 3,4	41 35 49

Table B.6.f. (contd.)

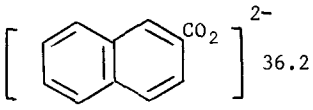
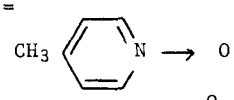
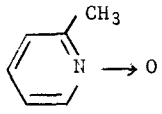
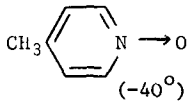
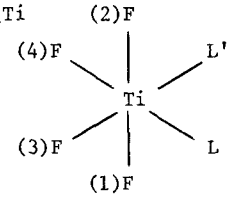
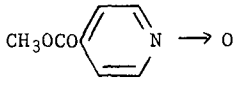
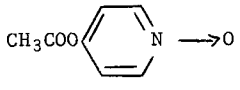
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J
853	5243	A	$C_{11}F_5H_7O_2Ti^{2-}$		36.2
1030	5244	M	$C_{12}F_4H_{14}N_2O_2Ti$	$F_2TiF_2(L)_2$	35
1032				L =	
1026					
1029				(-40°)	
1026	5245	M	$C_{12}F_4H_{14}N_2O_2Ti$	$F_2TiF_2(L)_2$	36
1030				L =	
					
				(-40°)	
1026	5246	S[4]	$C_{12}F_4H_{14}N_2O_4Ti$	$F_2TiF_2(L)_2$	35
1029				L =	
1032					
				(-40°)	
1031	5247		$C_{12}F_4H_{16}N_2O_4Ti$		1,3 39 2,4 34 3,4 48
				L' = $CH_3C(O)N(CH_3)_2$	
				L =	
					
1026	5248				
1029		S[4]	$C_{14}F_4H_{14}N_2O_6Ti$	$F_2TiF_2(L)_2$	34
1032				L =	
					
				(-40°)	

Table B.6.f. (contd.)

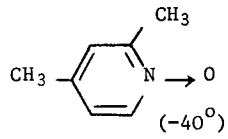
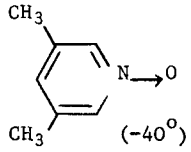
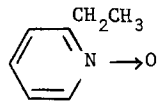
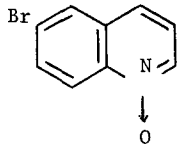
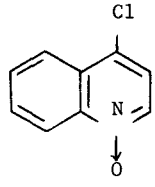
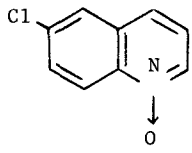
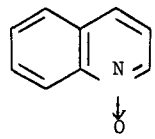
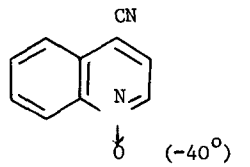
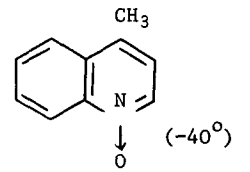
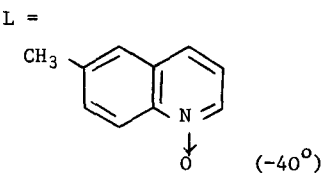
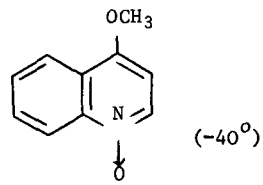
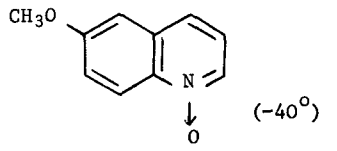
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J
1030	5249	M	$C_{14}F_4H_{18}N_2O_2Ti$	$F_2TiF_2(L)_2$ L =  (-40°)	36
1030	5250	M	$C_{14}F_4H_{18}N_2O_2Ti$	$F_2TiF_2(L)_2$ L =  (-40°)	35
1030	5251	M	$C_{14}F_4H_{18}N_2O_2Ti$	$F_2TiF_2(L)_2$ L = 	37
1029 1032	5252	S^4	$C_{18}F_4H_{12}Br_2N_2O_2Ti$	$F_2TiF_2(L)_2$ L =  (-40°)	37
1029 1032	5253	S^4	$C_{18}F_4H_{12}Cl_2N_2O_2Ti$	$F_2TiF_2(L)_2$ L =  (-40°)	36
1029 1032	5254	S^4	$C_{18}F_4H_{12}Cl_2N_2O_2Ti$	$F_2TiF_2(L)_2$ L =  (-40°)	36
1029 1030 1032	5255	S^4	$C_{18}F_4H_{14}N_2O_2Ti$	$F_2TiF_2(L)_2$ L =  (-40°)	36

Table B.6.f. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J
853	5256	A	$C_{18}F_5H_{35}O_2Ti^{2-}$	$F_4TiF(O_2C(CH_2)_{16}CH_3)^{2-}$	40.0
1029	5257	S^4	$C_{20}F_4H_{12}N_4O_2Ti$	$F_2TiF_2(L)_2$	36
1032				L =  (-40°)	
1029	5258	S^4	$C_{20}F_4H_{18}N_2O_2Ti$	$F_2TiF_2(L)_2$	37
1032				L =  (-40°)	
1029	5259	S^4	$C_{20}F_4H_{18}N_2O_2Ti$	$F_2TiF_2(L)_2$	36
1032				L =  (-40°)	
1029	5260	S^4	$C_{20}F_4H_{18}N_2O_4Ti$	$F_2TiF_2(L)_2$	37
1032				L =  (-40°)	
1029	5261	S^4	$C_{20}F_4H_{18}N_2O_4Ti$	$F_2TiF_2(L)_2$	38
1032				L =  (-40°)	

xvi) M = tungsten (W).

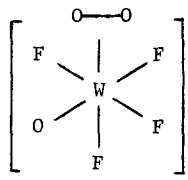
871	5262	B	F_3Cl_3W	mer WF_3Cl_3		62
871	5263	B	F_4Cl_2W	cis $F_2WF_2Cl_2$		66
1033	5264		$F_4O_3W^{2-}$		AB	±125
					BC	±52
					AC	±71

Table B.f.6. (contd.)

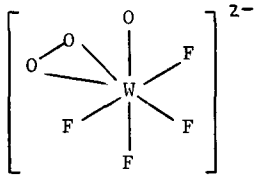
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J
				or	
					
				AB_2C	
871	5265 (6852)	B	F_5ClW	F_4WFCl	73
182	5266 (6853)	A^3	F_5OW^-	$[F_4WFO]^-$	±53
182	5267 (6858)	A^3	$F_9O_2W_2^-$	$[F_4OWFWOF_4]^-$	±58
182	5268	A^3	CF_5H_3OW	F_4WFOCH_3	66
535 558	(6859 2487)				
182	5269	B	$C_2F_4H_6O_2W$	cis $F_2WF_2(OCH_3)_2$	66
558	(2488 6860)	F			67
182	5270	A^3	$C_3F_3H_9O_3W$	trans $F_2WF(OCH_3)_3$	62
558	(2490 6863)				
558	5271	B	$C_4F_4H_{10}O_2W$	cis $F_2WF_2(OCH_2CH_3)_2$	68
535	5272 (6869)	M	$C_4F_5H_{12}O_4PW$	$[CH_3P(OCH_3)_3]^+[F_4WFO]^-$	53
182 535 558	5273 (6874)	A^3	$C_6F_5H_5OW$	$F_4WFOC_6H_5$	64
182 558	5274 (6875)	M	$C_{12}F_4H_{10}O_2W$	cis $F_2WF_2(OC_6H_5)_2$	62
744	5275 (6876)	M B^2	$C_{12}F_5H_{28}NOW$	$[CH_3(CH_2)_2]_4N^+(F_4WFO)^-$	53 52

Table B.6.g. Each fluorine bonded to an element other than carbon.

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^3J	^4J
1034	5276		F_2HNO_2S	$FNHSO_2F$	7.7	
1037	5277		F_3NO_3S	F_2NOSO_2F		4.6
645	5278 (5027)		F_7NOS	F_2NOSF_4F (1) (2)	1,2	3.8

Table B.6.g. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^3J	^4J
1038	5279		F_7NS	F_2NSF_4F	1,2	4.1	
				(1) (2)(3)	1,3	19.1	
970	5280		CF_9NOS	(2)F	1,2	21.8	
	(4804 5044)			(3)F, NF_2(1), S, (4)F, OCF_3, F	1,3	22.3	
					1,4	2.4	
968	5281		CF_9NS	trans $F_2NSF_4CF_3$	1,2	20	
				(1) (2)			
1035	5282		F_2O_3S	$FOSO_2F$		6.1	
1035	5283		F_6OS	$FOSF_4F$	1,2	17.4	
	(5023)			(1)(2)(3)	1,3	0.0	
685	5284		F_3O_4PS	$F_2P(O)OSO_2F$			3.3
	(5678)						
685	5285		$F_3O_7PS_2$	$FP(O)(OSO_2F)_2$			3.2
	(5679)						
691	5286		F_4NOPS	$F_2P(O)N{=}SF_2$			4.5
	(5694)						
683	5287	B	F_4NO_2PS	$F_3P{=}NSO_2F$			4
	(5695)						

C. Fluorine coupling to an element, M, other than hydrogen or fluorine.
(In alphabetical symbol order).

Table C.1. M = silver (Ag).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
81	5289	J-H	C_3F_6HAg	$(CF_3)_2CHAg$		20	
	(255)						

Table C.2. M = arsenic (As)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
612	5290	B	F_6AsK	$KAsF_6$		905		
643	5291	D	$F_{10}AsN$	$NF_4^+AsF_6^-$		~870		
	(5589)							
474	5292	J	$C_3F_5H_9AsN$	$(CH_3)_3NAsF_5$	1e,2	1048		
	(4860)			(2)(1)	1a,2	840		

Table C.3. M = boron (B).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J
591	5293		FBBrCl	BFBrCl		92		
592	5294	B[3]	FBBrCl	BFBrCl		95		
592	5295	B[3]	FBBrI	BFBrI		189		
591	5296		$FBBr_2$	$BFBr_2$		108		
592	5297	B[3]	$FBBr_2$	$BFBr_2$		121		
592	5298	B[3]	FBClI	BFClI		102		
591	5299		$FBCl_2$	$BFCl_2$		74		
592	5300	B	$FBCl_2$	$BFCl_2$		73		
593	5301		FH_8B_5	$2\text{-}FB_5H_8$		~60		
591	5302		F_2BBr	BF_2Br		56		
592	5303	B[3]	F_2BBr	BF_2Br		58		
591	5304		F_2BCl	BF_2Cl		34		
592	5305	B[3]	F_2BCl	BF_2Cl		33		
567	5306	F HB	F_2HB	BF_2H		84		
	(2518)							
591	5307		F_3B	BF_3		15		
592	5308	B	F_3B	BF_3		14.5		
594	5309		$F_3{}^{10}B$	$^{10}BF_3$ (-105°C)		8.07		
595	5310	A[2]	F_3HBNaO	$Na^+BF_3OH^-$		12.7		
475	5311		F_3H_3BN	NH_3BF_3		13.8		
596	5312	M	F_4AgB	$Ag^+BF_4^-$		0.39		
		A[2]				1.07		
595	5313	A[2]	F_4BNa	$Na^+BF_4^-$		1.37		
595	5314	A[2]	F_4H_4BN	$NH_4^+BF_4^-$		1.15		
1149	5315		F_7BSi_2	$SiF_3SiF_2BF_2$		122		
	(6671)							
597	5316		CF_2H_3B	CH_3BF_2		77		
598	5317	A	CF_2H_3B	CH_3BF_2		78		
475	5318		CF_3H_5BN	$CH_3NH_2BF_3$		15.7		
599	5319		CF_3H_5BN	$CH_3NH_2BF_3$		16.7		
600	5320		$CF_{10}B_2$	$\lvert CF_3BF_3\rvert^+\lvert BF_4\rvert^-$	1,4	39.0	3,4	34.0
				(3)(4)(1)(5)(2)	2,5	4.8		
598	5322	A	C_2FH_6B	$(CH_3)_2BF$		128		
601	5323	J	$C_2FH_6BBrClO$	$BFBrCl.O(CH_3)_2$		66.5		
601	5324	J	$C_2FH_6BBr_2O$	$BFBr_2.O(CH_3)_2$		76.1		
601	5325	J	$C_2FH_6BCl_2O$	$BFCl_2.O(CH_3)_2$		53.8		
597	5326		$C_2F_2H_3B$	$CH_2{=}CHBF_2$		57		
597	5327		$C_2F_2H_5B$	$CH_3CH_2BF_2$		81		
602	5328		$C_2F_2H_5B$	$CH_3CH_2BF_2$		81		
601	5329	J	$C_2F_2H_6BBrO$	$BF_2Br.O(CH_3)_2$		37.8		
601	5330	J	$C_2F_2H_6BClO$	$BF_2Cl.O(CH_3)_2$		27.0		
599	5331		$C_2F_2H_6BN$	$CH_3CH_2NHBF_2$		39.0		
475	5332		$C_2F_3H_7BN$	$(CH_3)_2NHBF_3$		15.5		

Table C.3. (contd.)

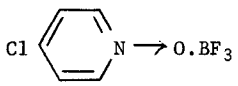
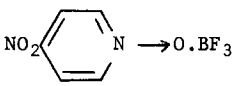
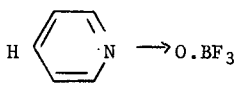
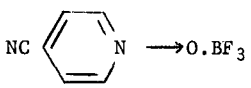
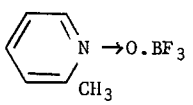
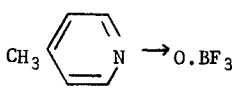
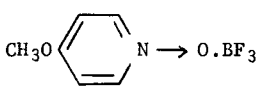
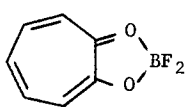
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	
603	5333	B	$C_2F_6H_8B_5P$	$(CF_3)_2P.B_5H_8$		6.0
604	5334		$C_3F_2H_5B$		72	6.0
597	5335		$C_3F_2H_7B$	$CH_3CH_2CH_2BF_2$	81	
599	5336		$C_3F_2H_8BN$	$(CH_3)_2CHNH.BF_2$	41.0	
475	5337		$C_3F_3H_9BP$	$(CH_3)_3P.BF_3$	52	
	(2199 5928)					
605	5338		$C_3F_3H_9BP$	$(CH_3)_3P.BF_3$	50	
	(2199 5928)					
602	5339		$C_4FH_{10}B$	$(CH_3CH_2)_2BF$	125	
606	5340	B	$C_4F_2H_9B$	$CH_3(CH_2)_3BF_2$	79	
607	5341		$C_4F_2H_{10}BN$	$(CH_3CH_2)_2NBF_2$	15	
606	5342	B	$C_5F_2H_{11}B$	$CH_3(CH_2)_4BF_2$	76	
608	5343	C	$C_5F_3H_4BClNO$		4.3	
608	5344	C[3]	$C_5F_3H_4BN_2O_3$		3.3	
608	5345	C[3]	$C_5F_3H_5BNO$			
606	5346	B	$C_6F_2H_{13}B$	$CH_3(CH_2)_5BF_2$	85	
608	5347	C[3]	$C_6F_3H_4BN_2O$		3.5	
608	5348	C[3]	$C_6F_3H_7BNO$		4.7	
608	5349	C[3]	$C_6F_3H_7BNO$		4.5	
608	5350	C	$C_6F_3H_7BNO_2$		5.0	
475	5351		$C_6F_3H_{15}BN$	$(CH_3CH_2)_3NBF_3$	18.4	
	(2201)					
605	5352	J	$C_6F_3H_{15}BP$	$(CH_3CH_2)_3PBF_3$	54.5	
	(6143)					
609	5353	G	$C_7FH_{19}BN$	$(CH_3CH_2)_2BFN(CH_3)_3$	67	
610	5354	A	$C_7F_2H_5BO_2$		5	

Table C.3. (contd.)

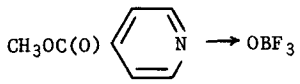
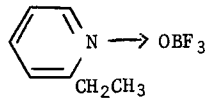
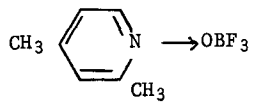
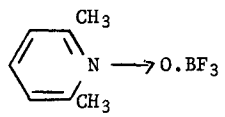
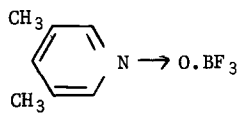
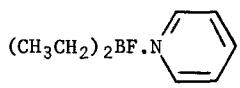
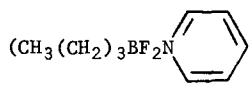
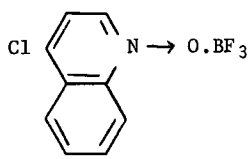
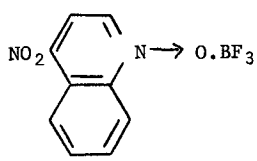
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J
609	5355	G	$C_7F_2H_{18}BN$	$CH_3(CH_2)_3BF_2.N(CH_3)_3$	67
608	5356	C^3	$C_7F_3H_7BNO_3$		3.8
608	5357	C^3	$C_7F_3H_9BNO$		4.5
608	5358	C^3	$C_7F_3H_9BNO$		5.2
608	5359	C^3	$C_7F_3H_9BNO$		4.9
608	5360	C^3	$C_7F_3H_9BNO$		4.6
607	5361		$C_8F_4H_{20}B_2N$	$\left[(CH_3CH_2)_2NBF_2\right]_2$	42
609	5362	G	$C_9FH_{15}BN$		77
609	5363	G	C_9FH_2BN	$(CH_3CH_2CH_2)_2BF.N(CH_3)_3$	58
609	5364	G	$C_9F_2H_{14}BN$		58
608	5365	C^3	$C_9F_3H_6BClNO$		4.1
608	5366	C^3	$C_9F_3H_6BN_2O$		3.3

Table C.3. (contd.)

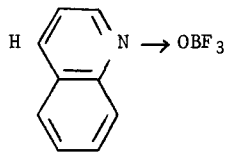
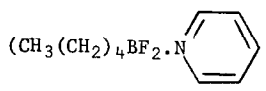
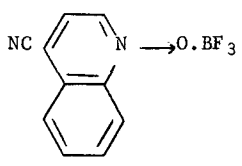
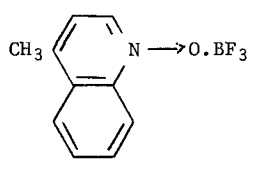
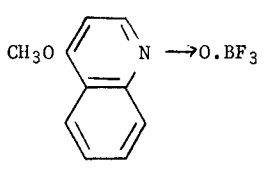
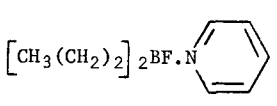
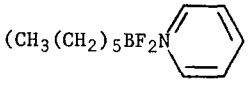
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J
608	5367	C[3]	$C_9F_3H_7BNO$		4.6
611	5368 (6273)		$C_9F_3H_{15}BP$	(cyclo C_3H_5)$_3$P.BF_3	52
611	5369 (6274)		$C_9F_3H_{21}BP$	$[(CH_3)_2CH]_3P.BF_3$	54.8
609	5370		$C_{10}F_2H_{16}BN$		58
608	5371		$C_{10}F_3H_6BN_2O$		3.4
608	5372		$C_{10}F_3H_9BNO$		4.8
608	5373		$C_{10}F_3H_9BNO_2$		5.3
609	5374	G	$C_{11}FH_{19}BN$		67
609	5375	G	$C_{11}FH_{27}BN$	$[CH_3(CH_2)_3]_2BF.N(CH_3)_3$	63
609	5376	G	$C_{11}F_2N_{18}BN$		58

Table C.3. (contd.)

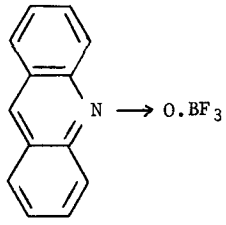
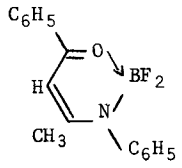
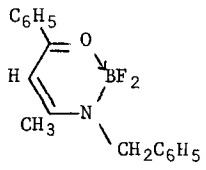
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J
608	5377	C[3]	$C_{13}F_3H_9BNO$		5.5
610	5378	A	$C_{16}F_2H_{14}BNO$		15.1
610	5379	A	$C_{17}F_2H_{16}BNO$		16.9

Table C.4. M = beryllium (Be)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J
613	5380	A[2]	$F_4H_8BeN_2$	$(NH_4)_2BeF_4$	33

Table C.5. M = bismuth (Bi)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J
979	5381		F_6BiK	$KBiF_6$	2700

Table C.6. M = carbon (C).

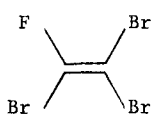
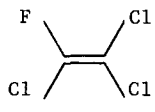
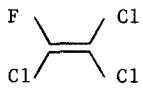
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	
614	5382		$CFBr_3$	$CFBr_3$	372	
615	5383		$CFCl_3$	$CFCl_3$	337	
615	5384		CFHO	HC(O)F	369	
6	5385		CFH_3	CFH_3	157.5	
	(6)					
5	5386	C	CFH_3	CFH_3	-161.9	
	(5)					
615	5387		CFH_3	CFH_3	158	
615	5388		CF_2Br_2	CF_2Br_2	358	
616	5389		CF_2Br_2	CF_2Br_2	357.8	
615	5390		CF_2Cl_2	CF_2Cl_2	325	
616	5391		CF_2Cl_2	CF_2Cl_2	324.7	
6	5392	D	CF_2H_2	CF_2H_2	235	
	(11)					
615	5393		CF_2H_2	CF_2H_2	232	
616	5394		CF_2H_2	CF_2H_2	233.4	
8	5395	D	CF_2H_2		-236.58	
	(12)	E			-232.78	
		F			-232.12	
615	5396		CF_3Br	CF_3Br	324	
615	5397		CF_3Cl	CF_3Cl	299	
615	5398		CF_3I	CF_3I	344	
6	5399	D	CF_3H	CF_3H	274.3	
	(14)					
615	5400		CF_3H	CF_3H	272	
8	5401	E	CF_3H	CF_3H	-274.12	
	(16)	F			-275.22	
		G			-274.22	
544	5402	B	CF_3H_3Si	CH_3SiF_3		+22.4
	(2442, 6680)					
615	5403		CF_4	CF_4	257	
615	5404		CF_5NS	$CF_3N{=}SF_2$	263	
617	5405		C_2FBr_3		323.6	39.9
618	5406		C_2FCl_3		303	43.7
617	5407		C_2FCl_3		303.1	44.2

Table C.6. (contd.)

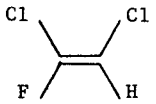
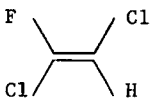
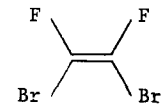
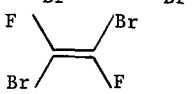
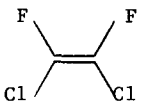
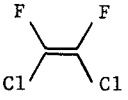
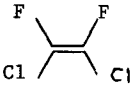
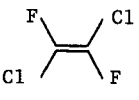
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
236	5408	A	C_2FHCl_2		300.0		
619	(989)	B	(50% v/v)		300.0	53.0	
		F			298.0		
		L			297.0		
		M			298.6		
		Q			300.0		
236	5409	A	C_2FHCl_2		306.2		
619	(990)	B	(50% v/v)		306.2	20.0	
		D			306.9		
		F			304.2		
		L			302.9		
		M			304.5		
		Q			306.6		
144	5410	B	$C_2FH_2NaO_2$	CFH_2CO_2Na	177.0	18.3	
615	5411		C_2FH_3O	$CH_3C(O)F$	353		
617	5412		$C_2F_2Br_2$	$CF_2{=}CBr_2$	289.9	43.1	
240	5413		$C_2F_2Br_2$		324.7	35.8	
617	(3406)						
240	5414		$C_2F_2Br_2$		355.0	102.5	
617	(3407)						
144	5415	A^2	$C_2F_2ClNaO_2$	CF_2ClCO_2Na	305.2	29.0	
618	5416		$C_2F_2Cl_2$	$CF_2{=}CCl_2$	-289	+44.2	
617	5417		$C_2F_2Cl_2$	$CF_2{=}CCl_2$	288.9	43.7	
620	5418		$C_2F_2Cl_2$		-299.26	+38.10	
	(3410)						
617	5419		$C_2F_2Cl_2$		299.3	38.1	
621	5420	B	$C_2F_2Cl_2$		-299.0	+37.0	
	(3411)						
620	5421		$C_2F_2Cl_2$		+289.57	-53.85	
	(3412)						
617	5422		$C_2F_2Cl_2$		289.6	53.9	
							

Table C.6. (contd.)

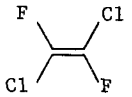
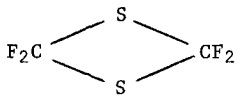
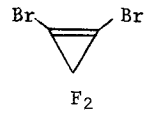
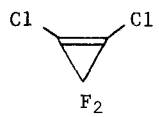
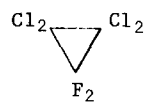
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
621	5423 (3413)	B	$C_2F_2Cl_2$		-291.0	+54.5	
615	5424		$C_2F_2D_2$	$CF_2=CD_2$	287		
144	5425	B	$C_2F_2HClO_2$	CF_2ClCO_2H	299.1	36.6	
616	5426		C_2F_2HN	CF_2HCN	243.5		
144	5427	A^2	$C_2F_2HNaO_2$	CF_2HCO_2Na	245.7	25.9	
144	5428	B	$C_2F_2H_2O_2$	CF_2HCO_2H	247.2	27.5	
615	5429		$C_2F_2H_3Cl$	CF_2ClCH_3	288		
618	5430		$C_2F_3Cl_3$	CF_3CCl_3	283	-43.1	
144	5431	A^2	$C_2F_3NaO_2$	CF_3CO_2Na	290.9	35.6	
618	5432		$C_2F_3HO_2$	CF_3CO_2H	283	-44.1	
144	5433	B	$C_2F_3HO_2$	CF_3CO_2H	283.8	41.7	
622	5434	A^3	$C_2F_3HO_2$	CF_3CO_2H	283		
615	5435		$C_2F_3H_2Br$	CF_3CH_2Br	272	-38.5	
615	5436		$C_2F_3H_2Cl$	CF_3CH_2Cl	274		
615	5437		$C_2F_3H_3$	CF_3CH_3	271		
615	5438		$C_2F_3H_3O$	CF_3CH_2OH	278		
1127	5439 (4087)	C	$C_2F_4S_2$		-315.31		13.49
623	5440	B	C_2F_6	CF_3CF_3 (-80^oC)	281.3	46.0	
615	5441		C_2F_6O	$(CF_3)_2O$	265		
624	5442		$C_3F_2Br_2$		320		
624	5443		$C_3F_2Cl_2$		292		
624	5444		$C_3F_2Cl_4$		313		
510	5445 (2330 5919)	S^2	$C_3F_2H_9P$	$(CH_3)_3PF_2$		+30.9	
615	5446		$C_3F_3Cl_3$	$CF_3CCl=CCl_2$	274	-39.2	
615	5447		$C_3F_3H_3O$	$CF_3C(O)CH_3$	289		

Table C.6. (contd.)

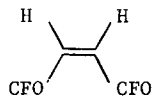
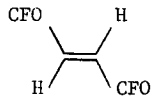
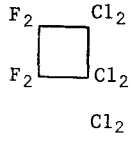
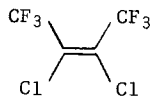
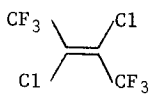
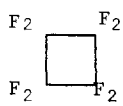
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J	^nJ
1059	5448 (3401)		C_3F_4	$CF_3C\equiv CF$ (2)(1)(3)	1,2	259.0	1,3	57.7	
615	5449		C_3F_8	$(CF_3)_2CF_2$	1,3	285	1,4	-40.0	
				(3)(1)(4)(2)	2,4	265	2,3	-32.5	
615	5450 (2771)		C_3F_9N	$(CF_3)_3N$		269			
472	5451 (2165)		C_4FH_3S			285			
472	5452 (2166)		C_4FH_3S			256			
615	5453		C_4FH_9	$(CH_3)_3CF$		167			
256	5454 (1130 3647)		$C_4F_2H_2O_2$			346			
256	5455 (1131 3648)		$C_4F_2H_2O_2$			345		72	
615	5456		$C_4F_3H_5O_2$	$CF_3CO_2CH_2CH_3$		284		-44.1	
280	5457	G	$C_4F_4Cl_4$			-299.67		+26.94	
615	5458		$C_4F_4Cl_4$	Cyclic $C_4F_4Cl_4$ (Structure not identified)		300			
615	5459		C_4F_6	$CF_3C\equiv CCF_3$		256		-57.2	
625	5460 (2795)		$C_4F_6Cl_2$			275.3			
625	5461 (2795)		$C_4F_6Cl_2$			275.7			
956	5462 (2796)	T^3	$C_4F_6Cl_4$	$CF_3CCl_2CCl_2CF_3$		285.6			
626	5463	B	$C_4F_6O_2S_2N_2$	$(CF_3SNCO)_2$		314			
615	5464		C_4F_8			298		-25.8	

Table C.6. (contd.)

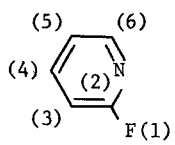
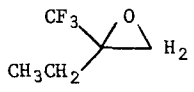
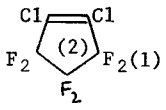
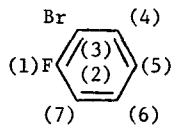
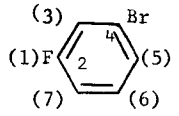
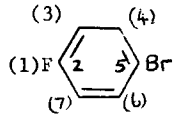
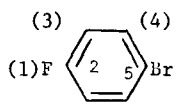
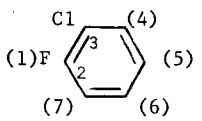
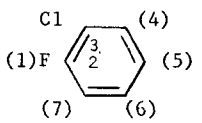
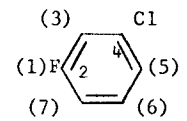
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
996	5465 (2830)		C_4F_{10}	$CF_3CF_2CF_2CF_3$ (1)(2)(3)(4)	1,2 3,4	286 267				
628	5466	*	C_5FH_4N		1,2	236.7	1,3	37.4	1,4 1,5 1,6	7.75 4.2 14.7
615	5467		$C_5F_3H_7O$			278				
627	5468		$C_5F_6Cl_2$		1,2	262				
628	5469 (1804)	*	C_6FH_4Br		1,2	247.0	1,3 1,7	20.7 21.95	1,4 1,5 1,6	0 3.35 7.1
628	5470 (1805)	*	C_6FH_4Br		1,2	250.4	1,3 1,7	24.5 21.1	1,4 1,5 1,6	9.3 3.4 8.4
628	5471 (1806)	*	C_6FH_4Br		1,2	246.7	1,3	23.7	1,4 1,5	8.0 3.3
615	5472 (1807)		C_6FH_4Br			247				
628	5473 (1808)	*	C_6FH_4Cl		1,2	248.7	1,3 1,7	17.5 20.8	1,4 1,5 1,6	0 4.05 7.2
615	5474 (1808)		C_6FH_4Cl			244				
628	5475 (1809)	*	C_6FH_4Cl		1,2	249.5	1,3 1,7	24.6 21.3	1,4 1,5 1,6	10.0 3.4 8.9

Table C.6. (contd.)

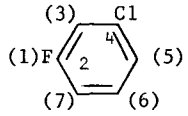
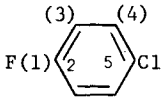
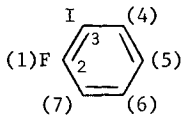
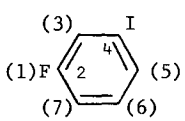
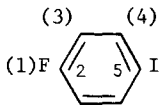
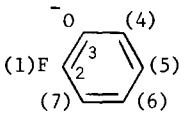
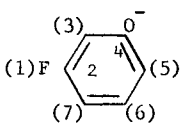
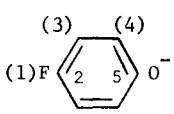
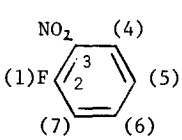
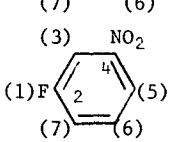
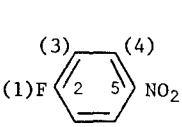
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
615	5476 (1809)		C_6FH_4Cl			248				
628	5477 (1810)	*	C_6FH_4Cl		1,2	245.5	1,3	23.1	1,4	8.2
									1,5	3.1
628	5478 (1813)	*	C_6FH_4I		1,2	245.6	1,3	25.2	1,4	1.46
							1,7	23.4	1,5	3.5
									1,6	7.2
628	5479 (1814)	*	C_6FH_4I		1,2	249.0	1,3	23.2	1,4	7.8
							1,7	20.8	1,5	3.3
									1,6	8.1
628	5480 (1815)	*	C_6FH_4I		1,2	247.4	1,3	22.2	1,4	7.6
									1,5	3.4
628	5481	E^2*	$C_6FH_4O^-$		1,2	235.8	1,3	12.15	1,4	3.4
							1,7	19.0	1,5	3.3
									1,6	7.0
628	5482	E^2*	$C_6FH_4O^-$		1,2	241.4	1,3	21.5	1,4	11.4
							1,7	21.4	1,5	2.4
									1,6	11.0
628	5483	E^2*	$C_6FH_4O^-$		1,2	236.1	1,3	22.7	1,4	8.0
									1,5	1.6
628	5484 (1816)	*	$C_6FH_4NO_2$		1,2	264.4	1,3		1,4	4.25
							1,7	20.6	1,5	2.8
									1,6	8.7
628	5485 (1817)	*	$C_6FH_4NO_2$		1,2	250.9	1,3	26.5	1,4	8.3
							1,7	24.5	1,5	3.3
									1,6	8.2
628	5486 (1819)	*	$C_6FH_4NO_2$		1,2	256.6	1,3	24.0	1,4	10.2

Table C.6. (contd.)

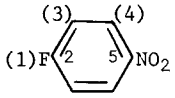
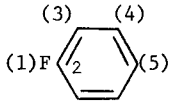
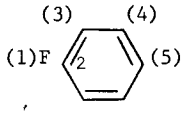
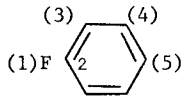
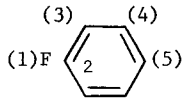
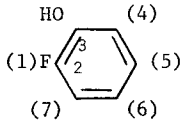
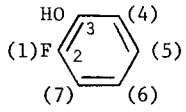
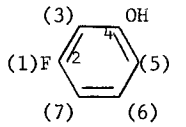
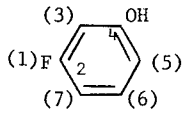
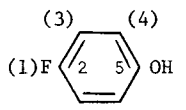
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
615	5487 (1819)		$C_6FH_4NO_2$			257				
615	5488		C_6FH_5			244				
389	5489 (1829)	*	C_6FH_5			265.5				
391	5490 (1823)	B*	C_6FH_5			252		17.5		
628	5491	*	C_6FH_5		1,2	245.3	1,3	21.0	1,4 1,5	7.7 3.3
628	5492	*	C_6FH_5O		1,2	238.8	1,3 1,7	13.7 18.0	1,4 1,5 1,6	1.94 3.78 6.6
629	5493		C_6FH_5O			241.6				
628	5494	*	C_6FH_5O		1,2	244.5	1,3 1,7	24.8 21.2	1,4 1,5 1,6	11.3 3.0 10.2
629	5495		C_6FH_5O			244.7				
628	5496	*	C_6FH_5O		1,2	237.4	1,3	23.0	1,4 1,5	7.9 2.14

Table C.6. (contd.)

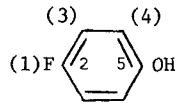
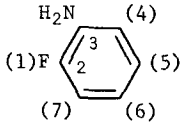
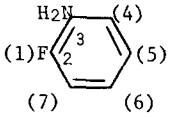
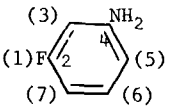
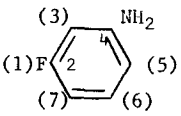
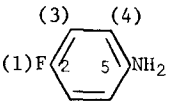
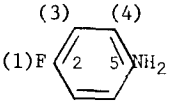
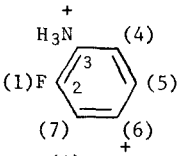
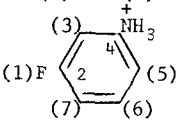
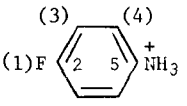
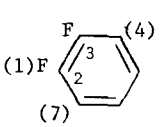
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
629	5497		C_6FH_5O			240.7				
628	5498	*	C_6FH_6N		1,2	237.5	1,3	12.7	1,4	3.8
							1,7	18.4	1,5	3.6
									1,6	6.7
629	5499		C_6FH_6N			236.7				
628	5500	*	C_6FH_6N		1,2	241.4	1,3	24.6	1,4	11.0
							1,7	21.3	1,5	2.3
									1,6	10.2
629	5501		C_6FH_6N			243.9				
628	5502	*	C_6FH_6N		1,2	233.2	1,3	22.4	1,4	7.5
									1,5	1.86
629	5503		C_6FH_6N			233.3				
628	5504	*	$C_6FH_7N^+$		1,2	248.6	1,3	13.8	1,4	0
							1,7	18.4	1,5	3.9
									1,6	7.5
628	5505	*	$C_6FH_7N^+$		1,2	247.5	1,3	25.6	1,4	9.8
							1,7	21.2	1,5	3.4
									1,6	8.9
628	5506	*	$C_6FH_7N^+$		1,2	246.8	1,3	23.7	1,4	9.1
									1,5	3.2
628	5507 [1894 1895 4132]	*	$C_6F_2H_4$		1,2	248.8	1,3	14.1	1,4	-3.0
							1,7	20.5		

Table C.6. (contd.)

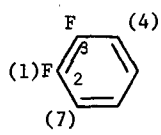
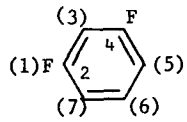
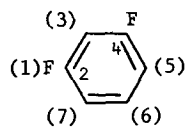
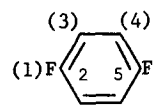
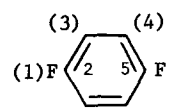
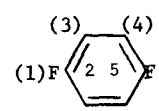
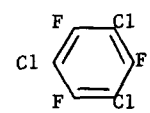
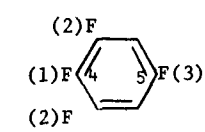
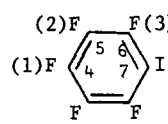
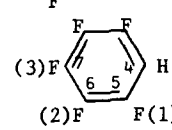
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
629	5508		$C_6F_2H_4$			254.5				
628	5509	*	$C_6F_2H_4$		1,2	245.4	1,3	25.3	1,4	12.1
	[4134						1,7	21.2	1,5	3.6
	1897								1,6	9.8
	1898]									
629	5510		$C_6F_2H_4$			250.8				
628	5511	*	$C_6F_2H_4$		1,2	242.0	1,3	24.3	1,4	8.5
	(1901)								1,5	3.8
629	5512		$C_6F_2H_4$			234.3				
418	5513	*	$C_6F_2H_4$			241.07				
	(1902									
	4137)									
615	5514		$C_6F_3Cl_3$			253				
628	5515		$C_6F_4H_2$				2,4	15.2	3,4	5.8
									2,5	13.0
									1,5	3.8
628	5516		C_6F_5I		1,4	255	3,7	28.4	2,7	1.3
					2,5	257	3,4	13.5	3,4	4.6
					3,6	254			1,7	4.8
628	5517		C_6F_5H				1,4	23.4	3,4	3.7
	(4343						2,7	13.2	1,7	5.2
	1986)									
630	5518		C_6F_6	C_6F_6		260				
112	5519		$C_6F_6H_{10}Sn$	$CF_3CFHCF_2Sn(CH_3)_3$	1,2	302				
	[423			(2) (1)						
	2918									
	6812]									

Table C.6. (contd.)

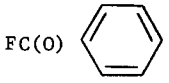
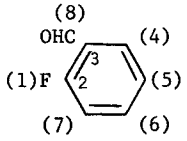
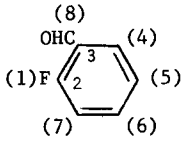
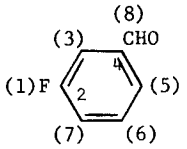
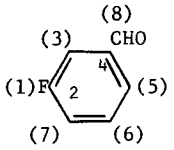
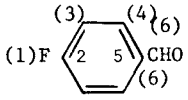
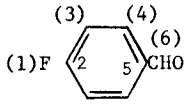
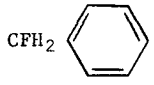
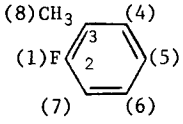
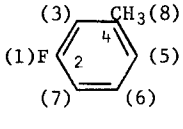
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
615	5520		C_7FH_5O			344				
628	5521 (1832)	*	C_7FH_5O		1,2	257.7	1,3	8.2	1,4	1.86
							1,7	20.45	1,5	3.75
									1,6	9.1
									1,8	6.4
629	5522		C_7FH_5O			256.4				
628	5523 (1833)		C_7FH_5O		1,2	248.2	1,3	21.7	1,4	6.3
							1,7	21.8	1,5	2.9
									1,6	7.8
									1,8	2.4
629	5524		C_7FH_5O			236.7				
628	5525 (1834)		C_7FH_5O		1,2	255.0	1,3	22.4	1,4	9.7
									1,5	2.6
									1,6	0
629	5526		C_7FH_5O			257.6				
615	5527		C_7FH_7			165				
628	5528	*	C_7FH_7		1,2	243.9	1,3	17.0	1,4	4.8
							1,7	22.1	1,5	3.7
									1,6	7.9
									1,8	3.8
628	5529	*	C_7FH_7		1,2	243.6	1,3	21.1	1,4	7.2
							1,7	21.2	1,5	2.2
									1,6	8.5
									1,8	1.75

Table C.6. (contd.)

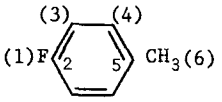
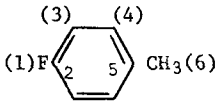
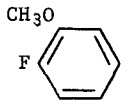
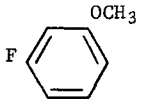
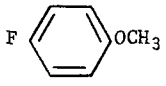
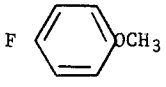
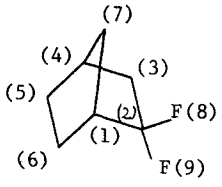
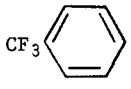
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
628	5530	*	C_7FH_7		1,2	243.5	1,3	21.1	1,4 1,5 1,6	7.75 2.9 0
615	5531		C_7FH_7			241				
629	5532		C_7FH_7O			246.2				
629	5533		C_7FH_7O			246.1				
629	5534		C_7FH_7O			236.8				
615	5535		C_7FH_7O			237				
631	5536	B	$C_7F_2H_{10}$		8,2 9,2	253.9 253.9	8,1 9,1 8,3 9,3	24.1 22.0 24.3 22.0	8,4 9,4 8,6 9,6 8,7 or 9,7	5.4 2.8 5.8 5.8 4.9
632	5537	P	$C_7F_3H_4NO_2$			275				
632	5538		$C_7F_3H_5$			272				
615	5539		$C_7F_3H_6N$			270		-32.4		

Table C.6. (contd.)

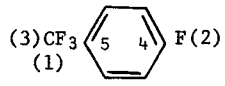
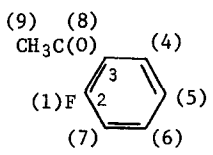
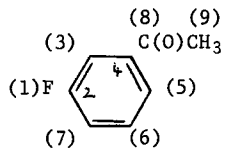
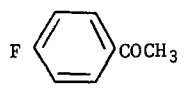
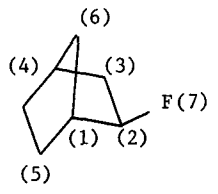
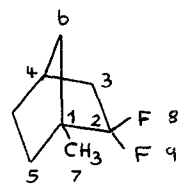
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
632	5540		$C_7F_3H_6N$			270				
615	5541		$C_7F_4H_4$		1,3 2,4	271 252	1,5	-33.2		
628	5542	*	C_8FH_7O		1,2	254.2	1,3 1,7	12.8 23.7	1,4 1,5 1,6 1,8 1,9	2.54 3.4 9.0 3.2 <0.4
628	5543	*	C_8FH_7O		1,2	246.3	1,3 1,7	22.2 21.6	1,4 1,5 1,6 1,8 1,9	5.9 2.9 7.75 1.9 0.68
615	5544		C_8FH_7O			253				
631	5545	B	C_8FH_{13}		7,2	182.0	7,1 7,3	20.2 20.4	7,4 7,5 7,6	2.3 9.8 <1
631	5546	B	$C_8F_2H_{12}$		8,2 9,2	256.5 256.5	8,1 9,1 8,3 9,3	21.9 21.9 24.7 22.7	8,4 9,4 8,5 9,5 8,6 or 9,6 8,7 or 9,7	4.5 2.6 6.3 4.2 5.3 4.0

Table C.6. (contd.)

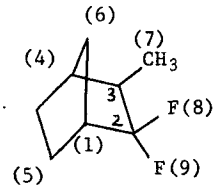
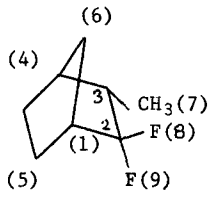
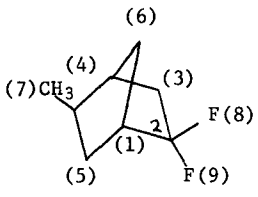
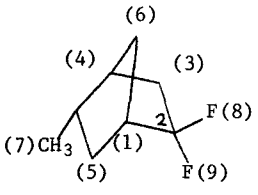
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
631	5547	B	$C_8F_2H_{12}$		8,2 258 9,2 258	8,1 {24.0 9,1 {21.8 8,3 {24.0 9,3 {20.3	8,4 {5.6 9,4 {1.2 8,5 5.8 9,5 5.8 8,6 or 9,6 4.7 8,7 14.1 9,7 2.7
631	5548	B	$C_8F_2H_{12}$		8,2 {259.9 9,2 {252.6	8,1 {24.2 9,1 {22.4 8,3 {22.4 9,3 {22.1	8,4 {4.4 9,4 {1.9 8,5 {6.9 9,5 {5.9 8,6 or 9,6 5.8 8,7 9.7 9,7 1.5
631	5549	B	$C_8F_2H_{12}$		8,2 {255.0 9,2 {250.2	8,1 {23.0 9,1 {21.8 8,3 {23.6 9,3 {21.6	8,4 3.2 9,4 3.2 8,5 6.0 9,5 6.0 8,6 or 9,6 5.0 8,7 <1 9,7
631	5550	B	$C_8F_2H_{12}$		8,2 {254.0 9,2 {251.6	8,1 {23.5 9,1 {21.3 8,3 {24.6 9,3 {21.8	8,4 {4.2 9,4 {2.2 8,5 6.0 9,5 6.0 8,6 or 9,6 4.0 8,7 <1 9,7

Table C.6. (contd.)

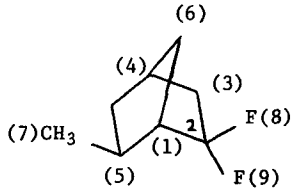
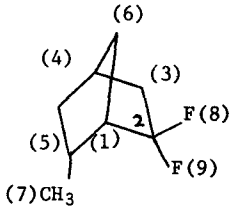
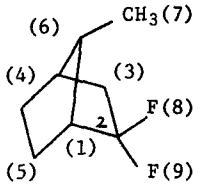
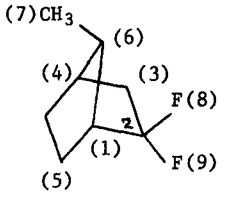
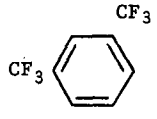
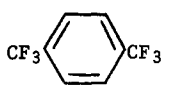
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ	
631	5551	B	$C_8F_2H_{12}$		8,2 9,2	255.0 250.2	8,1 9,1 8,3 9,3	22.3 20.9 23.1 21.1	8,4 9,4 8,5 9,5 8,6 or 9,6 8,7 or 9,7	4.6 2.0 5.8 5.8 5.0 ≈1
631	5552	B	$C_8F_2H_{12}$		8,2 9,2	257.3 250.3	8,1 9,1 8,3 9,3	22.3 19.1 21.8 21.8	8,5 9,5 8,6 or 9,6 8,7 or 9,7	3.4 3.4 5.2 7.0 <1
631	5553		$C_8F_2H_{12}$		8,2 9,2	253 253	8,1 9,1 8,3 9,3	20.7 20.7 25.4 21.6	8,4 9,4 8,5 9,5 8,6 or 9,6 8,7 9,7	4.0 3.0 8.1 6.8 5.5 4.5 <1
631	5554		$C_8F_2H_{12}$		8,2 9,2	254.5 254.5	8,1 9,1 8,3 9,3	22.6 20.6 24.1 21.7	8,4 9,4 8,5 9,5 8,6 or 9,6 8,7 or 9,7	3.5 2.6 5.8 5.8 4.3 <1
615	5555		$C_8F_6H_4$			272				
615	5556		$C_8F_6H_4$			271		-32.9		

Table C.7. M = cobalt (Co)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J
875	5556a	A^2	$C_{12}CoKP_4$	$K[Co(PF)_4]$	57

Table C.8. M = deuterium (D)

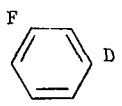
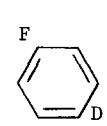
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^4J
571	5557 (5642)		F_2DOP	$DP(O)F_2$	18		
571	5558 (5642)		F_2DPS	$DP(S)F_2$	15.1		
1145	5559	D	C_6FH_4D			1.4	
		E^2				1.3	
		K^2				1.3	
1145	5560	D	C_6FH_4D				0.8
		E^2					0.9
		K^2					0.9
1145	5561	D	C_6FH_4D				<0.2
		E^2					<0.2
		K^2					<0.2

Table C.9. M = germanium (Ge).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^3J	^4J
860	5562		F_6Ge^{2-}	GeF_6^{2-}	98		

Table C.10. M = mercury (Hg).

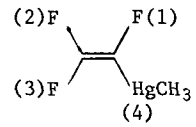
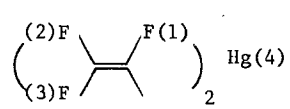
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^2J	^nJ
243	5563 (915)	B	$C_3F_3H_3Hg$		1,4 +584.6	2,4 +48.31 3,4 +118.5
243	5564 (3487)		C_4F_6Hg		1,4 +820.5	2,4 +33.31 3,4 +220.90

Table C.10 (contd.)

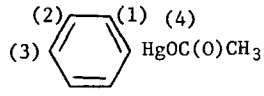
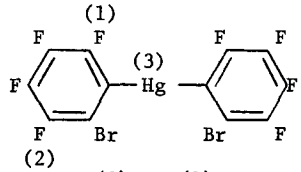
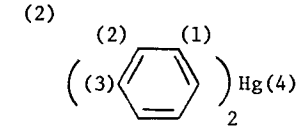
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
633	5565		$C_4F_6H_4Hg$	$(CF_3CH_2)_2Hg$			224
633	5566		$C_4F_8H_2Hg$	$(CF_3CHF)_2Hg$		480	161
633	5567		$C_4F_{10}Hg$	$(CF_3CF_2)_2Hg$		770	71
634	5568		$C_6F_{10}Hg$	$[CF_2=C(CF_3)]_2Hg$(4)			1,4 131.6
	(3293 3546)			(2,3) (1)			2,4 236.7
							3,4 323.7
634	5569		$C_6F_{11}HHg$	$(CF_3)_2CHHgC(CF_3)=CF_2$			1,5 131.6
	[431 3295 3547]			(4) (5) (1) (2,3)			2,5 236.7
							3,5 323.7
							4,5 188.4
634	5570		$C_6F_{12}H_2Hg$	$[(CF_3)_2CH]_2Hg$			1,2 188.4
	(433)			(1) (2)			
635	5571		$C_7F_3H_4BrHg$	ortho $CF_3C_6H_4HgBr$			28.8
635	5572		$C_7F_3H_4BrHg$	meta $CF_3C_6H_4HgBr$			18.3
635	5573		$C_7F_3H_4BrHg$	para $CF_3C_6H_4HgBr$			16.7
636	5574	F	$C_8F_5H_3HgO_2$				1,4 +597.0
	(4410)						2,4 +215.0
							3,4 +29.0
634	5575		$C_8F_{14}HgO_2$	$[(CF_3)_2C(COF)]_2Hg$			1,2 163
	(3660)			(1) (2)			
894	5576		$C_{12}F_8Br_2Hg$				1,3 462.0
							2,3 112.0
636	5577	F	$C_{12}F_{10}Hg$				1,4 +443.0
	(4453)						2,4 +116.0
							3,4 +14.4
635	5578		$C_{14}F_6H_8Hg$	(ortho $CF_3C_6H_4)_2Hg$			26.5
635	5579		$C_{14}F_6H_8Hg$	(meta $CF_3C_6H_4)_2Hg$			9.5
635	5580		$C_{14}F_6H_8Hg$	(para $CF_3C_6H_4)_2Hg$			8.0

Table C.11. M = nitrogen (N).

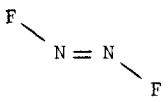
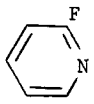
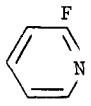
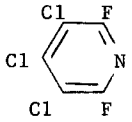
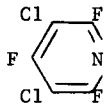
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
637	5581		FNO_2	FNO_2		113		
638	5582 (4889)		F_2N_2			145	37	
638	5583 (4889)		F_2N_2			136	73	
639	5584		F_3N	NF_3		160		
638	5585		F_3N	NF_3		155		
640	5586		F_3NO	F_3NO		135.5		
641	5587		F_3NO	F_3NO		136		
642	5588		F_7AsN_2	$FN{=}N^+AsF_6^-$		328		
643	5589 (5291)	D^2	$F_{10}AsN$	$NF_4^+AsF_6^-$		234		
644	5590		CFN	FCN			33	
21	5591		CFN_3O_6	$FC(NO_2)_3$			9.8	
645	5592 (4690)		CF_5NO	CF_3ONF_2		125.7		
646	5593		C_5FH_4N				43.8	
647	5594	B	C_5FH_4N				45.8	
		G					48.7	
		E^2	(50% Mole)				44.5	
		H^2					46.6	
		J^2					45.0	
		E^3					47.6	
		F^3					44.0	
648	5595	B	$C_5F_2Cl_3N$		^{15}N ^{15}N		52.24 37.2	
649	5596 (4613)	B	$C_5F_3Cl_2N$		^{15}N ^{15}N		52.60 37.50	

Table C.12. M = niobium (Nb)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
650	5597	J^2	F_6Nb^-	NbF_6^-	345		
651	5598		$C_2F_5H_6NbOS$	$NbF_5.2(CH_3)_2SO$	335		

Table C.12 (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
651	5599		$C_8F_5H_{16}NbS$	$NbF_5.2$ 	335		
651	5600		$C_{10}F_5H_{10}N_2Nb$	$NbF_5.$ 2N 	335		

Table C.13. M = oxygen (O).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
652	5601		C_2FH_3O	$CH_3C(O)F$		39	

Table C.14. M = phosphorus (P).

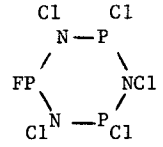
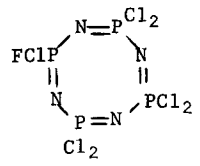
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
653	5602		FBr_2OP	$FPBr_2(O)$	1263		
654	5603		FBr_2P	$FPBr_2$	1292		
655	5604		FBr_2PS	$FPBr_2(S)$	1275		
656	5605		FCl_2OP	$FPCl_2(O)$	1175		
657	5606	B	FCl_2OP	$FPCl_2(O)$	1175		
658	5607	B	FCl_2OP	$FPCl_2(O)$	1180		
668	5608		FCl_2OP	$FPCl_2(O)$	1178		
657	5609	B	FCl_2P	$FPCl_2$	1320		
654	5610		FCl_2P	$FPCl_2$	1326		
655	5611	E^2	FCl_2PS	$FPCl_2(S)$	1240		
659	5612		FCl_4NOP_2	$FPCl(O)N{=}PCl_3$	1041		23
660	5613		FCl_4P	$FPCl_4$	992		
661	5614		$FCl_5N_3P_3$		1012		
674	5615		$FCl_7N_4P_4$		950		

Table C.14 (contd.)

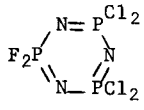
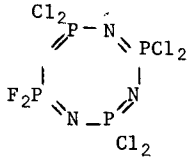
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
662	5616		FCl_9PSb	$FPCl_3.SbCl_6$	1296		
502	5617	A^2	FNa_2O_3P	Na_2PO_3F	863		
663	5618	A^2	FO_3P^{2-}	$FP(O_2)O^{2-}$	866		
663	5619	A^2	$FO_7P_3^{4-}$	$FP(O_2)OP(O_2)OPO_3^{4-}$	923		
664	5620		FH_2BrNPS	$FP(S)BrNH_2$	1141		
570	5621		FH_2O_2P	$H_2PF(O_2)$	1029		
	(2526)						
502	5622	A^2	$FH_8N_2O_3P$	$(NF_4)_2PO_3F$	895		
653	5623		F_2BrOP	$F_2P(O)Br$	1203		
654	5624		F_2BrP	F_2PBr	1395		
665	5625		F_2BrPS	$F_2P(S)Br$	1249		
657	5626	B	F_2ClOP	$F_2P(O)Cl$	1120		
668	5627		F_2ClOP	$F_2P(O)Cl$	1122		
657	5628	B	F_2ClP	F_2PCl	1390		
669	5629		F_2ClP	F_2PCl	1380		
665	5630		F_2ClPS	$F_2P(S)Cl$	1218		
670	5631		$F_2Cl_2NO_2PS$	$F_2PCl{=}NSO_2Cl$	1120		
656	5632		$F_2Cl_2O_3P$	$[FP(O)Cl]_2O$	1121		
659	5633		$F_2Cl_3NOP_2$	$F_2P(O)N{=}PCl_3$	973.5		21.5
671	5634		$F_2Cl_3NP_2S$	$F_2PCl{=}NP(S)Cl_2$	1091		5
660	5635		F_2Cl_3P	F_2PCl_3	1051		
672	5636		$F_2Cl_4N_3P_3$		934		-14
673	5637						
674	5638		$F_2Cl_6N_4P_4$		925		
675	5639	F	F_2CsO_2P	$Cs^+PF_2O_2^-$	952		
531	5640	F	F_2CsPS_2	$Cs^+PF_2S_2^-$	1152		
675	5641	F	F_2CsPS_2	$Cs^+PF_2S_2^-$	1164		
571	5642		F_2DOP	$DP(O)F_2$	1120		
	(5557)						
571	5643		F_2DPS	$DP(S)F_2$	1148		
	(5558)						
502	5644	A^2	F_2KO_2P	KPO_2F_2	960		
676	5645	A^2	$F_2K_2OP_2S$	$K_2[P_2F_2OS]$	940		-8
677	5646	B	F_2N_3PS	$F_2P(S)N_3$	1140		

Table C.14 (contd.)

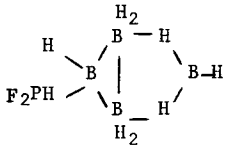
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
502	5647	A^2	F_2NaO_2P	$NaPO_2F_2$	959		
514	5648		$F_2O_2P^-$	$PO_2F_2^-$	954		
678	5649		F_2PS_2	PS_2F_2	1195		
571	5650		F_2HOP	$HP(O)F_2$	1121		
	(2528)						
570	5651		F_2HOP	$HP(O)F_2$	114		
679	5652		F_2HO_2P	$HP(O_2)F$	981		
680	5653		$F_2HO_2P_2$	$HP(O_2)F$	974		
681	5654		F_2HO_2P	$HP(O_2)F$	978		
682	5655		F_2HO_2P	$HP(O_2)F$	992		
572	5656		F_2HP	F_2PH	1134		
	(2530)						
544	5657	B	F_2HP	F_2PH	1136.7		
	(2529)						
571	5658		F_2HPS	$F_2PH(S)$	1153		
573	(2531)						
531	5659	B	F_2HPS_2	$HSP(S)F_2$	1214		
680	5660		F_2H_2NOP	$H_2NP(O)F_2$	984		
683	5661		F_2H_2NPS	$F_2P(S)NH_2$	1078		
574	5662		$F_2H_2P_2$	H_2PPF_2	1203	82	
	(2532)						
502	5663	A^2	$F_2H_4NO_2P$	$NH_4P(O_2)F_2$	960		
519	5664		$F_2H_8B_3P$	$F_2PH.B_3H_7$	1110		
	(2533)						
520	5665	B	$F_2H_9B_4P$		1120		
	(2534)						
507	5666		F_3Br_2P	F_3PBr_2 (<120°) 1a,2	1141		
530	(4923)			(1)(2) 1e,2	1143		
684							
990							
670	5667		F_3ClNO_2PS	$F_3P{=}NSO_2Cl$	1078		
671	5668		$F_3Cl_2NP_2S$	$F_3P{=}NP(S)Cl_2$	1044		
657	5669		F_3Cl_2P	F_3PCl_2 (-22°)	1048		
660				(-144°)	1032, 1092		
507	5670		F_3Cl_2P	F_3PCl_2 (25°)	1050		
530	(4924)			(-130°)	1023		
684					1085		

Table C.14. (contd.)

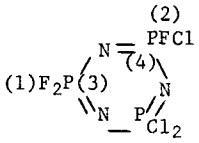
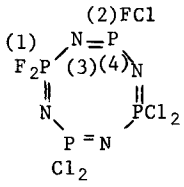
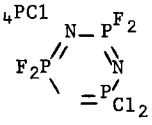
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
673	5671		$F_3Cl_3N_3P_3$		1,3 2,4	880 1000		
674	5672		$F_3Cl_5N_4P_4$		1,3 2,4	925 950		
668	5673		F_3OP	F_3PO		1057		
657	5674		F_3OP	F_3PO		1055		
658	5675	B	F_3OP	F_3PO		1080		
685	5676		F_3OP	F_3PO		1055		
686	5677		$F_3O_3PS_2$	$F_2P(S)OSO_2F$		1240		
685	5678		F_3O_4PS	$F_2P(O)OSO_2F$		1085		
	(5284)							
685	5679		$F_3O_7PS_2$	$FP(O)(OSO_2F)_2$		1100		
	(5285)							
668	5680		F_3P	PF_3		1402		
639	5681		F_3P	PF_3		1441		
657	5682	B	F_3P	PF_3		1400		
658	5683	B	F_3P	PF_3		1410		
688	5684	B	F_3P	PF_3		1441		
502	5685	B	F_3P	PF_3		1405		
689	5686	A	F_3P	PF_3		1418		
		B				1404		
		G				1423		
		G[3]				1411		
		H[3]				1415		
573	5687		F_3PS	F_3PS		1189		
665	5688		F_3PS	F_3PS		1180		
575	5689	M	$F_3H_4N_2P$	$F_3P(NH_2)_2$	1a,2	672		
	(2535 4925)			(1)(2)	1e,2	860		
671	5690		F_4ClNP_2S	$F_3P{=}NPFCl(S)$	1,3	1031	1,4	2.8
	(4926)			(1)(3)(4)(2)	2,4	1115	2,3	27
690	5691		F_4ClP	F_4PCl		1000		
673	5692		$F_4Cl_2N_3P_3$			860		

Table C.14. (contd.)

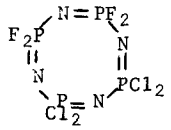
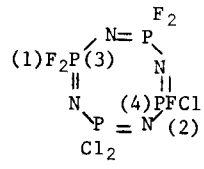
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
674	5693		$F_4Cl_4N_4P_4$		900		
691	5694 (5286)		F_4NOPS	$F_2P(O)N{=}SF_2$	1026		28
683	5695 (5287)	B	F_4NO_2PS	$F_3P{=}NSO_2F$	1090		16
692	5696		F_4OP_2	F_2POPF_2	1358		-14
693	5697 (4927)	B*	$F_4OP_2S_2$	$F_2P(S)OP(S)F_2$	1168.2		
694	5698	P	$F_4O_2P_2$	$F_2P(O)OPF_2$	1396.4 1032.5		
695	5699		$F_4O_3P_2$	$F_2P(O)OP(O)F_2$	1054		
693	5700 (4928)	B	$F_4O_3P_2$	$F_2P(O)OP(O)F_2$	1062.9		2.9
502	5701		$F_4O_3P_2$	$F_2P(O)OP(O)F_2$	980		
682	5702		$F_4O_3P_2$	$F_2P(O)OP(O)F_2$	1048		
696	5703	B	F_4P_2	F_2PPF_2	-1191.1	+64.0	
700	5704 (4929)	*	F_4P_2	F_2PPF_2	1198.5	67.5	
696	5705	B	F_4P_2S	F_2PSPF_2	-1306.3		+31.3
694	5706 (4930)	P	$F_4P_2S_2$	$F_2P(S)SPF_2$ (1)(3)(4)(2)	1,3 1217.9 2,4 1391.6	1,4 15.0 2,3 22.2	
531	5707	B	$F_4P_2S_4$	$(F_2PS_2)_2$	1268		
503	5708	R	$F_4H_2N_2O_2P_2$	$F_2P(O)NHNHP(O)F_2$	1024		
519	5709 (2537)		$F_4H_6B_2P_2$	$(F_2PH)_2B_2H_4$	1147		
674	5710	B	$F_5Cl_3N_4P_4$		1,3 900 2,4 975		
697	5711 (4931)		F_5NP_2	$F_3P{=}N{-}PF_2$ (1)(3)(4)(2)	1,3 1031 2,4 1279		2,3 24.1
671	5712		F_5NP_2S	$F_3P{=}N{-}PF_2(S)$ (1)(3)(4)(2)	1,3 1022 2,4 1080	1,4 2,3	30
683	5713	B	F_5NP_2S	$F_3P{=}N{-}PF_2(S)$ (1)(3)(4)(2)	1,3 1112 2,4 1045		

Table C.14. (contd.)

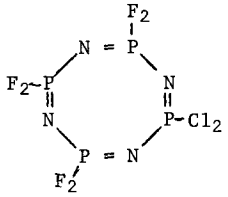
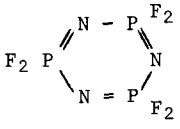
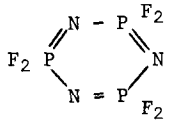
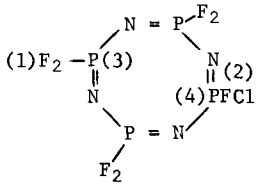
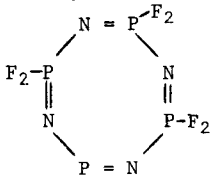
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
668	5714		F_5P	PF_5		929		
639	5715		F_5P	PF_5		916		
507								
657	5716	B	F_5P	PF_5		930		
658	5717	B	F_5P	PF_5		1010		
698	5718		F_5P	PF_5		938		
578	5719	M	F_5HKP	$K^+F_5PH^-$		1a,2 -729		
577	(2539)			(1)(2)		1e,2 -817		
562								
674	5720		$F_6Cl_2N_4P_4$			900 880		
668	5721	A^2	F_6KP	KPF_6		705		
502	5772	A^2	F_6KP	KPF_6		710		
514	5723	A	F_6KP	KPF_6		710		
699	5724		$F_6N_3P_3$			935		
502	5725		$F_6N_3P_3$			∿900		
668	5726		F_6HP	HPF_6		713		
639	5727		F_6HP	HPF_6		710		
658	5728		F_6HP	HPF_6		708		
502	5729	A^2	F_6H_4NP	NH_4PF_6		708		
674	5730	B	$F_7ClN_4P_4$		1,3 2,4	900 925		
701	5731		F_8AsOP	$F_3P(O).AsF_5$		1095		
674	5732	B	$F_8N_4P_4$			850		

Table C.14. (contd.)

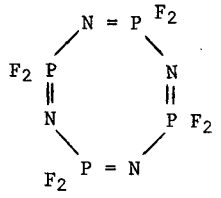
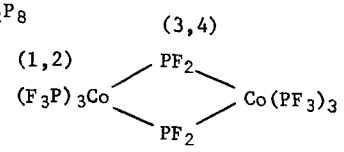
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
502	5733	E	$F_8N_4P_4$		∿900		
687	5734		$F_{12}NiP_4$	$Ni(PF_3)_4$	1300		
702	5735		$F_{12}NiP_4$	$Ni(PF_3)_4$	1260		
688	5736	B	$F_{12}NiP_4$	$Ni(PF_3)_4$	∿1320		
687	5737		$F_{12}P_4Pd$	$Pd(PF_3)_{12}$	1400		
1143	5738		$F_{22}Co_2P_8$		1,2 ∿1330 3,4 ∿1230		
718	5739		CFH_2Cl_2OP	$CH_2ClP(O)FCl$	1180		
703	5740		CFH_3BrOP	$CH_3P(O)FBr$	1153		
502	5741	F	CFH_3NaO_3P	$CH_3OP(O)FO^-Na^+$	896		
582	5742 (2546)		CFH_4O_2P	$CH_3OP(O)FH$	1056		
703	5743		CFH_4O_2P	$CH_3P(O)FOH$	1014		
658 704 720 719	5744	B	$CF_2Br_2Cl_3P$	$CCl_3PF_2Br_2$	1109		
658 704 705 509	5745	B	CF_2Cl_3P	CCl_3PF_2	1290		
658 704 719 720	5746		CF_2Cl_5P	$CCl_3PF_2Cl_2$	1106		
707	5747		CF_2NOP	$F_2P(NCO)$	1310		
708	5748	B	CF_2NOP	$F_2P(NCO)$	1361		
695	5749		CF_2NOPS	$F_2P(O)(NCS)$	1012		
677	5750	B	CF_2NOPS	$F_2P(S)(NCO)$	1176		
709	5751		CF_2NO_2P	$F_2P(O)(NCO)$	1007		
695	5752		CF_2NO_2P	$F_2P(O)(NCO)$	998		
692	5753		CF_2NP	F_2PCN	1267		
710	5754		CF_2NPS	$F_2P(NCS)$	1336		
677	5755	B	CF_2NPS	$F_2P(S)CN$	1148		
710	5756		CF_2NPS	$F_2P(S)(NCS)$	1123		

Table C.14 (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
677	5757	B	CF_2NPS_2	$F_2P(S)(NCS)$	1120		
658	5758	B	CF_2H_2ClOP	$ClCH_2P(O)F_2$	1142		
706	(2276)						
721							
718	5759	B	CF_2H_2ClOP	$ClCH_2P(O)F_2$	1140		
658	5760	B	CF_2H_2ClP	$ClCH_2PF_2$	1203		
500	(2277)						
509							
502	5761		CF_2H_2ClPS	$ClCH_2P(S)F_2$	1180		
	(2279)						
84	5762		CF_2H_3DNOP	$F_2P(O)NDCH_3$	986		
84	5763		CF_2H_3DNP	$F_2PN(D)CH_3$	1190		
84	5764		CF_2H_3DNPS	$F_2P(S)N(D)CH_3$	1083		
	(2279a)						
515	5765		CF_2H_3OP	$F_2P(O)CH_3$	1104		
502	(2280)						
706							
511	5766		CF_2H_3OP	$F_2P(O)CH_3$	1103		
503	5767		CF_2H_3OPS	$CH_3SP(O)F_2$	1174		
	(2282)						
502	5768		CF_2H_3OPS	$CH_3OP(S)F_2$	1121		
	(2281)						
502	6769		$CF_2H_3O_2P$	$CH_3OP(O)F_2$	1008		
	(2283)						
504	5770		CF_2H_3P	CH_3PF_2	1157		
	(2284)						
711	5771		CF_2H_3P	CH_3PF_2	1131		
502	5772		CF_2H_3PS	$CH_3P(S)F_2$	1147		
	(2286)						
84	5773		CF_2H_4NOP	$F_2P(O)NHCH_3$	991		
	(2547, 2287)						
84	5774	P	CF_2H_4NP	F_2PNHCH_3	1197		
	(2289)	H^2-P			1177		
505	5775		CF_2H_4NP	F_2PNHCH_3	1191		
	(2548, 2288)						
84	5776		CF_2H_4NPS	$F_2P(S)NHCH_3$	1083		
	(2549, 2290)						
712	5777		CF_3Br_2P	CF_3PBr_2		69.6	
36	5778	B	CF_3Br_2P	CF_3PBr_2		69.6	
713	5779	B	CF_3Cl_2OP	$CF_3P(O)Cl_2$		151	

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
712	5780		CF_3Cl_2P	CF_3PCl_2		79.9	
36	5781	B	CF_3Cl_2P	CF_3PCl_2		79.9	
712	5782		CF_3I_2P	CF_3PI_2		52.1	
36	5783	B	CF_3I_2P	CF_3PI_2		52.1	
36	5784	B	CF_3H_2P	CF_3PH_2		48.5	
	(2504)						
714	5785	A^2	$CF_3Na_2OPS_2$	$CF_3PS_2O^{2-}.2Na^+$		86.6	
714	5786	A^2	$CF_3Na_2O_2PS$	$CF_3PSO_2{}^{2-}.2Na^+$		89.9	
714	5787	A^2	$CF_3Na_2O_3P$	$CF_3PO_3{}^{2-}.2Na^+$		93.0	
714	5788	A^2	$CF_3HNaOPS_2$	$CF_3PS_2OH^-Na^+$		99.0	
714	5789	A^2	CF_3HNaO_2P	$CF_3P(H)O_2{}^-Na^+$		100.9	
714	5790	A	CF_3HNaO_2PS	$CF_3PSO_2H^-Na^+$		103.0	
506	5791	B	CF_3H_4P	CH_3PF_3H	1a,2	795	
	[2291			(2)(1)	1e,2	965	
	2550						
	4933]						
75	5792		CF_4ClP	CF_3PFCl	1178	84.6	
658	5793	B	CF_4Cl_3P	CCl_3PF_4	1120		
704							
507	5794		CF_4H_2ClP	$ClCH_2PF_4$	997		
706	(2292)						
658							
715	5795		$CF_4H_3NP_2$	$CH_3N(PF_2)_2$	1264		47
	(4934)						
507	5796	P-S[2]	CF_2H_3P	CH_3PF_4	-967.7		
509	(2294)						
510							
658							
706							
716	5797	T^2	CF_4H_3PS	CH_3SPF_4	1a,2 930		
717	(4935)			(2)(1)(-100°)	1a,2 1088		
					1e,2 1075		
				(Room temp.)	1032		
723	5798		CF_5Cl_2P	$CF_3PF_2Cl_2$	1085	165	
962	5799	B	CF_5OP	$CF_3P(O)F_2$	1215	162	
	(4756)						
658	5800	B	CF_5P	CF_3PF_2	1245	87.2	
712	5801						
	(4757)						
511	5802		$CF_5H_3P^-$	$CH_3PF_5{}^-$	691		
	(2295				830		
	4936)						

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J	^nJ
523	5803	A	$CF_5H_5P_2$	$CH_3P(H_2)PF_5$	1a,2	-800	1e,3	+220	
	(2551 4937)			(3) (2)(1)	1e,2	-867			
502	5804	B	CF_7P	CF_3PF_4		1103		170	
507									
720									
562	5805		CF_7HKP	(4)	1,5	767	4,5	124.5	
	[2505 4938 2552 4759]		K^+ [(1)F, (2)F, CF_3, H, (5), F(1), F]$^-$		2,5	~759			
				(3)	3,5	784			
583	5806		CF_7HKP	K^+ [F, F, F, F, CF_3, H, P]$^-$		858		156	
	[2505 4938 2552 4759]								
722	5807		CF_8CsP	$Cs^+[CF_3PF_5]^-$		802		133	
	(4760 4939)								
695	5808		$C_2FN_2OPS_2$	$FP(O)(NCS)_2$		957			
710									
707	5809		$C_2FN_2O_2P$	$FP(NCO)_2$		1226			
710	5810		$C_2FN_2PS_2$	$FP(NCS)_2$		1252			
710	5811		$C_2FN_2PS_3$	$FP(S)(NCS)_2$		1061			
512	5812		$C_2FH_4O_2P$			1226			
	(2296)			O, O, PF					
724	5813		C_2FH_6ClNP	$(CH_3)_2NPFCl$		1170			
502	5814	B	C_2FH_6OP	$(CH_3)_2P(O)F$		980			
658	(2297)								
503	5815		$C_2FH_6OPS_2$	$FP(O)(SCH_3)_2$		1164			
	(2298)								
502	5816		$C_2FH_6O_2P$	$FP(OCH_3)_2$		1210			
	(2299)								
502	5817		$C_2FH_6O_2P$	$CH_3P(O)F(OCH_3)$		1039			
	(2300)								
502	5818		$C_2FH_6O_2PS$	$FP(S)(OCH_3)_2$		1080			
	(2301)								
513	5819		C_2FH_6P	$(CH_3)_2PF$		823			
	(2302)								

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
502	5820 (2303)		C_2FH_6PS	$(CH_3)_2P(S)F$	985		
502	5821 (2304)		C_2FH_7NPS	$CH_3P(S)F(NHCH_3)$	1043		
582	5822 (2553)		$C_2FH_9NO_2P$	$(CH_3)_2{}^+NH_2HFPO_2{}^-$	986		
36	5823 (60)	B	$C_2F_2H_3Cl_2P$	$CF_2HCH_2PCl_2$			13.4
708	5824	B	$C_2F_2H_3O_2P$	$CH_3C(O)OPF_2$	1350		
658	5825	B	$C_2F_2H_5OP$	$CH_3CH_2P(O)F_2$	1130		
706	5826						
725	5827		$C_2F_2H_5OP$	$CH_3CH_2P(O)F_2$	1135		
502	5828	B	$C_2F_2H_5OP$	$CH_3CH_2OPF_2$	1284		
503	5829		$C_2F_2H_5OPS$	$F_2P(O)SCH_2CH_3$	1172		
658	5830	B	$C_2F_2H_5O_2P$	$F_2P(O)(OCH_2CH_3)$	1015		
680	5831		$C_2F_2H_5O_2P$	$F_2P(O)(OCH_2CH_3)$	1012		
718	5832		$C_2F_2H_5O_2P$	$F_2P(O)(OCH_2CH_3)$	1010		
706	5833		$C_2F_2H_5P$	$CH_3CH_2PF_2$	980		
711	5834		$C_2F_2H_5P$	$CH_3CH_2PF_2$	1114		
36	5835 (69)		$C_2F_2H_5P$	$CHF_2CH_2PH_2$			7.6
502	5836 (2305)		$C_2F_2H_5PS$	$CH_3CH_2P(S)F_2$	1163		
531	5837	B	$C_2F_2H_5PS_2$	$CH_3CH_2SP(S)F_2$	1206		
678	5838		$C_2F_2H_6ClPS_2Sn$	$(CH_3)_2SnClSP(S)F_2$	1210		
502	5839 (2306)		$C_2F_2H_6NOP$	$F_2P(O)N(CH_3)_2$	1004		
514	5840 (2307)		$C_2F_2H_6NOP$	$F_2P(O)N(CH_3)_2$	997.5		
512 516 688	5841 (2308)		$C_2F_2H_6NP$	$F_2PN(CH_3)_2$	1190		
516	5842 (2309)		$C_2F_2H_6NP$	$F_2PN(CH_3)_2$	1195		
502	5843 (2310)		$C_2F_2H_6NPS$	$F_2P(S)N(CH_3)_2$	1081		
518	5844 (2312)		$C_2F_2H_6NPS$	$F_2P(S)N(CH_3)_2$	1079		
517	5845 (2311)	B	$C_2F_2H_6NPS$	$F_2P(S)N(CH_3)_2$	1082		
519	5846 (2313)		$C_2F_2H_{13}B_3NP$	$F_2PN(CH_3)_2.B_3H_7$	1159		

Table C.14 (contd.)

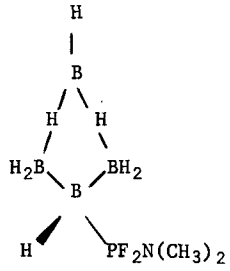
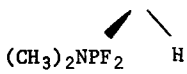
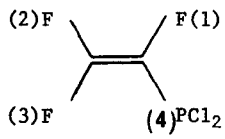
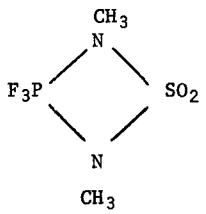
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
520	5847	B	$C_2F_2H_{14}B_4NP$			1110				
	(2314)					1150				
				and						
										
277	5848	B	$C_2F_3Cl_2P$				1,4	-17.2	2,4	+7.3
726	(3427)								3,4	+85.7
36	5849	B	$C_2F_3H_2Cl_2P$	$CH_2FCF_2PCl_2$				99		49.1
	(85, 2623)									
36	5850	B	$C_2F_3H_2Cl_2P$	$CF_2HCHFPCl_2$				83		7.5
	(86, 2624)									12.0
36	5851	B	$C_2F_3H_4P$	$CFH_2CF_2PH_2$				97		
	(100)									
727	5852	H	$C_2F_3H_6N_2O_2P$			968				
507	5853	B	$C_2F_3H_6P$	$(CH_3)_2PF_3$	1a,2	772				
706	(2315, 4940)			(2)(1)	1e,2	960				
658		P			1a,2	-781.6				
720					1e,2	-976.2				
510										
506	5854	B	$C_2F_3H_6P$	$CH_3CH_2PF_3H$	1a,2	810				
	(2317, 4941)			(2)(1)	1e,2	976				
717	5855		$C_2F_3H_6PS$	$CH_3PF_3(SCH_3)$	1a,2	925				
	(4942)				1e,2	1062				

Table C.14 (contd.)

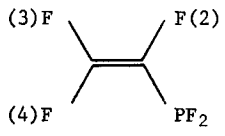
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
603	5856	B	$C_2F_3H_{11}B_5P$	$CF_3P(CH_3)B_5H_8$						
				Isomer with CF_3 group axial and CH_3 group equatorial				68		
				Isomer with above reversed				61		
36	5857 (1021, 2636)	B	$C_2F_4HCl_2P$	$CF_2HCF_2PCl_2$				81		26.9
512	5858 (2318)		$C_2F_4H_4O_2P_2$	$(F_2POCH_2)_2$		1301				
715	5859 (4943)		$C_2F_4H_5NP_2$	$CH_3CH_2N(PF_2)_2$		1261		52		
507	5860		$C_2F_4H_5P$	$CH_3CH_2PF_4$		1000				
530	(2319)									
706										
658										
720										
716	5861	T^2	$C_2F_4H_5PS$	$CH_3CH_2SPF_4$	1a,2	950				
717	(4944)			(2) (1)	1a,2	1082				
					1e,2	1074				
				(-70^o)						
				(Room tempt.)		1045				
521	5862		$C_2F_4H_6NP$	$F_4PN(CH_3)_2$		836				
735	(2320)									
708	5863	B	$C_2F_5O_2P$	$CF_3C(O)OPF_2$		1389				
227	5864		C_2F_5P		1,5	-1202	2,5	+20.9	3,5	+4.8
726	(3435, 4761)								4,5	+69.6
				(5) (1)						
728	5865		$C_2F_5H_3NP$	$CH_3CN.PF_5$		770				
474	5866	J	$C_2F_5H_6OP$	$(CH_3)_2O.PF_5$	1a,2	777				
	(4746)			(2) (1)	1e,2	820				
522	5867	M	$C_2F_5H_6CsNP$	$Cs^+[(CH_3)_2NPF_5]^-$	1a,2	664				
	(2321, 4945)			(2) (1)	1e,2	767				
521	5868		$C_2F_5H_7NP$	$(CH_3)_2NH.PF_5$	1a,2	752				
	(4947)			(2) (1)	1e,2	808				
523	5869	J	$C_2F_5H_7P_2$	$(CH_3)_2PHPF_5$	1a,2	-783	1,3	+184		
	[2322, 4948, 2555]			(3) (2) (1)	1e,2	-873				
729	5870		C_2F_6BrOP	$(CF_3)_2P(O)Br$				126		

Table C.14. (contd.)

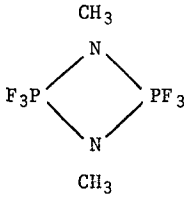
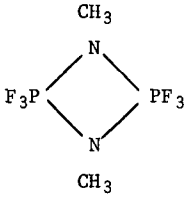
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
730	5871		C_2F_6BrP	$(CF_3)_2PBr$		80.6	
712							
100							
76	5872	P	C_2F_6BrPS	$(CF_3)_2P(S)Br$		119.7	
729	5873		C_2F_6ClOP	$(CF_3)_2P(O)Cl$		130	
730	5874		C_2F_6ClP	$(CF_3)_2PCl$		85.1	
712							
100							
76	5875		C_2F_6ClPS	$(CF_3)_2P(S)Cl$		123.1	
730	5876		$C_2F_6Cl_3P$	$(CF_3)_2PCl_3$		193.3	
730	5877		C_2F_6IP	$(CF_3)_2PI$		73.2	
712							
100							
76	5878		C_2F_6IPS	$(CF_3)_2P(S)I$		111.4	
714	5879	A^2	C_2F_6NaOPS	$Na^+(CF_3)_2PSO^-$		97.0	
714	5880	A^2	$C_2F_6NaO_2P$	$Na^+(CF_3)_2PO_2^-$		103.6	
714	5881	A^2	$C_2F_6NaPS_2$	$Na^+(CF_3)_2PS_2^-$		92.0	
731	5882	B	$C_2F_6NiO_2P_2$	$Ni(CO)_2(PF_3)_2$	±1357	∓34.5	
36	5883	B	C_2F_6HP	$(CF_3)_2PH$		68.6	
730	(2507)						
563	5884	A	C_2F_6HP	$(CF_3)_2PH$		67.4	
	(2506)	B				70.0	
		E				63.9	
		G				68.1	
		H				66.1	
		M				64.7	
		P				69.2	
		R				67.3	
		S^2				69.4	
732	5885		C_2F_6HPS	$(CF_3)_2PSH$		75.4	
76	5886	P	$C_2F_6HPS_2$	$(CF_3)_2P(S)SH$		110.0	
76	5887	P	$C_2F_6H_2NPS$	$(CF_3)_2P(S)NH_2$		111.0	
733	5888		$C_2F_6H_6N_2P_2$		±922		∓32
	(4949)						
727	5889	H	$C_2F_6H_6N_2P_2$		1083		

Table C.14. (contd.)

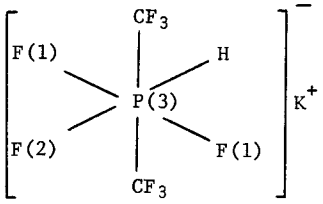
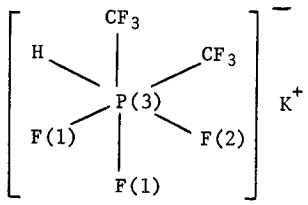
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
603	5890	B	$C_2F_6H_8B_5P$	$1\text{-}(CF_3)_2P.B_5H_8$			71.3	
729	5891	P	C_2F_7OP	$(CF_3)_2P(O)F$			136	
	(4762)							
730	5892		C_2F_7P	$(CF_3)_2PF$			89.6	
712	5893	B	C_2F_7P	$(CF_3)_2PF$		$\bar{+}1013$	± 89.6	
658	(2670							
734	4763)							
76	5894	P	C_2F_7PS	$(CF_3)_2P(S)F$		1174.6	128.6	
	(2671)							
736	5895		$C_2F_8Cl_2NP$	$(CF_3)_2NPF_2Cl_2$		985		1.8
	(4764)							
736	5896		C_2F_8NOP	$(CF_3)_2NP(O)F_2$		1065		0.5
	(4765)							
736	5897		C_2F_9ClNP	$(CF_3)_2NPF_3Cl$	1a,2	930		2.3
	(4766)			(2)(1)	1e,2	1030		
				(-70^o)				
507	5898	B	C_2F_9P	$(CF_3)_2PF_3$		1260	175	
658	(2682)							
564	5899	M	C_2F_9HKP		1,3	725	132	
562	[2509				2,3	834		
	2556							
	4950							
	4767]							
				or				
								
722	5900	M	$C_2F_{10}CsP$	$Cs^+[(CF_3)_2PF_4]^-$	1e,2	968	88	
				(2)(1)				
737	5901	M*	$C_2F_{10}CsP$	$Cs^+[(CF_3)_2PF_4]^-$	1e,2	$\bar{+}898$	± 148.5	
578	(4768)							
502	5902	A^2	$C_3FH_7NaO_3P$	$(CH_3)_2CHOP(O)FO^-Na^+$		920		
502	5903		$C_3FH_8PS_2$	$CH_3P(S)F(SCH_2CH_3)$		1093		
	(2323)							
502	5904		C_3FH_9NOP	$CH_3P(O)F[N(CH_3)_2]$		1017		
515	(2324)							
738	5905		C_3FH_9NOP	$CH_3P(O)F[N(CH_3)_2]$		998		

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
515	5906	B	C_3FH_9NP	$CH_3PFN(CH_3)_2$		920		
688	(2325)							
705								
738	5907		C_3FH_9NP	$CH_3PFN(CH_3)_2$		915		
502	5908		C_3FH_9NPS	$CH_3P(S)F[N(CH_3)_2]$		1046		
	(2326)							
671	5909		$C_3FH_{10}ClNPSSi$	$FP(S)Cl[NHSi(CH_3)_3]$		1120		
	(2558)							
590	5910		$C_3FH_{10}ClNPSSi$	$FP(S)Cl[NHSi(CH_3)_3]$		1118		
	(2557)							
582	5911		$C_3FH_{11}NO_2P$	$(CH_3)_3NH^+HFPO_2^-$		961		
	(2559)							
512	5912		$C_3F_2H_5OP$	$CH_2=CHCH_2OPF_2$		1290		
	(2327)							
512	5913	B	$C_3F_2H_7OP$	$CH_3CH_2CH_2OPF_2$		1288		
688	(2328)							
739	5914	B	$C_3F_2H_7OP$	$CH_3CH_2CH_2OPF_2$		1309		
740								
531	5915	B	$C_3F_2H_7PS$	$(CH_3)_2CHSP(S)F_2$		1206		
503	5916		$C_3F_2H_9N_2OP$	$F_2P(O)NCH_3N(CH_3)_2$		1000		
	(2329)							
680	5917		$C_3F_2H_9O_2PSi$	$(CH_3)_3SiOP(O)F_2$		984		
741	5918		$C_3F_2H_9O_3P$	$(CH_3O)_3PF_2$		706		
502	5919	S^2	$C_3F_2H_9P$	$(CH_3)_3PF_2$		-552.2		
507	(2330							
510	5445)							
532	5920	J	$C_3F_2H_9P$	$(CH_3)_3PF_2$		553		
678	5921		$C_3F_2H_9PS_2Si$	$F_2P(S)SSi(CH_3)_3$		1200		
659	5922		$C_3F_2H_{10}NOPSi$	$F_2P(O)NHSi(CH_3)_3$		997		
671	5923		$C_3F_2H_{10}NPSSi$	$F_2P(S)NHSi(CH_3)_3$		1088		
590	5924		$C_3F_2H_{10}NPSSi$	$F_2P(S)NHSi(CH_3)_3$		1089		
	(2560)							
189	5925	B	$C_3F_3H_6PS_2$	$(CH_3S)_2PCF_3$			68.3	
	(196)							
725	5926		$C_3F_3H_8OP$	$F_3PCH_3(OCH_2CH_3)$	1a,2	850		
	(4951)			(1)(2)	1e,2	990		
717	5927		$C_3F_3H_8PS$	$F_3PCH_3(SCH_2CH_3)$	1a,2	897		
	(4952)			(1)(2)	1e,2	1022		
605	5928	J	$C_3F_3H_9BP$	$(CH_3)_3P.BF_3$			240	
	(2199							
	5338)							
515	5929		$C_3F_3H_9NP$	$F_3PCH_3[N(CH_3)_2]$	1a,2	808		
705	(2332			(1)(2)	1e,2	965		
	4953)							

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
742	5930		$C_3F_3H_9NP$	$CH_3CH_2CH_2NH_2.PF_3$		1247				
742	5931		$C_3F_3H_9NP$	$(CH_3)_2CHNH_2.PF_3$		1280				
565	5932 (3441)		$C_3F_4Cl_3OP$	(3)F, Cl; (1)F, $CF_2P(O)Cl_2$; (2)(4)			2,4	146	1,4 3,4	11.6 16.2
75	5933 (2333, 4769)		$C_3F_4H_6NP$	$CF_3PFN(CH_3)_2$		1010		86.7		
76	5934 (2334)	P	$C_3F_4H_6NPS$	$CF_3P(S)FN(CH_3)_2$		1084		121.5		
474	5935 (2325, 4954)	J	$C_3F_5H_9NP$	$F_5PN(CH_3)_3$	1a,2	747				
				(1)(2)	1e,2	848				
523	5936 (2336, 4955)	M	$C_3F_5H_9P_2$	$F_5PP(CH_3)_3$	1a,2	-784	1e,3	+183		
				(1)(2)(3)	1e,2	-900				
525	5937 (2337, 4956)		$C_3F_5H_{11}NP$	$[(CH_3)_2NH_2]^+[F_5PCH_3]^-$	1a,2	668				
				(1)(2)	1e,2	833				
731	5938	B	$C_3F_6FeO_3P_2$	$Fe(CO)_3(PF_3)_2$		±1322				∓26
730	5939		C_3F_6NOP	$(CF_3)_2PNCO$				88.0		
730	5940		C_3F_6NP	$(CF_3)_2PCN$				85.6		
84	5941 (240)		$C_3F_6H_3DNOP$	$(CF_3)_2P(O)NDCH_3$				112		
84	5942 (241)		$C_3F_6H_3DNP$	$(CF_3)_2PNDCH_3$				82.0		
84	5943 (242)		$C_3F_6H_3DNPS$	$(CF_3)_2P(S)NDCH_3$				106		
86	5944 (247)		$C_3F_6H_3OP$	$(CF_3)_2POCH_3$				85.4		
86	5945 (248)		$C_3F_6H_3OP$	$(CF_3)_2P(O)CH_3$				99		
86	5946		$C_3F_6H_3O_2P$	$CH_3OP(O)(CF_3)_2$				120		
36	5947 (250)	B	$C_3F_6H_3P$	$(CF_3)_2PCH_3$				76.7		
86	5948		$C_3F_6H_3P$	$(CF_3)_2PCH_3$				75		
732	5949		$C_3F_6H_3PS$	$(CF_3)_2PSCH_3$				77.8		
84	5950		$C_3F_6H_4NOP$	$(CF_3)_2P(O)NHCH_3$				111		
84	5951		$C_3F_6H_4NP$	$(CF_3)_2PNHCH_3$				82.4		
743	5952		$C_3F_6H_4NP$	$(CF_3)_2PNHCH_3$				82		
84	5953		$C_3F_6H_4NPS$	$(CF_3)_2P(S)NHCH_3$				106		
744	5954 (6866)	M B^2	$C_3F_6H_9PW$	$(CH_3)_3PWF_6$				73 73		

Table C.14. (contd.)

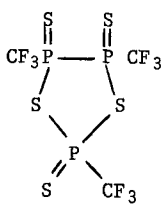
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ
712	5955		$C_3F_7Cl_2P$	$CF_3CF_2CF_2PCl_2$		1,4	58.2	2,4	36.2
	(2746)			(3)(2)(1)(4)				3,4	9.6
712	5956		$C_3F_7I_2P$	$CF_3CF_2CF_2PI_2$		1,4	25.3	2,4	37.2
	(2747)							3,4	9.7
708	5957	B	$C_3F_7O_2P$	$CF_3CF_2C(O)OPF_2$	1389				
	(2752)								
745	5958	B	C_3F_8BrOP	$(CF_3)_2C(OPF_2)Br$	1384				12
	(4771)								
745	5959	B	C_3F_8IOP	$(CF_3)_2C(OPF_2)I$	1384				8
	(4772)								
658	5960	B	$C_3F_9Cl_2P$	$CF_3CF_2CF_2PF_2Cl_2$	1105		128		
723									
720									
688	5961	H	$C_3F_9MoO_3P_3$	$(PF_3)_3Mo(CO)_3$	-1296				+2.4
746									
730	5962		C_3F_9OP	$(CF_3)_3P(O)$			113.4		
730	5963		C_3F_9P	$(CF_3)_3P$			85.5		
658	5964	B	C_3F_9P	$CF_3CF_2CF_2PF_2$	1,5 1257	2,5	90.5	3,5	19.3
712	(2776)			(4)(3)(2)(5)(1)				4,5	9.3
747	5965		C_3F_9PS	$(CF_3)_3P(S)$			108.7		
100	5966		C_3F_9PS	$(CF_3)_2PSCF_3$			83.8		
730	5967		C_3F_9PS	$(CF_3)_2PSCF_3$			83.8		
734	5968		C_3F_9PS	$(CF_3)_2PSCF_3$			83.8		21.9
	(2777)								
730	5969		C_3F_9PSe	$(CF_3)_2PSeCF_3$			77.2		
100	5970		C_3F_9PSe	$(CF_3)_2PSeCF_3$			77.2		
748	5971	G	$C_3F_9P_3S_5$				131		
507	5972		$C_3F_{11}P$	$(CF_3)_3PF_2$	988				
658									
723	5973		$C_3F_{11}P$	$CF_3CF_2CF_2PF_4$	1090		124		
720									
749	5974		$C_4FCl_2FeO_4P$	$FPCl_2Fe(CO)_4$	1215.2				
738	5975		C_4FH_9NP	$CH_3PFNHCH_2CH{=}CH_2$	873				
502	5976		C_4FH_9NPS	$CH_2{=}CHP(S)F[N(CH_3)_2]$	1045				
724	5977		$C_4FH_{10}ClNP$	$FPClN(CH_2CH_3)_2$	1164				
502	5978		$C_4FH_{10}OPS$	$CH_3CH_2P(S)F(OCH_2CH_3)$	1100				
	(2338)								
502	5979		$C_4FH_{10}O_2P$	$FP(OCH_2CH_3)_2$	1209				

Table C.14. (contd.)

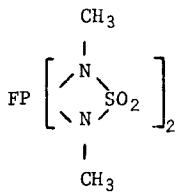
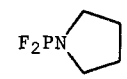
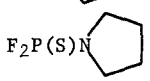
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
739	5980	B	$C_4FH_{10}O_2P$	$FP(OCH_2CH_3)_2$	1225		
740							
725	5981		$C_4FH_{10}O_2P$	$CH_3CH_2P(O)F(OCH_2CH_3)$	1055		
502	5982		$C_4FH_{10}O_3P$	$FP(O)(OCH_2CH_3)_2$	970		
742	5983		$C_4FH_{11}NP$	$CH_3PFNHCH(CH_3)_2$	1065		
502	5984		$C_4FH_{12}N_2OP$	$FP(O)[N(CH_3)_2]_2$	941		
514	5985		$C_4FH_{12}N_2OP$	$FP(O)[N(CH_3)_2]_2$	948.0		
	(2340)						
512	5986	B	$C_4FH_{12}N_2P$	$FP[N(CH_3)_2]_2$	1046		
515	(2342)						
688							
754	5987		$C_4FH_{12}N_2P$	$FP\ N(CH_3)_2\ _2$	1023		
518	5988		$C_4FH_{12}N_2PS$	$FP(S)[N(CH_3)_2]_2$	1016		
	(2344)						
502	5989		$C_4FH_{12}N_2PS$	$FP(S)[N(CH_3)_2]_2$	1014		
	(2343)						
727	5990	H	$C_4FH_{12}N_4O_4PS_2$		894		
749	5991		$C_4F_2BrFeO_4P$	$F_2PBrFe(CO)_4$	1253.5		
749	5992		$C_4F_2ClFeO_4P$	$F_2PClFe(CO)_4$	1258.3		
749	5993	J	$C_4F_2N_3O_4P$	$F_2PN_3Fe(CO)_4$	1219.3		
95	5994	B	$C_4F_2H_7Cl_3NP$	$CHCl_2CF_2PCl[N(CH_3)_2]$ (1,2)(3)		1,3	93
	(284 2781)					2,3	53
527	5995		$C_4F_2H_8NP$		1198		
	(2345)						
517	5996	B	$C_4F_2H_8NPS$		1086.2		
750	5997	B	$C_4F_2H_9OP$	$F_2P(O)C(CH_3)_3$	1195		
526	(2346)						
512	5998	B	$C_4F_2H_9OP$	$CH_3(CH_2)_3OPF_2$	1288		
	(2347)						
739	5999	B	$C_4F_2H_9OP$	$CH_3(CH_2)_3OPF_2$	1309		
740							
658	6000	B	$C_4F_2H_9OP$	$CH_3(CH_2)_3P(O)F_2$	1140		
526	6001	B	$C_4F_2H_9P$	$F_2PC(CH_3)_3$	1212		
	(2348)						
526	6002		$C_4F_2H_9PS$	$F_2P(S)C(CH_3)_3$	1209		
	(2349)						
502	6003	B	$C_4F_2H_{10}NOP$	$F_2P(O)N(CH_2CH_3)_2$	1004		
658							

Table C.14. (contd.)

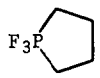
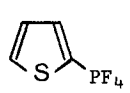
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J	^nJ
512	6004	B	$C_4F_2H_{10}NP$	$F_2PN(CH_2CH_3)_2$		1194			
688	(2350)								
527	6005		$C_4F_2H_{10}NP$	$F_2PN(CH_2CH_3)_2$		1191			
	(2351								
738	6006		$C_4F_2H_{10}NP$	$F_2PHCH_3(HNCH_2CH{=}CH_2)$		609			
502	6007		$C_4F_2H_{10}NPS$	$F_2P(S)N(CH_2CH_3)_2$		1082			
517	6008	B	$C_4F_2H_{10}NPS$	$F_2P(S)N(CH_2CH_3)_2$		1084.7			
522	6009	M	$C_4F_2H_{12}NP$	$(CH_3)_2PF_2N(CH_3)_2$		654			
	(2352)								
95	6010		$C_4F_3H_7Cl_2NP$	$CHCl_2CF_2PF[N(CH_3)_2]$			1,3	97	
	(292)			(1,2) (3)			2,3	51	
502	6011		$C_4F_3H_8P$			915			
507	(2353								
658	4957)								
706									
36	6012	B	$C_4F_3H_9NP$	$CF_2HCH_2PFN(CH_3)_2$		890			18.3
	(295)								
751	6013		$C_4F_3H_9P_2$	$(CH_3)_3PPCF_3$				36.0	22.7
725	6014		$C_4F_3H_{10}OP$	$CH_3CH_2PF_3OCH_2CH_3$	1a,2	875			
	(4958)			(2) (1)	1e,2	1005			
507	6015	B	$C_4F_3H_{10}P$	$(CH_3CH_2)_2PF_3$	1a,2	815			
658	2354			(2) (1)	1e,2	980			
	4959)								
706	6016		$C_4F_3H_{10}P$	$(CH_3CH_2)_2PF_3$	1a,2	830			
					1e,2	1000			
751	6017		$C_4F_3H_{12}BP_2$	$(CH_3)_3PPCF_3BH_3$				41.4	15.3
512	6018		$C_4F_3H_{12}N_2P$	$F_3P[N(CH_3)_2]_2$	1a,2	752			
	(4960)			(1) (2)	1e,2	871			
751	6019		$C_4F_3H_{15}B_2P_2$	$(CH_3)_3PPCF_3(BH_3)_2$				42.0	6.9
502	6020		$C_4F_4H_3PS$			928			
227	6021		$C_4F_4H_6NP$	$CF_2{=}CFPFN(CH_3)_2$		995			
	(916)								
507	6022		$C_4F_4H_9P$	$CH_3(CH_2)_3PF_4$		990			
705	(2356)								
526	6023	B	$C_4F_4H_9P$	$(CH_3)_3CPF_4$		1060			
530	6024		$C_4F_4H_{10}NP$	$F_4PN(CH_2CH_3)_2$					
752	(4961)			(1) (2) (25°)		851			
705				(-85°)	1a,2	793			
					1e,2	916			
521	6025		$C_4F_4H_{10}NP$	$F_4PN(CH_2CH_3)_2$		868			

Table C.14. (contd.)

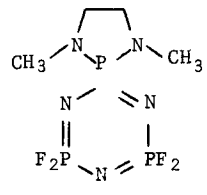
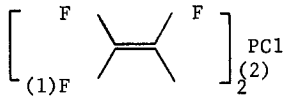
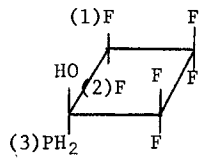
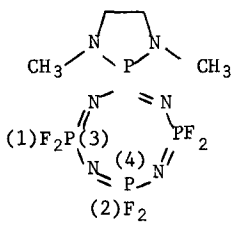
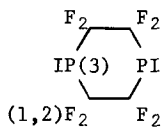
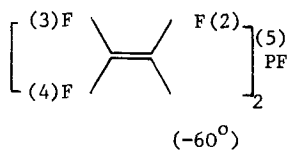
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
753	6026	H	$C_4F_4H_{10}N_5P_3$		930		
519	6027		$C_4F_4H_{16}B_2N_2P_2$	$[(CH_3)_2NPF_2]_2B_2H_4$	1140		
	(2357)						
521	6028		$C_4F_5H_{11}NP$	$PF_5.NH(CH_2CH_3)_2$	1a,2 756		
	(4962)			(2)(1)	1e,2 813		
227	6029		C_4F_6ClP			1,2	70
	(3485)						
755	6030		$C_4F_6CoO_3P$	$CF_3Co(CO)_3PF_3$ (25°)	1368		58
	[4773			At -70° trans isomer	1351		80
	4774			cis isomer	1373		38
	4775]						
756	6031		$C_4F_6CrO_4P_2$	$Cr(CO)_4(PF_3)_2$			
	(4963)			trans isomer	1318		11.5
				cis isomer	1312		2.5
731	6032	B	$C_4F_6CrO_4P_2$	cis $Cr(CO)_4(PF_3)_2$	±1306		∓1.5
757	6033	B	$C_4F_6D_6PS$	$(CD_3CF_3P)_2S$			
	(2797)			High field isomer		66.1	4.3
				Low field isomer		66.1	4.8
731	6034	B	$C_4F_6MoO_4P_2$	$Mo(CO)_4(PF_3)_2$			
				trans	±1320		∓3.7
				cis	±1306		∓2.5
758	6035	B	$C_4F_6MoO_4P_2$	cis $Mo(CO)_4(PF_3)_2$	1305		2
730	6036		C_4F_6NPS	$(CF_3)_2P.NCS$		87.3	
731	6037	B	$C_4F_6O_4P_2W$	$W(CO)_4(PF_3)_2$			
	(6870			trans	±1286		∓39
	6871)			cis	±1281		∓1.5
759	6038		$C_4F_6H_3OP$			1,3	1.0
	(3723)					2,3	5.3
730	6039		$C_4F_6H_5OP$	$(CF_3)_2POCH_2CH_3$		86.6	
36	6040	B	$C_4F_6H_5P$	$(CF_3)_2PCH_2CH_3$		71.2	

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ
99	6041 (303)		$C_4F_6H_6AsP$	$(CF_3)_2PAs(CH_3)_2$			61.5		
99	6042 (302)		$C_4F_6H_6AsP$	$(CF_3)_2AsP(CH_3)_2$					7.5
729	6043	P	$C_4F_6H_6NOP$	$(CF_3)_2P(O)N(CH_3)_2$			106		
100	6044 (305)		$C_4F_6H_6NP$	$(CF_3)_2PN(CH_3)_2$			85.6		
730	6045		$C_4F_6H_6NP$	$(CF_3)_2PN(CH_3)_2$			85.6		
76	6046 (306)	P	$C_4F_6H_6NPS$	$(CF_3)_2P(S)N(CH_3)_2$			102.9		
760	6047	B	$C_4F_6H_6P_2$	$(CF_3)_2PP(CH_3)_2$			64.1		7.9
99	6048 (307)		$C_4F_6H_6P_2$	$(CF_3)_2PP(CH_3)_2$			64.2		7.8
757	6049	B	$C_4F_6H_6P_2$	$(CH_3CF_3P)_2$			$^2J + {}^3J$		
				High field isomer			79.1		
				Low field isomer			73.1		
753	6050	H	$C_4F_6H_{10}N_6P_4$		1,3 2,4	840 835			
502	6051	A^2	$C_4F_6H_{12}NP$	$[(CH_3)_4N]^+[PF_6]^-$		711			
702	6052		$C_4F_8Cl_{12}NiP_4$	$Ni(CCl_3PF_2)_4$		1116			
761	6053 (4090)		$C_4F_8I_2P_2$				1,3 2,3	54 128	
762	6054		$C_4F_8H_5N_2P$	$CH_3PF_2{=}NC(CF_3)_2NH_2$		1115			
500	6055		$C_4F_8H_8Cl_4NiP_4$	$Ni(ClCH_2PF_2)_4$		1149			~38
708	6056 (2822)	B	$C_4F_9O_2P$	$CF_3CF_2CF_2C(O)OPF_2$		1388			
763	6057 [3505 4776 4964]		C_4F_9P		1a,5 1e,5	641 975	2,5	91	3,5 4,5	31 15

(-60°)

Table C.14. (contd.)

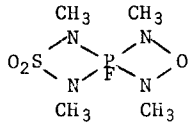
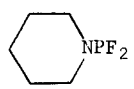
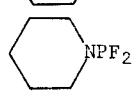
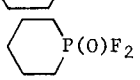
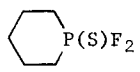
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
99	6058		$C_4F_{12}AsP$	$(CF_3)_2PAs(CF_3)_2$		65.1	12.3
	(2842)						
764	6059		$C_4F_{12}NP$	$(CF_3)_2PN(CF_3)_2$		113.7	14.4
	(2843)						
757	6060	B	$C_4F_{12}OP$	$(CF_3)_2POP(CF_3)_2$		94.3	4.4
729	6061	P	$C_4F_{12}O_3P_2$	$[(CF_3)_2P(O)]_2O$		137	
757	6062	B	$C_4F_{12}P_2$	$(CF_3)_2PP(CF_3)_2$		84.9	
757	6063	B	$C_4F_{12}P_2S$	$(CF_3)_2PSP(CF_3)_2$		76.7	8.2
765	6064		$C_4F_{12}P_2S_2$	$(CF_3)_2PSP(S)(CF_3)_2$	1,3 81.3	1,4	0.6
	(2844)			(1) (3)(4) (2)	2,4 111.7	2,3	4.9
766	6065		$C_4F_{13}OP$	$(CF_3)_3COPF_4$	919		
	(4777)						
530	6066		$C_4F_{13}P$	$(CF_3CF_2)_2PF_3$	1245		
702	6067		$C_4F_{20}NiP_4$	$Ni(CF_3PF_2)_4$	1205	118	39
727	6068	H	$C_5FH_{12}N_4O_3P$		1035		
658	6069		$C_5FH_{12}OP$	$CH_3CH_2P(O)FCH(CH_3)_2$	1045		
706	6070		$C_5FH_{12}O_2P$	$CH_3CH_2P(O)FOCH(CH_3)_2$	1062		
750	6071		$C_5FH_{12}O_2P$	$(CH_3)_3CP(O)FOCH_3$	1803		
767	6072		$C_5FH_{12}PS$	$CH_3PFS(CH_2)_3CH_3$	960		
502	6073		$C_5FH_{13}NOP$	$FP(OCH_3)[N(CH_2CH_3)_2]$	1120		
	(2360)						
742	6074		$C_5FH_{13}NP$	$CH_3PFNHCH_2CH(CH_3)_2$	1040		
738	6075		$C_5FH_{13}NP$	$CH_3PFN(CH_2CH_3)_2$	914		
749	6076		$C_5F_2NO_4PS$	$F_2P(SCN)Fe(CO)_4$	1303.8		
512	6077		$C_5F_2H_{10}NP$		1193		
527	6078		$C_5F_2H_{10}NP$		1199		
	(2361)						
502	6079		$C_5F_2H_{10}OP$		1016		
502	6080		$C_5F_2H_{10}PS$		1009		
658	6081		$C_5F_2H_{11}OP$	$F_2P(O)CH_2CH_2CH(CH_3)_2$	1126		
706							
739	6082		$C_5F_2H_{11}OP$	$F_2PO(CH_2)_4CH_3$	1309		
725	6083		$C_5F_2H_{13}PS_2$	$CH_3.PF_2(SCH_2CH_3)_2$	690		
738	6084		$C_5F_2H_{14}NP$	$CH_3PF_2HNHCH_2CH(CH_3)_2$	622		
741	6085		$C_5F_2H_{15}N_2OP$	$F_2P(OCH_3)[N(CH_3)_2]_2$	715		
731	6086	B	$C_5F_3CrO_5P$	$Cr(CO)_5PF_3$	1315		
731	6087	B	$C_5F_3MoO_5P$	$Mo(CO)_5PF_3$	1310		
731	088	B	$C_5F_3O_5PW$	$W(CO)_5PF_3$	1245		

Table C.14. (contd.)

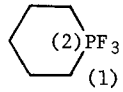
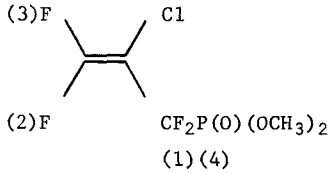
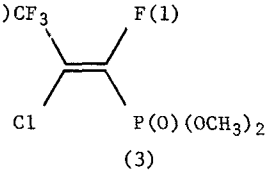
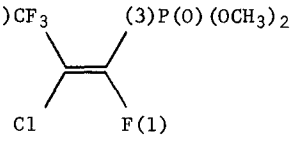
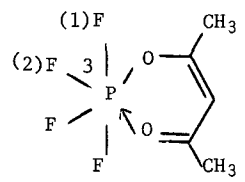
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
502	6089		$C_5F_3H_{10}P$		1a,2	801				
507	(4965)				1e,2	998				
189	6090 (356)	D	$C_5F_3H_{12}As_2P$	$CF_3P[As(CH_3)_2]_2$				33.9		
189	6091	B	$C_5F_3H_{12}AsP_2$	$(CH_3)_2PP(CF_3)As(CH_3)_2$				37.7		7.3
189	6092		$C_5F_3H_{12}NP_2$	$(CH_3)_2PP(CF_3)N(CH_3)_2$				53.0		11.3
189	6093		$C_5F_3H_{12}NP_2$	$(CH_3)_2P(PCF_3)N(CH_3)_2$				23.4 or 35.8		35.8 or 23.4
75	6094 (357)		$C_5F_3H_{12}N_2P$	$CF_3P[N(CH_3)_2]_2$				87.4		
189 760	6095	B	$C_5F_3H_{12}P_3$	$CF_3P[P(CH_3)_2]_2$				42.1		7.1
584	6096		$C_5F_3H_{13}NP$	$CH_3PF_3N(CH_2CH_3)_2$	1a,2	793				
	(4966)			(2)(1)	1e,2	945				
584	6097		$C_5F_3H_{13}NP$	$CH_3PF_3NHCH_2CH(CH_3)_2$	1a,2	838				
	(4967)				1e,2	970				
565	6098 (3262 3511)		$C_5F_4H_6ClO_3P$	 (3)F, Cl; (2)F, $CF_2P(O)(OCH_3)_2$; (1)(4)			1,4	109	2,4 3,4	6.9 9.8
768	6099 (3264)		$C_5F_4H_6ClO_3P$	 (2)CF_3, F(1); Cl, $P(O)(OCH_3)_2$; (3)			1,3	90.0	2,3	1.0
768	6100 (3263)		$C_5F_4H_6ClO_3P$	 (2)CF_3, (3)$P(O)(OCH_3)_2$; Cl, F(1)			1,3	91.9	2,3	3.2
769	6101 (4968)		$C_5F_4H_7O_2P$	 (1)F, CH_3; (2)F, 3, O, P, F, O, F, CH_3	1,3 2,3	824 741				

Table C.14. (contd.)

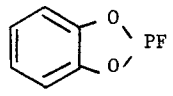
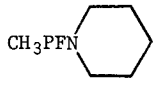
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
83	6102		$C_5F_6H_7O_3P$	$(CF_3)_2CHP(O)(OCH_3)_2$			10
	(368)						
36	6103	B	$C_5F_6H_7P$	$(CF_3)_2PCH_2CH_2CH_3$		71.2	
	(369)						
764	6104		$C_5F_{15}N_2P$	$[(CF_3)_2N]\ PCF_3$		149.4	23.2
	(2899)						
749	6105		$C_6FFeN_2O_4PS_2$	$FP(SCN)_2Fe(CO)_4$	1233.1		
386	6106		$C_6FH_4Cl_2P$	$pFC_6H_4PCl_2$			5.4
	(1811)						
512	6107		$C_6FH_4O_2P$		1307		
688							
502	6108		C_6FH_5ClOP	$C_6H_5P(O)FCl$	1135		
738	6109		C_6FH_5ClP	C_6H_5PFCl	1050		
770	6110		C_6FH_5ClPS	$C_6H_5P(S)FCl$	1243		
671	6111		$C_6FH_5Cl_3NP_2S$	$FP(S)ClN{=}PCl_2(C_6H_5)$	1107		
502	6112		$C_6FH_{12}O_2PS$	$CH_3CH_2SCH{=}CHP(O)F(OCH_2CH_3)$	1013		
738	6113		$C_6FH_{13}NP$		927		
							
739	6114		$C_6FH_{14}O_2P$	$FP(OCH_2CH_2CH_3)_2$	1227		
740							
502	6115		$C_6FH_{14}O_3P$	$FP(O)[OCH(CH_3)_2]_2$	968		
529	6116	B-H	$C_6FH_{14}O_3P$	$FP(O)[OCH(CH_3)_2]_2$	955		
	(2362)						
750		G	$C_6FH_{15}NOP$	$(CH_3)_3CP(O)F[N(CH_3)_2]$			
	6117			Rotational isomer A	1077		
	6118			Rotational isomer B	1011		
771	6119		$C_6FH_{18}Cl_2N_3P_3$	gem $P_3N_3FCl_2[N(CH_3)_2]_3$	910		
711	6120		$C_6F_2H_4ClP$	para $ClC_6H_4PF_2$	1118.5		
772							
658	6121	B	$C_6F_2H_5OP$	$C_6H_5P(O)F_2$	1115		
706							
515							
511	6122		$C_6F_2H_5OP$	$C_6H_5P(O)F_2$	1102		
512	6123	B	$C_6F_2H_5OP$	$C_6H_5OPF_2$	1326		
688	(2363)						
502	6124		$C_6F_2H_5OPS$	$C_6H_5OP(S)F_2$	1140		
770	6125	B	$C_6F_2H_5OPS$	$C_6H_5SP(O)F_2$	1201		
658	6126	B	$C_6F_2H_5O_2P$	$C_6H_5OP(O)F_2$	1030		
502							

Table C.14. (contd.

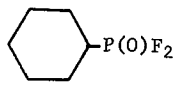
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
509	6127	B	$C_6F_2H_5P$	$C_6H_5PF_2$		1174		
658								
688								
532	6128	A	$C_6F_2H_5P$	$C_6H_5PF_2$		1180		
711	6129		$C_6F_2H_5P$	$C_6H_5PF_2$		1100		
772								
502	6130		$C_6F_2H_5PS$	$C_6H_5P(S)F_2$		1140		
773	6131	B	$C_6F_2H_7N_2PS$	$C_6H_5NHNHP(S)F_2$		1113.5		
517	(2561)	T[2]				1109.6		
502	6132		$C_6F_2H_{10}NP$	$F_2PN(CH_2CH{=}CH_2)_2$		1202		
	( )							
502	6133		$C_6F_2H_{11}OP$			1153		
	(2365)							
517	6134		$C_6F_2H_{14}NPS$	$(CH_3CH_2CH_2)_2NP(S)F_2$		1085.5		
36	6135	B	$C_6F_2H_{15}N_2P$	$CF_2HCH_2P[N(CH_3)_2]_2$				17.9
	(401)							
507	6136		$C_6F_2H_{15}P$	$(CH_3CH_2)_3PF_2$		575		
	(2366)							
522	6137	M	$C_6F_2H_{16}NP$	$(CH_3)_2PF_2N(CH_2CH_3)_2$		663		
	(2367)							
528	6138		$C_6F_2H_{18}N_3P$	$F_2P[N(CH_3)_2]_3$		700		
	(2368)							
741	6139		$C_6F_2H_{18}N_3P$	$F_2P[N(CH_3)_2]_3$		707		
502	6140		$C_6F_3H_4OP$	meta $FC_6H_4P(O)F_2$		1100		
530	6141		$C_6F_3H_5ClP$	$C_6H_5PF_3Cl$	1a,2	956		
	(4969)			(2)(1)	1e,2	1035		
530	6142		$C_6F_3H_5P$	$C_6H_5PF_3H$	1a,2	831		
	(2562, 4970)				1e,2	969		
605	6143		$C_6F_3H_{15}BP$	$(CH_3CH_2)_3PBF_3$			217	
	(5352)							
774	6144		$C_6F_3H_{15}NP$	$CH_3CH_2PF_3N(CH_2CH_3)_2$	1a,2	830		
	(2369, 4971)			(2)(1)	1e,2	984		
771	6145		$C_6F_3H_{18}N_3P_3$	gem $P_3N_3F_3[N(CH_3)_2]_3$		~900		
						~900		
						905		
771	6146		$C_6F_3H_{18}N_3P_3$	trans $P_3N_3F_3[N(CH_3)_2]_3$		~860		
						~885		
771	6147		$C_6F_3H_{18}N_3P_3$	cis $P_3N_3F_3[N(CH_3)_2]_3$		907		
758	6148		$C_6F_4Cl_6MoP_2O_4$	cis$(CCl_3PF_2)_2Mo(CO)_4$		1196		

Table C.14. (contd.)

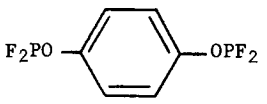
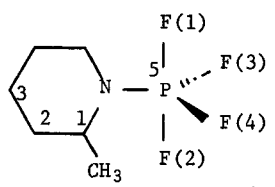
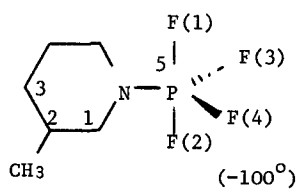
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
715	6149 (4972)		$C_6F_4H_4ClNP_2$	meta $ClC_6H_4N(PF_2)_2$	1285		41.5
507	6150 (2370)		$C_6F_4H_4ClP$	meta $ClC_6H_4PF_4$	960		
507	6151 (2371)		$C_6F_4H_4ClP$	para $ClC_6H_4PF_4$	960		
758	6152		$C_6F_4H_4Cl_2MoO_4P_2$	cis $(ClCH_2PF_2)_2Mo(CO)_4$	1120		5
512	6153 (2372)		$C_6F_4H_4O_2P_2$		1328		
775	6154 (4973)	B*	$C_6F_4H_5CrO_4P_2$	$(F_2P)_2NCH_2CH_3.Cr(CO)_4$	-1301		+56.5
775	6155 (4974	B*	$C_6F_4H_5MoO_4P_2$	$(F_2P)_2NCH_2CH_3.Mo(CO)_4$	-1284		+40
715	6156 (4975)		$C_6F_4H_5NP_2$	$(F_2P)_2NC_6H_5$	1252		40
775	6157 (4976)	B*	$C_6F_4H_5O_4P_2W$	$(F_2P)_2NCH_2CH_3.W(CO)_4$	-1277		+46.0
507	6158 (2373)	B	$C_6F_4H_5P$	$C_6H_5PF_4$	973		
658							
706							
716	6159	T^2	$C_6F_4H_5PS$	$C_6H_5SPF_4$	1a,2	1071	
717	(4977)			(2)(1)	1a,2	943	
				(-80°)	1e,2	1064	
				Room temp.		1060	
531	6160	J	$C_6F_4H_{10}P_2S_4$	c-$C_6H_{10}(SP(S)F_2)_2$		1208	
776	6161 (4978)	T^2	$C_6F_4H_{12}NP$	 (-100°)	1,5	781	
					2,5	781	
					3,5	921	
					4,5	905	
776	6162 (4979)	T^2	$C_6F_4H_{12}NP$	 (-100°)	1,5	763	
					2,5	763	
					3,5	940	
					4,5	940	

Table C.14. (contd.)

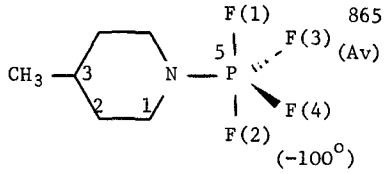
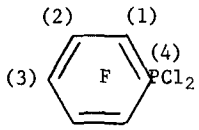
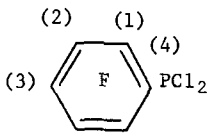
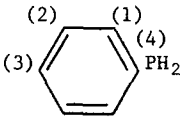
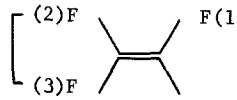
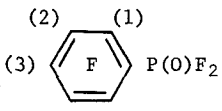
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
776	6163	T^2	$C_6F_4H_{12}NP$		F(1) 865 F(3) (Av) F(4) F(2) (-100°)		
688	6164	B	$C_6F_4H_{12}N_2NiO_2P_2$	$[(CH_3)_2NPF_2]_2Ni(CO)_2$	1150		
521	6165		$C_6F_4H_{14}NP$	$F_4PN(CH_2CH_2CH_3)_2$	856		
735							
777	6166		$C_6F_5Cl_2P$			1,4 2,4 3,4	63.2 0.8 1.0
	(4329)						
778	6167	H*	$C_6F_5Cl_2P$			1,4 2,4 3,4	63.2 0.9 1.1
	(4330)						
777	6168		$C_6F_5H_2P$			1,4 2,4	3.9 1.3
	(4362)						≈0
511	6169		$C_6F_5H_5P^-$	$C_6H_5PF_5^-$ (2)(1)	1a,2 680 1e,2 830		
	(4980)						
502	6170	M	$C_6F_5H_{17}NP$	$[(CH_3CH_2)_2NH_2]^+[CH_3CH_2PF_5]^-$ (2)(1)	1a,2 710 1e,2 835		
658	6171	M	$C_6F_6H_4ClN_2P$	$[pClC_6H_4N_2]^+PF_6^-$ (4)	707		
227	6172		$C_6F_6H_6NP$			1,4 24	2,4 8
	950						3,4 53
	3540						
83	6173		$C_6F_6H_9O_3P$	$(CF_3)_2C=P(OCH_3)_3$			13
83	6174		$C_6F_6H_9O_3P$	$(CF_3)_2C(CH_3)P(O)(OCH_3)_2$			5
510	6175		$C_6F_6H_{18}N_2P_2$	$[CH_3PF[N(CH_3)_2]_2]^+[CH_3PF_5]^-$ (4)(2) (3)(1)			
525	(2374 4981)						
515		H-M			1a,3 675.7 1e,3 832.4 2,4 1032		
778	6176	H*	C_6F_7OP			1,4 2,4 3,4	1.0 9.5 3.5
	(4366)						

Table C.14. (contd.)

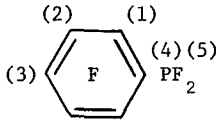
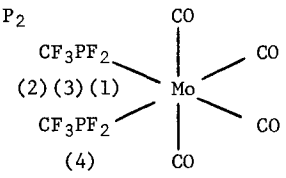
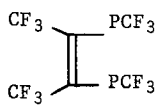
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
777	6177		C_6F_7P		4,5	1222			1,4	43.6
	(4367 4778)								2,4	2.5
									3,4	2.1
758	6178		$C_6F_{10}MoO_4P_2$		1,3	1155	2,3	106	1,4	4
	(4779)									
779	6179		$C_6F_{12}P_2$					59		18
780	6180		$C_6F_{13}H_3P_2$	$(CF_3)_2PCH_2CHFP(CF_3)_2$			1,3	77		
	(2937)			(1)(3) (4)(2)			2,4	76.7		
862	6181		$C_6F_{14}ClP$	$(CF_3CF_2CF_2)_2PCl$			1,4	58.4	2,4	36.5
	(2939)			(3)(2)(1) (4)					3,4	9.6
712	6182		$C_6F_{14}ClP$	$(CF_3CF_2CF_2)_2PCl$			1,4	54.8	2,4	36.0
	(2940)			(3)(2)(1) (4)					3,4	8.2
780	6183		$C_6F_{14}Cl_2P_2$	$(CF_3)_2PCF_2CCl_2P(CF_3)_2$			1,4	86	1,5	1
	(2941)			(1) (4)(3) (5)(2)			2,5	86	2,4	1
							3,4	40		
712	6184		$C_6F_{14}IP$	$(CF_3CF_2CF_2)_2PI$			1,4	47	2,4	37.4
	(2942a)			(3)(2)(1) (4)				20	3,4	7.8
862	6185		$C_6F_{14}IP$	$(CF_3CF_2CF_2)_2PI$			1,4	23.6	2,4	36.2
	(2942)			(3)(2)(1) (4)					3,4	9.2
780	6186		$C_6F_{14}H_2P_2$	$(CF_3)_2PCF_2CH_2P(CF_3)_2$			1,4	80	1,5	<1
	(2947)			(1) (4)(3)(5)(2)			2,5	80	2,4	1
							3,4	54		
658	6187	B	$C_6F_{15}P$	$(CF_3CF_2CF_2)_2PF$	1,5	1025	2,5	62.1	3,5	33.5
712				(4)(3)(2)(5)(1)					4,5	8.3
723	6188		$C_6F_{17}P$	$(CF_3CF_2CF_2)_2PF_3$		1172		125		
764	6189		$C_6F_{18}N_3P$	$[(CF_3)_2N]_3P$						14.0
502	6190		C_7FH_8OP	$C_6H_5P(O)FCH_3$		997				
	(2375)									
502	6191		C_7FH_8OPS	$C_6H_5P(S)F(OCH_3)$		1084				
770	6192	B	$C_7FH_8OPS_2$	$C_6H_5SP(S)F(OCH_3)$		1171				
502	6193		$C_7FH_8O_2P$	$C_6H_5P(O)F(OCH_3)$		1035				
	(2377)									
502	6194		C_7FH_8PS	$C_6H_5P(S)FCH_3$		1003				
	(2378)									
502	6195		$C_7FH_{10}ClNO_2P$	$ClCH_2P(O)FO^-C_6H_5NH_3^+$		980				
	(2379)									

Table C.14. (contd.)

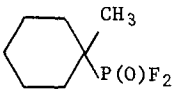
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
502	6196		$C_7FH_{11}NO_2P$	$CH_3P(O)FO^-C_6H_5NH_3^+$		962		
	(2380)							
133	6197	A^2	$C_7FH_{11}NO_3P$	$FCH_2P(O)(OH)O^-C_6H_5NH_3^+$			61	
	(443)							
781	6198		$C_7F_2H_5N_2P$	$C_6H_5PF_2NCN$		1132		
711	6199		$C_7F_2H_7P$	p $CH_3C_6H_4PF_2$		1099		
772								
711	6200		$C_7F_2H_7P$	$C_6H_5CH_2PF_2$		1190		
772								
531	6201	B	$C_7F_2H_7PS_2$	$C_6H_5CH_2SP(S)F_2$		1215		
	(2381)							
533	6202	H	$C_7F_2H_9NiO_3P$	$(CH_3)_3CPF_2Ni(CO)_3$		1135		
502	6203		$C_7F_2H_{13}OP$			1167		
231	6204		$C_7F_2H_{18}N_3P$	$[(CH_3)_2N]_3P{=}CF_2$			700	
	(954)							
584	6205		$C_7F_3H_7ClP$	p $CH_3C_6H_4PF_3Cl$	1a,2	970		
	(4982)			(2)(1)	1e,2	1047		
507	6206	B	$C_7F_3H_8P$	$CH_3PF_3C_6H_5$	1a,2	785		
658	(2382)			(2)(1)	1e,2	935		
706	(4983)							
584	6207		$C_7F_3H_8P$	para $CH_3C_6H_4PF_3H$	1a,2	815		
	(2563)			(2)(1)	1e,2	950		
	(4984)							
717	6208		$C_7F_3H_8PS$	$C_6H_5PF_3SCH_3$	1a,2	942		
789	(4985)			(2)(1)	1e,2	1042		
774	6209		$C_7F_3H_9NP$	$C_6H_5PF_3NHCH_3$	1a,2	770		
	(4986)			(2)(1)	1e,2	953		
502	6210		$C_7F_4H_7OP$	para $CH_3OC_6H_4PF_4$		951		
507	6211		$C_7F_4H_7P$	meta $CH_3C_6H_4PF_4$		960		
	(2384)							
507	6212		$C_7F_4H_7P$	para $CH_3C_6H_4PF_4$		960		
	(2385)							
507	6213		$C_7F_4H_7P$	$C_6H_5CH_2PF_4$		1002		
	(2383)							
762	6214		$C_7F_5H_{19}NP$	$[(CH_3CH_2)_3NH]^+[CH_3PF_5]^-$				
					1a,2	680		
					1e,2	835		
502	6215	A^2	$C_7F_6H_{10}NP$	$[C_6H_5CH_2NH_3]^+[PF_6]^-$		710		
502	6216		$C_7F_7H_4P$	meta $CF_3C_6H_4PF_4$		964		
780	6217		$C_7F_{12}H_6P_2$	$(CF_3)_2PCH_2CH(CH_3)P(CF_3)_2$			1,3	69
				(1) (3) (4)(2)			2,4	76

Table C.14. (contd.)

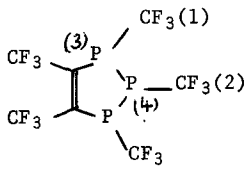
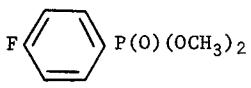
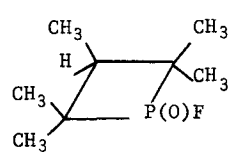
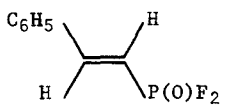
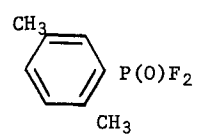
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
779	6218		$C_7F_{15}P_3$		1,3 2,4	65 60	1,4 2,3	25 20
400	6219 (1844)	B	$C_8FH_{10}OP$					1.54
770	6220	B	$C_8FH_{10}OPS_2$	$C_6H_5SP(S)F(OCH_2CH_3)$	1168			
502	6221		$C_8FH_{10}O_2P$	$C_6H_5P(O)F(OCH_2CH_3)$	1035			
502	6222 (2386)		$C_8FH_{11}NOP$	$C_6H_5P(O)F[N(CH_3)_2]$	1019			
515 705	6223 (2387)		$C_8FH_{11}NP$	$C_6H_5PF_3N(CH_3)_2$	989			
770	6224	B	$C_8FH_{11}NPS_2$	$C_6H_5SP(S)FN(CH_3)_2$	1112			
502	6225	A	$C_8FH_{16}OP$		1200			
502	6226 (2388)		$C_8FH_{18}OP$	$[CH_3(CH_2)_3]_2P(O)F$	1009			
526	6227 (2389)	B	$C_8FH_{18}OP$	$[(CH_3)_3C]_2P(O)F$	1090			
739 740	6228	B	$C_8FH_{18}O_2P$	$[CH_3(CH_2)_3O]_2PF$	1230			
526	6229 (2390)	B	$C_8FH_{18}P$	$[(CH_3)_3C]_2PF$	848			
502	6230 (2391)		$C_8FH_{18}PS$	$[CH_3(CH_2)_3]_2P(S)F$	1009			
526	6231 (2392)	H	$C_8FH_{18}PS$	$[(CH_3)_3C]_2P(S)F$	1093			
724	6232		$C_8FH_{20}N_2P$	$[(CH_3CH_2)_2N]_2PF$	1037			
502	6233		$C_8F_2H_7OP$		1084			
502	6234		$C_8F_2H_7PS$	$C_6H_5CH{=}CHP(S)F_2$ (Unknown configuration)	1118			
502	6235		$C_8F_2H_9OP$		1118			

Table C.14. (contd.)

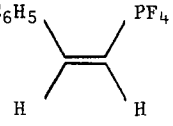
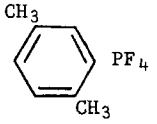
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
749	6236		$C_8F_2H_{10}FeNO_4P$	$F_2PN(CH_2CH_3)_2Fe(CO)_4$		1119.6		
790	6237	B	$C_8F_2H_{11}OP$	$(CH_3)_2PF_2(OC_6H_5)$		736		
502	6238		$C_8F_2H_{11}P$	$(CH_3)_2PF_2C_6H_5$		586		
532	6239	A	$C_8F_2H_{11}P$	$(CH_3)_2PF_2C_6H_5$		589		
	(2393)							
502	6240		$C_8F_2H_{17}PS$	$CH_3(CH_2)_4CH=(CH_3)CH_2P(S)F_2$				
				Isomer A		1135		
				Isomer B		1125		
688	6241	B	$C_8F_2H_{18}N_2NiO_2P_2$	$[CH_3PFN(CH_3)_2]_2Ni(CO)_2$		940		
716	6242	T[2]	$C_8F_3H_{10}PS$	$C_6H_5PF_3SCH_2CH_3$	1a,2	871		
717	(4987			(2)(1) (-60°)	1a,2	1015		
789	4988)				1e,2	1049		
				(Room temp.)	1a,2	938		
					1e,2	1049		
515	6243		$C_8F_3H_{11}NP$	$C_6H_5PF_3N(CH_3)_2$	1a,2	818		
530	(4989)			(2)(1)	1e,2	959		
750								
752								
774								
779								
507	6244		$C_8F_3H_{18}P$	$[CH_3(CH_2)_3]_2PF_3$	1a,2	810		
	(4990)			(2)(1)	1e,2	985		
526	6245		$C_8F_3H_{18}P$	$[(CH_3)_3C]_2PF_3$	1a,2	910		
	(2396			(2)(1)	1e,2	980		
	4991)							
530	6246		$C_8F_3H_{20}N_2P$	$F_3P[N(CH_2CH_3)_2]_2$	1a,2	751		
752	(4992)			(1)(2)	1e,2	875		
774								
521	6247		$C_8F_3H_{20}N_2P$	$F_3P[N(CH_2CH_3)_2]_2$	1a,2	753		
	(4993)			(1)(2)	1e,2	876		
771	6248		$C_8F_3H_{24}N_3P_3$	cis $P_3N_3F_3[N(CH_3)_2]_4$		920		
771	6249		$C_8F_3H_{24}N_3P_3$	trans $P_3N_3F_3[N(CH_3)_2]_4$		905		
507	6250		$C_8F_4H_7P$			940		
	(2397)							
502	6251		$C_8F_4H_9P$			980		
507	(2398)							
758	6252		$C_8F_4H_{12}MoN_2O_4P_2$	cis $[F_2PN(CH_3)_2]_2Mo(CO)_4$		1118		4

Table C.14. (contd.)

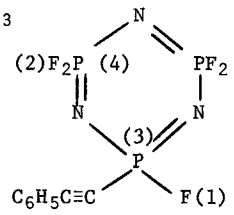
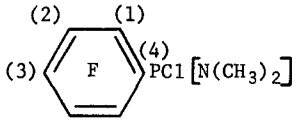
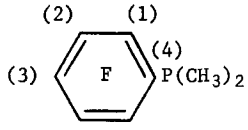
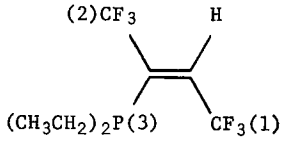
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J	^nJ	
507	6253		$C_8F_4H_{15}P$	$CH_3(CH_2)_3CH{=}C(CH_3)CH_2PF_4$					
	(2399)			Isomer A		955			
				Isomer B		955			
792	6254	G	$C_8F_5H_5N_3P_3$		1,3 2,4	900 910			
777	6255		$C_8F_5H_6ClNP$				1,4	51.0	2,4 1.7 3,4 1.3
777 778	6256 (4414)	H*	$C_8F_5H_6P$				1,4	30.1	2,4 1.7 3,4 ~0
206	6257	B	$C_8F_6H_{11}P$						1,3 53 2,3 ~0
	(867)								
502	6258	A^2	$C_8F_6H_{22}N_2P_2$	$[CH_3CH_2PF]N(CH_3)_2]_2]^+[CH_3CH_2PF_5]^-$ (3)(1) (4)(2)	1,3 2a,4 2e,4	1051 693 853			
790	6259	M	$C_8F_7H_6OP$	$(CH_3)_2PF_2(OC_6F_5)$		747			
688	6260	B	$C_8F_8H_{24}N_4NiP$	$[F_2PN(CH_3)_2]_4Ni$		1104			
780	6261		$C_8F_{12}H_8P_2$	$[(CF_3)_2PCH(CH_3)]_2$				78 or 69	
794	6262		$C_8F_{13}H_6O_4P$	$(CH_3O)_2PF.2(CF_3)_2CO$		915			
758	6263		$C_8F_{14}MoO_4P_2$	cis $[FP(CF_3)_2]_2Mo(CO)_4$		976		96	~2
	(4780)								
730	6264		$C_8F_{18}NiO_2P_2$	$[(CF_3)_3P]_2Ni(CO)_2$				91.4	
766	6265		$C_8F_{22}O_2P$	$[(CF_3)_3CO]_2PF_4$		892			1.2
	(4781)								
702	6266		$C_8F_{28}NiP_4$	$[(CF_3)_2PF]_4Ni$		1005		107	40

Table C.14. (contd.

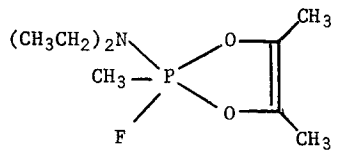
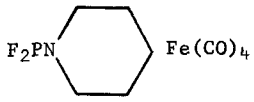
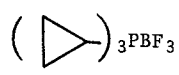
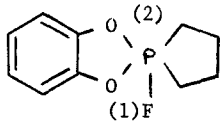
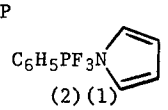
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
795	6267		$C_9FH_{19}NO_2P$			785	
738	6268		$C_9FH_{21}NP$	$CH_3PF[N(CH_2CH_2CH_2CH_3)_2]$		924	
533	6269	H	$C_9F_2H_9CrO_5P$	$(CH_3)_3CPF_2Cr(CO)_5$		1184	
533	6270	H	$C_9F_2H_9MoO_5P$	$(CH_3)_3CPF_2Mo(CO)_5$		1114	
533	6271	H	$C_9F_2H_9O_5PW$	$(CH_3)_3CPF_2W(CO)_5$		1104	
749	6272		$C_9F_2H_{10}FeNO_4P$			1117.2	
611	6273 (5368)		$C_9F_3H_{15}BP$				210.0
611	6274 (5369)		$C_9F_3H_{21}BP$	$[(CH_3)_2CH]_3PBF_3$			195.0
502	6275		$C_9F_4H_{11}P$	meta $(CH_3)_2CHC_6H_4PF_4$		964	
507	(2400)						
502	6276		$C_9F_4H_{11}P$	para $(CH_3)_2CHC_6H_5PF_4$		964	
507	(2401)						
796	6277		$C_{10}FH_{12}O_2P$		1a,2	829.2	
502	6278		$C_{10}FH_{14}O_2P$	$C_6H_5P(O)F[O(CH_2)_3CH_3]$		1037	
515	6279		$C_{10}FH_{15}NP$	$C_6H_5PF[N(CH_2CH_3)_2]$		990	
688	(2402)						
738	6280		$C_{10}FH_{15}NP$	$C_6H_5PF[N(CH_2CH_3)_2]$		964	
738	6281		$C_{10}FH_{15}NP$	$C_6H_5PF[HNCH_2CH(CH_3)_2]$		920	
502	6282		$C_{10}FH_{15}NPS$	$C_6H_5P(S)F[N(CH_2CH_3)_2]$		1059	
770	6283	B	$C_{10}FH_{15}NPS_2$	$C_6H_5SP(S)F[N(CH_2CH_3)_2]$		1115	
749	6284		$C_{10}F_2H_5FeO_4P$	$C_6H_5PF_3Fe(CO)_4$		1110.0	
688	6285	B	$C_{10}F_2H_{24}N_4NiO_2P_2$	$[FP[N(CH_3)_2]_2]_2Ni(CO)_2$		1041	
752	6286		$C_{10}F_3H_9NP$		1a,2	860	
					1e,2	978	
515	6287		$C_{10}F_3H_{15}NP$	$C_6H_5PF_3N(CH_2CH_3)_2$	1a,2	823	
530	(4994)			(2)(1)	1e,2	966	
705							
774							

Table C.14. (contd.)

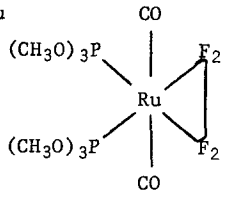
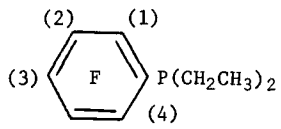
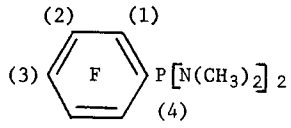
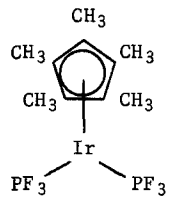
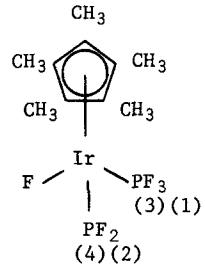
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ
797	6288	A	$C_{10}F_4H_{18}O_8P_2Ru$						46.5 26.1
688	6289	B	$C_{10}F_4H_{20}N_2NiO_2P_2$	$[F_2PN(CH_2CH_3)_2]_2Ni(CO)_2$	1140				
777	6290 (4433)		$C_{10}F_5H_{10}P$			1,4	35.8	2,4 3,4	1.0 0.8
777	6291 (4435)		$C_{10}F_5H_{12}N_2P$			1,4	∿5	2,4 3,5	6.6 2.6
774	6292 (4995)		$C_{10}F_5H_{17}NP$	$[(CH_3CH_2)_2NH_2]^+[C_6H_5PF_5]^-$ (2)(1)					
				1a,2	700				
				1e,2	820				
100	6293		$C_{10}F_6BrMn_2O_8P$	$(CF_3)_2PBrMn_2(CO)_8$			53.1		
100	6294		$C_{10}F_6ClMn_2O_8P$	$(CF_3)_2PClMn_2(CO)_8$			54.0		
100	6295		$C_{10}F_6IMn_2O_8P$	$(CF_3)_2PIMn_2(CO)_8$			51.6		
100	6296		$C_{10}F_6HMn_2O_8P$	$(CF_3)_2PHMn_2(CO)_8$			67.4		
798	6297 (4996)		$C_{10}F_6H_{15}IrP_2$		1250				2
798	6298		$C_{10}F_6H_{15}IrP_2$			1,3	1280		
						2,4	1177		

Table C.14. (contd.)

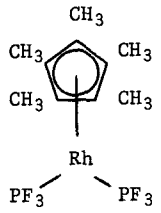
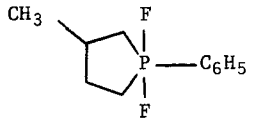
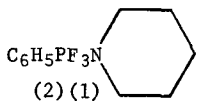
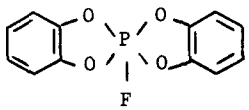
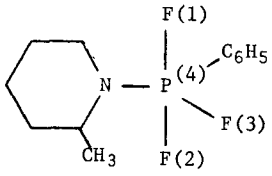
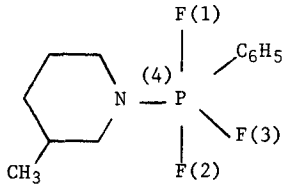
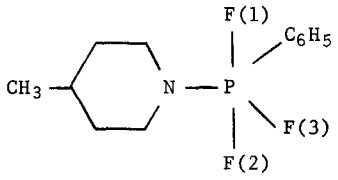
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
798	6299 (4997 6637)		$C_{10}F_6H_{15}P_2Rh$		1334		~6
794	6300		$C_{10}F_{14}H_{10}NO_2P$	$(CH_3CH_2)_2NPF_2.2(CF_3)_2CO$	810		
533	6301	H	$C_{11}FH_{18}NiO_3P$	$[(CH_3)_3C]_2PFNi(CO)_3$	870		
502	6302		$C_{11}F_2H_{15}P$		613		
522	6303 (2404)	M	$C_{11}F_2H_{18}NP$	$CH_3PF_2(C_6H_5)N(CH_2CH_3)_2$	693		
774	6304 (4998)		$C_{11}F_3H_{15}NP$		1a,2 820 1e,2 964		
100	6305		$C_{11}F_9Mn_2O_8PS$	$(CF_3)_2PSCF_3Mn_2(CO)_8$	544		
100	6306		$C_{11}F_9Mn_2O_8PSe$	$(CF_3)_2PSeCF\ Mn_2(CO)_8$	53.8		
796	6307		$C_{12}FH_8O_4P$		1018		
671	6308		$C_{12}FH_{10}Cl_2NP_2S$	$FP(S)ClN{=}PCl(C_6H_5)_2$	1100		13.7
658 706	6309		$C_{12}FH_{10}OP$	$(C_6H_5)_2P(O)F$	1020		
503	6310	B	$C_{12}FH_{10}OPS_2$	$FP(O)(SC_6H_5)_2$ (at 100°)	1201		
502	6311		$C_{12}FH_{10}O_2PS$	$(C_6H_5O)_2P(S)F$	1105		
502	6312		$C_{12}FH_{10}O_3P$	$(C_6H_5O)_2P(O)F$	1001		
770	6313	B	$C_{12}FH_{10}PS_3$	$(C_6H_5S)_2P(S)F$	1205		
502 658	6314	F	$C_{12}FH_{13}NO_2P$	$C_6H_5NH_3^+C_6H_5PFO_2^-$	963		
749	6315		$C_{12}FH_{20}FeN_2O_4P$	$FP[N(CH_2CH_3)_2]_2Fe(CO)_4$	1032.6		
386	6316 (1858)		$C_{12}F_2H_8ClP$	(para $FC_6H_4)_2PCl$			5.2
680	6317		$C_{12}F_2H_{27}O_2PSn$	$[CH_3(CH_2)_3]_3SnOP(O)F_2$	966		
507 658 706	6318 (2405)	B	$C_{12}F_2H_{27}P$	$[CH_3(CH_2)_3]_3PF_2$	553		
741	6319		$C_{12}F_2H_{27}P$	$[CH_3(CH_2)_3]_3PF_2$	588		

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
526	6320	B	$C_{12}F_2H_{27}P$	$[(CH_3)_3C]_3PF_2$		808		
741	6321		$C_{12}F_2H_{27}PS_3$	$[CH_3(CH_2)_3S]_3PF_2$		713		
799	6322		$C_{12}F_2H_{28}NOPS$	$(CH_3CH_2CH_2)_4N^+F_2P(O)S^-$		1096		
531	6323	M	$C_{12}F_2H_{28}NPS_2$	$(CH_3CH_2CH_2)_4N^+F_2PS_2^-$		1150		
658	6324	B	$C_{12}F_3H_{10}P$	$(C_6H_5)_2PF_3$	1a,2	838		
507				(2)(1)	1e,2	970		
706								
789	6325		$C_{12}F_3H_{10}PS$	$C_6H_5PF_3SC_6H_5$	1a,2	970		
717	(5000)			(2)(1)	1e,2	1066		
776	6326	T^2	$C_{12}F_3H_{17}NP$		1,4	828		
	(5001)				2,4	814		
					3,4	965		
776	6327	T^2	$C_{12}F_3H_{17}NP$		1,4	823		
	(5002)				2,4	820		
					3,4	1066		
776	6328	T^2	$C_{12}F_3H_{17}NP$		1,4	820		
	(5003)				2,4	820		
					3,4	965		
688	6329	B	$C_{12}F_3H_{27}MoN_3O_3P_3$	$[CH_3PFN(CH_3)_2]_3Mo(CO)_3$		930		
522	6330	M	$C_{12}F_4H_{10}CsP$	$Cs^+[(C_6H_5)_2PF_4]^-$		947		
744	6331	T^2	$C_{12}F_4H_{10}NP$	$F_4PN(C_6H_5)_2$	1a,2	788		
	(5004)			(1)(2) (-72°)	1e,2	941		
				(Room temp)		865		
802	6332	J	$C_{12}F_4H_{10}N_3P_3$	$(C_6H_5)_2$		~890		

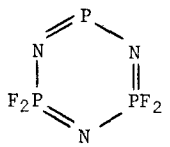


Table C.14. (contd.)

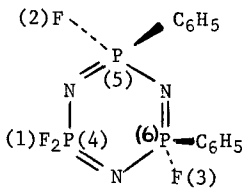
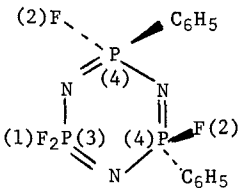
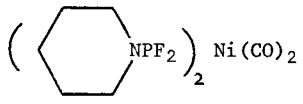
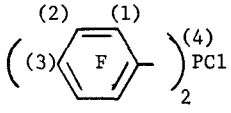
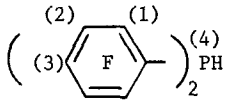
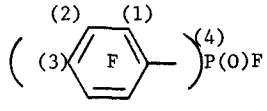
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J		^nJ
803	6333 (5005)	J	$C_{12}F_4H_{10}N_3P_3$		1,4 2,5 3,6	965 898 879			
803	6334 (5006)	J	$C_{12}F_4H_{10}N_3P_3$		1,3 2,4	939 879			
533	6335 (2406)	H	$C_{12}F_4H_{18}MoO_4P_2$	$[(CH_3)_3CPF_2]_2Mo(CO)_4$		1104 (^1J + ^3J)			
758	6336		$C_{12}F_4H_{20}MoN_2O_4P_2$	cis $((CH_3CH_2)_2NPF_2)_2Mo(CO)_4$		1100			~4
688	6337	T[2]	$C_{12}F_4H_{20}N_2NiO_2P_2$			1147			
688	6338	B	$C_{12}F_6H_{21}MoO_6P_3$	$[CH_3(CH_2)_2OPF_2]_3Mo(CO)_3$		~1220			
688	6339	B	$C_{12}F_8H_{28}NiO_4P_4$	$[CH_3(CH_2)_2OPF_2]_4Ni$		1230			
740	6340	B	$C_{12}F_8H_{28}NiO_4P_4$	$[CH_3(CH_2)_2OPF_2]_4Ni$		~1250			
777	6341	H*	$C_{12}F_{10}ClP$				1,4	38.7	2,4	1.5
778	(4452)								3,4	1.8
777	6342 (4457)		$C_{12}F_{10}HP$				1,4	12.3	2,4 3,4	1.6 ~0
778	6343 (4458)	H	$C_{12}F_{11}OP$						2,4 3,4	7.0 3.0
100	6344		$C_{12}F_{12}Mn_2O_8P_2$	$[(CF_3)_2P]_2Mn_2(CO)_8$				53.3		
794	6345		$C_{12}F_{13}H_{14}O_4P$	$[(CH_3)_2CHO]_2PF.2(CF_3)_2CO$		930				
781	6346		$C_{13}FH_{10}N_2P$	$(C_6H_5)_2PFNCN$		1064				
533	6347	H	$C_{13}FH_{18}CrO_5P$	$[(CH_3)_3C]_2PFCr(CO)_5$		865				
533	6348	H	$C_{13}FH_{18}MoO_5P$	$[(CH_3)_3C]_2PFMo(CO)_5$		853				
533	6349	H	$C_{13}FH_{18}O_5PW$	$[(CH_3)_3C]_2PFW(CO)_5$		848				

Table C.14. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
789	6350	H	$C_{13}F_2H_{13}O_2P$	$CH_3PF_2(OC_6H_5)_2$	825		
790							
502	6351		$C_{13}F_2H_{13}P$	$CH_3PF_2(C_6H_5)_2$	636		
532	6352	J	$C_{13}F_2H_{13}P$	$CH_3PF_2(C_6H_5)_2$	638		
717	6353		$C_{13}F_2H_{13}PS$	$(C_6H_5)_2PF_2SCH_3$	760		
789							
805	6354		$C_{13}F_2H_{20}BrClNPPt$	(1)F, Cl; (2)F, $PtBr[P(CH_2CH_3)_3]$, C_5H_5N		1,3	1
	(3606 6565)					2,3	2
231	6355		$C_{13}F_2H_{30}N_3P$	$CF_2=P[N(CH_2CH_3)_2]_3$	677		
	(977)						
806	6356		$C_{13}F_3H_{10}P$	$CF_3P(C_6H_5)_2$		73.3	
100	6357		$C_{13}F_6H_6Mn_2NO_9P$	$(CF_3)_2PN(CH_3)_2Mn_2(CO)_9$		74.5	
790	6358	M	$C_{13}F_{12}H_3O_2P$	$CH_3PF_2(OC_6F_5)_2$	870		
717	6359		$C_{14}F_2H_{15}PS$	$(C_6H_5)_2PF_2SCH_2CH_3$	752		
789							
522	6360	M	$C_{14}F_2H_{16}NP$	$(C_6H_5)_2PF_2N(CH_3)_2$	709		
	(2407)						
805	6361		$C_{14}F_3H_{30}BrNiP_2$	(1)F, F(3); (2)F, L(4), Ni, (4)L, Br		1,4	7.0
	(3608)					2,4	7.0
						3,4	5.5
		L =	$(CH_3CH_2)_3P$				
807	6362		$C_{14}F_3H_{30}BrP_2Pt$	(1)F, F(3); (2)F, (4) $P(CH_2CH_3)_3$, Pt, Br, $P(CH_2CH_3)_3$		1,4	23
	(3609 6569)					2,4	0
						3,4	34
807	6363		$C_{14}F_3H_{30}ClP_2Pt$	(1)F, F; F; $P(CH_2CH_3)_3$, Pt, (2) $(CH_3CH_2)_3P$, Cl		1,2	4.8
173	(3611 6570)						

Table C.14. (contd.)

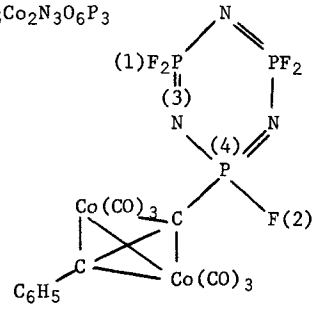
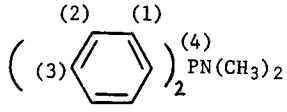
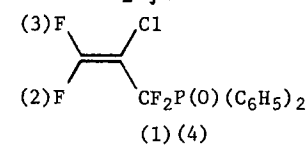
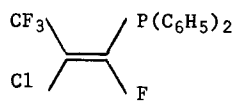
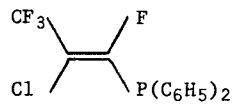
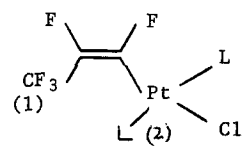
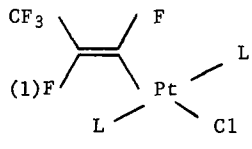
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ
792	6364	H	$C_{14}F_5H_5Co_2N_3O_6P_3$		1,3 2,4	910 970			
777	6365 (4468)		$C_{14}F_{10}H_6NP$				1,4	29	2,4 3,4	3.0 1.7
808	6366		$C_{14}F_{12}H_{10}O_2P_2Ti$	$(C_5H_5)_2Ti[OP(CF_3)_2]_2$				77		
741	6367		$C_{15}F_2H_{36}N_3P$	$F_2P[CH_2N(CH_2CH_3)_2]_3$		688				
809	6368	H	$C_{15}F_3H_{30}INiP$	$[(CH_3CH_2)_3P]_2NiI(C{\equiv}CCF_3)$						6.2
688	6369	A	$C_{15}F_3H_{36}MoN_6O_3P_3$	$[FP[N(CH_3)_2]_2]_3Mo(CO)_3$		1034				
565	6370 (3347 3613)		$C_{15}F_4H_{10}ClOP$				1,4	88	2,4 3,4	5.5 7.5
768	6371 (3349)		$C_{15}F_4H_{10}ClP$					14.2		63.7
768	6372 (3348)		$C_{15}F_4H_{10}ClP$					24.0		5.5
173	6373 [3350 3615 6575]		$C_{15}F_5H_{30}ClP_2Pt$	 L = $P(CH_2CH_3)_3$					1,2	3.2
173	6374 [3351 3616 6576]		$C_{15}F_5H_{30}ClP_2Pt$	 L = $P(CH_2CH_3)_3$					1,2	3.5

Table C.14. (contd.)

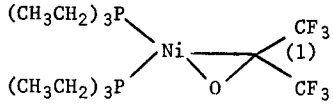
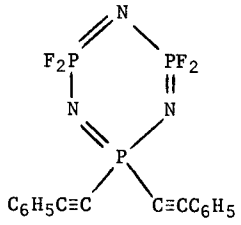
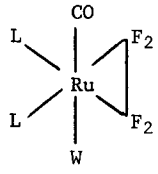
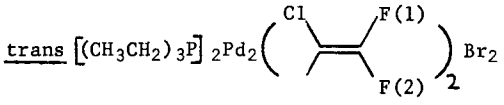
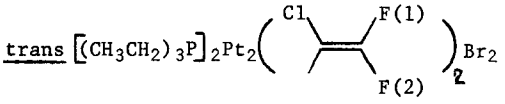
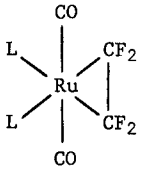
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
533	6375 (2408)	H	$C_{15}F_6H_{27}MoO_3P_3$	$[(CH_3)_3CPF_2]_3Mo(CO)_3$	1087		
688	6376	G	$C_{15}F_6H_{30}MoN_3O_3P_3$	$[(CH_3CH_2)_2NPF_2]_3Mo(CO)_3$	1104		
810	6377	J	$C_{15}F_6H_{30}NiOP_2$	 (2)		1,2	8.7
522	6378	B	$C_{16}F_2H_{20}NP$	$(C_6H_5)_2PF_2N(CH_2CH_3)_2$	730		
792	6379	G	$C_{16}F_4H_{10}N_3P_3$		860		
797	6380	A	$C_{16}F_4H_{22}O_8P_2Ru$	 L = $CH_3CH_2C(CH_2O)_3P$			49.0 30.0
805	6381 (3618)		$C_{16}F_4H_{30}Br_2Cl_2P_2Pd_2$			1,3 2,3	4 4
805	6382 (3619 6578)		$C_{16}F_4H_{30}Br_2Cl_2P_2Pt_2$			1,3 2,3	1
797	6383	A	$C_{16}F_4H_{30}O_8P_2Ru$	 L = $(CH_3CH_2O)_3P$			45.7 25.8
740	6384	B	$C_{16}F_4H_{40}NiO_8P$	$[FP(OCH_2CH_3)_2]_4Ni$	~1142		

Table C.14. (contd.)

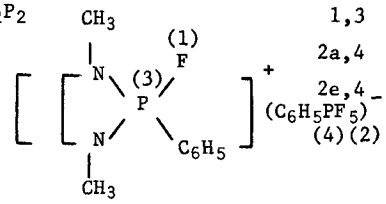
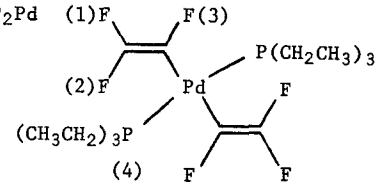
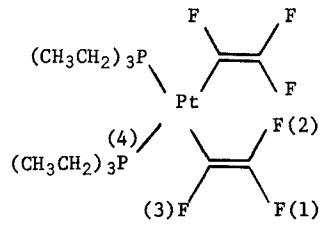
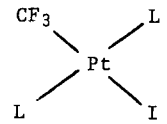
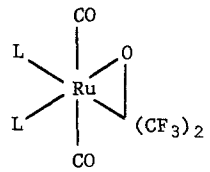
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
793	6385	M	$C_{16}F_6H_{20}N_2P_2$		1,3 1136 2a,4 691 2e,4 820		
515 525 658 791	6386 (5007)		$C_{16}F_6H_{22}N_2P_2$	$[C_6H_5PF[N(CH_3)_2]_2]^+[C_6H_5PF_5]^-$ (3)(1) (4)(2)	1,3 1042 2a,4 687 2e,4 820		
805	6387 (3623)		$C_{16}F_6H_{30}P_2Pd$			1,4 6.0 2,4 4.5 3,4 1.0	
805	6388 (3624 6577)		$C_{16}F_6H_{30}P_2Pt$			1,4 17 2,4 0 3,4 33	
740	6389	B	$C_{16}F_8H_{36}NiO_4P_4$	$[F_2PO(CH_2)_3CH_3]_4Ni$	1250		
688	6390	B	$C_{16}F_8H_{40}N_4NiP_4$	$[F_2PN(CH_2CH_3)_2]_4Ni$	1115		
702	6391		$C_{16}F_8H_{40}N_4NiP_4$	$[F_2PN(CH_2CH_3)_2]_4Ni$	1095		
177	6392 (6581)		$C_{17}F_3H_{22}IP_2Pt$	 L = $(CH_3)_2PC_6H_5$			20.5
797	6393	A	$C_{17}F_6H_{22}O_9P_2Ru$	 L = $CH_3CH_2C(CH_2O)_3P$			13.0

Table C.14. (contd.)

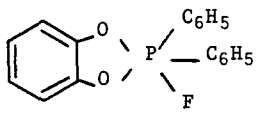
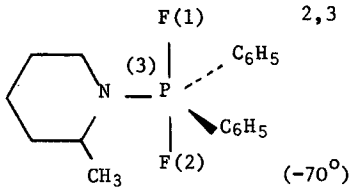
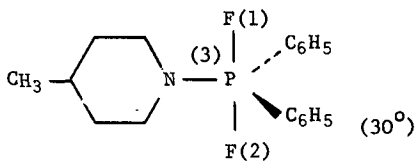
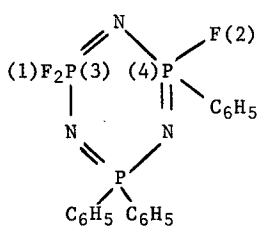
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
796	6394		$C_{18}FH_{14}O_2P$		797		
789	6395	H	$C_{18}F_2H_{15}OP$	$(C_6H_5)_2PF_2(OC_6H_5)$	797		
790							
789	6396	H	$C_{18}F_2H_{15}O_2P$	$C_6H_5PF_2(OC_6H_5)_2$	829		
790							
790	6397	H	$C_{18}F_2H_{15}O_3P$	$F_2P(OC_6H_5)_3$	768		
741			$C_{18}F_2H_{15}O_3P$	$F_2P(OC_6H_5)_3$	721		
502	6398	A	$C_{18}F_2H_{15}P$	$(C_6H_5)_3PF_2$	660		
741	6399		$C_{18}F_2H_{15}P$	$(C_6H_5)_3PF_2$	664		
811	6400	H	$C_{18}F_2H_{15}P$	$(C_6H_5)_3PF_2$	667		
717	6401		$C_{18}F_2H_{15}PS$	$(C_6H_5)_2PF_2(SC_6H_5)$	796		
789							
776	6402	T^2	$C_{18}F_2H_{22}NP$		1,3	689	
	(5008)				2,3	689	
							
					(-70°)		
776	6403	T^2	$C_{18}F_2H_{22}NP$			715 (av)	
							
					(30°)		
400	6404	E	$C_{18}F_3H_{12}OP$	(para $FC_6H_4)_3P(O)$			1.95
	(1871)						
386	6405		$C_{18}F_3H_{12}P$	(para $FC_6H_4)_3P$			4.5
	(1872)						
407	6406	J	$C_{18}F_3H_{12}P$	(para $FC_6H_4)_3P$			-4.5
	(1873)						
407	6407	J	$C_{18}F_3H_{12}PS$	(para $FC_6H_4)_3P(S)$			+2.4
	(1874)						
802	6408	J	$C_{18}F_3H_{15}N_3P_3$		1,3	895	
	(5009)				2,4	958	

Table C.14. (contd.)

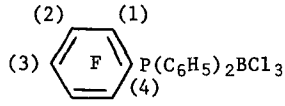
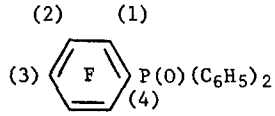
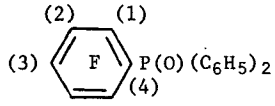
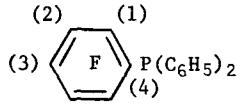
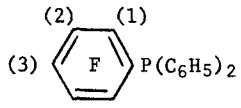
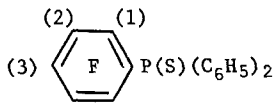
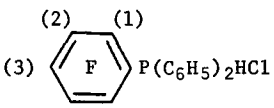
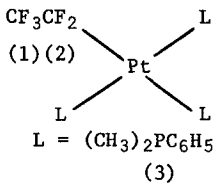
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
177	6409 (6582)		$C_{18}F_3H_{25}I_2P_2Pt$	$CH_3PtI_2(CF_3)[P(CH_3)_2C_6H_5]_2$				14.5
778	6410 (4478)	H*	$C_{18}F_5H_{10}BCl_3P$		1,4	14.0	2,4 3,4	2.7 3.1
778	6411 (4479)	H*	$C_{18}F_5H_{10}OP$		1,4	2.0	2,4 3,4	3.4 2.3
812	6412 (4480)	A*	$C_{18}F_5H_{10}OP$		1,4	6.5	2,4 3,4	3.6 2.3
812	6413 (4482)	A*	$C_{18}F_5H_{10}P$		1,4	38.0	2,4 3,4	<0.5 <0.5
778	6414 (4481)	H*	$C_{18}F_5H_{10}P$		1,4	38.9	2,4 3,4	0.6 0.6
778	6415 (4483)	H*	$C_{18}F_5H_{10}PS$		1,4	0	2,4 3,4	3.8 3.0
778	6416 (4485)	H*	$C_{18}F_5H_{11}ClP$		1,4	13.0	2,4 3,4	4.0 2.7
177	6417 (6584)	A	$C_{18}F_5H_{22}IP_2Pt$	 (3)			1,3 2,3	27.5 2.3

Table C.14. (contd.)

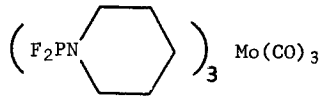
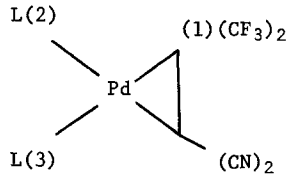
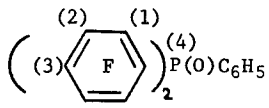
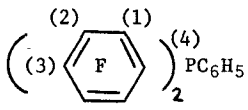
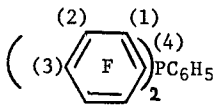
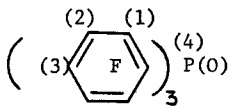
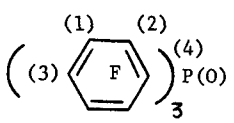
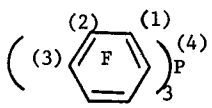
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
688	6418	B	$C_{18}F_6H_{30}MoN_3O_3P_3$		1120			
813	6419	R	$C_{18}F_6H_{30}N_2P_2Pd$	 (L = $(CH_3CH_2)_3P$			1,2 1,3	2.0 11.0
809	6420	G	$C_{18}F_6H_{30}P_2Pd$	$[(CH_3CH_2)_3P]_2\,Pd(C{\equiv}CCF_3)_2$				3.4
809	6421 (6585)	G	$C_{18}F_6H_{30}P_2Pt$	$[(CH_3CH_2)_3P]_2\,Pt(C{\equiv}CCF_3)_2$				3.3
790	6422	M	$C_{18}F_7H_{10}OP$	$(C_6H_5)_2PF_2(OC_6F_5)$	812			
812	6423 (4490)	A*	$C_{18}F_{10}H_5OP$			1,4 15.0	2,4 3,4	4.9 2.7
812	6424 (4492)	A*	$C_{18}F_{10}H_5P$			1,4 31.0	2,4 3,4	< 0.5 < 0.5
778	6425 (4491)	H*	$C_{18}F_{10}H_5P$			1,4 31.1	2,4 3,4	1.1 0
790	6426	M	$C_{18}F_{12}H_5O_2P$	$C_6H_5PF_2(OC_6F_5)_2$	817			
778	6427 (4501)	H*	$C_{18}F_{15}OP$				3,4	3.0
812	6428 (4502)	A*	$C_{18}F_{15}OP$			1,4 37.4	2,4 3,4	<1.0 <1.0
814	6429		$C_{18}F_{15}P$			1,4 36		

Table C.14. (contd.)

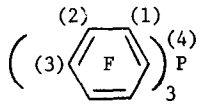
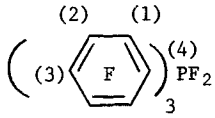
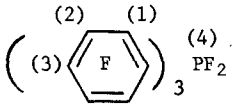
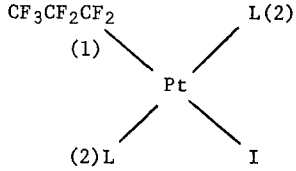
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ
812	6430	A*	$C_{18}F_{15}P$			1,4	36.5	2,4	<1.0
	(4504)							3,4	<1.0
812	6431	H*	$C_{18}F_{15}PS$					3,4	3.2
	(4505)								
790	6432	M	$C_{18}F_{17}O_3P$	$F_2P(OC_6F_5)_3$	809				
778	6433	H*	$C_{18}F_{17}P$					2,4	10.3
	(4509)							3,4	3.6
799	6434		$C_{19}F_2H_{18}OP_2S$	$[(C_6H_5)_3PCH_3]^+F_2P(O)S^-$	1098				
815	6435	I^3	$C_{19}F_3H_{14}P$	ortho $CF_3C_6H_4P(C_6H_5)_2$					
				(-12^o)					52.50
				(25.3^o)					53.41
				(72.4^o)					54.44
				(112^o)					55.20
407	6436	J	$C_{19}F_3H_{15}BrP$	(para $FC_6H_4)_3PBrCH_3$					+1.3
	(1875)								
177	6437	A	$C_{19}F_3H_{28}IP_2Pt$	$(CH_3)_2PtICF_3[P(CH_3)_2C_6H_5]_2$					14
	(6587)								
177	6438	A	$C_{19}F_5H_{25}I_2P_2Pt$	$CH_3PtI_2CF_2CF_3[P(CH_3)_2C_6H_5]_2$				1,2	22
	(746, 6588)			(1) (2)					
177	6439	A	$C_{19}F_7H_{22}IP_2Pt$					1,2	28
	(3176, 6589)			L = $(CH_3)_2PC_6H_5$					
533	6440	H	$C_{20}F_2H_{36}MoO_4P_2$	$[[(CH_3)_3C]_2PF]_2Mo(CO)_4$	855	$(^1J + {}^3J)$			
	(2409)								
177	6441	A	$C_{20}F_5H_{28}IP_2Pt$	$(CH_3)_2PtI(CF_2CF_3)[P(CH_3)_2C_6H_5]_2$				1,2	33
	(6593)			(1) (2)					
815	6442	I^3	$C_{20}F_6H_{13}P$	(ortho $CF_3C_6H_4)_2PC_6H_5$					
				(-43^o)					51.10
				(24.6^o)					52.82
				(69.5^o)					52.72
				(117^o)					54.50

Table C.14. (contd.)

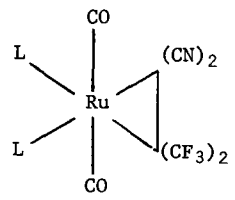
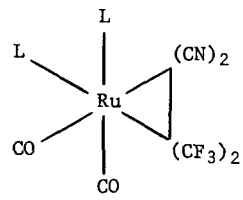
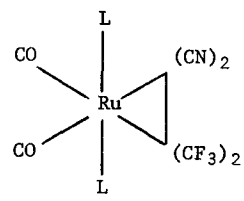
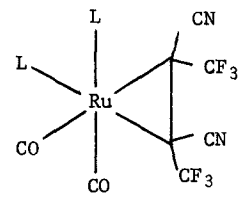
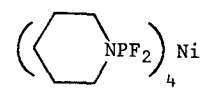
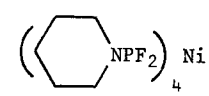
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
797	6443	A	$C_{20}F_6H_{22}N_2O_8P_2Ru$	 L = $CH_3CH_2C(CH_2O)_3P$			11.5
797	6444	A	$C_{20}F_6H_{22}N_2O_8P_2Ru$	 or  L = $CH_3CH_2C(CH_2O)_3P$			11.5
797	6445	A	$C_{20}F_6H_{22}N_2O_8P_2Ru$	 L = $CH_3CH_2C(CH_2O)_3P$			6.0
688	6446	H	$C_{20}F_8H_{40}N_4NiP_4$		1123		
702	6447		$C_{20}F_8H_{40}N_4NiP$		1120		
740	6448	B	$C_{20}F_8H_{44}NiO_4P_4$	$[F_2PO(CH_2)_4CH_3]_4Ni$	~1260		

Table C.14. (contd.)

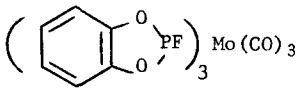
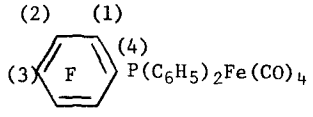
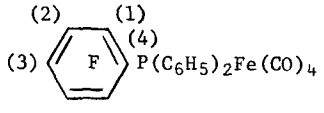
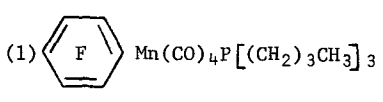
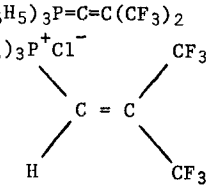
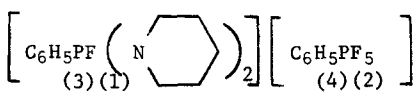
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ	
688	6449	H	$C_{21}F_3H_{12}MoO_9P_3$		1270			
688	6450	B	$C_{21}F_6H_{15}MoO_3P_3$	$(C_6H_5PF_2)_3Mo(CO)_3$	1113			
746		H			-1096			+6.7
688	6451	B	$C_{21}F_6H_{15}MoO_6P_3$	$(C_6H_5OPF_2)_3Mo(CO)_3$	1240			
746		H			-1243			+2.5
177	6452 (3181, 6597)	A	$C_{21}F_7H_{26}BrP_2Pt$	$(CH_3)_2PtBr(CF_2CF_2CF_3)[P(CH_3)_2C_6H_5]_2$ (1) (2)			1,2	31
177	6453 (3182, 6598)	A	$C_{21}F_7H_{28}IP_2Pt$	$(CH_3)_2PtI(CF_2CF_2CF_3)[P(CH_3)_2C_6H_5]_2$ (1) (2)			1,2	30
815	6454	I[3]	$C_{21}F_9H_{12}P$	(ortho $CF_3C_6H_4)_3P$				
				(-15.5°)				54.23
				(24.1°)				55.00
				(73.5°)				55.98
				(117°)				56.73
778	6455 (4514)	H*	$C_{22}F_5H_{10}FeO_4P$		1,4	0	2,4	1.1
							3,4	1.8
928	6456 (4513)		$C_{22}F_5H_{10}FeO_4P$		1,4	<3	3,4	1.8
816	6457		$C_{22}F_5H_{27}MnO_4P$				1,2	0.8
817	6458		$C_{22}F_6H_{15}P$	$(C_6H_5)_3P{=}C{=}C(CF_3)_2$				3.5
210	6459 (3183)	A	$C_{22}F_6H_{16}ClP$					≈0.5
502	6460	M	$C_{22}F_6H_{30}N_2P_2$		1,3	1042		
					2a,4	690		
					2e,4	825		
								

Table C.14. (contd.)

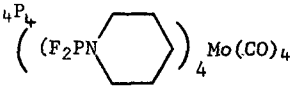
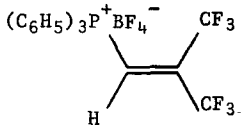
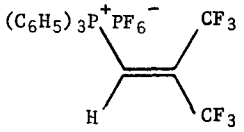
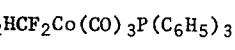
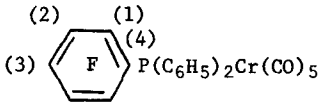
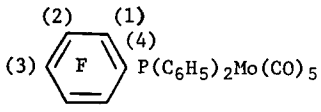
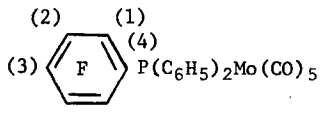
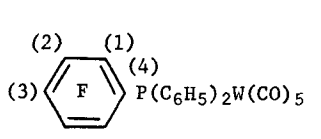
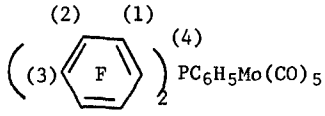
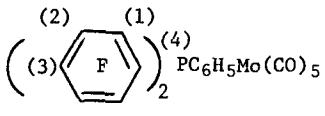
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
688	6461	B	$C_{22}F_8H_{40}MoN_4O_4P_4$		1079			
210	6462 (3184)	A	$C_{22}F_{10}H_{16}BP$					1.1
210	6463 (3185)	A	$C_{22}F_{12}H_{16}P_2$		714			
124	6464 (762 3187)		$C_{23}F_4H_{16}CoO_3P$				1,2	30.5
778	6465 (4519)	H*	$C_{23}F_5H_{10}CrO_5P$		1,4	0	2,4 3,4	0.9 1.7
928	6466 (4521)		$C_{23}F_5H_{10}MoO_5P$		1,4	<2	3,4	1.6
778	6467 (4522)	H*	$C_{23}F_5H_{10}MoO_5P$		1,4	0	2,4 3,4	0.9 1.6
778	6468 (4523)	H*	$C_{23}F_5H_{10}O_5PW$		1,4	0	2,4 3,4	1.3 1.9
778	6469 (4526)	H*	$C_{23}F_{10}H_5MoO_5P$		1,4	5.0	2,4 3,4	1.3 1.4
928	6470 (4525)		$C_{23}F_{10}H_5MoO_5P$		1,4	5	3,4	1.4
655	6471	E^2	$C_{24}FH_{20}ClOP_2S$	$(C_6H_5)_4P^+FP(O)ClS^-$	1056			

Table C.14. (contd.)

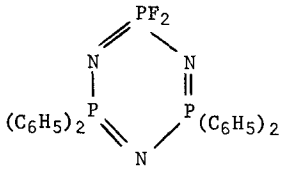
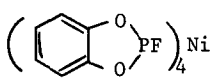
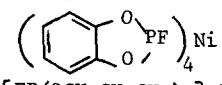
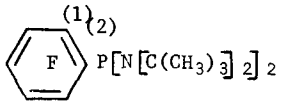
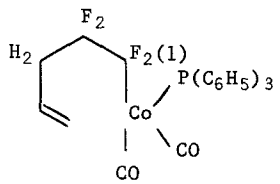
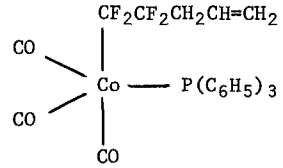
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
802	6472	J	$C_{24}F_2H_{20}N_3P_3$		896			
531	6473	M	$C_{24}F_2H_{56}N_2P_2S_5$	$[(CH_3CH_2CH_2)_4N]_2(FPS_2)_2S$	1160			
531	6474	M	$C_{24}F_2H_{56}N_2P_2S_6$	$[(CH_3CH_2CH_2)_4N]_2(FPS_2)_2S_2$	1170			
818	6475 (5010)	*	$C_{24}F_4H_{16}NiO_8P_4$		-1290			+29.2
688	6476	H	$C_{24}F_4H_{16}NiO_8P$		1280			
740	6477		$C_{24}F_4H_{56}NiO_8P_4$	$[FP(OCH_2CH_2CH_3)_2]_4Ni$	~1143			
777	6478		$C_{24}F_5H_{36}N_2P$			1,2	39	
688	6479	B	$C_{24}F_8H_{20}NiO_8P_4$	$(C_6H_5OPF_2)_4Ni$	1258			
688	6480	A	$C_{24}F_8H_{20}NiP_4$	$(C_6H_5PF_2)_4Ni$	1113			
819	6481	J	$C_{25}F_3H_{20}FeOP$	$CF_3Fe(CO)[P(C_6H_5)_3](C_5H_5)$				1.6
806	6482		$C_{25}F_3H_{38}Br_3NPPd$	$[(CH_3CH_2CH_2)_4N]^+([CF_3P(C_6H_5)_2]PdBr_3)^-$		56.0		
806	6483		$C_{25}F_3H_{38}Cl_3NPPd$	$[(CH_3CH_2CH_2)_4N]^+([CF_3P(C_6H_5)_2]PdCl_3)^-$		65.8		
806	6484		$C_{25}F_3H_{38}I_3NPPd$	$[(CH_3CH_2CH_2)_4N]^+([CF_3P(C_6H_5)_2]PdI_3)^-$		47.6		
806	6485 (6601)		$C_{25}F_3H_{38}I_3NPPt$	$[(CH_3CH_2CH_2)_4N]^+([CF_3P(C_6H_5)_2]PtI_3)^-$		53.6		
200	6486		$C_{25}F_4H_{20}CoO_2P$				1,2	33.0
1056	6487 (3189)		$C_{25}F_5H_{20}NiP$	$CF_3CF_2Ni[P(C_6H_5)_3]\pi C_5H_5$ (1) (2)			1,2	38.0
820	6488 (4782)	J	$C_{25}F_8H_{20}AsP$	$[(C_6H_5)_4As]^+[CF_3PF_5]^-$	810	145		
819	6489	J	$C_{26}F_3H_{20}MoO_2P$	$CF_3Mo(CO)_2[P(C_6H_5)_3](C_5H_5)$				1.5
200	6490 (765)	A	$C_{26}F_4H_{20}CoO_3P$					34.0
806	6491		$C_{26}F_6H_{20}Br_2P_2Pd$	trans $[CF_3P(C_6H_5)_2]_2PdBr_2$		72.6 (^2J + ^4J)		
806	6492 (6605)		$C_{26}F_6H_{20}Br_2P_2Pt$	trans $[CF_3P(C_6H_5)_2]_2PtBr_2$		69.2 (^2J + ^4J)		

Table C.14. (contd.)

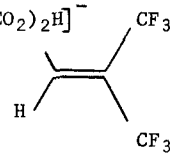
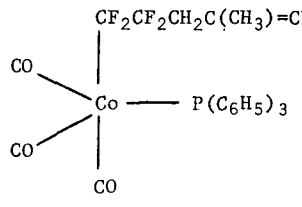
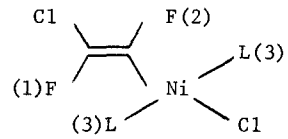
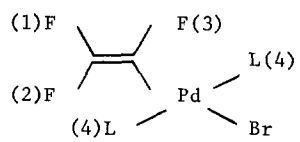
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
806	6493 (6606)		$C_{26}F_6H_{20}Br_2P_2Pt$	cis $[CF_3P(C_6H_5)_2]_2PtBr_2$		68.4		
806	6494		$C_{26}F_6H_{20}Cl_2P_2Pd$	trans $[CF_3P(C_6H_5)_2]_2PdCl_2$		71.0	($^2J + {}^4J$)	
806	6495 (6607)		$C_{26}F_6H_{20}Cl_2P_2Pt$	trans $[CF_3P(C_6H_5)_2]_2PtCl_2$		73.2	($^2J + {}^4J$)	
806	6496 (6608)		$C_{26}F_6H_{20}Cl_2P_2Pt$	cis $[CF_3P(C_6H_5)_2]_2PtCl_2$		68.5		
806	6497		$C_{26}F_6H_{20}I_2P_2Pd$	trans $[CF_3P(C_6H_5)_2]_2PdI_2$		62.7	($^2J + {}^4J$)	
806	6498		$C_{26}F_6H_{20}Br_4P_2Pd_2$	$[CF_3P(C_6H_5)_2]_2Pd_2Br_4$		69.7		
806	6499		$C_{26}F_6H_{20}Cl_4P_2Pd$	$[CF_3P(C_6H_5)_2]_2Pd_2Cl_4$		72.2		
806	6500		$C_{26}F_6H_{20}I_4P_2Pd_2$	$[CF_3P(C_6H_5)_2]_2Pd_2I_4$		62.0		
806	6501 (6609)		$C_{26}F_6H_{20}I_4P_2Pt_2$	$[CF_3P(C_6H_5)_2]_2Pt_2I_4$		66.9		
820	6502 (4783)	J	$C_{26}F_{10}H_{20}AsP$	$[(C_6H_5)_4As]^+[(CF_3)_2PF_4]^-$	884	145		
821	6503 (3193)		$C_{26}F_{11}H_{20}CoOP_2$	$[\pi C_5H_5Co(CO)[P(C_6H_5)_3]CF_2CF_3]^+PF_6^-$ (4) (2) (3)(1)	1,3 699		2,4	12.3 32.9
210	6504 (3194)	A	$C_{26}F_{12}H_{17}O_4P$	$(C_6H_5)_3P^+[(CF_3CO_2)_2H]^-$ 				1.2
200	6505 (769)	A	$C_{27}F_4H_{22}CoO_3P$ 					29.0
821	6506 (3176)		$C_{27}F_5H_{23}ClCoNO_4P$	$[\pi C_5H_5Co(CH_3CN)[P(C_6H_5)_3]CF_2CF_3]^+ClO_4^-$ (2) (1)			1,2	10.1 30.8
822	6507	J	$C_{28}F_2H_{26}Cl_2NiP_2$  L = $P(C_6H_5)_2CH_3$				1,3 2,3	7.0 7.0
823	6508 (3630)	A	$C_{28}F_3H_{26}BrP_2Pd$  L = $P(C_6H_5)_2CH_3$				1,4 2,4 3,4	7.5 5.5 6.5

Table C.14. (contd.)

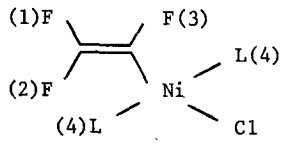
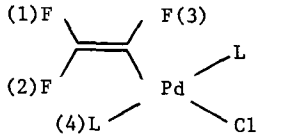
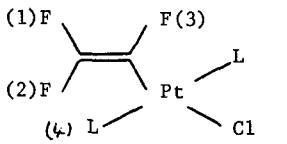
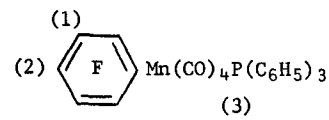
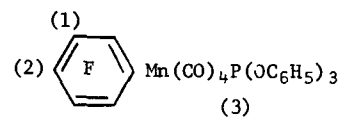
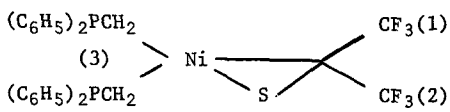
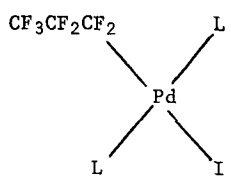
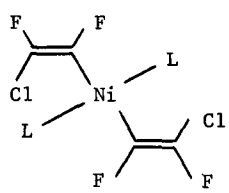
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
822	6509 (3629)	J	$C_{28}F_3H_{26}ClNiP_2$	 $L = P(C_6H_5)_2CH_3$		1,4 2,4 3,4	7.0 7.0 5.5
823	6510 (3630)	A	$C_{28}F_3H_{26}ClP_2Pd$	 $L = P(C_6H_5)_2CH_3$		1,4 2,4 3,4	8.0 5.6 7.0
807	6511 (3631 / 6610)	A	$C_{28}F_3H_{26}ClP_2Pt$	 $L = P(C_6H_5)_2CH_3$		1,4 2,4	5.8 3.8
816	6512 (4544)		$C_{28}F_5H_{15}MnO_4P$			1,3 2,3	0.9 1.8
816	6513 (4546)		$C_{28}F_5H_{15}MnO_7P$			1,3 2,3	1.4 2.4
810	6514	A	$C_{29}F_6H_{24}NiP_2S$			1,3 2,3	2.0 10.0
823	6515 (3203)	A	$C_{29}F_7H_{26}IP_2Pd$	 $L = P(C_6H_5)_2CH_3$		1,2	18.5
822	6516 (3633)	J	$C_{30}F_4H_{26}Cl_2NiP_2$	 $L = P(C_6H_5)_2CH_3$			7.0

Table C.14. (contd.)

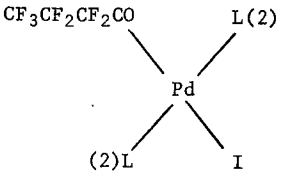
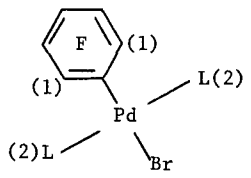
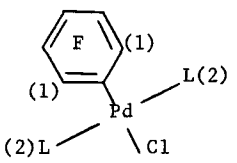
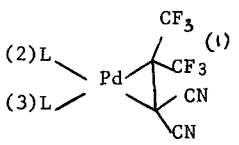
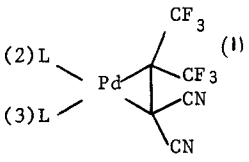
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
823	6517 (3205)	A	$C_{30}F_7H_{26}IOP_2Pd$	 L = $P(C_6H_5)_2CH_3$		1,2	8.0
740	6518	B	$C_{32}F_4H_{72}NiO_8P_4$	$[FP[O(CH_2)_3CH_3]_2]_4Ni$	~1145		
823	6519 (4548)	A	$C_{32}F_5H_{26}BrP_2Pd$	 L = $P(C_6H_5)_2CH_3$		1,2	<0.5
823	6520 (4549)	A	$C_{32}F_5H_{26}ClP_2Pd$	 L = $P(C_6H_5)_2CH_3$		1,2	<0.5
813	6521	J	$C_{32}F_6H_{24}N_2P_2Pd$	 L = $CH_2P(C_6H_5)_2$		1,2 1,3	5.0 11.0
813	6522	R	$C_{32}F_6H_{26}N_2P_2Pd$	 L = $P(C_6H_5)_2CH_3$		1,2 1,3	4.0 10.0
688	6523	B	$C_{33}F_3H_{45}MoN_3O_3P_3$	$[C_6H_5PF[N(CH_2CH_3)_2]]_3Mo(CO)_3$			

Table C.14. (contd.)

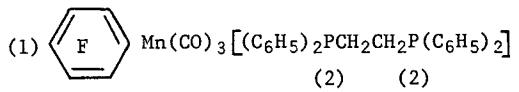
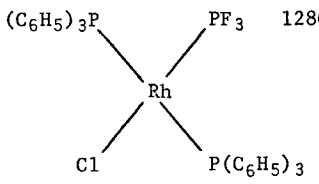
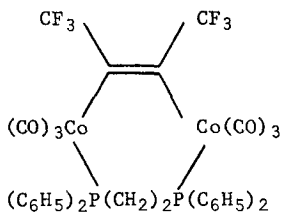
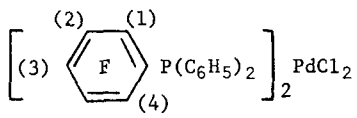
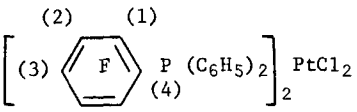
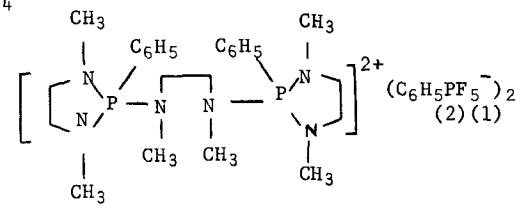
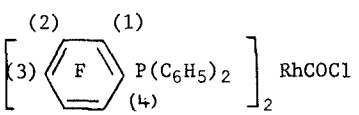
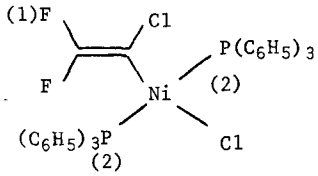
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
816	6524 (4551)		$C_{35}F_5H_{24}MnO_3P_2$			1,2	1.1
824	6525 (6638)	H	$C_{36}F_3H_{30}ClP_3Rh$		1286		7
825	6526	A	$C_{36}F_6H_{24}Co_2O_2P_2$				
778	6527 (4553)	H	$C_{36}F_{10}H_{20}Cl_2P_2Pd$			2,4 3,4	0 0
812	6528 (4554)	A	$C_{36}F_{10}H_{20}Cl_2P_2Pt$			1,4 2,4 3,4	<1.0 <0.5 <0.5
793	6529	M	$C_{36}F_{10}H_{50}N_6P_4$		1a,2 693 1e,2 822		
812	6530 (4556)	A	$C_{37}F_{10}H_{20}ClOP_2Rh$			1,4 2,4 3,4	<1.0 <0.5 <0.5
822	6531 (3634)		$C_{38}F_2H_{30}Cl_2NiP_2$			1,2	2.0

Table C.14. (contd.)

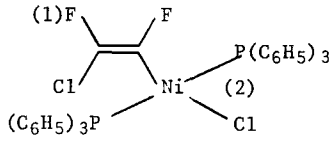
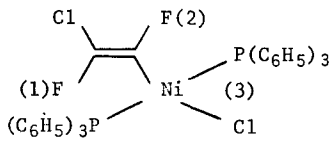
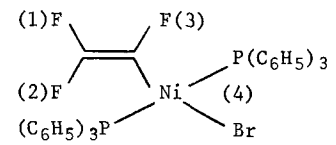
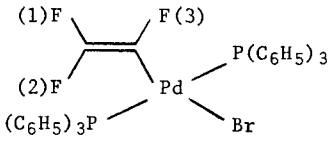
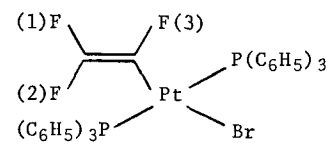
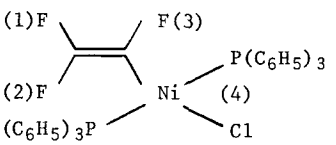
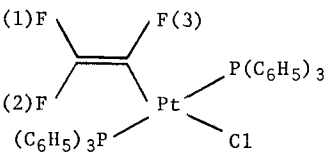
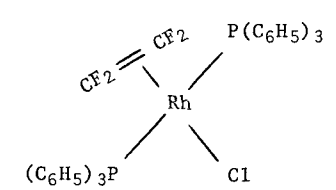
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
822	6532 (3635)		$C_{38}F_2H_{30}Cl_2NiP_2$	 (2)			1,2 7.5
822	6533 (3636)		$C_{38}F_2H_{30}Cl_2NiP_2$	 (3)			1,3 5.5 2,3 7.5
822	6534 (3637)		$C_{38}F_3H_{30}BrNiP_2$	 (4)			1,4 7.0 2,4 7.0 3,4 5.5
823	6535 (3638)	A	$C_{38}F_3H_{30}BrP_2Pd$	 (4)			1,4 5.0 2,4 5.0 3,4 7.0
807	6536 (3639, 6614)	A	$C_{38}F_3H_{30}BrP_2Pt$	 (4)			1,4 5.8 2,4 3.8
822	6537 (3640)		$C_{38}F_3H_{30}ClNiP_2$	 (4)			1,4 7.0 2,4 7.0 3,4 5.5
807	6538 (3641, 6615)	A	$C_{38}F_3H_{30}ClP_2Pt$	 (4)			1,4 5.6 2,4 3.5
141	6539 (6640)		$C_{38}F_4H_{30}ClP_2Rh$			24.3	

Table C.14. (contd.)

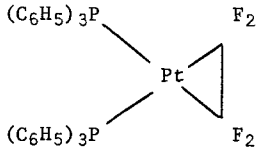
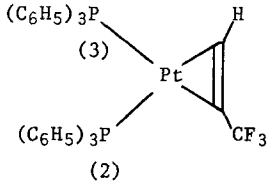
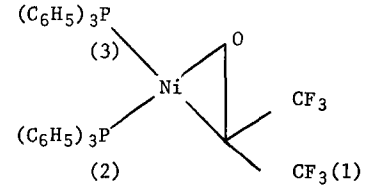
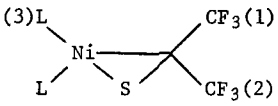
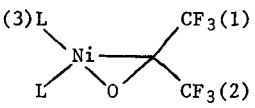
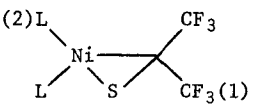
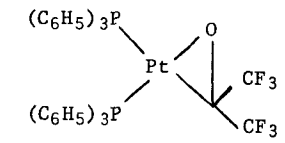
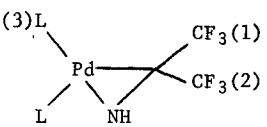
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
807	6540	A	$C_{38}F_4H_{30}P_2Pt$				24.5
826	(4063 / 6617)						38.0
749	6541	H	$C_{39}F_3H_{30}MoO_3P_3$	fac $[(C_6H_5O)_2PF]_3Mo(CO)_3$	-1269		+1.2
168	6542		$C_{39}F_3H_{31}P_2Pt$			1,2	2.8
	(900 / 6619)					1,3	12.5
822	6543	J	$C_{39}F_6H_{30}NiOP_2$			1,2	<1.0
						1,3	12.2
810	6544		$C_{39}F_6H_{30}NiO_6P_2S$			1,3	1.0
						2,3	12.0
				L = $P(OC_6H_5)_3$			
810	6545	A	$C_{39}F_6H_{30}NiO_7P_2$			1,3	3.4
						2,3	12.2
				L = $P(OC_6H_5)_3$			
810	6546	A	$C_{39}F_6H_{30}NiP_2S$			1,2	7.5
				L = $P(C_6H_5)_3$			
826	6547		$C_{39}F_6H_{30}OP_2Pt$				11.6
	(6620)						1
813	6548	R	$C_{39}F_6H_{31}P_2NPd$			1,3	3.0
						2,3	12.0
				L = $P(C_6H_5)_3$			

Table C.14. (contd.)

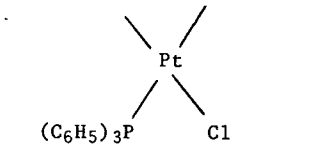
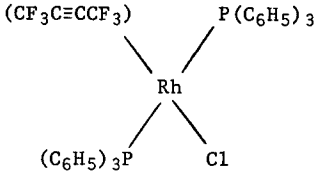
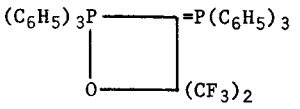
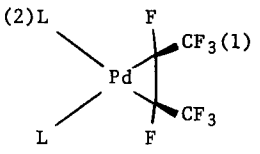
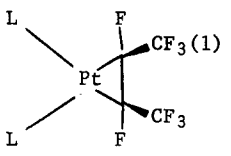
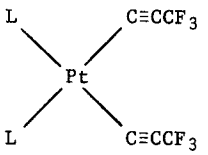
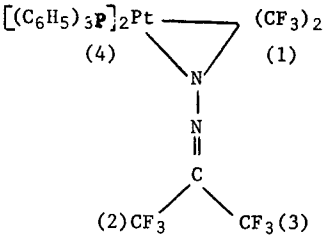
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
827	6549 (6624)		$C_{40}F_6H_{30}ClP_2Pt$				10.3
141	6550 (6641)		$C_{40}F_6H_{30}ClP_2Rh$				<1
210	6551	J	$C_{40}F_6H_{30}OP_2$				~ 0.8
825	6552	A	$C_{40}F_8H_{30}P_2Pd$	 L = $P(C_6H_5)_3$		1,2	9.5
825	6553	A	$C_{40}F_8H_{30}P_2Pt$	 L = $P(C_6H_5)_3$		1,2	9.2
817 210	6554	M	$C_{40}F_{12}H_{31}OP_2$	$(CF_3)_2C(OH)^+C[P(C_6H_5)_3]_2PF_6^-$	709		
828	6555 (6629)		$C_{42}F_6H_{30}P_2Pt$	 L = $P(C_6H_5)_3$			3.8
832	6556 (3215 6631)		$C_{42}F_{12}H_{30}N_2P_2Pt$			1,4 2,4 3,4	10.0 2.5 6.0

Table C.15. M = platinum (Pt)

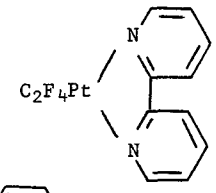
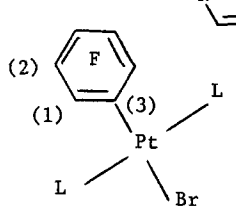
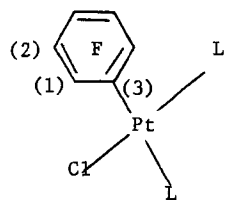
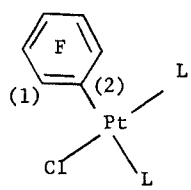
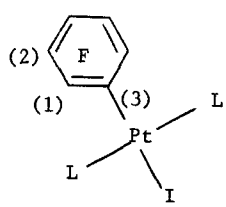
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
829	6557	D[3]	F_6K_2Pt	K_2PtF_6	2080			
831	6558	L	$C_4F_4H_8N_2Pt$	$C_2F_4Pt(H_2NCH_2CH_2NH_2)$		501		
831	6559	L	$C_{12}F_4H_8N_2Pt$			494		
830	6560		$C_{12}F_5H_{30}BrP_2Pt$				1,3 2,3	461 99
				L = $P(CH_2CH_3)_3$				
830	6561		$C_{12}F_5H_{30}ClP_2Pt$				1,3 2,3	463 100
				L = $P(CH_2CH_3)_3$				
830	6562		$C_{12}F_5H_{30}ClP_2Pt$				1,2	339
				L = $P(CH_2CH_3)_3$				
830	6563		$C_{12}F_5H_{30}IP_2Pt$				1,3 2,3	441 94
				L = $P(CH_2CH_3)_3$				

Table C.1 . (contd.)

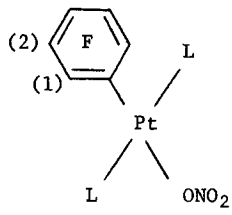
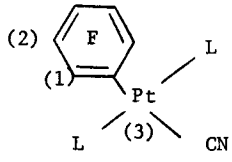
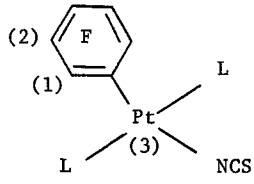
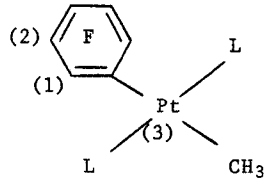
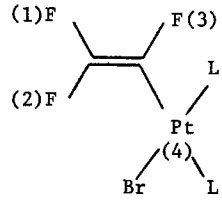
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
830	6564		$C_{12}F_5H_{30}NO_3P_2Pt$	 L = $P(CH_2CH_3)_3$			1,3 2,3	472 101
805	6565 (3606 6354)		$C_{13}F_2H_{20}BrClNPPt$	$(CH_3CH_2)_3PPtD(Br)(CCl{=}CF_2)$ (3) (1,2) D = 			1,3 2,3	87 145
830	6566		$C_{13}F_5H_{30}NP_2Pt$	 L = $P(CH_2CH_3)_3$			1,3 2,3	348 71
830	6567		$C_{13}F_5H_{30}NP_2PtS$	 L = $P(CH_2CH_3)_3$			1,3 2,3	443 96
830	6568		$C_{13}F_5H_{33}P_2Pt$	 L = $P(CH_2CH_3)_3$			1,3	282
805 807	6569 (3609 6362)		$C_{14}F_3H_{30}BrP_2Pt$	 L = $P(CH_2CH_3)_3$	3,4	348	1,4 2,4	188 51

Table C.15. (contd.)

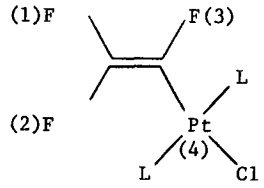
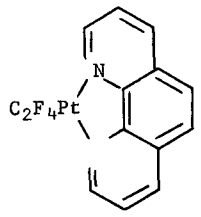
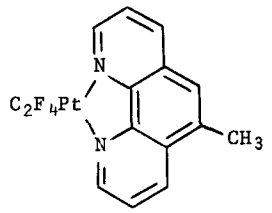
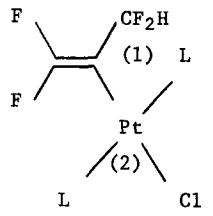
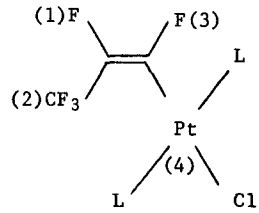
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
173	6570 (3611 6364)		$C_{14}F_3H_{30}ClP_2Pt$	 $L = P(CH_2CH_3)_3$	3,4	574	1,4 59.7 2,4 62.4
831	6571	L	$C_{14}F_4H_8N_2Pt$			491	
168	6572 (890)		$C_{15}F_3H_{32}ClP_2Pt$	$CH_2=C(CF_3)PtCl[P(CH_2CH_3)_3]_2$			72.7
831	6573	L	$C_{15}F_4H_{10}N_2Pt$			485	
173	6574 (732 3614)		$C_{15}F_4H_{31}ClP_2Pt$	 $L = P(CH_2CH_3)_3$			1,2 240
173	6575 [3350 3615 6373]		$C_{15}F_5H_{30}ClP_2Pt$	 $L = P(CH_2CH_3)_3$			1,4 12.8 2,4 13.5 3,4 479

Table C.15. (contd.)

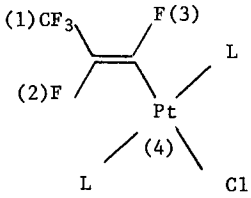
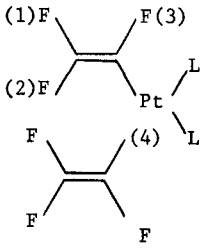
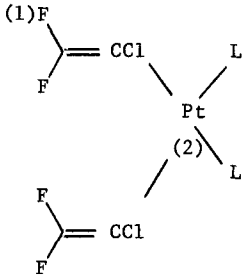
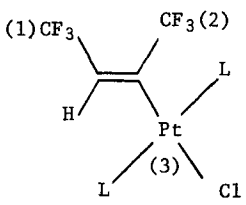
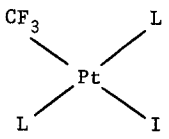
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J		^nJ
173	6576 [3351 3616 6374]		$C_{15}F_5H_{30}ClP_2Pt$	 L = $P(CH_2CH_3)_3$			1,4 2,4 3,4	5.8 186.1 501
805	6577 (3624 6388)		$C_{16}F_3H_{30}P_2Pt$	 L = $P(CH_2CH_3)_3$	3,4	395	1,4 2,4	167 42
805	6578 (3619 6382)		$C_{16}F_4H_{30}Br_2Cl_2P_2Pt_2$	trans $[(CH_3CH_2)_3P]_2Pt_2(CCl{=}CF_2)_2Br_2$				145 90
805	6579 (3620)		$C_{16}F_4H_{30}Cl_2P_2Pt$	 L = $P(CH_2CH_3)_3$			1,2	140
173	6580 (896 3163)		$C_{16}F_6H_{31}ClP_2Pt$	 L = $P(CH_2CH_3)_3$			1,3 2,3	5.8 142.3
177	6581 (6392)	A	$C_{17}F_3H_{22}IP_2Pt$	 L = $P(CH_3)_2C_6H_5$		753		

Table C.15. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
177	6582 (6409)	A	$C_{18}F_3H_{25}I_2P_2Pt$	$CF_3PtI_2(CH_3)[P(CH_3)_2C_6H_5]_2$		505	
831	6583	J	$C_{18}F_4H_{22}P_2Pt$	$C_2F_4Pt[P(CH_3)_2C_6H_5]_2$		286	
177	6584 (6417)	A	$C_{18}F_5H_{22}IP_2Pt$	$CF_3CF_2PtI[P(CH_3)_2C_6H_5]_2$		445	54
809	6585 (6421)	G	$C_{18}F_6H_{30}P_2Pt$	$(CF_3C{\equiv}C)_2Pt[P(CH_2CH_3)_3]_2$			25.4
177	6586	A	$C_{19}F_3H_{28}As_2IPt$	$CF_3PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$		539	
177	6587 (6437)	A	$C_{19}F_3H_{28}IP_2Pt$	$CF_3PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$		517	
177	6588 (746 / 6438)	A	$C_{19}F_5H_{25}I_2P_2Pt$	$CF_3CF_2PtI_2(CH_3)[P(CH_3)_2C_6H_5]_2$		364	
177	6589 (3176 / 6439)	A	$C_{19}F_7H_{22}IP_2Pt$	$CF_3CF_2CF_2$ (3)(2)(1) — L, L, L, L around Pt (4); L = $P(CH_3)_2C_6H_5$	1,4	442	2,4 105 3,4 25
177	6590 (750)	A	$C_{20}F_3H_{30}As_2IPt$	$CF_3CH_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$			94
177	6591 (751)	A	$C_{20}F_3H_{30}IP_2Pt$	$CF_3CH_2PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$			100
177	6592	A	$C_{20}F_5H_{28}As_2IPt$	$CF_3CF_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$		277	13.5
177	6593 (6441)	A	$C_{20}F_5H_{28}IP_2Pt$	$CF_3CF_2PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$		273	12
177	6594 (756)	A	$C_{21}F_5H_{30}As_2IPt$	$CF_3CF_2CH_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$ (2)(1) (3)			2,3 19
177	6595 (757)	A	$C_{21}F_5H_{30}IP_2Pt$	$CF_3CF_2CH_2PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$ (2)(1) (3)			1,3 48 2,3 20
177	6596 (758 / 3180)	A	$C_{21}F_7H_{28}As_2IPt$	$CF_3CF_2CF_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$ (2) (1)(3)	1,3	274	2,3 20.5
177	6597 (3181 / 6452)	A	$C_{21}F_7H_{28}BrP_2Pt$	$CF_3CF_2CF_2PtBr(CH_3)_2[P(CH_3)_2C_6H_5]_2$	1,3	260	2,3 21
177	6598 (3182 / 6453)	A	$C_{21}F_7H_{28}IP_2Pt$	$CF_3CF_2CF_2PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$ (2) (1)(3)	1,3	260	2,3 22
831	6599	J	$C_{22}F_4H_{30}P_2Pt$	$C_2F_4Pt[P(CH_2CH_3)_2C_6H_5]_2$		290	

Table C.15. (contd.)

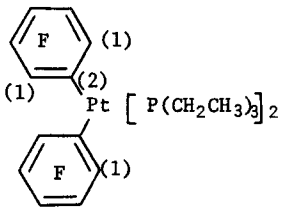
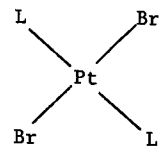
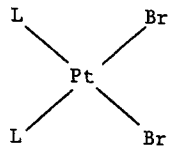
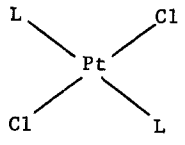
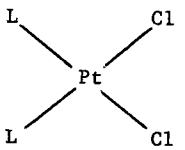
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
830	6600		$C_{24}F_{10}H_{30}P_2Pt$		1,2		354
806	6601 (6485)		$C_{25}F_3H_{38}I_3NPPt$	$(CH_3CH_2CH_2)_4N^+CF_3P(C_6H_5)_2PtI_3^-$			33.5
177	6602 (763 / 3191)	A	$C_{25}F_{15}H_{28}As_2IPt$	$CF_3(CF_2)_5CF_2PtI(CH_3)_2[As(CH_3)_2C_6H_5]_2$ (1)(2)	1,2	285	
177	6603	A	$C_{25}F_{15}H_{28}IP_2Pt$	$CF_3(CF_2)_5CF_2PtI(CH_3)_2[P(CH_3)_2C_6H_5]_2$	1,2	285	
831	6604	J	$C_{26}F_4H_{54}P_2Pt$	$C_2F_4Pt[P(CH_2CH_2CH_2CH_3)_3]_2$		281	
806	6605 (6492)		$C_{26}F_6H_{20}Br_2P_2Pt$	 L = $P(C_6H_5)_2CF_3$			25.3
806	6606 (6493)		$C_{26}F_6H_{20}Br_2P_2Pt$	 L = $P(C_6H_5)_2CF_3$			39.0
806	6607 (6495)		$C_{26}F_6H_{20}Cl_2P_2Pt$	 L = $P(C_6H_5)_2CF_3$			27.0
806	6608 (6496)		$C_{26}F_6H_{20}Cl_2P_2Pt$	 L = $P(C_6H_5)_2CF_3$			38.0
806	6609 (6501)		$C_{26}F_6H_{20}I_4P_2Pt_2$	$[CF_3P(C_6H_5)_2]_2Pt_2I_4$			40.5

Table C.15. (contd.)

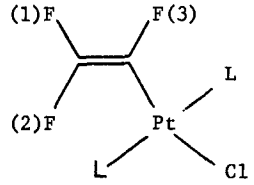
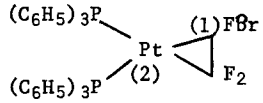
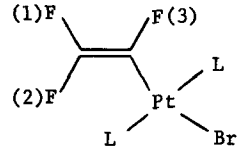
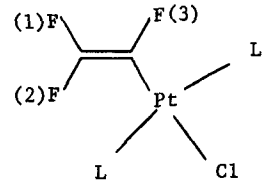
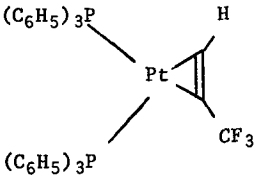
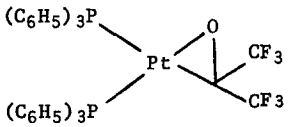
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ
807	6610 (3631, 6511)	A	$C_{28}F_3H_{26}ClP_2Pt$	 L = $P(C_6H_5)_2CH_3$	3,4		475	1,4 2,4	61.6 46.0
831	6611	J	$C_{28}F_4H_{24}P_2Pt$	$C_2F_4Pt[(C_6H_5)_2PCH_2CH_2P(C_6H_5)_2]$			316		
831	6612	J	$C_{28}F_4H_{26}P_2Pt$	$C_2F_4Pt[P(C_6H_5)_2CH_3]_2$			284		
807	6613	A	$C_{38}F_3H_{30}BrP_2Pt$		1,2		181		
807	6614 (3639, 6536)	A	$C_{38}F_3H_{30}BrP_2Pt$	 L = $P(C_6H_5)_3$	3,4		464	1,4 2,4	62.0 52.0
807	6615 (3641, 6538)	A	$C_{38}F_3H_{30}ClP_2Pt$						
				L = $P(C_6H_5)_3$	3,4		452	1,4 2,4	63.6 49.0
831	6616	J	$C_{38}F_4H_{30}As_2Pt$	$C_2F_4Pt[As(C_6H_5)_3]_2$			343		
807	6617	J	$C_{38}F_4H_{30}P_2Pt$	$C_2F_4Pt[P(C_6H_5)_3]_2$			278		
826	(4063, 6540)								
831	4064	J	$C_{38}F_4H_{30}P_2Pt$	$C_2F_4Pt[P(C_6H_5)_3]_2$			278		
168	6619 (900, 6542)		$C_{39}F_3H_{31}P_2Pt$						88.4
826	6620 (6547)		$C_{39}F_6H_{30}OP_2Pt$						71.5

Table C.15. (contd.)

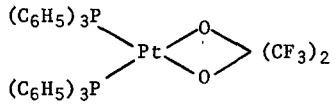
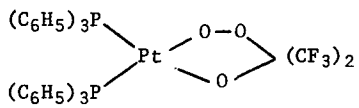
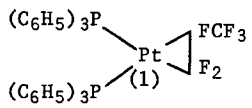
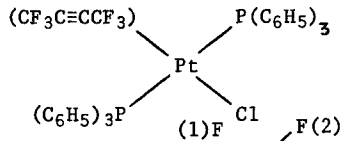
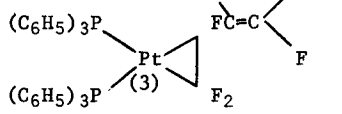
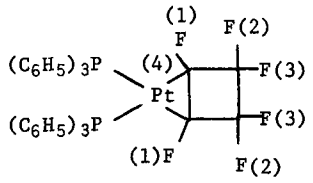
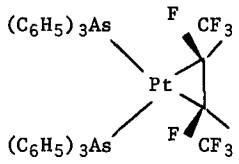
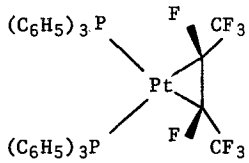
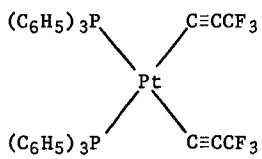
Ref. No..	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
181	6621	J	$C_{39}F_6H_{30}O_2P_2Pt$				6.8
181	6622	J	$C_{39}F_6H_{30}O_3P_2Pt$				6.1
807	6623 (4064)	A	$C_{39}F_6H_{30}P_2Pt$				1,2 105
827	6624 (6549)		$C_{40}F_6H_{30}ClP_2Pt$				65.1
807	6625 (3353 3642)	A	$C_{40}F_6H_{30}P_2Pt$				1,3 265 2,3 40
807	6626	A	$C_{40}F_6H_{30}P_2Pt$		1,4	160	2,4 300 3,4 70
825	6627	A	$C_{40}F_8H_{30}As_2Pt$				93.0
825	6628	A	$C_{40}F_8H_{30}P_2Pt$				77.6
828	6629 (6555)		$C_{42}F_6H_{30}P_2Pt$				29.8

Table C.15. (contd.)

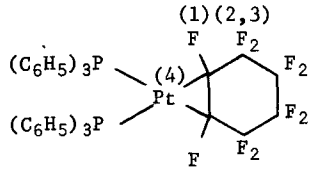
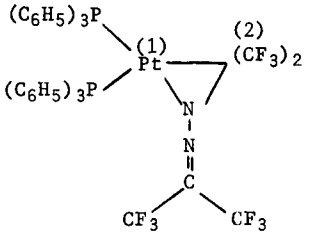
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J		^2J		^nJ
807	6630	A	$C_{42}F_{10}H_{30}P_2Pt$		1,4	100	2,4 3,4	200 100
832	6631 (3215 6556)		$C_{42}F_{12}H_{30}N_2P_2Pt$				1,2	79.0

Table C.16. M = Rhodium (Rh)

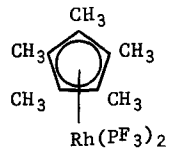
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
51	6632 (113 2643)	A^2	$C_2F_4H_{15}N_4O_5SRh$	$[Rh(CF_2HCF_2)(NH_3)_4H_2O]SO_4$		6.9	
51	6633 (114 2644)	A^2	$C_2F_4H_{16}N_5O_4SRh$	$[Rh(CF_2HCF_2)(NH_3)_5]SO_4$		6	~0.5
833	6634		$C_7F_3H_5IORh$	$CF_3Rh(CO)I\ C_5H_5$		11.7	
142	6634a		$C_7F_4HN_5Rh^{3-}$	$[Rh(CN)_5CF_2HCF_2]^{3-}$		11.1	1.9
142	6635		$C_8F_5H_5IORh$	$\pi C_5H_5Rh(CO)I(CF_2CF_3)$		9.7	
833	(3002)					6.1	
142	6636		$C_9F_7H_5IORh$	$C_5H_5Rh(CO)I(CF_2CF_2CF_3)$		4.3	
833	(3065)						
798	6637 (4997 6299)		$C_{10}F_6H_{15}P_2Rh$			~30	

Table C.16. (contd.)

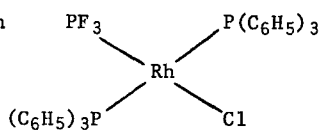
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
824	6638 (6525)	H	$C_{36}F_3H_{30}ClP_3Rh$			32	
834	6639		$C_{38}F_4H_{30}As_2ClRh$	$C_2F_4RhCl[As(C_6H_5)_3]_2$		8	
141	6640 (6539)		$C_{38}F_4H_{30}ClP_2Rh$	$C_2F_4RhCl[P(C_6H_5)_3]_2$ (trans)		9.6	
141	6641 (6550)		$C_{40}F_6H_{30}ClP_2Rh$	$(CF_3C{\equiv}CCF_3)RhCl[P(C_6H_5)_3]_2$ (trans)			1.6

Table C.17. M = antimony (Sb)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
857	6642	D	F_6KSbF_6	$KSbF_6$	1945		
612	6643	B	F_6KSb	$K^{121}SbF_6$	1820		
650	6644	J^2	F_2KSb	$K^+ \left[{}^{121}SbF_6^-, {}^{123}SbF_6^-\right]$	1945		
		DD			1950		
		J^2			1055		
		D^3			1050		

Table C.18. M = selenium (Se).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
835	6645	B	$FClOSe$	$SeOFCl$	647.5		
835	6646	B	FHO_3Se	$HSeO_3F$	1454		
836							
835	6647	B	F_2OSe	$SeOF_2$	837.1		
836							
835	6648	B	F_2O_2Se	SeO_2F_2	1583.9		
836							
835	6649	B	F_6Se	SeF_6	1420.9		
836							
542	6650 (2436)		CFH_3O_3Se	$FSeO_2OCH_3$	1454		
835	6651	B	$CF_3ClHgSe$	$CF_3SeHgCl$		35.8	

Table C.18. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
835	6652	B	$C_2F_6HgSe_2$	$(CF_3Se)_2Hg$		39.5	
835	6652	B	C_2F_6Se	$(CF_3)_2Se$		11.1	
835	6653	B	$C_2F_6Se_2$	$(CF_3Se)_2$		6.4	

Table C.19. M = scandium (Sc).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
837	6654	A[2]	$F_6H_{12}N_3Sc$	$(NH_4)_3ScF_6$	172		

Table C.20. M = silicon (Si).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
838	6655	J[3]	FBr_3Si	$SiFBr_3$	368.7		
838	6656	J[3]	FCl_3Si	$SiFCl_3$	311.5		
838	6657	B	FCl_5Si_2	$SiFCl_2SiCl_3$	384.9		
838	6658	J[3]	F_2Br_2Si	SiF_2Br_2	318.8		
838	6659	J[3]	F_2Cl_2Si	SiF_2Cl_2	273.6		
838	6660	J[3]	F_3BrSi	SiF_3Br	252.7		
838	6661	J[3]	F_3ClSi	SiF_3Cl	228.0		
544	6662	B	F_3HSi	SiF_3H	275.1		
	(2574)						
585	6663		$F_3H_3Si_2$	SiF_3SiH_3	356		
	(2575)						
839	6664		F_4OSi_2	$(SiF_2)_2O$	167.63		<2.5
840	6665	A	F_4Si	SiF_4	176.12		
838		D			176.88		
		G	(15 mole %)		176.83		
		H			176.98		
		J			175.23		
		P			175.03		
		R			173.70		
		A[3]			173.44		
		K[3]			170.51		
		L[3]			170.66		
		M[3]			170.78		
		N[3]			171.12		

Table C.20. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J		^2J		^nJ
		O[3]				171.51				
		P[3]				172.01				
		Q[3]				172.05				
		R[3]				172.35				
		S[3]				173.06				
		T[3]				173.67				
		U[3]				174.51				
		V[3]				174.68				
		W[3]				176.45				
		X[3]				178.0				
		Y[3]				178.61				
545	6666	B	F_4Si	SiF_4		178				
838	6667	J[3]	F_6OSi_2	$(SiF_3)_2O$		167.6				
839	(5103)									
853	6668		F_6Si^{2-}	SiF_6^{2-}		109.8				
838	6669	J[3]	F_6Si_2	SiF_3SiF_3		±321.83		∓90.48		
839	(5104)									
838	6670	A[2]	$F_6H_8N_2Si$	$(NH_4)_2SiF_6$		108.1				
1149	6671		F_7BSi_2	$SiF_3SiF_2BF_2$	1,2	351				
	(5315)			(2)(1)						
545	6672	A[2]	$F_7H_{12}N_3Si$	$(NH_4)_3SiF_6.NH_4F$		110				
838	6673	B	F_8Si_3	$SiF_3SiF_2SiF_3$	1,3	+344.4	2,3	-50.1	1,5	-15.7
854	(5105)			(3)(1)(2)(5)	2,4	+356.61	1,4	-64.35		
1148	6674		F_8Si_3	$SiF_3SiF_2SiF_3$	1,3	345	1,4	66		
	(5106)									
1149	6675		F_9BSi_3	$SiF_3SiF_2SiF_2BF_2$	1,2	355				
	(5107)			(2)(1)						
543	6676		CF_2H_4Si	CH_3SiF_2H		293.4				
	(2438)									
14	6677	B	CF_3Cl_3Si	CCl_3SiF_3		264				
	(2439)									
14	6678	B	CF_3HCl_2Si	$CHCl_2SiF_3$		266				
	(2440)									
14	6679	B	CF_3H_2ClSi	CH_2ClSiF_3		267				
544	6680		CF_3H_3Si	CH_3SiF_3		267.2				
	(5402, 2442)									
543	6681		CF_3H_3Si	CH_3SiF_3		267.9				
	(2441)									
838	6682	J	CF_3H_3Si	CH_3SiF_3		267.2				
545	6683	B	CF_3H_3Si	CH_3SiF_3		260				
	(2443)									
546	6684	P	$CF_6H_3NSi_2$	$(SiF_3)_2NCH_3$		204				
	(2444)									

Table C.20. (contd.)

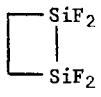
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
543	6685 (2447 2581)		C_2FH_7Si	$(CH_3)_2SiFH$	278		
545	6686 (2454)	B	$C_2F_2H_6Si$	$(CH_3)_2SiF_2$	289		
543	6687 (2453)		$C_2F_2H_6Si$	$(CH_3)_2SiF_2$	291		
838	6688	J[2]	$C_2F_2H_6Si$	$(CH_3)_2SiF_2$	287.8		
838	6689		$C_2F_3H_3Si$	$CH_2{=}CHSiF_3$	259.8		
838	6690		$C_2F_3H_5Si$	$CH_3CH_2SiF_3$	280.5		
855	6691		$C_2F_3H_6NSi$	$(CH_3)_2NSiF_3$	201.4		
546	6692 (2458)		$C_2F_3H_6NSi$	$(CH_3)_2NSiF_3$	202		
853	6693 (5108)		$C_2F_4O_4Si^{2-}$	$[Si(CO_2CO_2)F_4]^{2-}$	118.5 137.7		
549	6694 (2459)		$C_2F_4H_4Si_2$		488		
856	6695		$C_2F_6O_2Si$	$CF_3CO_2SiF_3$	194		
14	6696 (122a 2461 4854 2672)	B	C_2F_7HSi	$CF_2HCF_2SiF_3$	278		
550	6697 (2463)		C_3FH_9Si	$(CH_3)_3SiF$	280		
543	6698 (2465)		C_3FH_9Si	$(CH_3)_3SiF$	274		
545	6699 (2466)	B	C_3FH_9Si	$(CH_3)_3SiF$	266		
838	6700		C_3FH_9Si	$(CH_3)_3SiF$	274.5		
855	6701		$C_3F_3H_9OSi_2$	$(CH_3)_3SiOSiF_3$	184.2		
838	6702	A[3]	$C_3F_3H_{10}NSi_2$	$(CH_3)_3SiNHSiF_3$	202		
14	6703	B	$C_3F_6H_4Si$	$CF_3CH_2CH_2SiF_3$	274		
546	6704 (2468)	P	$C_3F_6H_9N_3Si_3$	$(F_2SiNCH_3)_3$	218		
856	6705		$C_3F_8O_2Si$	$CF_3CF_2CO_2SiF_3$	195		
853	6706		$C_4F_2O_8Si^{2-}$	$[Si(CO_2CO_2)_2F_2]^{2-}$	142.9		
846	6707 (2471)	P	$C_4F_2H_{12}N_2Si$	$[(CH_3)_2N]_2SiF_2$	219		
838	6708	B	$C_4F_3CoO_4Si$	$SiF_3Co(CO)_4$	370.0		
855	6709		$C_4F_3H_9N_2Si_2$	$(CH_3)_3SiN{=}C{=}NSiF_3$	187.6		

Table C.20. (contd.)

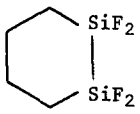
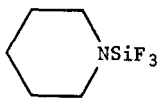
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
545	6710 (2472)	B	$C_4F_3H_9Si$	$CH_3(CH_2)_3SiF_3$	282		
546	6711 (2473)	P	$C_4F_3H_{10}NSi$	$(CH_3CH_2)_2NSiF_3$	206		
546	6712	P	$C_4F_3H_{10}NSi$	$CH_3(CH_2)_3NHSiF_3$	204		
549	6713		$C_4F_4H_8Si_2$		380		
856	6714 (2835)		$C_4F_{10}O_2Si$	$CF_3CF_2CF_2CO_2SiF_3$	197		
546	6715 (2474)	P	$C_5F_3H_{10}NSi$		202		
545	6716	B	$C_6F_3H_5Si$	$C_6H_5SiF_3$	266		
838	6717	A[3]	$C_6F_3H_5Si$	$C_6H_5SiF_3$	249.4		
926	6718 (4368, 4856)		C_6F_8Si	$C_6F_5SiF_3$	250		
545	6719	F	$C_{10}F_4H_{17}NSi$	$[(CH_3)_4N][C_6H_5SiF_4]$	205		
545	6720	B	$C_{12}F_2H_{10}Si$	$(C_6H_5)_2SiF_2$	290		
545	6721	J	$C_{12}F_5H_{28}NSi$	$[(CH_3CH_2CH_2)_4N][SiF_5]$	148		
545	6722 (2478)	J	$C_{13}F_4H_{31}NSi$	$[(CH_3CH_2CH_2)_4N][CH_3SiF_4]$	218		
545	6723 (2479)	J	$C_{16}F_4H_{37}NSi$	$[(CH_3CH_2CH_2)_4N][CH_3(CH_2)_3SiF_4]$	223		
545	6724 (2480)	J	$C_{17}F_4H_{39}NSi$	$[(CH_3(CH_2)_3)_4N][CH_3SiF_4]$	218		
545	6725	B	$C_{18}FH_{15}Si$	$(C_6H_5)_3SiF$	292		
545	6726	A	$C_{18}F_4H_{33}NSi$	$[(CH_3CH_2CH_2)_4N][C_6H_5SiF_4]$	206		
545	6727	J	$C_{20}F_3H_{30}NSi$	$[(CH_3CH_2)_4N][(C_6H_5)_2SiF_3]$	254, 212		

Table C.21. M = tin (Sn).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
858	6728	E^2	$F_2N_{12}Sn^{2-}$	$[SnF_2(N_3)_4]^{2-}$		2224	
858	6729	E^2	$F_3Br_3Sn^{2-}$	$[SnF_3Br_3]^{2-}$		2197	
858	6730	E^2	$F_3Cl_3Sn^{2-}$	$[SnF_3Cl_3]^{2-}$		2033	
858	6731	A	$F_3I_3Sn^{2-}$	$[SnF_3I_3]^{2-}$		∿2440	
858	6732	E^2	$F_3N_9Sn^{2-}$	$[SnF_3(N_3)_3]^{2-}$		2014	
858	6733	E^2	$F_3N_9Sn^{2-}$	$[FSnF_2(N_3)_3]^{2-}$	1,2	2331	
	(5111)			(2)(1)			
858	6734	A^2	$F_3H_3O_3Sn^{2-}$	$[SnF_3(OH)_3]^{2-}$		1605	
859				^{117}Sn-F		1553	
858	6735	A^2	$F_3H_3O_3Sn^{2-}$	$[FSnF_2(OH)_3]^{2-}$	1,3	∿1670	
	(5112)			(1)(3)(2)	2,3	1909	
858	6736	A	$F_4BrClSn^{2-}$	$[FSnF_2FBrCl]^{2-}$	1,2	2253	
	(5113)			(2)(1)			
858	6737	E^2	$F_4Br_2Sn^{2-}$	$[F_2SnF_2Br_2]^{2-}$		1918	
	(5114)					2406	
		A				1924	
						1833	
858	6738	E^2	$F_4Cl_2Sn^{2-}$	$[SnF_4Cl_2]^{2-}$		2240	
858	6739	E^2	$F_4Cl_2Sn^{2-}$	$[F_2SnF_2Cl_2]^{2-}$		1779	
	(5115)					2114	
		A				1802	
						2122	
858	6740	A	$F_4I_2Sn^{2-}$	$[F_2SnF_2I_2]^{2-}$		2139	
	(5116)					2804	
858	6741	E^2	$F_4N_6Sn^{2-}$	$[SnF_4(N_3)_2]^{2-}$		2151	
858	6742	E^2	$F_4N_6Sn^{2-}$	$[F_2SnF_2(N_3)_2]^{2-}$		1794	
	(5117)					2100	
858	6743	A^2	$F_4H_2O_2Sn^{2-}$	$[SnF_4(OH)_2]^{2-}$		1956	
859				^{117}Sn-F		1870	
858	6744	A^2	$F_4H_2O_2Sn^{2-}$	$[F_2SnF_4(OH)_2]^{2-}$		1518	
859	(5118)					1820	
				^{117}Sn-F		1452	
						1750	
858	6745	E^2	F_5BrSn^{2-}	$[FSnF_4Br]^{2-}$	1,3	1492	
	(5119)			(1)(3)(2)	2,3	2063	
858	6746	A	F_5BrSn^{2-}	$[FSnF_4Br]^{2-}$	1,3	1505	
	(5119)			(1)(3)(2)	2,3	2068	
858	6747	A	F_5ClSn^{2-}	$[FSnF_4Cl]^{2-}$	1,3	1529	
	(5120)			(1)(3)(2)	2,3	1899	
858	6748	F	F_5ClSn^{2-}	$[FSnF_4Cl]^{2-}$	1,2	1885	
	(5120)						
858	6749	E^2	F_5ClSn^{2-}	$[FSnF_4Cl]^{2-}$	1,3	1501	
				(1)(3)(2)	2,3	1892	

Table C.21. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
858	6750	A	F_5ISn^{2-}	$[FSnF_4I]^{2-}$	1,3 ~1500		
	(5121)			(1)(3)(2)	2,3 2400		
858	6751	E^2	$F_5N_3Sn^{2-}$	$[FSnF_4N_3]^{2-}$	1,3 ~1550		
	(5122)			(1)(3)(2)	2,3 1869		
858	6752	A^2	F_5HOSn^{2-}	$[FSnF_4OH]^{2-}$	1,3 1278		
	(5123)			(1)(3)(2)	2,3 1776		
				$^{117}Sn-F$	1,3 1222		
					2,3 1698		
858	6753	A^2	$F_5H_2OSn^{2-}$	$[FSnF_4(H_2O)]^{2-}$	1,2 ~1620		
				(2)(1)			
858	6754	H^4	$F_5H_2O_4PSn^{2-}$	$[FSnF_4(OPO(OH)_2)]^{2-}$	1,2 1564		
	(5125)			(2)(1)			
858	6755	A	F_6Sn^{2-}	SnF_6^{2-}		1601	
859		F				1603	
860		L (10% w/v)				1589	
		A^2				1557	
		E^2				1577	
		J^2				1584	
		I^4				1590	
		J^4				1570	
		K^4				1603	
		L^4				1602	
		A^2		$^{117}Sn-F$		1486	
861	6756	J^2	F_6Sn^{2-}	SnF_6^{2-}		1550	
858	6757	E^2	CF_5NOSn^{2-}	$[FSnF_4(NCO)]^{2-}$	1,3 1536		
	(5126)			(1)(3)(2)	2,3 1614		
858	6758	F	CF_5NSSn^{2-}	$[FSnF_4(NCS)]^{2-}$	1,3 1714		
	(5127)			(1)(3)(2)	2,3 1623		
858	6759	E^2	CF_5NSeSn^{2-}	$[FSnF_4(NCSe)]^{2-}$	1,2 1620		
	(5128)			(2)(1)			
858	6760	A	CF_5NSn^{2-}	$[FSnF_4(CN)]^{2-}$	1,3 1534		
	(5129)			(1)(3)(2)	2,3 1787		
858	6761	J^4	$CF_5HO_2Sn^{2-}$	$[FSnF_4(OOCH)]^{2-}$	1,2 1704		
	(5130)			(2)(1)			
858	6762	E^2	$CF_5H_3OSn^{2-}$	$[FSnF_4(OCH_3)]^{2-}$	1,3 1401		
	(5131)			(1)(3)(2)	2,3 1786		
861	6763	E^2	$CF_5H_4OSn^-$	$[SnF_5MeOH]^-$		1700	
	(5132)						
858	6764	E^2	$C_2F_4N_2O_2Sn^{2-}$	$[SnF_4(NCO)_2]^{2-}$		1648	
858	6765	E^2	$C_2F_4N_2O_2Sn^{2-}$	$[F_2SnF_2(NCO)_2]^{2-}$		1572	
	(5138)					1639	
858	6766	F	$C_2F_4N_2S_2Sn^{2-}$	$[SnF_4(NCS)_2]^{2-}$		1640	

Table C.21. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
858	6767	F	$C_2F_4N_2S_2Sn^{2-}$	$[F_2SnF_2(NCS)_2]^{2-}$		1724	
	(5139)					1646	
858	6768	E^2	$C_2F_4O_4Sn^{2-}$	$[F_2SnF_2(CO_2CO_2)]^{2-}$		1780	
	(5140)					1854	
858	6769	A	$C_2F_5HCl_2O_2Sn^{2-}$	$[FSnF_4(OOCCHCl_2)]^{2-}$ (2)(1)	1,2	1720	
858	6770	A	$C_2F_5H_2ClO_2Sn^{2-}$	$[FSnF_4(OOCCH_2Cl)]^{2-}$ (2)(1)	1,2	1727	
	(5145)						
858	6771	K^4	$C_2F_5H_3OSSn^{2-}$	$[FSnF_4(SOCCH_3)]^{2-}$ (2)(1)	1,2	2325	
	(5146)						
858	6772	A	$C_2F_5H_3O_2Sn^{2-}$	$[FSnF_4(OOCCH_3)]^{2-}$ (1)(3)(2)	1,3	∿1590	
	(5147)				2,3	1731	
858	6773	L^4	$C_2F_5H_3S_2Sn^{2-}$	$[FSnF_4(SSCCH_3)]^{2-}$ (2)(1)	1,2	2356	
858	6774	J^2	$C_2F_5H_5OSn^{2-}$	$[FSnF_4(OCH_2CH_3)]^{2-}$ (1)(3)(2)	1,3	1420	
	(5148)				2,3	1798	
861	6775		$C_2F_5H_6OSn^-$	$[SnF_5(CH_3CH_2OH)]^-$		1700	
	(5149)						
858	6776	F	$C_2F_5H_6OSSn^-$	$[FSnF_4(CH_3)_2SO]^-$ (1)(3)(2)	1,3	1788	
	(5150)				2,3	1729	
858	6777	A	$C_2F_8O_2Sn^{2-}$	$[FSnF_4(OOCCF_3)]^{2-}$ (2)(1)	1,2	1719	
	(5152)						
858	6778	E^2	$C_3F_3N_3O_3Sn^{2-}$	$[SnF_3(NCO)_3]^{2-}$		1628	
858	6779	E^2	$C_3F_3N_3O_3Sn^{2-}$	$[FSnF_2(NCO)_3]^{2-}$ (2)(1)	1,2	∿1670	
	(5153)						
858	6780	F	$C_3F_3N_3S_3Sn^{2-}$	$[FSnF_2(NCS)_3]^{2-}$ (2)(1)	1,2	1669	
	(5154)						
71	6781	H	$C_3F_3H_4Cl_3Sn$	$CF_3CH_2CH_2SnCl_3$			2.3
	(181)						
858	6782	E^2	$C_3F_4H_2O_4Sn^{2-}$	$[F_2SnF_2(CO_2CH_2CO_2)]^{2-}$		1703	
	(5159)					1806	
858	6783	A	$C_3F_5H_2NO_2Sn^{2-}$	$[FSnF_4(OOCCH_2CN)]^{2-}$ (2)(1)		1722	
	(5160)						
858	6784	A	$C_3F_5H_4ClO_2Sn^{2-}$	$[FSnF_4(OOCCHClCH_3)]^{2-}$ (2)(1)	1,2	1740	
	(5161)						
858	6785	A	$C_3F_5H_5O_2Sn^{2-}$	$[FSnF_4(OOCCH_2CH_3)]^{2-}$ (2)(1)	1,3	∿1580	
	(5162)				2,3	1750	
858	6786	I^4	$C_3F_5H_7OSn^{2-}$	$[FSnF_5(OCH_2CH_2CH_3)]^{2-}$ (1)(3)(2)	1,3	1414	
	(5164)				2,3	1797	
858	6787	E^2	$C_4F_2N_4O_4Sn^{2-}$	$SnF_2(NCO)_4^{2-}$ Tentative assignment		1634	
858	6788	E^2	$C_4F_2O_8Sn^{2-}$	$[SnF_2(CO_2CO_2)_2]^{2-}$		2054	
858	6789	A	$C_4F_4H_2Cl_4O_4Sn^{2-}$	$[SnF_4(OOCCHCl_2)_2]^{2-}$		1856	

Table C.21. (contd.)

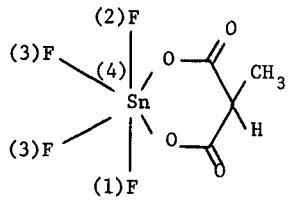
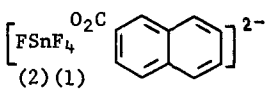
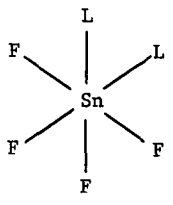
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
858	6790	A	$C_4F_4H_2Cl_4O_4Sn^{2-}$	$[F_2SnF_2(OOCCHCl_2)_2]^{2-}$		1756		
	(5166)					1841		
858	6791	E^2	$C_4F_4H_4O_4Sn^{2-}$		1,4	1722		
	(5168)				2,4	1863		
					3,4	1686		
858	6792	A	$C_4F_4H_6O_4Sn^{2-}$	$[SnF_4(OOCCH_3)_2]^{2-}$		1850		
858	6793	A	$C_4F_4H_6O_4Sn^{2-}$	$[F_2SnF_2(OOCCH_3)_2]^{2-}$		1691		
	(5169)					1841		
858	6794	F	$C_4F_4H_{12}O_2S_2Sn^{2-}$	$[F_2SnF_2((CH_3)_2SO)_2]^{2-}$		1937		
	(5170)					1856		
861	6795	J^2	$C_4F_4H_{12}O_2Sn$	$[F_2SnF_2(CH_3CH_2OH)_2]^{2-}$		1850		
861	6796	J^2	$C_4F_4H_{12}O_2Sn$	$[SnF_4(CH_3CH_2OH)_2]^{2-}$		1800		
858	6797	A	$C_4F_5H_6ClO_2Sn^{2-}$	$[FSnF_4(O_2CCH_2CHClCH_3)]^{2-}$		1731		
	(5171)							
858	6798	A	$C_4F_{10}O_4Sn^{2-}$	$[SnF_4(OOCCF_3)_2]^{2-}$		1837		
858	6799	A	$C_4F_{10}O_4Sn^{2-}$	$[F_2SnF_2(OOCCF_3)_2]^{2-}$		1780		
	(5173)					1826		
858	6800	E^2	$C_5F_4H_6O_4Sn^{2-}$	$[F_2SnF_2((CH_3)_2C(CO_2)_2)]^{2-}$		1667		
	(5175)					1769		
112	6801		$C_5F_4H_{10}Sn$	$CF_2HCF_2Sn(CH_3)_3$			249.5	
	(358)			^{117}Sn-F			237.6	
858	6802	A	$C_5F_5H_9O_2Sn^{2-}$	$[FSnF_4(OOCC(CH_3)_3]^{2-}$	1,3	~1570		
	(5176)			(1)(3)(2)	2,3	1759		
858	6803	E^2	$C_5F_5H_{10}NS_2Sn^{2-}$	$[FSnF_4(SSCN(CH_2CH_3)_2)]^{2-}$				
	(5177)			(2)(1)	1,2	1880		
858	6804	E^2	$C_6F_2H_4O_8Sn^{2-}$	$[SnF_2(CO_2CH_2CO_2)_2]^{2-}$		1952		
71	6805	B-H	$C_6F_3H_{13}Sn$	$CF_3CH_2CH_2Sn(CH_3)_3$				~0
	(411)							
858	6806	A	$C_6F_4H_4N_2O_4Sn^{2-}$	$[SnF_4(OOCCH_2CN)_2]^{2-}$		1851		
858	6807	A	$C_6F_4H_4N_2O_4Sn^{2-}$	$[F_2SnF_2(OOCCH_2CN)_2]^{2-}$		1755		
	(5178)					1846		
858	6808	A	$C_6F_4H_8Cl_2O_4Sn^{2-}$	$[SnF_4(OOCCHClCH_3)_2]^{2-}$		1878		
858	6809	A	$C_6F_4H_8Cl_2O_4Sn^{2-}$	$[F_2SnF_2(OOCCHClCH_3)_2]^{2-}$		1734		
	(5179)					1848		
858	6810	A	$C_6F_4H_{10}O_4Sn^{2-}$	$[F_2SnF_2(OOCCH_2CH_3)_2]^{2-}$		1698		
	(5180)					1857		
71	6811	B-H	$C_6F_6H_8Cl_2Sn$	$(CF_3CH_2CH_2)_2SnCl_2$				5.0
	(417)							

Table C.21. (contd.)

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
112	6812 [423 2918 5519]		$C_6F_6H_{10}Sn$	$CF_3CFHCF_2Sn(CH_3)_3$		222.0	
858	6813 (5181)	A	$C_7F_5H_4NO_4Sn^{2-}$	$[FSnF_4(\text{ortho } NO_2C_6H_4CO_2)]^{2-}$ (2)(1)	1,2 1725		
858	6814 (5182)	A	$C_7F_5H_4NO_4Sn^{2-}$	$[FSnF_4(\text{para } NO_2C_6H_4CO_2)]^{2-}$ (2)(1)	1,2 1706		
858	6815 (5183)	A	$C_7F_5H_5O_2Sn^{2-}$	$[FSnF_4(C_6H_5CO_2)]^{2-}$ (2)(1)	1,2 1720		
858	6816 (5185)	A	$C_8F_4H_{14}O_4Sn^{2-}$	$[F_2SnF_2(OOCCH(CH_3)_2)_2]^{2-}$ (1)(3)(2)	1,3 1706 2,3 1866		
71	6817 (561)	B-H	$C_8F_6H_{14}Sn$	$(CF_3CH_2CH_2)_2Sn(CH_3)_2$			~0
71	6818 (617)	B-H	$C_9F_9H_{12}ClSn$	$(CF_3CH_2CH_2)_3SnCl$			4.0
858	6819	E^2	$C_{10}F_2H_{12}O_8Sn^{2-}$	$[SnF_2((CH_3)_2C(CO_2)_2)_2]^{2-}$ (Structure uncertain)	1863		
858	6820 (5186)	A	$C_{10}F_4H_{18}O_4Sn^{2-}$	$[F_2SnF_2(OOCC(CH_3)_3)_2]^{2-}$	1714 1866		
71	6821 (664)	B-H	$C_{10}F_9H_{15}OSn$	$(CF_3CH_2CH_2)_3SnOCH_3$			2.8
71	6822 (665)	B-H	$C_{10}F_9H_{15}Sn$	$(CF_3CH_2CH_2)_3SnCH_3$			~0
858	6823 (5187)	A	$C_{11}F_5H_7O_2Sn^{2-}$	 (2)(1)	1,2 1743		
866	6824		$C_{12}F_4H_{14}N_2O_2Sn$		1965		

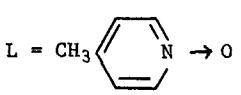


Table C.21. (contd.)

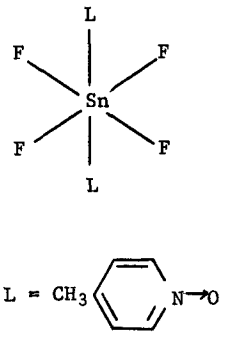
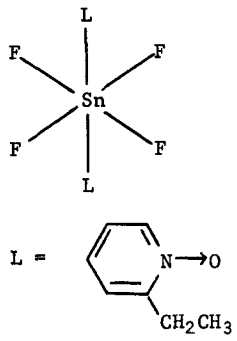
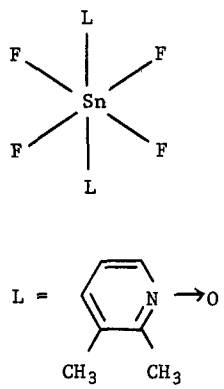
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
866	6825		$C_{12}F_4H_{14}N_2O_2Sn$		1964		
71	6826 (712)	B-H	$C_{12}F_{12}H_{16}Sn$	$(CF_3CH_2CH_2)_4Sn$			~0
858	6827 (5188)	A	$C_{14}F_4H_8N_2O_8Sn^{2-}$	$[F_2SnF_2(o\ NO_2C_6H_4CO_2)_2]^{2-}$ (2)(1)	1,2	1842	
858	6828 (5189)	A	$C_{14}F_4H_8N_2O_8Sn^{2-}$	$[F_2SnF_2(p\text{-}NO_2C_6H_4CO_2)_2]^{2-}$ (2)(1)	1,2	1706	
858	6829 (5190)	A	$C_{14}F_4H_{10}O_4Sn^{2-}$	$[F_2SnF_2(OOCC_6H_5)_2]^{2-}$		1706 1846	
866	6830		$C_{14}F_4H_{18}$			2002	
866	6831		$C_{14}F_4H_{18}N_2O_2Sn$			1992	

Table C.21. (contd.)

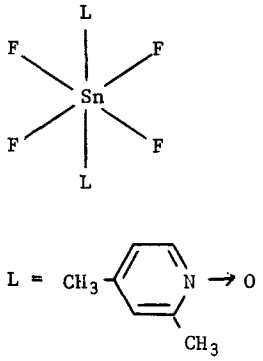
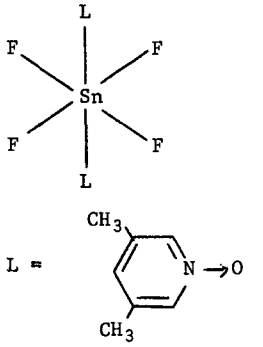
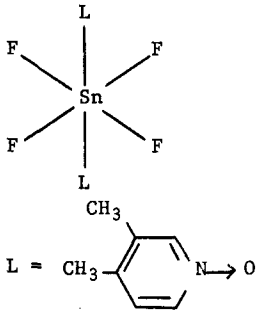
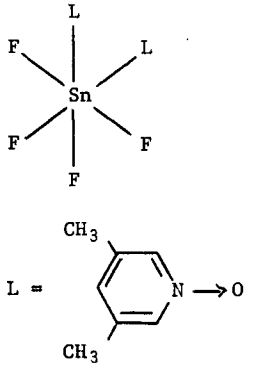
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
866	6832		$C_{14}F_4H_{18}N_2O_2Sn$		1989		
866	6833		$C_{14}F_4H_{18}N_2O_2Sn$		1972		
866	6834		$C_{14}F_4H_{18}N_2O_2Sn$		1977		
866	6835		$C_{14}F_4H_{18}N_2O_2Sn$		1956		

Table C.21. (contd.)

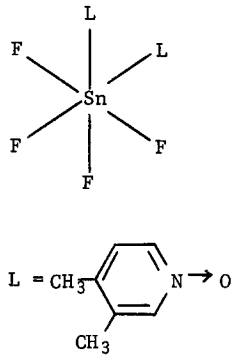
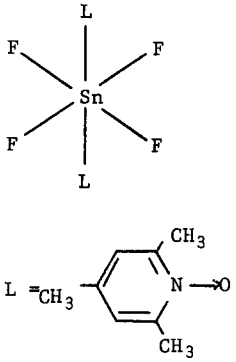
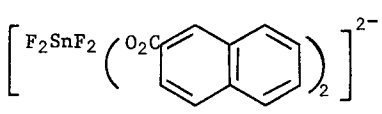
Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
866	6836		$C_{14}F_4H_{18}N_2O_2Sn$		1978		
866	6837		$C_{15}F_4H_{22}N_2O_2Sn$		2056		
71	6838 (734)	B-H	$C_{15}F_9H_{17}Sn$	$(CF_3CH_2CH_2)_3SnC_6H_5$			1.9
858	6839 (5191)	A	$C_{18}F_5H_{15}PSn^-$	$[FSnF_4P(C_6H_5)_3]^-$ (2)(1)	1,2	1640	
858	6840 (5192)	A	$C_{18}F_5H_{35}O_2Sn^{2-}$	$[FSnF_4OOC(CH_2)_{16}CH_3]^{2-}$ (2)(1)	1,2	1753	
71	6841 (742)	B-H	$C_{18}F_6H_{18}Sn$	$(CF_3CH_2CH_2)_2Sn(C_6H_5)_2$			1.5
858	6842 (5193)	A	$C_{20}F_5H_{15}O_2Sn^{2-}$	$[FSnF_4OOCC(C_6H_5)_3]^{2-}$ (2)(1)	1,2	1767	
71	6843 (755)	B-H	$C_{21}F_3H_{19}Sn$	$CF_3CH_2CH_2Sn(C_6H_5)_3$			~0
858	6844 (5194)	A	$C_{22}F_4H_{14}O_4Sn^{2-}$			1734 1856	
555	6845 (2482)		$C_{30}FH_{39}Sn$	$FSn[CH_2C(CH_3)_2C_6H_5]_3$		2298	
585	6846 (5195)	A	$C_{36}F_4H_{70}O_4Sn^{2-}$	$[F_2SnF_2(OOC(CH_2)_{16}CH_3)_2]^{2-}$		1702 1858	

Table C.22. M = tellurium (Te).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
557	6847 (2485 5201)	B	$C_4F_5H_{10}NTe$	$FTeF_4N(CH_2CH_3)_2$ (1)(3)(2)	1,3 +3060 2,3 +3970		

Table C.23. M = titanium (Ti).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
860	6848		F_6Ti^{2-}	$^{49}TiF_6^{2-}$	33.0		

Table C.24. M = vanadium (V).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
650	6849	D[3]	F_4OV^-	$^{51}VOF_4^-$	116		

Table C.25. M = tungsten (W).

Ref. No.	Serial No.	Solvent	Molecular formula	Structure	^1J	^2J	^nJ
871	6850	B	F_4Cl_2W	trans WF_4Cl_2		20	
744	6851	B[2]	F_4OW	WOF_4		64	
871	6852 (5265)	B	F_5ClW	WF_5Cl		25	
182	6853 (5266)	A[3]	F_5OW^-	FWF_4O^- (1)(3)(2)	1,3 ∓58 2,3 ±71		
872	6854		F_6W	WF_6		43.8	
744	6855	D	F_6W	WF_6		41	
		M				48	
		P				44	
		B[2]				44	
		M[4]				39	
871	6856	B	F_6W	WF_6		44	
182	6857	A[3]	F_6W	WF_6		44	
182	6858 (5267)	A[3]	$F_9O_2W_2^-$	$(F_4OWFWOF_4)^-$ (2)(3)(1)	1,3 ∓49 2,3 ±70		

Table C.25. (contd.)

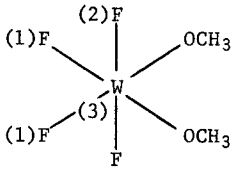
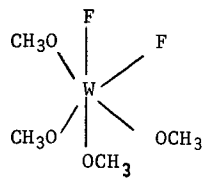
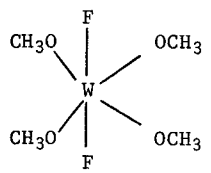
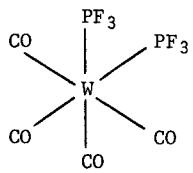
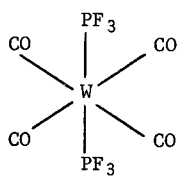
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
182	6859	A^3	CF_5H_3OW	FWF_4OCH_3	1,3	±33		
535	(2487			(1)(3)(2)	2,3	±43		
558	5268)							
182	6860	B	$C_2F_4H_6O_2W$		1,3	25		
558	(2488				2,3	46		
	5269)	A^3			1,3	±25		
					2,3	±45		
182	6861	A^3	$C_2F_4H_6O_2W$	$WOF_4.O(CH_3)_2$		67		
182	6862	A^3	$C_2F_4H_6O_4SW$	$WOF_4.OS(OCH_3)_2$		67.5		
182	6863	A^3	$C_3F_3H_9O_3W$	trans $WF_3(OCH_3)_3$		45		
	(2490							
	5270)							
558	6864	A^3	$C_3F_3H_9O_3W$	cis $WF_3(OCH_3)_3$		18		
	(2489)							
182	6865	B	$C_3F_4H_9O_4PW$	$WOF_4.OP(OCH_3)_2CH_3$		70		
535		A^3				67		
744	6866	B^2	$C_3F_6H_9PW$	$F_6WP(CH_3)_3$		38		
	(5954)							
182	6867	A^3	$C_4F_2H_{12}O_4W$			12		
558	6868	A^3	$C_4F_2H_{12}O_4W$			14		
535	6869	M	$C_4F_5H_{12}O_4PW$	$(CH_3O)_3{}^+PCH_3(FWOF_4)^-$ (2)(1)	1,2	72		
	(5272)							
731	6870	B	$C_4F_6O_4P_2W$				30	
	(6037)							
731	6871	B	$C_4F_6O_4P_2W$				32	
	(6037)							

Table C.25. (contd.)

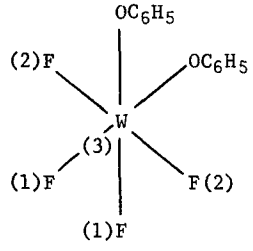
Ref. No.	Serial No.	Solvent	Molecular formula	Structure		^1J	^2J	^nJ
731	6872	B	$C_5F_3O_5PW$	$W(CO)_5PF_3$			31	
775	6873	B*	$C_6F_4H_5O_4P_2W$	$CH_3CH_2N(PF_2)_2W(CO)_4$			27	
182	6874	A	$C_6F_5H_5OW$	$FWF_4OC_6H_5$	1,3	±38		
535	(5273)			(1) (3) (2)	2,3	±42		
558								
182	6875	A	$C_{12}F_4H_{10}O_2W$		1,3	38		
	(5274)				2,4	35		
744	6876	M	$C_{12}F_5H_{28}NOW$	$(CH_3CH_2CH_2)_4N^+ WOF_5^-$		70		
	(5275)	B				71		

Table C.26. M = xenon (Xe)

Ref. No.	Serial No.	Solventq	Molecular formula	Structure	^1J
873	6877	B	F_2O_2Xe	XeO_2F_2	1178
873	6878	B	F_4OXe	$XeOF_4$	1124

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