

# Tables of Molecular Vibrational Frequencies

## Consolidated Volume II

T. Shimanouchi\*

*Department of Chemistry, University of Tokyo, Tokyo, Japan*

The compilations of fundamental vibrational frequencies of molecules previously published as Tables of Molecular Vibrational Frequencies Part 5, Part 6, Part 7, and Part 8, which appeared in the Journal of Physical and Chemical Reference Data in 1972, 1973, and 1974, have been revised. This Consolidated Volume II includes data on a total of 212 molecules in addition to those on 223 molecules included in Volume I (NSRDS-NBS 39). Selected values of the fundamental vibrational frequencies are given for each molecule, together with observed infrared and Raman spectral data and citations to the original literature. The selection of vibrational fundamentals has been based on careful studies of the spectral data and comprehensive normal-coordinate analyses. An estimate of the accuracy of the selected values is included. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

Key words. Fundamental frequencies; infrared spectra; polyatomic molecules; Raman spectra; vibrational frequencies.

### 1. Introduction

Establishing the assignment of molecular vibrational frequencies has fundamental importance in elucidating various problems in physics and chemistry. The information concerning the force field and motion of atoms in a molecule can be most directly derived from its vibrational frequencies. If all the vibrational frequencies of a molecule are known, as well as the molecular structure, thermodynamic quantities can be easily computed on the ideal gas model. Thus, the need for a tabulation of evaluated reference data on molecular vibrational frequencies has often been felt by many investigators. In 1964 a project for producing such tables was initiated at the University of Tokyo in cooperation with the National Standard Reference Data System of the National Bureau of Standards. The evaluated data resulting from this project were first published in the three parts of Tables of Molecular Vibrational Frequencies [1]<sup>1</sup>. A Consolidated Volume [2] of these tables appeared in 1972 which includes revised versions of all the tables in [1] plus tables for 52 additional molecules (a total of 223 molecules). Tables covering 160 more molecules have appeared as Parts 5, 6, 7, and 8 of the series in earlier issues [3, 4, 5, 6] of this journal.

The present volume consists of Parts 5, 6, 7, and 8 after extensive revision in the light of new experimental data.

### 2. Molecules Selected and Their Ordering

The present volume contains tables of fundamental vibrational frequencies for 212 molecules. The molecules were selected from basic organic and inorganic molecules for which the vibrational assignments have been established with little

ambiguity. The effort of extending the tables to many other important molecules is continuing in this laboratory. Diatomic molecules and electronically excited species are not included in this volume, since [7, 8, 9] contain good compilations of data for them. Rotational isomers are treated as independent molecular species, and a separate table is made for each of the isomers. When the gas and liquid state spectra are significantly different from each other, they are tabulated separately.

The molecules are ordered according to the following rules:

(a) Number of carbon atoms.

(b) Total number of atoms.

(c) Molecular shape: linear, planar, and non-planar.

(d) Molecular symmetry, in descending order of the number of symmetry elements. Isotopically substituted molecules directly follow the normal species regardless of their symmetry.

(e) Atomic number of main atoms.

(f) Atomic number of the other atoms.

Molecules are first divided into groups by the items (a) and (b) and the ordering of molecules in each group is given by the items (c), (d), (e), and (f). A complete list in the order presented is given at the beginning of the tables. Indices by compound name and empirical formula follow the tables.

### 3. Description of the Tables

#### 3.1. Symmetry

The symmetry (point group) of each molecule is given by the Schoenflies notation. Detailed discussions of symmetry properties will be found in [10] and [11].

#### 3.2. Symmetry Number

The symmetry number,  $\sigma$ , is used in the calculation of thermodynamic quantities. It is the number of indistinguishable positions into which the molecule can be transformed by simple rigid rotations. A general discussion and pertinent formulas may be found in [11], page 508.

<sup>1</sup> Figures in brackets indicate the literature references in section 5.

\*Present address: College of Information Sciences, Third Cluster of Colleges, The University of Tsukuba, Sakura, Ibaraki 300-31, Japan.

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### 3.3. Symmetry Species

In the table the normal modes are divided into the symmetry species of the point group to which the molecule belongs. The ordering of species in each point group is given in table I, which is a summary of tables 12–30 of [11]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be defined uniquely. In such cases we generally follow the notation adopted in [11].

TABLE I. Ordering of symmetry species

(In the present article small letters are used to designate the species of fundamental frequencies)

Point group	Symmetry species
$C_2$	A, B
$C_\infty$	A', A''
$C_i$	$A_g, A_u$
$C_{2v}$	$A_1, A_2, B_1, B_2$
$C_{2h}$	$A_g, A_u, B_g, B_u$
$D_2$	A, B <sub>1</sub> , B <sub>2</sub> , B <sub>3</sub>
$D_{2h}$	$A_g, A_u, B_{1g}, B_{1u}, B_{2g}, B_{2u}, B_{3g}, B_{3u}$
$C_{3v}$	$A_1, A_2, E$
$D_3$	$A_1, A_2, E$
$C_{6v}$	$A_1, A_2, E_1, E_2$
$C_{\infty v}$	$\Sigma^+, \Sigma^-, \pi, \Delta, \Phi, \dots$
$C_{4v}, D_4, D_{2d}$	$A_1, A_2, B_1, B_2, E$
$C_{6v}, D_6$	$A_1, A_2, B_1, B_2, E_1, E_2$
$D_{3d}$	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u$
$D_{4d}$	$A_1, A_2, B_1, B_2, E_1, E_2, E_3$
$D_{3h}$	$A_1', A_1'', A_2', A_2'', E', E''$
$D_{6h}$	$A_1', A_1'', A_2', A_2'', E_1', E_1'', E_2', E_2''$
$D_{4h}$	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_g, E_u$
$D_{6h}$	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_{1g}, E_{1u}, E_{2g}, E_{2u}$
$D_{\infty h}$	$\Sigma_g^+, \Sigma_u^+, \Sigma_g^-, \Sigma_u^-, \pi_g, \pi_u, \Delta_g, \Delta_u, \Phi_g, \Phi_u, \dots$
$C_3$	A, E
$C_6$	A, B, E <sub>1</sub> , E <sub>2</sub>
$S_6$	$A_g, A_u, E_g, E_u$
$C_{3h}$	$A', A'', E', E''$
$C_{4h}$	$A_g, A_u, B_g, B_u, E_g, E_u$
$C_{6h}$	$A_g, A_u, B_g, B_u, E_{1g}, E_{1u}, E_{2g}, E_{2u}$
$T_d, O$	$A_1, A_2, E, F_1, F_2$
$O_h$	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u, F_{1g}, F_{1u}, F_{2g}, F_{2u}$
T	A, E, F

### 3.4. Numbering of Frequencies

The numbering is indicated by  $\nu_i$  given in the second column of each table. The normal modes are first grouped into symmetry species, and then those in each species are ordered from higher to lower values of the frequency. However, we

always denote the bending vibration of a linear triatomic molecule as  $\nu_2$ , following the widely accepted nomenclature [12]. For the  $C_{2v}$  type of molecule we adopt the numbering given in [11], although it is based on  $D_{3h}$  symmetry. For some deuterated compounds the frequencies are arranged so that the same  $\nu_i$  numbering is given to the corresponding vibrational modes of deuterated and normal compounds.

### 3.5. Approximate Type of Mode

The approximate type of mode given in the third column of each table is the local symmetry coordinate which makes the maximum contribution to the normal mode. Local symmetry coordinates are defined for several chemical groups in table II. It should be emphasized that two or more local symmetry coordinates are often coupled strongly in a normal coordinate, and the approximate type of mode given in the table has only limited significance in such a case.

TABLE II. Definition of local symmetry coordinates

(a) Local symmetry coordinates for the CH <sub>3</sub> group (see fig. 1a)
CH <sub>3</sub> symmetrical stretching: $(\Delta r_1 + \Delta r_2 + \Delta r_3) / \sqrt{3}$
CH <sub>3</sub> degenerate stretching: $(2\Delta r_1 - \Delta r_2 - \Delta r_3) / \sqrt{6}$
$(\Delta r_2 - \Delta r_3) / \sqrt{2}$
CH <sub>3</sub> symmetrical deformation:
$(\Delta \alpha_{23} + \Delta \alpha_{31} + \Delta \alpha_{12} - \Delta \beta_1 - \Delta \beta_2 - \Delta \beta_3) / \sqrt{6}$
CH <sub>3</sub> degenerate deformation: $(2\Delta \alpha_{23} - \Delta \alpha_{31} - \Delta \alpha_{12}) / \sqrt{6}$
$(\Delta \alpha_{31} - \Delta \alpha_{12}) / \sqrt{2}$
CH <sub>3</sub> rocking: $(2\Delta \beta_1 - \Delta \beta_2 - \Delta \beta_3) / \sqrt{6}$
$(\Delta \beta_2 - \Delta \beta_3) / \sqrt{2}$
(b) Local symmetry coordinates for the CH <sub>2</sub> group (see fig. 1b)
CH <sub>2</sub> symmetrical stretching: $(\Delta r_1 + \Delta r_2) / \sqrt{2}$
antisymmetrical stretching: $(\Delta r_1 - \Delta r_2) / \sqrt{2}$
CH <sub>2</sub> scissors: $(4\Delta \alpha - \Delta \beta_{1x} - \Delta \beta_{2x} - \Delta \beta_{3y}) / \sqrt{20}$
CH <sub>2</sub> wagging: $(\Delta \beta_{1x} + \Delta \beta_{2x} - \Delta \beta_{1y} - \Delta \beta_{2y}) / 2$
CH <sub>2</sub> twisting: $(\Delta \beta_{1x} - \Delta \beta_{2x} - \Delta \beta_{1y} + \Delta \beta_{2y}) / 2$
CH <sub>2</sub> rocking: $(\Delta \beta_{1x} - \Delta \beta_{2x} + \Delta \beta_{1y} - \Delta \beta_{2y}) / 2$
(c) Local symmetry coordinates for the CH group (see fig. 1c)
CH stretching: $\Delta r_{CH}$
CH bending: $(2\Delta \beta_{HX} - \Delta \beta_{HY} - \Delta \beta_{HZ}) / \sqrt{6}$
$(\Delta \beta_{HY} - \Delta \beta_{HZ}) / \sqrt{2}$
(d) Local symmetry coordinates for the planar CH <sub>2</sub> group (see fig. 1d)
CH <sub>2</sub> symmetrical stretching: $(\Delta r_1 + \Delta r_2) / \sqrt{2}$
CH <sub>2</sub> antisymmetrical stretching: $(\Delta r_1 - \Delta r_2) / \sqrt{2}$
CH <sub>2</sub> scissors: $(2\Delta \alpha - \Delta \beta_1 - \Delta \beta_2) / \sqrt{6}$
CH <sub>2</sub> rocking: $(\Delta \beta_1 - \Delta \beta_2) / \sqrt{2}$
CH <sub>2</sub> wagging: $\Delta \theta \cdot \sin \alpha$
(e) Local symmetry coordinates for the planar CH group (see fig. 1e)
CH stretching: $\Delta r_{CH}$
in-plane CH bending: $(\Delta \beta_{HX} - \Delta \beta_{HY}) / \sqrt{2}$
out-of-plane CH bending: $\Delta \theta_H \cdot \sin \gamma_{XY}$

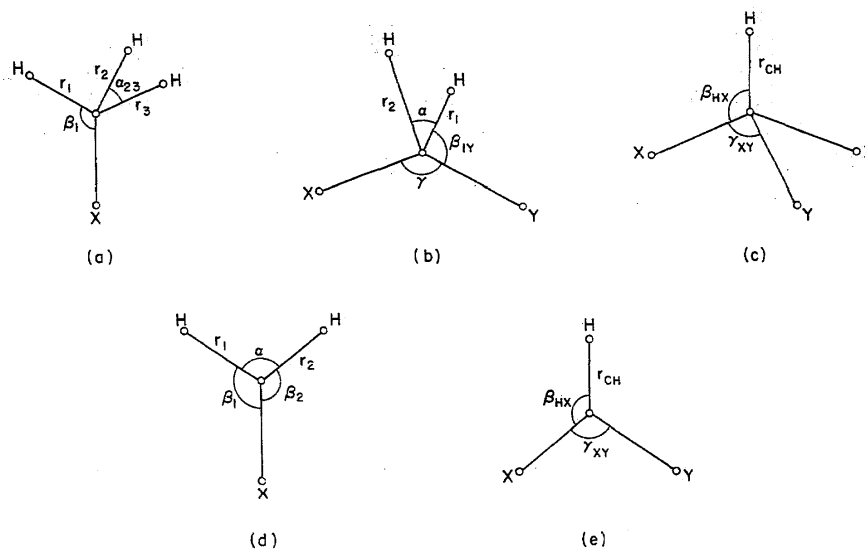


FIGURE 1. Parameters of methyl, methylene, and methine groups.

The following abbreviations are used for the type of mode:

stretch.	stretching
deform.	deformation
rock.	rocking
twist.	twisting
wag.	wagging
scis.	scissors
bend.	bending
sym. or s-	symmetrical
anti. or a-	antisymmetrical
deg. or d-	degenerate
ip-	in-plane
op-	out-of-plane

The plane to which the in-plane and out-of-plane expressions refer is the molecular plane of a planar molecule or the symmetry plane of a general molecule belonging to point group  $C_s$ . Local symmetry coordinates of the  $CX_3$  groups attached to a relatively large molecule are designated as s-stretch, s-deform., d-stretch., and d-deform. In such a molecule with low symmetry none of the normal vibrations are genuinely "symmetrical" or "degenerate" with respect to the three-fold symmetry axis of the  $CX_3$  group. However, the

notation is retained because it is convenient for indicating the correspondence between similar modes in large and small molecules.

### 3.6. Selected Value of Frequency<sup>2</sup>

The fundamental frequency  $\nu_i$  is defined as the difference between the term values  $G(\nu_i = 1, \text{ all other } \nu_j = 0)$  and  $G(\nu_i = 0, \text{ and other } \nu_j = 0)$  expressed in  $\text{cm}^{-1}$ . Fundamental frequencies rather than harmonic frequencies ( $\omega_j$ ) are listed in the table. Although harmonic frequencies are of greater physical significance, they are accurately known only for a small number of polyatomic molecules. The selected values are rounded to the nearest  $1 \text{ cm}^{-1}$ .

The letter code, A, B, C, D, or E following the selected value of frequency indicates the evaluator's judgment of the accuracy of the value. The basis for estimating accuracy of an observed frequency is given in table III, together with the range of uncertainty in  $\text{cm}^{-1}$  for each grade.

<sup>2</sup> In keeping with the universally accepted convention in molecular spectroscopy, the fundamental frequencies are expressed in their wavenumber ( $\text{cm}^{-1}$ ) equivalents. The actual frequency in units of hertz may be obtained by multiplying the numbers in these tables by the speed of light expressed in centimeters per second.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis <sup>a</sup>
	cm <sup>-1</sup>	
A	0 ~ 1	(i) Gas, grating spectrometer, rotational fine structure accurately analyzed. (ii) Gas, grating spectrometer, a sharp <i>Q</i> branch.
B	1 ~ 3	(i) Gas, grating spectrometer, rotational fine structure partly analyzed. (ii) Gas, prism spectrometer, fairly high resolution (e.g., 700 ~ 1000 cm <sup>-1</sup> for NaCl prism).
C	3 ~ 6	(i) Gas, prism spectrometer, low resolution (e.g., 1000 ~ 2000 cm <sup>-1</sup> for NaCl prism). (ii) Solid, liquid or solution, accurate measurement.
D	6 ~ 15	(i) Gas, prism spectrometer, very low resolution (e.g., > 2000 cm <sup>-1</sup> for NaCl prism). (ii) Solid, liquid or solution, inaccurate measurement.
E	15 ~ 30	(i) Value estimated from Fermi resonance doublet. (ii) Value estimated from overtone or combination tone. (iii) Calculated frequency.

<sup>a</sup> The uncertainty assigned here to each method of measurement is a typical value; greater accuracy is often achieved with some of the methods.

Frequencies derived from infrared and Raman measurements in the gaseous state are chosen unless otherwise mentioned. When a detailed analysis of the rotational fine structure of an infrared band is available, the band center  $\nu_0$  is chosen as the fundamental frequency and given the uncertainty code A (see below). For a well-analyzed perpendicular band of a symmetric top molecule, the frequency listed contains the nonvibrational part  $A' \zeta^2$ , where  $A'$  is the rotational constant of the vibrational level and  $\zeta$  is the Coriolis coupling constant. This is in accord with the definition of  $\nu_0$  given in [11], page 404 and equation (IV, 60).

When the spectra in the gaseous state are not available, the frequencies observed in the liquid or solid state are listed. When no spectral data have been obtained, the results of normal vibration calculations or of some other methods of estimating frequencies are listed with the grade D or E.

The torsional frequency may be calculated using the barrier height and reduced moment derived from microwave spectroscopy. The value obtained in this way is given as MW (frequency in cm<sup>-1</sup>) in the "Comments" column or as a footnote for comparison with the value observed or calculated by the normal coordinate treatment. Microwave data are taken from [13] unless otherwise noted.

For many molecules the assignments given in the literature have been checked by normal vibration calculations carried out in this laboratory as part of the project. Revisions in some assignments have been made as a result of these calculations. The details of the normal coordinate treatment and evaluation of force constants may be found in [14].

Thermodynamic quantities may be computed in most cases by employing the harmonic oscillator partition function and by assuming that the harmonic frequencies are not much different from the fundamental frequencies given here. Such an approximation is not adequate, however, for molecules with highly anharmonic motions such as internal rotation, inversion, and ring-puckering. The vibrational partition function

should be formed for these molecules by summing the terms due to the individual energy levels.

### 3.7. Infrared and Raman Spectra

The observed infrared and Raman frequencies are given in the fifth and sixth columns of each table. Rough estimates of relative intensities, band shapes, and polarization characteristics are also given. An additional significant figure is included here when warranted. The abbreviations used here are as follows:

VS	very strong
S	strong
M	medium
W	weak
VW	very weak
ia	inactive
b	broad
vb	very broad
sh	shoulder
p	polarized
dp	depolarized

For some molecules the relative intensities of Raman lines are indicated by the numbers from one to ten in accordance with the tradition widely used. These estimates of intensity are taken from the original references without any attempt at critical evaluation.

### 3.8. Comments

In the last column of each table brief comments are added to give special information which is not indicated in the preceding columns. The abbreviations used in this column are as follows:

- FR Fermi resonance with an overtone or a combination tone indicated in the parentheses.
- OC Frequency estimated from an overtone or a combination tone indicated in the parentheses.
- CF Calculated frequency.
- SF Calculation shows that frequency approximately equals that of the vibration indicated in the parentheses.
- OV Overlapped by the band indicated in the parentheses.
- MW Torsional frequency calculated from microwave spectroscopic data.
- RP Frequency determined by the Ritz principle.
- EL Derived from analysis of electronic transitions.

### 3.9. Footnotes and References

The footnote is used to supply other necessary information which cannot be placed simply in the column of Comments. The references accompanying the table are not comprehensive. Only the papers relevant to the present tabulation are cited. The abbreviations IR, R, MW, and Th stand for infrared, Raman, microwave, and theoretical, respectively.

### 4. Acknowledgments

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### 5. References

- [1] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 6, Part 1, 56 pages (March 1967); Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 11, Part 2, 38 pages (October 1967); Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 17, Part 3, 39 pages (March 1968).
- [2] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Consolidated Volume, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 39, 160 pages (June 1972).
- [3] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 5, J. Phys. Chem. Ref. Data 1, 189 (1972).
- [4] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 6, J. Phys. Chem. Ref. Data 2, 121 (1973).
- [5] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 7, J. Phys. Chem. Ref. Data 2, 225 (1973).
- [6] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 8, J. Phys. Chem. Ref. Data 3, 269 (1974).
- [7] Herzberg, G., Electronic Spectra of Diatomic Molecules (D. Van Nostrand, Inc., New York, 1950).
- [8] Herzberg, G., Electronic Spectra of Polyatomic Molecules (D. Van Nostrand, Inc., New York, 1966).
- [9] Rosen, B., Ed., Selected Constants, Spectroscopic Data Relative to Diatomic Molecules (Pergamon Press, New York, 1955).
- [10] Wilson, E. Bright, Jr., Decius, J. C., and Cross, Paul C., Molecular Vibrations (McGraw-Hill Book Co., New York, 1955).
- [11] Herzberg, G., Infrared and Raman Spectra of Polyatomic Molecules (D. Van Nostrand, Inc., New York, 1945).
- [12] Report on Notation for the Spectra of Polyatomic Molecules, J. Chem. Phys. 23, 1997 (1955).
- [13] Starck, B., Landolt-Bornstein Numerical Data and Functional Relationships in Science and Technology, New Series, Group II, Vol. 4 (Springer-Verlag, Berlin, 1967).
- [14] Shimanouchi, T., The Molecular Force Field. Chapter in Physical Chemistry, An Adv. Treatise, Vol. 4, Molecular Properties, pp. 233-306, D. Henderson, Ed. (Academic Press, New York, 1970).

### List of Tables of Molecular Vibrational Frequencies

#### C<sub>0</sub>-triatomic molecules

No. 1	Krypton difluoride	KrF <sub>2</sub>
No. 2	Nitrogen dioxide	<sup>14</sup> NO <sub>2</sub>
No. 3	Nitrogen dioxide	<sup>15</sup> NO <sub>2</sub>
No. 4	Ozone	<sup>16</sup> O <sub>3</sub>
No. 5	Ozone	<sup>18</sup> O <sub>3</sub>
No. 6	Water	H <sub>2</sub> <sup>18</sup> O
No. 7	Sulfur dioxide	S <sup>18</sup> O <sub>2</sub>
No. 8	Sulfur dichloride	SCl <sub>2</sub>
No. 9	Germanium (II) chloride	GeCl <sub>2</sub>
No. 10	Tin (II) fluoride	SnF <sub>2</sub>
No. 11	Tin (II) chloride	SnCl <sub>2</sub>
No. 12	Tin (II) bromide	SnBr <sub>2</sub>
No. 13	Lead (II) fluoride	PbF <sub>2</sub>
No. 14	Lead (II) chloride	PbCl <sub>2</sub>
No. 15	Nitrosyl fluoride	<sup>16</sup> O <sup>14</sup> NF
No. 16	Nitrosyl fluoride	<sup>16</sup> O <sup>15</sup> NF
No. 17	Nitrosyl fluoride	<sup>18</sup> O <sup>14</sup> NF
No. 18	Nitrosyl fluoride	<sup>18</sup> O <sup>15</sup> NF
No. 19	Nitrosyl chloride	<sup>16</sup> O <sup>14</sup> NCl
No. 20	Nitrosyl chloride	<sup>16</sup> O <sup>15</sup> NCl
No. 21	Nitrosyl chloride	<sup>18</sup> O <sup>14</sup> NCl
No. 22	Nitrosyl chloride	<sup>18</sup> O <sup>15</sup> NCl

No. 23	Nitrosyl bromide	<sup>16</sup> O <sup>14</sup> NBr
No. 24	Nitrosyl bromide	<sup>16</sup> O <sup>15</sup> NBr
No. 25	Nitrosyl bromide	<sup>18</sup> O <sup>15</sup> NBr
No. 26	Hypofluorous acid	HO <sup>16</sup> F
No. 27	Hypochlorous acid	HO <sup>16</sup> Cl
No. 28	Hypochlorous acid-d	DO <sup>16</sup> Cl
No. 29	Thionitrosyl-S-fluoride	NS <sup>16</sup> F
No. 30	Thionitrosyl-S-chloride	NS <sup>16</sup> Cl

#### C<sub>0</sub>-four-atomic molecules

No. 31	Boron trifluoride	<sup>10</sup> B <sup>19</sup> F <sub>3</sub>
No. 32	Boron trifluoride	<sup>11</sup> B <sup>19</sup> F <sub>3</sub>
No. 33	Sulfur trioxide	SO <sub>3</sub>
No. 34	Ammonia-t <sub>3</sub>	NT <sub>3</sub>
No. 35	Nitrogen trifluoride	<sup>15</sup> N <sup>19</sup> F <sub>3</sub>
No. 36	Aluminum trichloride	Al <sup>35</sup> Cl <sub>3</sub>
No. 37	Phosphorus triiodide	PI <sub>3</sub>
No. 38	Arsenic trifluoride	As <sup>75</sup> F <sub>3</sub>
No. 39	Arsenic triiodide	As <sup>127</sup> I <sub>3</sub>
No. 40	trans-1,2-Difluorodiazine	N <sub>2</sub> F <sub>2</sub>
No. 41	Nitryl fluoride	F <sup>14</sup> N <sup>16</sup> O <sub>2</sub>
No. 42	Nitryl fluoride	F <sup>15</sup> N <sup>16</sup> O <sub>2</sub>
No. 43	Nitryl chloride	Cl <sup>14</sup> N <sup>16</sup> O <sub>2</sub>
No. 44	Nitryl chloride	Cl <sup>15</sup> N <sup>16</sup> O <sub>2</sub>

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<b>C<sub>1</sub>-eight-atomic molecules</b>			<b>C<sub>2</sub>-ten-atomic molecules</b>		
No. 155	Methylsilane	CH <sub>3</sub> SiH <sub>3</sub>	No. 185	Azomethane	CH <sub>3</sub> NNCH <sub>3</sub>
No. 156	Methylsilane-d <sub>3</sub>	CH <sub>3</sub> SiD <sub>3</sub>	No. 186	Azomethane-d <sub>6</sub>	CD <sub>3</sub> NNCD <sub>3</sub>
No. 157	Methylgermane	CH <sub>3</sub> GeH <sub>3</sub>	<b>C<sub>3</sub>-five-atomic molecules</b>		
No. 158	Methyl-d <sub>3</sub> -germane	CD <sub>3</sub> GeH <sub>3</sub>	No. 187	Carbon suboxide	C <sub>3</sub> O <sub>2</sub>
No. 159	Methyltriiodogermane	CH <sub>3</sub> GeI <sub>3</sub>	No. 188	Carbon subsulfide	C <sub>3</sub> S <sub>2</sub>
No. 160	Methylstannane	CH <sub>3</sub> SnH <sub>3</sub>	No. 189	Chloro cyanoacetylene	ClCCCN
No. 161	Methylstannane-d <sub>3</sub>	CH <sub>3</sub> SnD <sub>3</sub>	No. 190	Bromo cyanoacetylene	BrCCCN
No. 162	Methyl-d <sub>3</sub> -stannane	CD <sub>3</sub> SnH <sub>3</sub>	No. 191	Iodo cyanoacetylene	ICCCN
<b>C<sub>2</sub>-four-atomic molecules</b>			<b>C<sub>3</sub>-seven-atomic molecules</b>		
No. 163	Cyanogen	C <sub>2</sub> N <sub>2</sub>	No. 192	Chloropropadiene	CH <sub>2</sub> CCHCl
No. 164	Dichloroacetylene	C <sub>2</sub> Cl <sub>2</sub>	No. 193	Bromopropadiene	CH <sub>2</sub> CCHBr
No. 165	Dibromoacetylene	C <sub>2</sub> Br <sub>2</sub>	No. 194	Iodopropadiene	CH <sub>2</sub> CCHI
No. 166	Diiodoacetylene	C <sub>2</sub> I <sub>2</sub>	No. 195	Trifluoropropyne	CF <sub>3</sub> CCH
No. 167	Bromochloroacetylene	C <sub>2</sub> BrCl	No. 196	Trifluoropropyne-d	CF <sub>3</sub> CCD
No. 168	Chloriodoacetylene	C <sub>2</sub> ClI	No. 197	1-Chloro-3,3,3-trifluoropropyne	CF <sub>3</sub> CCCl
No. 169	Bromiodoacetylene	C <sub>2</sub> BrI	No. 198	1-Bromo-3,3,3-trifluoropropyne	CF <sub>3</sub> CCBr
<b>C<sub>2</sub>-six-atomic molecules</b>			No. 199	1-Iodo-3,3,3-trifluoropropyne	CF <sub>3</sub> CCI
No. 170	Trifluoroacetonitrile	CF <sub>3</sub> CN	No. 200	Propargyl fluoride	CHCCH <sub>2</sub> F
No. 171	trans-1,2-Difluoroethylene	CHFCHF	No. 201	Propargyl chloride	CHCCH <sub>2</sub> Cl
No. 172	trans-1,2-Difluoroethylene-d <sub>1</sub>	CHFCDf	No. 202	Propargyl bromide	CHCCH <sub>2</sub> Br
No. 173	trans-1,2-Difluoroethylene-d <sub>2</sub>	CDfCDF	No. 203	Propargyl iodide	CHCCH <sub>2</sub> I
No. 174	Glyoxal	C <sub>2</sub> H <sub>2</sub> O <sub>2</sub>	<b>C<sub>4</sub>-six-atomic molecules</b>		
No. 175	Glyoxal-d <sub>1</sub>	C <sub>2</sub> HDO <sub>2</sub>	No. 204	Chlorodiacetylene	ClCCCCH
No. 176	Glyoxal-d <sub>2</sub>	C <sub>2</sub> D <sub>2</sub> O <sub>2</sub>	No. 205	Bromodiacetylene	BrCCCCH
<b>C<sub>2</sub>-seven-atomic molecules</b>			No. 206	Iododiacetylene	ICCCCCH
No. 177	Acetyl fluoride	CH <sub>3</sub> COF	<b>C<sub>4</sub>-fourteen-atomic molecules</b>		
No. 178	Acetyl fluoride-d <sub>3</sub>	CD <sub>3</sub> COF	No. 207	1,4-Dioxane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>
<b>C<sub>2</sub>-nine-atomic molecules</b>			<b>C<sub>5</sub>-eight-atomic molecules</b>		
No. 179	Dimethylzinc	CH <sub>3</sub> ZnCH <sub>3</sub>	No. 208	Diethynyl ketone	(HC≡C) <sub>2</sub> CO
No. 180	Dimethylzinc-d <sub>6</sub>	CD <sub>3</sub> ZnCD <sub>3</sub>	<b>C<sub>6</sub>-eight-atomic molecules</b>		
No. 181	Dimethylcadmium	CH <sub>3</sub> CdCH <sub>3</sub>	No. 209	Dicyanodiacetylene	NCCCCCN
No. 182	Dimethylcadmium-d <sub>6</sub>	CD <sub>3</sub> CdCD <sub>3</sub>	<b>C<sub>6</sub>-thirteen-atomic molecules</b>		
No. 183	Dimethylmercury	CH <sub>3</sub> HgCH <sub>3</sub>	No. 210	Hexacarbonylchromium(0)	Cr( <sup>12</sup> C <sup>16</sup> O) <sub>6</sub>
No. 184	Dimethylmercury-d <sub>6</sub>	CD <sub>3</sub> HgCD <sub>3</sub>	No. 211	Hexacarbonylmolybdenum(0)	Mo( <sup>12</sup> C <sup>16</sup> O) <sub>6</sub>
			No. 212	Hexacarbonyltungsten(0)	W( <sup>12</sup> C <sup>16</sup> O) <sub>6</sub>

**No. 1      Krypton difluoride    KrF<sub>2</sub>**  
**Symmetry D<sub>∞h</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Gas)	
$\sigma_g^+$	$\nu_1$	Sym. stretch.	449 B	ia	449	
$\pi_u$	$\nu_2$	Bend.	233 B	232.6 S	ia	
$\sigma_u^+$	$\nu_3$	Antisym. stretch.	590 A	589.89 VS	ia	

**References**

- [1] IR.R. H. H. Classen, G. L. Goodman, J. G. Malm, and F. Schreiner, J. Chem. Phys. **42**, 1229 (1965).  
 [2] IR. C. Murchison, S. Reichman, D. Anderson, J. Overend, and F. Schreiner, J. Amer. Chem. Soc. **90**, 5690 (1968).

**No. 2      Nitrogen dioxide    <sup>14</sup>NO<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
$a_1$	$\nu_1$	Sym. stretch.	1318 B	1318 W		
	$\nu_2$	Bend.	750 A	749.650 S		
$b_1$	$\nu_3$	Antisym. stretch.	1618 B	1617.8 VS		

**References**

- [1] IR. E. T. Arakawa and A. H. Nielsen, J. Mol. Spectry. **2**, 413 (1958).  
 [2] IR. J. W. Keller and A. H. Nielsen, J. Chem. Phys. **29**, 252 (1958).  
 [3] IR. S. C. Hurlock, K. N. Rao, L. A. Weller, and P. K. L. Yin, J. Mol. Spectry. **48**, 372 (1973).

**No. 3      Nitrogen dioxide    <sup>15</sup>NO<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
$a_1$	$\nu_1$	Sym. stretch.	1306 B	1306 W		
	$\nu_2$	Bend.	740 B	740.2 S		
$b_1$	$\nu_3$	Antisym. stretch.	1580 B	1580.3 VS		

**Reference**

- [1] IR. E. T. Arakawa and A. H. Nielsen, J. Mol. Spectry. **2**, 413 (1958).



**No. 4 Ozone  $^{16}\text{O}_3$** Symmetry  $\text{C}_{2v}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	1103 A	1103.157 VW		
	$\nu_2$	Bend.	701 B	701.42 W		
$b_1$	$\nu_3$	Antisym. stretch.	1042 A	1042.096 S		

**References**

- [1] IR. S. A. Clough and F. X. Kneizys, J. Chem. Phys. **44**, 1855 (1966).  
 [2] IR. D. J. McCaa and J. H. Shaw, J. Mol. Spectry. **25**, 374 (1968).  
 [3] IR. J. L. Brumant, A. Barve, and P. Jouve, Comptes Rendus **B268**, 459 (1969).

**No. 5 Ozone  $^{18}\text{O}_3$** Symmetry  $\text{C}_{2v}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Xe Matrix)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	1038 C	1038 W		
	$\nu_2$	Bend.	660 C	660 W		
$b_1$	$\nu_3$	Antisym. stretch.	974 C	974 S		

**References**

- [1] IR. L. Brewer and J. Ling-Fai Wang, J. Chem. Phys. **56**, 759 (1972).  
 [2] IR.Th. M. Spoliti, S. N. Cesaro, and B. Mariti, J. Chem. Phys. **59**, 985 (1973).

**No. 6 Water  $\text{H}_2^{18}\text{O}$** Symmetry  $\text{C}_{2v}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	3650 A	3649.68		
	$\nu_2$	Bend	1588 A	1588.275		
$b_1$	$\nu_3$	Antisym. stretch.	3742 A	3741.58		

**References**

- [1] IR. W. S. Benedict, Mem. Soc. Roy. Sci. Liege, **18**, 557 (1957).  
 [2] IR. P. E. Fraley, K. N. Rao, and L. H. Jones, J. Mol. Spectry. **29**, 312 (1969).  
 [3] IR. J. G. Williamson, K. N. Rao, and L. H. Jones, J. Mol. Spectry. **40**, 372 (1971).

**No. 7 Sulfur dioxide  $S^{18}O_2$**   
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	1101 B	1100.65		
	$\nu_2$	Bend.	497 B	496.7		
$b_1$	$\nu_3$	Antisym. stretch.	1318 B	1317.9		

**Reference**

- [1] IR. A. Barbe and P. Jauve, J. Mol. Spectry. **38**, 273 (1971).

**No. 8 Sulfur dichloride  $SCl_2$**   
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
$a_1$	$\nu_1$	Sym. stretch.	525 D	525 VS	514 (10), p	
	$\nu_2$	Bend.	208 B		208 (5), p	
$b_1$	$\nu_3$	Antisym. stretch.	535 D		535 (1)	

**References**

- [1] R. H. Stammerich, R. Forneris, and K. Sone, J. Chem. Phys. **23**, 972 (1955).  
 [2] IR. G. M. Barrow, Can. J. Chem. **59**, 987 (1955).  
 [3] IR. Y. Morino, Y. Murata, T. Ito, and J. Nakamura, J. Phys. Soc. Japan **17**, Supplement B-II, 37 (1962)

**No. 9 Germanium (II) chloride  $GeCl_2$**   
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Ar Matrix)	$cm^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.	399 C	399	399 p	
	$\nu_2$	Bend.	159 C		159 p	
$b_1$	$\nu_3$	Antisym. stretch.	374 D	374	362 dp (Ar Matrix)	

**References**

- [1] R. I. R. Beattie and R. O. Perry, J. Chem. Soc. **A1970**, 2429.  
 [2] IR. L. Andrews and D. L. Frederick, J. Amer. Chem. Soc. **92**, 775 (1970).  
 [3] R. C. A. Ozin and A. Vander Voet, J. Chem. Phys. **56**, 4768 (1972).

**No. 10      Tin (II) fluoride       $\text{SnF}_2$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Ar Matrix)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	593 D	592.7		
	$\nu_2$	Bend.	197 D	197		
$b_1$	$\nu_3$	Antisym. stretch.	571 D	570.9		

**Reference**[1] IR.      R. H. Hauge, J. W. Hastie, and J. L. Margrave, J. Mol. Spectry. **45**, 420 (1973).

**No. 11      Tin (II) chloride       $\text{SnCl}_2$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Ar Matrix)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.	352 C	354	352 p	
	$\nu_2$	Bend.	120 C		120 p	
$b_1$	$\nu_3$	Antisym. stretch.	334 D	334	332 (Ar Matrix)	

**References**See No. 9( $\text{GeCl}_2$ ).

**No. 12      Tin (II) bromide       $\text{SnBr}_2$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.	244 D		244 (Ar Matrix)	
	$\nu_2$	Bend.	80 C		80	
$b$	$\nu_3$	Antisym. stretch.	231 D		231 (Ar Matrix)	

**References**See No. 9( $\text{GeCl}_2$ ).

No. 13		Lead (II) fluoride	PbF <sub>2</sub>	Symmetry number $\sigma = 2$		
Symmetry C <sub>2v</sub>						
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Ar Matrix)	cm <sup>-1</sup>	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	531 D	531.2		
	$\nu_2$	Bend.	165 D	165		
b <sub>1</sub>	$\nu_3$	Antisym. stretch.	507 D	507.2		

**Reference**See No. 10(SnF<sub>2</sub>).

No. 14		Lead (II) chloride	PbCl <sub>2</sub>	Symmetry number $\sigma = 2$		
Symmetry C <sub>2v</sub>						
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Ar Matrix)	cm <sup>-1</sup> (Gas)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	314 C	322	314 p	
	$\nu_2$	Bend.	99 C		99 p	
b <sub>1</sub>	$\nu_3$	Antisym. stretch.	299 D	299	300 dp (Ar Matrix)	

**References**See No. 9(GeCl<sub>2</sub>).

No. 15		Nitrosyl fluoride	<sup>16</sup> O <sup>14</sup> NF	Symmetry number $\sigma = 1$		
Symmetry C <sub>s</sub>						
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a'	$\nu_1$	NO stretch.	1844 B	1843.5 VS		
	$\nu_2$	NF stretch.	766 B	765.8 VS		
	$\nu_3$	Bend.	520 C	519.9 VS		

**References**

- [1] IR. P. J. H. Woltz, E. A. Jones, and A. H. Nielsen, J. Chem. Phys. **20**, 378 (1952).  
 [2] IR. D. W. Magnuson, J. Chem. Phys. **20**, 380 (1952).  
 [3] IR. L. H. Jones, L. B. Asprey, and R. R. Ryan, J. Chem. Phys. **47**, 3371 (1967).

No. 16		Nitrosyl fluoride		$^{16}\text{O}^{15}\text{NF}$		
Symmetry $C_s$				Symmetry number $\sigma = 1$		
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NO stretch.	1812 C	1811.8 VS		
	$\nu_2$	NF stretch.	749 C	748.7 VS		
	$\nu_3$	Bend.	517 C	517.4 VS		

**Reference**

[1] IR. L. H. Jones, L. B. Asprey, and R. R. Ryan, J. Chem. Phys. **47**, 3371 (1967).

No. 17		Nitrosyl fluoride		$^{18}\text{O}^{14}\text{NF}$		
Symmetry $C_s$				Symmetry number $\sigma = 1$		
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NO stretch.	1796 C	1795.6 VS		
	$\nu_2$	NF stretch.	758 C	757.8 VS		
	$\nu_3$	Bend.	511 C	511.3 VS		

**Reference**

See No. 16( $^{16}\text{O}^{15}\text{NF}$ ).

No. 18		Nitrosyl fluoride		$^{18}\text{O}^{15}\text{NF}$		
Symmetry $C_s$				Symmetry number $\sigma = 1$		
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NO stretch.	1763 C	1763.0 VS		
	$\nu_2$	NF stretch.	740 C	740.4 VS		
	$\nu_3$	Bend.	509 C	509.3 VS		

**Reference**

See No. 16( $^{16}\text{O}^{15}\text{NF}$ ).

No. 19		Nitrosyl chloride		$^{16}\text{O}^{14}\text{NCl}$		Symmetry number $\sigma = 1$	
Symmetry		Symmetry $C_s$					
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$		
$a'$	$\nu_1$	NO stretch.	1800 C	1799.7 VS			
	$\nu_2$	NCl stretch.	596 C	595.8 VS			
	$\nu_3$	Bend.	332 C	331.9 VS			

**References**

- [1] IR. W. G. Burns, and H. J. Bernstein, J. Chem. Phys. **18**, 1669 (1950).  
 [2] IR. A. G. Pulford and A. Walsh, Trans. Faraday Soc. **47**, 347 (1951).  
 [3] IR. W. H. Eberhardt and T. G. Burke, J. Chem. Phys. **20**, 529 (1952).  
 [4] IR. L. Landau and W. H. Fletcher, J. Mol. Spectry. **4**, 276 (1960).  
 [5] IR. L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Chem. Phys. **49**, 581 (1968).

No. 20		Nitrosyl chloride		$^{16}\text{O}^{15}\text{NCl}$		Symmetry number $\sigma = 1$	
Symmetry		Symmetry $C_s$					
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$		
$a'$	$\nu_1$	NO stretch.	1769 C	1768.9 VS			
	$\nu_2$	NCl stretch.	582 C	581.7 VS			
	$\nu_3$	Bend.	330 C	329.9 VS			

**References**

- [1] IR. L. Landau and W. H. Fletcher, J. Mol. Spectry. **4**, 276 (1960).  
 [2] IR. L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Chem. Phys. **49**, 581 (1968).

No. 21		Nitrosyl chloride		$^{18}\text{O}^{14}\text{NCl}$		Symmetry number $\sigma = 1$	
Symmetry		Symmetry $C_s$					
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$		
$a'$	$\nu_1$	NO stretch.	1751 C	1752.7 VS 1749.0 VS		FR( $3\nu_2$ )	
	$\nu_2$	NCl stretch.	588 C	588.4 VS			
	$\nu_3$	Bend.	325 C	324.9 VS			

**Reference**

- [1] IR. L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Chem. Phys. **49**, 581 (1968).

No. 22		Nitrosyl chloride		$^{18}\text{O}^{15}\text{NCl}$		Symmetry number $\sigma = 1$	
Symmetry $C_s$							
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$		
$a'$	$\nu_1$	NO stretch.	1721 C	1720.6 VS			
	$\nu_2$	NCl stretch.	574 C	573.9 VS			
	$\nu_3$	Bend.	323 C	323.2 VS			

**Reference**See No. 21( $^{18}\text{O}^{14}\text{NCl}$ )

No. 23		Nitrosyl bromide		$^{16}\text{O}^{14}\text{NBr}$		Symmetry number $\sigma = 1$	
Symmetry $C_s$							
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$		
$a'$	$\nu_1$	NO stretch.	1799 C	1799.0 VS			
	$\nu_2$	NBr stretch.	542 C	542.0 VS			
	$\nu_3$	Bend.	266 C	266.4 S			

**References**

- [1] IR. W. G. Burns and H. J. Bernstein, J. Chem. Phys. **18**, 1669 (1950).  
 [2] IR. J. Laane, L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Mol. Spectry. **30**, 485 (1969).

No. 24		Nitrosyl bromide		$^{16}\text{O}^{15}\text{NBr}$		Symmetry number $\sigma = 1$	
Symmetry $C_s$							
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$		
$a'$	$\nu_1$	NO stretch.	1768 C	1768.3 VS			
	$\nu_2$	NBr stretch.	528 D	527.8 VS			
	$\nu_3$	Bend.	264 C	264 S			

**Reference**

- [1] IR. J. Laane, L. H. Jones, R. R. Ryan, and L. B. Asprey, J. Mol. Spectry. **30**, 485 (1969).

**No. 25 Nitrosyl bromide  $^{18}\text{O}^{15}\text{NBr}$**   
**Symmetry  $C_s$  Symmetry number  $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NO stretch.	1720 C	1719.5 VS		
	$\nu_2$	NBr stretch.	522 C	521.5 VS		
	$\nu_3$	Bend.	257 C	257.0 S		

**Reference**

See No. 24( $^{16}\text{O}^{15}\text{NBr}$ ).

**No. 26 Hypofluorous acid HOF**  
**Symmetry  $C_s$  Symmetry number  $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ ( $\text{N}_2$ Matrix)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	OH stretch.	3537 C	3537.1		
	$\nu_2$	OF stretch.	1393 C	1393.0		
	$\nu_3$	Bend.	886 C	886.0		

**References**

- [1] IR. P. N. Noble and G. C. Pimentel, *Spectrochim. Acta* **24A**, 797 (1968).  
 [2] IR. J. A. Golb, H. H. Claassen, M. H. Studier, and E. H. Appelman, *Spectrochim. Acta* **28A**, 65 (1972).

**No. 27 Hypochlorous acid HOCl**  
**Symmetry  $C_s$  Symmetry number  $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	OH stretch.	3609 A	3609 M		
	$\nu_2$	Bend.	1242 C	1242 S		
	$\nu_3$	OCl stretch.	725 C	725 M		

**References**

- [1] IR. K. Hedberg and R. M. Badger, *J. Chem. Phys.* **19**, 508 (1951).  
 [2] IR. R. A. Ashby, *J. Mol. Spectry.* **23**, 439 (1967).  
 [3] IR. I. Schwager and A. Arkell, *J. Amer. Chem. Soc.* **89**, 6006 (1967).  
 [4] IR. R. A. Ashby, *J. Mol. Spectry.* **40**, 639 (1971).



**No. 28 Hypochlorous acid-d DOCl**  
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	OD stretch.	2666 B	2666 M		
	$\nu_2$	Bend.	911 C	911 S		
	$\nu_3$	OCl stretch.	739 C	739 M		

**References**

- [1] IR. K. Hedberg and R. M. Badger, J. Chem. Phys. **19**, 508 (1951).  
 [2] IR. R. A. Ashby, J. Mol. Spectry. **23**, 439 (1967).

**No. 29 Thionitrosyl-S-fluoride NSF**  
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NS stretch.	1372 C	1372 VS		
	$\nu_2$	SF stretch.	640 C	640 VS		
	$\nu_3$	Bend.	366 C	366 S		

**References**

- [1] IR. H. Richert and O. Glemser, Z. Anorg. Alleg. Chem. **307**, 328 (1961).  
 [2] IR. I. Schwager and A. Arkell, J. Amer. Chem. Soc. **89**, 6006 (1967).

**No. 30 Thionitrosyl-S-chloride NSCl**  
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NS stretch.	1325 C	1325		
	$\nu_2$	SCl stretch.	414 C	414		
	$\nu_3$	Bend.	273 D			$OC(\nu_2 + \nu_3, 2\nu_3)$ .

**Reference**

- [1] IR. A. Müller, G. Nagarajan, O. Glemser, S. F. Cyvin, and J. Wegener, Spectrochim. Acta **23A**, 2683 (1967).

**No. 31      Boron trifluoride       $^{10}\text{BF}_3$**   
**Symmetry  $D_{3h}$       Symmetry number  $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1'$	$\nu_1$	Sym. stretch.	888 B	ia	888 VS	
$a_2''$	$\nu_2$	Op-deform.	719 A	719.3 S	ia	
$e'$	$\nu_3$	Deg. stretch.	1503 A	1502.5 S	1481 VW	
	$\nu_4$	Deg. deform.	482 B	482.0 M	482 W, b	

**References**

- [1] R. D. M. Yost, D. DeVault, T. F. Anderson, E. N. Lassettre, J. Chem. Phys. **6**, 424 (1938).  
 [2] IR. L. P. Lindeman and M. K. Wilson, J. Chem. Phys. **24**, 242 (1956).  
 [3] IR. M. N. Dreska, K. N. Rao, and L. H. Jones, J. Mol. Spectry. **18**, 404 (1965).  
 [4] IR. S. W. Ginn, J. K. Kenney, and J. Overend, J. Chem. Phys. **48**, 1571 (1968).  
 [5] IR. S. W. Ginn, C. W. Brown, J. K. Kenney, and J. Overend, J. Mol. Spectry. **28**, 509 (1968).

**No. 32      Boron trifluoride       $^{11}\text{BF}_3$**   
**Symmetry  $D_{3h}$       Symmetry number  $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1'$	$\nu_1$	Sym. stretch.	888 B	ia	888 VS	
$a_2''$	$\nu_2$	Op-deform.	691 A	691.2 S	ia	
$e'$	$\nu_3$	Deg. stretch.	1449 B	1449 S	1448 VW	
	$\nu_4$	Deg. deform.	480 B	480.4 M	482 b	

**References**

See No. 31( $^{10}\text{BF}_3$ ).

**No. 33 Sulfur trioxide SO<sub>3</sub>**  
**Symmetry D<sub>3h</sub>**

Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Gas)	
<i>a</i> <sub>1</sub> '	$\nu_1$	Sym. stretch.	1065 B	ia	1065 VS, p	
<i>a</i> <sub>2</sub> '	$\nu_2$	Op deform.	498 B	497.55 M	ia	
<i>e</i> '	$\nu_3$	Deg. stretch.	1391 A	1391.3 VS	1390 W	
	$\nu_4$	Deg. deform.	530 B	530.2 S	528 W	

**References**

- [1] R. H. Gerding and W. J. Nijverd, *Rec. Trav. Chim.* **59**, 1206 (1940).  
 [2] IR. R. W. Lovejoy, J. H. Colwell, D. F. Eggers, and G. D. Halsey, *J. Chem. Phys.* **36**, 612 (1962).  
 [3] IR. R. Bent and W. R. Lander, *Spectrochim. Acta* **19**, 931 (1963).  
 [4] R. K. Stopperka, *Z. Anorg. Allegem. Chem.* **345**, 277 (1966).  
 [5] IR. J. B. Milne and A. Ruoff, *J. Mol. Spectry.* **23**, 408 (1967).  
 [6] IR. R. K. Thomas and H. Thompson, *Proc. Roy. Soc. London* **A314**, 329 (1970).  
 [7] IR.R.Th. A. Kaldar, A. G. Maki, A. J. Dorney, and L. M. Mills, *J. Mol. Spectry.* **45**, 247 (1973).

**No. 34 Ammonia-t<sub>3</sub> NT<sub>3</sub>**  
**Symmetry C<sub>3v</sub>**

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)		
<i>a</i> <sub>1</sub>	$\nu_1$	Sym. stretch.	2014 A	2014.1		
	$\nu_2$	Sym. deform.	657 B	656.4 s <sup>a</sup> 657.2 a <sup>a</sup>		
<i>e</i>	$\nu_3$	Deg. stretch.	2185 A	2184.8		
	$\nu_4$	Deg. deform.	996 A	996.3		

<sup>a</sup>"s" and "a" refer to symmetric and antisymmetric levels [1].**References**

- [1] IR. K. N. Rao, W. W. Brim, J. M. Hoffman, L. H. Jones, and R. S. McDowell, *J. Mol. Spectry.* **7**, 362 (1961).  
 [2] IR. L. H. Jones, W. W. Brim, and K. N. Rao, *J. Mol. Spectry.* **11**, 389 (1963).

No. 35 Nitrogen trifluoride  $^{15}\text{NF}_3$   
Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	1009 A	1008.93		
	$\nu_2$	Sym. deform.	645 B	644.84		
$e$	$\nu_3$	Deg. stretch.	886 A	886.34		
	$\nu_4$	Deg. deform.	492 B	492.02		

## References

- [1] MW. M. Otake, C. Matsumura, and Y. Morino, J. Mol. Spectry. **28**, 316 (1968).  
 [2] IR.MW.Th. M. Otake, E. Hirota, and Y. Morino, J. Mol. Spectry. **28**, 325 (1968).  
 [3] IR.Th. A. Allan, J. L. Duncan, J. H. Holloway, and D. C. McKean, J. Mol. Spectry. **31**, 368 (1969).

No. 36 Aluminum trichloride  $\text{AlCl}_3$   
Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Ar Matrix)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.	375 C	380.2	375 p	
	$\nu_2$	Sym. deform.	183 C	182.8		
$e$	$\nu_3$	Deg. stretch.	595 C	594.7		
	$\nu_4$	Deg. deform.	150 C	149.2	150	

## References

- [1] IR. W. Klemperer, J. Chem. Phys. **24**, 353 (1956).  
 [2] R. I. R. Beatie and J. R. Horder, J. Chem. Soc. **B1969**, 2655.  
 [3] IR. M. L. Lesiecki and J. S. Shirk, J. Chem. Phys. **56**, 4171 (1972).

**No. 37 Phosphorus triiodide  $\text{PI}_3$** Symmetry  $\text{C}_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ ( $\text{CS}_2$ , $\text{C}_6\text{H}_6$ , $\text{CH}_2\text{Cl}_2$ soln.)	$\text{cm}^{-1}$ $\text{C}_6\text{H}_6$ , $\text{CCl}_4$ soln.)	
$a_1$	$\nu_1$	Sym. stretch.	303 D	306 M	303 (3) p	
	$\nu_2$	Sym. deform.	111 D	112 VW	111 (7) p	
$e$	$\nu_3$	Deg. stretch.	325 D	328 VS	325 (1b) dp	
	$\nu_4$	Deg. deform.	79 D	80 VW, b	79 (10) dp	

**References**

- [1] R. R. H. Stammreich, R. Forneris, and Y. Tavares, J. Chem. Phys. **25**, 580 (1956).  
 [2] IR. S. G. Frankiss, F. A. Miller, H. Stammreich and Th. T. Sans, Spectrochim. Acta **23A**, 543 (1967).

**No. 38 Arsenic trifluoride  $\text{AsF}_3$** Symmetry  $\text{C}_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	Sym. stretch.	741 A	740.5 S	707 (10)	
	$\nu_2$	Sym. deform.	337 B	336.5 M	341 (2)	
$e$	$\nu_3$	Deg. stretch.	702 B	702.2 S	644 (9)	
	$\nu_4$	Deg. deform.	262 B	262.3 M	274 (4)	

**References**

- [1] R. D. M. Yost and J. E. Sherborne, J. Chem. Phys. **2**, 125 (1934).  
 [2] IR. L. C. Hoskins and R. C. Lord, J. Chem. Phys. **43**, 155 (1965).  
 [3] IR.Th. I. W. Levin and S. Abramowitz, J. Chem. Phys. **44**, 2562 (1966).  
 [4] IR.Th. L. C. Hoskins, J. Chem. Phys. **45**, 4594 (1966).  
 [5] Th. A. M. Mirri, J. Chem. Phys. **47**, 2823 (1967).  
 [6] IR. S. Reichman and J. Overend, Spectrochim. Acta **26A**, 379 (1970).  
 [7] Th. S. Reichman, D. F. Smith, Jr. and J. Overend, Spectrochim. Acta **26A**, 927 (1970).

**No. 39      Arsenic triiodide      AsI<sub>3</sub>**  
**Symmetry C<sub>3v</sub>**

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Solid)	cm <sup>-1</sup> (CHBr <sub>3</sub> , CS <sub>2</sub> soln.)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	219 C	225.7	218.5 p	
	$\nu_2$	Sym. deform.	94 C	101.6	94 p	
e	$\nu_3$	Deg. stretch.	224 C	201.2 VVS,b	223.5 dp	
	$\nu_4$	Deg. deform.	71 C	73.6	71 dp	

**References**

- [1] R. R. H. Stammreich, R. Forneris, and Y. Tavares, *J. Chem. Phys.* **25**, 580 (1956).  
 [2] IR. T. R. Marley and D. A. Williams, *Spectrochim. Acta* **21**, 1773 (1968).  
 [3] R. M. A. Hooper and D. N. James, *Austral. J. Chem.* **21**, 2379 (1968).  
 [4] R. W. Kiefer, *Z. Naturforsch.* **A25**, 1101 (1970).

**No. 40      trans-1,2-Difluorodiazine      N<sub>2</sub>F<sub>2</sub>**  
**Symmetry C<sub>2h</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Gas)	
a <sub>g</sub>	$\nu_1$	NN stretch.	1523 C	ia	1523 (2)	
	$\nu_2$	NF stretch.	1018 C	ia	1018 (5)	
	$\nu_3$	FNN deform.	603 C	ia	603 (10)	
a <sub>v</sub>	$\nu_4$	Torsion	364 B	363.5 M	ia	
b <sub>u</sub>	$\nu_5$	NF stretch.	991 A	991.01 VS	ia	
	$\nu_6$	FNN deform.	423 C	423 M	ia	

**References**

- [1] IR. R. H. Sanborn, *J. Chem. Phys.* **33**, 1855 (1960).  
 [2] IR.R. S-T. King and J. Overend, *Spectrochim. Acta* **22**, 689 (1966).  
 [3] IR. S-T. King and J. Overend, *Spectrochim. Acta* **23A**, 2875 (1967).  
 [4] IR.R. J. Shamir and H. H. Hyman, *Spectrochim. Acta*, **23A**, 1191 (1967).

**No. 41 Nitryl fluoride  $F^{14}NO_2$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$a_1$	$\nu_1$	$NO_2$ s-stretch.	1310 B	1309.6 VS		
	$\nu_2$	NF stretch.	822 B	822.4 VS		
	$\nu_3$	$NO_2$ scis.	568 C	567.8 S		
$b_1$	$\nu_4$	$NO_2$ a-stretch.	1792 B	1791.5 VS		
	$\nu_5$	$NO_2$ rock.	560 C	559.6 S		
$b_2$	$\nu_6$	Op-deform.	742 B	742.0 M		

**References**

- [1] IR. R. E. Dodd, J. A. Roufe, and L. A. Woodward, Trans. Farad. Soc. **52**, 145 (1956).  
 [2] IR. D. L. Bernitt, R. H. Miller, and I. C. Hisatsune, Spectrochim. Acta **22A**, 237 (1967).  
 [3] Th. T. Tanaka and Y. Morino, J. Mol. Spectry. **32**, 430 (1969).

**No. 42 Nitryl fluoride  $F^{15}NO_2$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$a_1$	$\nu_1$	$NO_2$ s-stretch.	1298 B	1298.0 VS		
	$\nu_2$	NF stretch.	809 B	808.5 VS		
	$\nu_3$	$NO_2$ scis.	567 C	567.1 S		
$b_1$	$\nu_4$	$NO_2$ a-stretch.	1751 B	1750.5 VS		
	$\nu_5$	$NO_2$ rock.	559 C	558.9 S		
$b_2$	$\nu_6$	Op-deform.	722 B	722.0 M		

**References**See No. 41( $F^{14}NO_2$ ).

**No. 43 Nitryl chloride  $\text{Cl}^{14}\text{NO}_2$**   
**Symmetry  $C_{2v}$  Symmetry number  $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{NO}_2$ s-stretch.	1286 C	1318.5 S 1267.1 VS		FR( $2\nu_6$ ).
	$\nu_2$	NCl stretch.	793 B	792.6 VS		
	$\nu_3$	$\text{NO}_2$ scis.	370 C	369.6 VS		
$b_1$	$\nu_4$	$\text{NO}_2$ a-stretch.	1685 B	1684.6 VS		
	$\nu_5$	$\text{NO}_2$ rock.	408 C	408.1 VW		
$b_2$	$\nu_6$	Op-deform.	652 C	652.3 M		

**References**

- [1] IR. R. Ryason and M. K. Wilson, J. Chem. Phys. **22**, 2000 (1954).  
 [2] IR. D. L. Bernitt, R. H. Miller, and I. C. Hisatsune, Spectrochim. Acta **23A**, 237 (1967).

**No. 44 Nitryl chloride  $\text{Cl}^{15}\text{NO}_2$**   
**Symmetry  $C_{2v}$  Symmetry number  $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{NO}_2$ s-stretch.	1286 D	1318.5 S 1267.1 VS		FR( $2\nu_6$ ).
	$\nu_2$	NCl stretch.	793 B	792.6 VS		
	$\nu_3$	$\text{NO}_2$ scis.	370 C	369.6 VS		
$b_1$	$\nu_4$	$\text{NO}_2$ a-stretch.	1685 B	1684.6 VS		
	$\nu_5$	$\text{NO}_2$ rock.	408 C	408.1 VW		
$b_2$	$\nu_6$	Op-deform.	652 C	652.3 M		

**References**

See No. 43( $\text{Cl}^{14}\text{NO}_2$ ).



**No. 45 Chlorine trifluoride  $\text{ClF}_3$**   
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{ClF}$ stretch.	752 C	751 S	752.1 S, p	
	$\nu_2$	$\text{ClF}_2$ s-stretch.	529 C	530 M	529.3 VS, p	
	$\nu_3$	$\text{ClF}_2$ ip-deform.	328 C	328 S	337 W, p 321	$\text{OV}(\nu_6)$ .
$b_1$	$\nu_4$	$\text{ClF}_2$ a-stretch.	702 C	702 VS		
	$\nu_5$	$\text{ClF}_2$ ip-deform.	442 C	442 W	431 W, dp	
$b_2$	$\nu_6$	$\text{ClF}_2$ op-deform.	328 D	328 S		$\text{OV}(\nu_3)$ .

**References**

- [1] IR.R. H. Selig, H. H. Claassen, and J. H. Holloway, J. Chem. Phys. **52**, 3517 (1970).  
 [2] Th. K. Ramaswamy and P. Muthusbramanian, J. Mol. Structure **9**, 193 (1971).

**No. 46 Bromine trifluoride  $\text{BrF}_3$**   
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{BrF}$ stretch.	675 C	675 S	675 S, p	
	$\nu_2$	$\text{BrF}_2$ s-stretch.	552 C	552 W	552 VS, p	
	$\nu_3$	$\text{BrF}_2$ ip-deform.	242 C	242 S	233 W, p	$\text{OV}(\nu_6)$ .
$b_1$	$\nu_4$	$\text{BrF}_2$ a-stretch.	614 C	614 VS	612 VW	
	$\nu_5$	$\text{BrF}_2$ ip-deform.	350 C	350 VW		
$b_2$	$\nu_6$	$\text{BrF}_2$ op-deform.	242 D	242 S		$\text{OV}(\nu_3)$ .

**References**

- [1] IR.R. H. Selig, H. H. Claassen, and J. H. Holloway, J. Chem. Phys. **52**, 3517 (1970).  
 [2] IR. K. O. Christe, E. C. Curtis, and D. Pilipovich, Spectrochim. Acta **27A**, 931 (1971).  
 [3] Th. K. Ramaswamy and P. Muthusbramanian, J. Mol. Structure **9**, 193 (1971).

**No. 47 Hydrogen peroxide  $\text{H}_2\text{O}_2$** Symmetry  $\text{C}_2$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
<i>a</i>	$\nu_1$	OH stretch.	3599 B	3599.2	3364 p	
	$\nu_2$	OH bend.	1402 E		1402 p	
	$\nu_3$	OO stretch.	877 C	877	880 p	
	$\nu_4$	Torsion	371 B	370.7		
			243 C	242.8		
<i>b</i>	$\nu_5$	OH stretch.	3608 B	3607.9		
	$\nu_6$	OH bend.	1266 D	1266		

**References**

- [1] IR. P. A. Giguère, J. Chem. Phys. **18**, 88 (1950).  
 [2] IR. P. A. Giguère and O. Bain, J. Phys. Chem. **56**, 340 (1952).  
 [3] IR. O. Bain and P. A. Giguère, Can. J. Chem. **33**, 527 (1956).  
 [4] R. R. C. Tylor and P. C. Cross, J. Chem. Phys. **24**, 41 (1956).  
 [5] IR. R. L. Redington, W. B. Olson, and P. C. Cross, J. Chem. Phys. **36**, 1311 (1962).  
 [6] IR. R. H. Hunt, R. A. Leacock, C. W. Peters and K. T. Hecht, J. Chem. Phys. **42**, 1931 (1965).

**No. 48 Hydrogen persulfide  $\text{H}_2\text{S}_2$** Symmetry  $\text{C}_2$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
<i>a</i>	$\nu_1$	SH stretch.	2556 A	2555.78	2509 (2), dp	
	$\nu_2$	SH bend.	883 D		883 (2), dp	
	$\nu_3$	SS stretch.	509 D		509 (9)	
	$\nu_4$	Torsion	416 B	416		
<i>b</i>	$\nu_5$	SH stretch.	2559 A	2558.64		
	$\nu_6$	SH bend.	886 C	886		

**References**

- [1] IR. M. K. Wilson and R. M. Badger, J. Chem. Phys. **17**, 1232 (1949).  
 [2] R. F. Fehér, W. Laue, and G. Winkhaus, Z. Anorg. Allg. Chem. **288**, 113 (1956).  
 [3] IR. R. L. Redington, J. Mol. Spectry. **9**, 469 (1962).  
 [4] IR. B. P. Winnwischer, J. Mol. Spectry. **36**, 414 (1970).

**No. 49      Difluoro disulphane      F<sub>2</sub>S<sub>2</sub>****Symmetry C<sub>2</sub>****Symmetry number  $\sigma = 2$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
<i>a</i>	$\nu_1$	SF stretch.	717 B	717.0		
	$\nu_2$	SS stretch.	615 B	614.6	623 p	
	$\nu_3$	SF bend.	320 B	319.8	322 p	
	$\nu_4$	Torsion	183 C	182.5	193 p	
<i>b</i>	$\nu_5$	SF stretch.	681 B	680.8	683	
	$\nu_6$	SF bend.	301 C	301	297 dp	

**References**

- [1] IR. F. Seel and R. Budenz, Chem. Ber. **98**, 251 (1965).  
 [2] IR.R. R. D. Brown and G. P. Pez, Spectrochim. Acta **26A**, 1375 (1970).

**No. 50      Hydrazoic acid      HN<sub>3</sub>****Symmetry C<sub>s</sub>****Symmetry number  $\sigma = 1$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a'</i>	$\nu_1$	NH stretch.	3336 B	3336 M		
	$\nu_2$	N $\equiv$ N stretch.	2140 B	2139.8 VS		
	$\nu_3$	NH bend.	1264 B	1263.7 M		
	$\nu_4$	N-N stretch.	1151 B	1150.5 VS		
	$\nu_5$	NNN bend.	534 B	534.2 W		
<i>a''</i>	$\nu_6$	NNN bend.	607 B	607.0 VW		

**References**

- [1] IR. D. A. Dows and G. C. Pimentel, J. Chem. Phys. **23**, 1258 (1955).  
 [2] IR. G. C. Pimentel, S. W. Charles, and K. J. Rosengren, J. Chem. Phys. **44**, 3029 (1966).  
 [3] IR. G. B. Moore and K. J. Rosengren, J. Chem. Phys. **44**, 4108 (1966).  
 [4] IR. D. M. Levine and D. A. Dows, J. Chem. Phys. **46**, 1168 (1967).

**No. 51      Hydrazoic acid    DN<sub>3</sub>**  
**Symmetry C<sub>s</sub>**

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a'</i>	$\nu_1$	ND stretch.	2478 B	2478 M		FR( $\nu_3 + \nu_4$ ).
	$\nu_2$	N≡N stretch.	2112 C	2112 VS		
	$\nu_3$	ND bend.	954 B	953.8 S		
	$\nu_4$	N-N stretch.	1184 B	1183.7 M		
<i>a''</i>	$\nu_5$	NNN bend.	492 B	492.2 W		
	$\nu_6$	NNN bend.	588 B	588.4 VW		

**References**See No. 50(NH<sub>3</sub>).

**No. 52      Difluoroamine    NF<sub>2</sub>H**  
**Symmetry C<sub>s</sub>**

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a'</i>	$\nu_1$	NH stretch.	3193 C	3193 W		
	$\nu_2$	NH bend.	1307 B	1307 S		
	$\nu_3$	NF <sub>2</sub> s-stretch.	972 B	972 S		
	$\nu_4$	NF <sub>2</sub> scis.	500 C	500 M		
<i>a''</i>	$\nu_5$	NH bend.	1424 B	1424 S		
	$\nu_6$	NF <sub>2</sub> a-stretch.	888 C	888 VS		

**Reference**

- [1] IR. J. J. Comeford, D. E. Mann, J. L. Schoen, and D. R. Lide, Jr.,  
 J. Chem. Phys. **38**, 461 (1963).

**No. 53      Chlorodifluoroammonia    NClF<sub>2</sub>**  
**Symmetry C<sub>s</sub>**

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a'</i>	$\nu_1$	NF <sub>2</sub> s-stretch.	930 C	930.2		
	$\nu_2$	NCl stretch.	697 C	696.9		
	$\nu_3$	NF <sub>2</sub> deform.	556 C	555.5		
	$\nu_4$	NClF s-deform.	377 C	377		
<i>a''</i>	$\nu_5$	NF <sub>2</sub> a-stretch.	855 C	855.4		
	$\nu_6$	NClF a-deform.	382 D	382 <sup>a</sup>		

<sup>a</sup> An average of two splitting bands.**References**

- [1] IR. R. Ettinger, J. Chem. Phys. **38**, 2427 (1963).  
 [2] IR. J. J. Comeford, J. Chem. Phys. **45**, 3463 (1966).

**No. 54 Dichlorofluoroammonia  $\text{NCl}_2\text{F}$** Symmetry  $\text{C}_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NF stretch.	825 C	825 S		
	$\nu_2$	$\text{NCl}_2$ s-stretch.	615 C	615 M		
	$\nu_3$	NFCl s-deform.	409 C	409 W		
	$\nu_4$	$\text{NCl}_2$ deform.	274 C	274 W		
$a''$	$\nu_5$	$\text{NCl}_2$ a-stretch.	692 C	692 S		
	$\nu_6$	NFCl a-deform.	344 C	344 M		

**References**

- [1] IR. D. E. Milligan, NBS Report 8149.  
 [2] IR. R. P. Hirschmann, L. R. Anderson, D. F. Harnish, and W. B. Fox, Spectrochim. Acta **24A**, 1267 (1968).

**No. 55 Thionyl fluoride  $\text{SOF}_2$** Symmetry  $\text{C}_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a'$	$\nu_1$	SO stretch.	1333 D	1340.8 S	1339.3 VS	FR( $\nu_2 + \nu_3$ ).
	$\nu_2$	$\text{SF}_2$ s-stretch.	808 B	1330.9 S	1329.9 VS	
	$\nu_3$	OSF deform.	530 B	808.2 VS	808.3 VS	
	$\nu_4$	$\text{SF}_2$ scis.	378 D	530.4 M	529.6 S	
$a''$				377.8 W	379.5 W	
	$\nu_5$	$\text{SF}_2$ a-stretch.	747 C	747.0 VS	746.8 W	
	$\nu_6$	OSF deform.	393 D	392.5 W	398.6 M	

**References**

- [1] IR. J. K. O'Loane and M. K. Wilson, J. Chem. Phys. **23**, 1313 (1955).  
 [2] R. P. Bender and J. M. Wood, Jr., J. Chem. Phys. **23**, 1316 (1955).  
 [3] IR. F. Seel and R. Budenz, Chem. Ber. **98**, 251 (1965).  
 [4] IR.R. E. L. Pace and H. V. Samuelson, J. Chem. Phys. **44**, 3682 (1966).

**No. 56      Thionyl chloride      SOCl<sub>2</sub>**  
**Symmetry C<sub>s</sub>** **Symmetry number  $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
<i>a'</i>	$\nu_1$	SO stretch.	1251 C	1251 VS	1230 W, p	
	$\nu_2$	SCl <sub>2</sub> s-stretch.	492 C	492 VS	490 M, p	
	$\nu_3$	OSCl deform.	344 D		344 S, p	
	$\nu_4$	SCl <sub>2</sub> scis.	194 D		194 M, p	
<i>a''</i>	$\nu_5$	SCl <sub>2</sub> a-stretch.	455 C	455 VS	445 W, dp	
	$\nu_6$	OSCl deform.	284 D		284 M, dp	

**References**

- [1] R. R. Vogel-Hogler, *Acta. Phys. Austriaca* **1**, 323 (1948).  
 [2] R. C. A. McDowell, *Trans. Faraday Soc.* **49**, 371 (1953).  
 [3] IR. D. E. Martz and R. T. Lagemann, *J. Chem. Phys.* **22**, 1193 (1954).  
 [4] R. G. Allen and C. A. McDowell, *J. Chem. Phys.* **23**, 209 (1955).  
 [5] Th. A. Mueller and G. Nagarajan, *Z. Phys. Chem. (Leipzig)* **235**, 57 (1967).  
 [6] Th. K. Ramaswamy and S. Jayaraman, *J. Mol. Structure* **7**, 470 (1971).

**No. 57      Thionyl bromide      SOBr<sub>2</sub>**  
**Symmetry C<sub>s</sub>** **Symmetry number  $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup> (Liquid)	
<i>a'</i>	$\nu_1$	SO stretch.	1121 D	1121 (2) p		
	$\nu_2$	SBr s-stretch.	405 D		405 (7) p	
	$\nu_3$	OSBr deform.	267 D		267 (10) p	
	$\nu_4$	SBr <sub>2</sub> scis.	120 D		120 (10) p	
<i>a''</i>	$\nu_5$	SBr <sub>2</sub> a-stretch.	379 D		379 (5) dp	
	$\nu_6$	OSBr deform.	223 D		223 (7) dp	

**Reference**

- [1] R. H. Stammreich, R. Forneris, and Y. Tavares, *J. Chem. Phys.* **25**, 1277 (1956).

**No. 58**      **Titanium tetrachloride**    **TiCl<sub>4</sub>****Symmetry T<sub>d</sub>****Symmetry number  $\sigma = 12$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Gas)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	389 B	ia, 388 <sup>a</sup>	389	
e	$\nu_2$	Deg. deform.	114 B	ia, 119 <sup>a</sup>	114	
f <sub>2</sub>	$\nu_3$	Deg. stretch.	498 C	498.5	498	
	$\nu_4$	Deg. deform.	136 C	136	136	

<sup>a</sup> Estimated from combination bands.**References**

- [1] IR.      N. J. Hawkins and D. R. Carpenter, J. Chem. Phys. **23**, 1700 (1955).  
 [2] IR.      H. Bürger and A. Ruoff, Spectrochim. Acta **24A**, 1863 (1968).  
 [3] R.      R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

**No. 59**      **Titanium tetrabromide**    **TiBr<sub>4</sub>****Symmetry T<sub>d</sub>****Symmetry number  $\sigma = 12$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Liquid)	cm <sup>-1</sup> (Gas)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	232 B	ia	231.5	
e	$\nu_2$	Deg. deform.	69 B	ia	68.5	
f <sub>2</sub>	$\nu_3$	Deg. stretch.	393 C	383 VS	393	
	$\nu_4$	Deg. deform.	88 C		88	

**References**

- [1] IR.R.      F. A. Miller and G. L. Carlson, Spectrochim. Acta **16**, 6 (1960).  
 [2] R.      R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

**No. 60**      **Titanium tetraiodide**      **TiI<sub>4</sub>****Symmetry T<sub>d</sub>****Symmetry number  $\sigma = 12$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (C <sub>6</sub> H <sub>12</sub> soln.)	cm <sup>-1</sup> (C <sub>6</sub> H <sub>12</sub> soln.)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	162 D	ia	162 VS, p	
e	$\nu_2$	Deg. deform.	51 D	ia	51 M, dp	
f <sub>2</sub>	$\nu_3$	Deg. stretch.	322 D	322 VS	324 M, dp	
	$\nu_4$	Deg. deform.	67 D	67 M		

**Reference**

- [1] IR. R.      R. J. H. Clark and C. J. Willis, J. Chem. Soc. A **1971**, 838.

**No. 61 Zirconium tetrachloride  $\text{ZrCl}_4$** Symmetry  $T_d$ Symmetry number  $\sigma = 12$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.	377 B	ia, 388 <sup>a</sup>	377 VS, p	
$e$	$\nu_2$	Deg. deform.	98 B	ia, 102 <sup>a</sup>	98	
$f_2$	$\nu_3$	Deg. stretch.	418 C	421	418 VW	
	$\nu_4$	Deg. deform.	113 C	112 <sup>a</sup>	113	

<sup>a</sup> Estimated from combination bands.**References**

- [1] IR. J. K. Wilmschurst, J. Mol. Spectry. **5**, 343 (1960).  
 [2] IR. A. Büchler, J. B. Berkowitz-Mattuck, and D. H. Dugre, J. Chem. Phys. **34**, 2202 (1961).  
 [3] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

**No. 62 Zirconium tetrabromide  $\text{ZrBr}_4$** Symmetry  $T_d$ Symmetry number  $\sigma = 12$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.	223 B	ia	222.5	
$e$	$\nu_2$	Deg. deform.	60 B	ia	60	
$f_2$	$\nu_3$	Deg. stretch.	315 C		315	
	$\nu_4$	Deg. deform.	72 C		72	

**Reference**

- [1] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

**No. 63 Zirconium tetraiodide  $\text{ZrI}_4$** Symmetry  $T_d$ Symmetry number  $\sigma = 12$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.	158 B	ia	158	
$e$	$\nu_2$	Deg. deform.	43 B	ia	43	
$f_2$	$\nu_3$	Deg. stretch.	254 C		254	
	$\nu_4$	Deg. deform.	55 C		55	

**Reference**See No. 62( $\text{ZrBr}_4$ ).



**No. 64 Ruthenium tetroxide RuO<sub>4</sub>**  
Symmetry T<sub>d</sub>

Symmetry number  $\sigma = 12$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	885 C	ia	885.3 S	
					(Gas)	
e	$\nu_2$	Deg. deform.	322 C	ia	322.4 M	
f <sub>2</sub>	$\nu_3$	Deg. stretch.	921 C	921.0	912.9 W	
	$\nu_4$	Deg. deform.	336 C	336.0	333 W	

**References**

- [1] IR. R. E. Dodd, Trans. Faraday Soc. **55**, 1480 (1959).  
 [2] IR. M. H. Ortner, J. Chem. Phys. **34**, 559 (1961).  
 [3] R. G. Davidson, N. Logan, and A. Morris, Chem. Commun. **1968**, 1044.  
 [4] R. W. P. Griffith, J. Chem. Soc. **A1968**, 1663.  
 [5] IR. A. Müller and B. Krebs, J. Mol. Spectry. **26**, 136 (1968).  
 [6] IR.R. I. W. Levin and S. Abramowitz, J. Chem. Phys. **50**, 4860 (1969).  
 [7] Th. R. S. McDowell, J. Chem. Phys. **53**, 4407 (1970).  
 [8] IR.R. R. S. McDowell, L. B. Aspery and L. C. Hoskins, J. Chem. Phys. **56**, 5712 (1972).

**No. 65 Hafnium tetrachloride HfCl<sub>4</sub>**  
Symmetry T<sub>d</sub>

Symmetry number  $\sigma = 12$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Gas)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	382 B	ia	382	
e	$\nu_2$	Deg. deform.	102 B	ia	101.5	
f <sub>2</sub>	$\nu_3$	Deg. stretch.	390 C	393	390	
	$\nu_4$	Deg. deform.	112 C		112	

**References**

- [1] IR. A. Büchler, J. B. Berkowitz-Mattuck, and D. H. Dugre, J. Chem. Phys. **34**, 2202 (1961).  
 [2] R. R. J. H. Clark, B. K. Hunter, and D. M. Rippon, Inorg. Chem. **11**, 56 (1972).

**No. 66 Hafnium tetrabromide HfBr<sub>4</sub>**  
Symmetry T<sub>d</sub>

Symmetry number  $\sigma = 12$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
					(Gas)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	236 B	ia	235.5	
e	$\nu_2$	Deg. deform.	63 B	ia	63	
f <sub>2</sub>	$\nu_3$	Deg. stretch.	273 C		273	
	$\nu_4$	Deg. deform.	71 C		71	

**Reference**See No. 62(ZrBr<sub>4</sub>).

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**No. 67 Hafnium tetraiodide  $\text{HfI}_4$**   
**Symmetry  $T_d$**  **Symmetry number  $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
					(Gas)	
$a_1$	$\nu_1$	Sym. stretch.	158 B	ia	158	
$e$	$\nu_2$	Deg. deform.	55 C	ia	55	
$f_2$	$\nu_3$	Deg. stretch.	224 C		224	
	$\nu_4$	Deg. deform.	63 C		63	

**Reference**See No. 62( $\text{ZrBr}_4$ ).

**No. 68 Osmium tetroxide  $\text{Os}^{16}\text{O}_4$**   
**Symmetry  $T_d$**  **Symmetry number  $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Gas)	
$a_1$	$\nu_1$	Sym. stretch.	965 B	ia	965.2	
$e$	$\nu_2$	Deg. deform.	333 B	ia	333.1	
$f_2$	$\nu_3$	Deg. stretch.	960 B	960.5	960.1	
	$\nu_4$	Deg. deform.	329 B	329.0	322.7	

**References**

- [1] IR. N. J. Hawkins and W. W. Sabal, *J. Chem. Phys.* **25**, 775 (1956).  
 [2] IR. R. E. Dodd, *Trans. Faraday Soc.* **55**, 1480 (1959).  
 [3] IR. I. W. Levin and S. Abramowitz, *Inorg. Chem.* **5**, 2024 (1966).  
 [4] IR. R. S. McDowell, *Inorg. Chem.* **6**, 1759 (1967).  
 [5] R. W. P. Griffith, *J. Chem. Soc. A* **1968**, 1663.  
 [6] R. C. Davidson, N. Logan, and A. Morris, *Chem. Commun.* **1968**, 1044.  
 [7] R. I. W. Levin, *Inorg. Chem.* **8**, 1018 (1969).  
 [8] R. J. L. Huston and H. H. Claassen, *J. Chem. Phys.* **52**, 5646 (1970).  
 [9] IR. C. G. Barraclough and M. M. Sinclair, *Spectrochim. Acta* **26A**, 207 (1970).  
 [10] IR.R. R. S. McDowell and M. Goldblatt, *Inorg. Chem.* **10**, 625 (1971).

**No. 69 Osmium tetroxide  $\text{Os}^{18}\text{O}_4$**   
**Symmetry  $T_d$**  **Symmetry number  $\sigma = 12$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	( $\text{CCl}_4$ soln.)	
$a_1$	$\nu_1$	Sym. stretch.	910 C	ia	909.7	
$e$	$\nu_2$	Deg. deform.	317 C	ia	316.6	
$f_2$	$\nu_3$	Deg. stretch.	912 B	911.8		
	$\nu_4$	Deg. deform.	313 B	312.7		

**References**

- [1] IR. C. G. Barraclough and M. M. Sinclair, *Spectrochim. Acta* **26A**, 207 (1970).  
 [2] IR.R. R. S. McDowell and M. Goldblatt, *Inorg. Chem.* **10**, 625 (1971).

No. 70 Thionitrosyl trifluoride NSF<sub>3</sub>  
Symmetry C<sub>3v</sub> Symmetry number  $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
a <sub>1</sub>	$\nu_1$	NS stretch.	1515 B	1515	1512 p	
	$\nu_2$	NF <sub>3</sub> s-stretch.	775 B	775	768 p	
	$\nu_3$	NF <sub>3</sub> s-deform.	521 B	521	520 dp	
e	$\nu_4$	NF <sub>3</sub> d-stretch.	811 B	811	812 dp	
	$\nu_5$	NF <sub>3</sub> d-deform.	429 B	429	430 dp	
	$\nu_6$	NF <sub>3</sub> rock.	342 B	342	340 dp	

## References

- [1] IR. H. Richert and O. Glemser, Z. Anorg. Alleg. Chem. **307**, 328 (1961).  
 [2] R. A. Müller, A. Ruoff, B. Krebs, O. Glemser, and W. Koch, Spectrochim. Acta **25A**, 199 (1969).

No. 71 Trifluorosilane SiHF<sub>3</sub>  
Symmetry C<sub>3v</sub> Symmetry number  $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a <sub>1</sub>	$\nu_1$	SiH stretch.	2316 B	2315.6 M		
	$\nu_2$	SiF <sub>3</sub> s-stretch.	858 B	858.25 S		
	$\nu_3$	SiF <sub>3</sub> s-deform.	425 B	425.2 M		
e	$\nu_4$	SiF <sub>3</sub> d-stretch.	998 B	997.83 VS		
	$\nu_5$	SiH bend.	844 B	843.6 S		
	$\nu_6$	SiF <sub>3</sub> d-deform.	306 B	306.2 M		

## References

- [1] IR. C. Newman, S. R. Polo, and M. K. Wilson, Spectrochim. Acta **15**, 793 (1959).  
 [2] IR. H. Bürger und S. Biedermann, Spectrochim. Acta **27A**, 1687 (1971)

No. 72 Trifluorosilane-d SiDF<sub>3</sub>  
Symmetry C<sub>3v</sub> Symmetry number  $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a <sub>1</sub>	$\nu_1$	SiD stretch.	1691 B	1690.72		
	$\nu_2$	SiF <sub>3</sub> s-stretch.	854 B	853.84 S		
	$\nu_3$	SiF <sub>3</sub> s-deform.	422 B	422.1 M		
e	$\nu_4$	SiF <sub>3</sub> d-stretch.	992 B	991.76 VS		
	$\nu_5$	SiD bend.	628 B	628.41 M		
	$\nu_6$	SiF <sub>3</sub> d-deform.	303 B	302.8 M		

## References

See No. 71(SiHF<sub>3</sub>).

**No. 73 Trichlorosilane  $\text{SiHCl}_3$**   
**Symmetry  $C_{3v}$  Symmetry number  $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	SiH stretch.	2261 B	2260.9 S	2258 p	
	$\nu_2$	$\text{SiCl}_3$ s-stretch.	499 B	498.6 S	489 p	
	$\nu_3$	$\text{SiCl}_3$ s-deform.	254 B	253.7 M	250 p	
$e$	$\nu_4$	SiH bend.	811 B	810.8 VS	799 dp	
	$\nu_5$	$\text{SiCl}_3$ d-stretch.	600 B	600.1 VS	587 dp	
	$\nu_6$	$\text{SiCl}_3$ d-deform.	176 B	175.5 M	179 dp	

**References**

- [1] R. M. L. Delwaulle and M. F. François, *Comptes Rendus* **228**, 1007 (1949).  
 [2] IR.Th. H. Bürger and A. Ruoff, *Spectrochim. Acta* **26**, 1449 (1970).

**No. 74 Trichlorosilane-d  $\text{SiDCl}_3$**   
**Symmetry  $C_{3v}$  Symmetry number  $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	SiD stretch.	1647 B	1647.1 S		
	$\nu_2$	$\text{SiCl}_3$ s-stretch.	496 B	495.9 S		
	$\nu_3$	$\text{SiCl}_3$ s-deform.	252 B	252.0 M		
$e$	$\nu_4$	SiD bend.	634 B	633.8 VS		
	$\nu_5$	$\text{SiCl}_3$ d-stretch.	550 B	550.0 VS		
	$\nu_6$	$\text{SiCl}_3$ d-deform.	175 B	174.5 M		

**Reference**

- [1] IR.Th. H. Bürger and A. Ruoff, *Spectrochim. Acta* **26**, 1449 (1970).

**No. 75 Tribromosilane  $\text{SiHBr}_3$**   
**Symmetry  $C_{3v}$  Symmetry number  $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	SiH stretch.	2239 B	2239.2 S	2236 p	
	$\nu_2$	$\text{SiBr}_3$ s-stretch.	362 C	362 M, b	362 p	
	$\nu_3$	$\text{SiBr}_3$ s-deform.	168 B	168.5 M	166 p	
$e$	$\nu_4$	SiH bend.	774 C	774 VS	770 dp	
	$\nu_5$	$\text{SiBr}_3$ d-stretch.	484 C	483.5 VS	470 dp	
	$\nu_6$	$\text{SiBr}_3$ d-deform.	117 C	116.8 W	115 dp	

**References**

- [1] R. M. L. Delwaulle and M. F. François, *Comptes Rendus* **230**, 743 (1950).  
 [2] IR.Th. H. Bürger und J. Cichon, *Spectrochim. Acta* **27A**, 2191 (1971).

**No. 76 Phosphoryl fluoride  $\text{POF}_3$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	PO stretch.	1417 B	1415 M	1416.8 p	
	$\nu_2$	$\text{PF}_3$ s-stretch.	873 B	873 M	872.7 p	
	$\nu_3$	$\text{PF}_3$ s-deform.	472 B	473 S	472.4	OV(5) in Raman.
$e$	$\nu_4$	$\text{PF}_3$ d-stretch.	991 C	990 VS	991.0 dp	
	$\nu_5$	$\text{PF}_3$ d-deform.	482 C	485 M	482.0 dp	
	$\nu_6$	PO bend.	336 C		335.5 dp	

**References**

- [1] R. M. L. Delwaulle and M. F. François, *Comptes Rendus* **222**, 550 (1946).  
 [2] IR. H. S. Gutowsky and A. D. Liehr, *J. Chem. Phys.* **20**, 1652 (1952).  
 [3] R.Th. R. J. H. Clark and D. M. Rippon, *Mol. Phys.* **28**, 305 (1974).

**No. 77 Phosphoryl chloride  $\text{POCl}_3$** Symmetry  $C_2$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	PO stretch.	1322 C		1321.5	
	$\nu_2$	$\text{PCl}_3$ s-stretch.	481 C		480.5	
	$\nu_3$	$\text{PCl}_3$ s-deform.	266 C		265.5	
$e$	$\nu_4$	$\text{PCl}_3$ d-stretch.	590 C		589.5	
	$\nu_5$	PO bend.	333 C		332.5	
	$\nu_6$	$\text{PCl}_3$ d-deform.	187 C		187.0	

**References**

- [1] R. M. L. Delwaulle and M. F. François, *J. Chim. Physique* **45**, 50 (1948).  
 [2] R.Th. R. J. H. Clark and D. M. Rippon, *Mol. Phys.* **28**, 305 (1974).

**No. 78 Phosphoryl bromide  $\text{POBr}_3$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	PO stretch.	1261 D		1261	
	$\nu_2$	$\text{PBr}_3$ s-stretch.	340 D		340	
	$\nu_3$	$\text{PBr}_3$ s-deform.	173 D		173	
$e$	$\nu_4$	$\text{PBr}_3$ d-stretch.	488 D		488	
	$\nu_5$	PO bend.	267 D		267	
	$\nu_6$	$\text{PBr}_3$ d-deform.	118 D		118	

**Reference**See No. 77( $\text{POCl}_3$ ).

No. 79 Thiophosphoryl trifluoride  $\text{PSF}_3$ Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{PF}_3$ s-stretch.	981 B	981 VS	969 (4.5) p	
	$\nu_2$	PS stretch.	695 B	695 M	696 (100) p	
	$\nu_3$	$\text{PF}_3$ s-deform.	440 B	440 M	441 (20) p	
$e$	$\nu_4$	$\text{PF}_3$ d-stretch.	945 B	945 VS	937 (6.0) dp	
	$\nu_5$	$\text{PF}_3$ d-deform.	402 C	402 M	404 (13) dp	
	$\nu_6$	$\text{PF}_3$ rock.	275 B	275 W	276 (37) dp	

## References

- [1] R. M. L. Delwaulle and F. Francois, *Comptes Rendus* **226**, 894 (1948).  
 [2] R. M. L. Delwaulle and F. Francois, *J. Chim. Phys.* **46**, 87 (1949).  
 [3] IR. R. G. Cavell, *Spectrochim. Acta* **23A**, 249 (1968).  
 [4] IR.R. J. R. Durig and J. W. Clark, *J. Chem. Phys.* **46**, 3057 (1967).

No. 80 Thiophosphoryl trichloride  $\text{PSCl}_3$ Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	PS stretch.	767 B	770	767.2 p	
	$\nu_2$	$\text{PCl}_3$ s-stretch.	432 B	431	431.6 p	
	$\nu_3$	$\text{PCl}_3$ s-deform.	246 C	252	246.0 dp	OV( $\nu_5$ ).
$e$	$\nu_4$	$\text{PCl}_3$ d-stretch.	544 C	547	543.7 dp	
	$\nu_5$	$\text{PCl}_3$ d-deform.	246 C	252	246 dp	OV( $\nu_3$ ).
	$\nu_6$	$\text{PCl}_3$ rock.	167 C	174 (liquid)	167.3 dp	

## References

- [1] IR. G. Cilento, D. A. Ramsay, and R. N. Jones *J. Amer. Chem. Soc.* **71**, 2753 (1949).  
 [2] IR.R. J. R. Durig and J. W. Clark, *J. Chem. Phys.* **46**, 3057 (1967).  
 [3] R.Th. R. J. H. Clark and D. M. Rippon, *Mol. Phys.* **28**, 305 (1974).

**No. 81**      **Perchlorylfluoride**       $^{35}\text{ClO}_3\text{F}$   
**Symmetry  $C_{3v}$**

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{ClO}_3$ s-stretch.	1063 B	1061 S	1062.5 VS	
	$\nu_2$	ClF stretch.	716 B	714 S	716.0 S	
	$\nu_3$	$\text{ClO}_3$ s-deform.	550 B	549 W	549.5 M	
$e$	$\nu_4$	$\text{ClO}_3$ d-stretch.	1318 B	1315 VS	1317.5 W	
	$\nu_5$	$\text{ClO}_3$ d-deform.	590 B	590.55 M	589.5 W	
	$\nu_6$	$\text{ClO}_3$ rock.	405 B	405 W	404.5 W	

**References**

- [1] IR. R. P. Madden and W. S. Benedict, J. Chem. Phys. **25**, 594 (1956).  
 [2] IR. D. R. Lide, Jr. and D. E. Mann, J. Chem. Phys. **25**, 1128 (1956).  
 [3] R. F. X. Powell and E. R. Lippincott, J. Chem. Phys. **32**, 1883 (1960).  
 [4] R. H. H. Claassen and E. H. Appleman, Inorg. Chem. **9**, 622 (1970).  
 [5] R.Th. R. J. H. Clark and D. M. Rippon, Mol. Phys. **28**, 305 (1974).

**No. 82**      **Vanadyl(V) chloride**       $\text{VOCl}_3$   
**Symmetry  $C_{3v}$**

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	VO stretch.	1042 C	1035 VS	1042.5 (1.8) p	
	$\nu_2$	$\text{VCl}_3$ s-stretch.	408 C	408 S	409.5 (10.0) p	
	$\nu_3$	$\text{VCl}_3$ s-deform.	163 C		163.0 (0.8)	
$e$	$\nu_4$	$\text{VCl}_3$ d-stretch.	502 C	502 VS	503 (20) dp	
	$\nu_5$	$\text{VCl}_3$ d-deform.	246 C		246.0 (1.5) dp	
	$\nu_6$	$\text{VCl}_3$ rock.	125 C		124.5 (3.8)	

**References**

- [1] R. H. J. Eichoff and F. Weigel, Z. Allg. Chem. **275**, 267 (1954).  
 [2] IR.R. F. A. Miller and L. R. Cousins, J. Chem. Phys. **26**, 329 (1957).  
 [3] R. J. R. Beattie, K. M. S. Livingston, D. J. Reynolds, and G. A. Ozin, J. Chem. Soc. **1970**, 1210 (1970).  
 [4] R.Th. R. J. H. Clark and D. M. Rippon, Mol. Phys. **28**, 305 (1974).

**No. 83 Permanganyl fluoride  $\text{MnO}_3\text{F}$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{MnO}_3$ s-stretch.	905 B	905.2 M		
	$\nu_2$	MnF stretch.	721 B	720.7 M		
	$\nu_3$	$\text{MnO}_3$ s-deform.	338 B	337.7 W		
$e$	$\nu_4$	$\text{MnO}_3$ d-stretch.	953 B	952.5 S		
	$\nu_5$	$\text{MnO}_3$ d-deform.	374 B	373.9 W		
	$\nu_6$	MnF bend.	264 B	264.3 W		

**Reference**[1] IR. M. J. Reisfeld, L. B. Asprey, and N. A. Matuiyoff, *Spectrochim. Acta* **27A**, 765 (1971).**No. 84 Germyl fluoride  $\text{GeH}_3\text{F}$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{GeH}_3$ s-stretch.	2121 C	2120.6 S		
	$\nu_2$	$\text{GeH}_3$ s-deform.	859 C	859.0 VS		
	$\nu_3$	GeF stretch.	689 B	689.1 S		
$e$	$\nu_4$	$\text{GeH}_3$ d-stretch.	2132 B	2131.7 S		
	$\nu_5$	$\text{GeH}_3$ d-deform.	874 B	874.0 S		
	$\nu_6$	$\text{GeH}_3$ rock.	643 B	642.6 M		

**References**[1] IR. J. E. Griffiths, T. N. Srivastava, and M. Onyszchuk, *Can. J. Chem.* **40**, 579 (1962).[2] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, *J. Chem. Phys.* **39**, 2908 (1963).[3] IR. K. H. Rhee and M. K. Wilson, *J. Chem. Phys.* **43**, 331 (1965).**No. 85 Germyl fluoride- $d_3$   $\text{GeD}_3\text{F}$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{GeD}_3$ s-stretch.	1525 C	1525		
	$\nu_2$	$\text{GeD}_3$ s-deform.	696 B	696		
	$\nu_3$	GeF stretch.	618 C	618		
$e$	$\nu_4$	$\text{GeD}_3$ d-stretch.	1535 B	1535		
	$\nu_5$	$\text{GeD}_3$ d-deform.	635 C	635		
	$\nu_6$	$\text{GeD}_3$ rock.	466 C	466		

**Reference**[1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, *J. Chem. Phys.* **39**, 2908 (1963).



**No. 86**      **Germyl chloride**   **GeH<sub>3</sub>Cl****Symmetry C<sub>3v</sub>****Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	GeH <sub>3</sub> s-stretch.	2120 C	2119.9		
	$\nu_2$	GeH <sub>3</sub> s-deform.	848 B	847.5		
	$\nu_3$	GeCl stretch.	422 C	421.7		
<i>e</i>	$\nu_4$	GeH <sub>3</sub> d-stretch.	2129 B	2128.9		
	$\nu_5$	GeH <sub>3</sub> d-deform.	874 B	874.1		
	$\nu_6$	GeH <sub>3</sub> rock.	602 B	602.2		

**References**

- [1] IR. R. C. Lord, Jr., and C. M. Steese, J. Chem. Phys. **22**, 542 (1954).  
 [2] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).  
 [3] IR. K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).

**No. 87**      **Germyl chloride-d<sub>3</sub>**   **GeD<sub>3</sub>Cl****Symmetry C<sub>3v</sub>****Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				(Gas)		
<i>a</i> <sub>1</sub>	$\nu_1$	GeD <sub>3</sub> s-stretch.	1518 C	1518		
	$\nu_2$	GeD <sub>3</sub> s-deform.	609 C	609		
	$\nu_3$	GeCl stretch.	422 C	422		
<i>e</i>	$\nu_4$	GeD <sub>3</sub> d-stretch.	1530 C	1530		
	$\nu_5$	GeD <sub>3</sub> d-deform.	630 C	630		
	$\nu_6$	GeD <sub>3</sub> rock.	434 C	434		

**Reference**

- [1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).

**No. 88**      **Germyl bromide**   **GeH<sub>3</sub>Br****Symmetry C<sub>3v</sub>****Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	GeH <sub>3</sub> s-stretch.	2115 C	2115.2		
	$\nu_2$	GeH <sub>3</sub> s-deform.	833 C	832.7		
	$\nu_3$	GeBr stretch.	308 C	307.7		
<i>e</i>	$\nu_4$	GeH <sub>3</sub> d-stretch.	2127 B	2126.7		
	$\nu_5$	GeH <sub>3</sub> d-deform.	871 B	870.9		
	$\nu_6$	GeH <sub>3</sub> rock.	578 B	578.2		

**References**See No. 84(GeH<sub>3</sub>F).

**No. 89**      **Germyl bromide-d<sub>3</sub> GeD<sub>3</sub>Br****Symmetry C<sub>3v</sub>****Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	GeD <sub>3</sub> s-stretch.	1514 C	1514		
	$\nu_2$	GeD <sub>3</sub> s-deform.	596 C	596		
	$\nu_3$	GeBr stretch.	305 C	305		
<i>e</i>	$\nu_4$	GeD <sub>3</sub> d-stretch.	1530 C	1530		
	$\nu_5$	GeD <sub>3</sub> d-deform.	621 C	621		
	$\nu_6$	GeD <sub>3</sub> rock.	420 C	420		

**Reference**[1] IR.      D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).**No. 90**      **Germyl iodide GeH<sub>3</sub>I****Symmetry C<sub>3v</sub>****Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	GeH <sub>3</sub> s-stretch.	2110 C	2110.1		
	$\nu_2$	GeH <sub>3</sub> s-deform.	808 C	808.2		
	$\nu_3$	GeI stretch.	248 C	248.2		
<i>e</i>	$\nu_4$	GeH <sub>3</sub> d-stretch.	2121 B	2120.8		
	$\nu_5$	GeH <sub>3</sub> d-deform.	854 B	853.6		
	$\nu_6$	GeH <sub>3</sub> rock.	558 B	558.3		

**References**[1] IR.      D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).[2] IR.      K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).**No. 91**      **Germyl iodide-d<sub>3</sub> GeD<sub>3</sub>I****Symmetry C<sub>3v</sub>****Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	GeD <sub>3</sub> s-stretch.	1508 C	1508		
	$\nu_2$	GeD <sub>3</sub> s-deform.	582 C	582		
	$\nu_3$	GeI stretch.	249 C	249		
<i>e</i>	$\nu_4$	GeD <sub>3</sub> d-stretch.	1525 C	1525		
	$\nu_5$	GeD <sub>3</sub> d-deform.	603 C	603		
	$\nu_6$	GeD <sub>3</sub> rock.	404 C	404		

**Reference**[1] IR.      D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).

**No. 92 Trichlorogermane  $\text{GeHCl}_3$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	GeH stretch.	2159 D		(Liquid) 2159 p	
	$\nu_2$	$\text{GeCl}_3$ s-stretch.	409 D		409 p	
	$\nu_3$	$\text{GeCl}_3$ s-deform.	181 D		181 p	
$e$	$\nu_4$	GeH bend.	699 D		699 dp	
	$\nu_5$	$\text{GeCl}_3$ d-stretch.	438 D		438 dp	
	$\nu_6$	$\text{GeCl}_3$ d-deform.	149 D		149 dp	

**Reference**[1] R. M. L. Delwaulle and M. F. François, *Comptes Rendus* **228**, 1007 (1949).**No. 93 Tribromogermane  $\text{GeHBr}_3$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	GeH stretch.	2116 D		(Liquid) 2116 p	
	$\nu_2$	$\text{GeBr}_3$ s-stretch.	273 D		273 p	
	$\nu_3$	$\text{GeBr}_3$ s-deform.	128 D		128 p	
$e$	$\nu_4$	Ge H bend.	674 D		674 dp	
	$\nu_5$	$\text{GeBr}_3$ d-stretch.	325 D		325 dp	
	$\nu_6$	$\text{GeBr}_3$ d-deform.	95 E		95 dp	

**Reference**[1] R. M. L. Delwaulle and M. F. François, *Comptes Rendus* **230**, 743 (1950).**No. 94 Rhenium (VII) oxide chloride  $\text{ReO}_3\text{Cl}$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{ReO}_3$ s-stretch.	1001 C	(Liquid) 1001.5 VS	(Liquid) 1001 S, p	
	$\nu_2$	$\text{ReO}_3$ s-deform.	434 C	434 VS	435 M, p	
	$\nu_3$	ReCl stretch.	293 C	293 S		
$e$	$\nu_4$	$\text{ReO}_3$ d-stretch.	960 C	960 VS	962.5 M, dp	
	$\nu_5$	$\text{ReO}_3$ d-deform.	344 C	343.5 S	344 M, dp	
	$\nu_6$	ReCl bend.	196 C	196 M	196 S, dp	

**References**

- [1] R. H. J. Eichhoff and F. Weigel, *Z. Anorg. Allg. Chem.* **275**, 267 (1954).  
 [2] IR.R. F. A. Miller and G. L. Carlson, *Spectrochim. Acta* **16**, 1148 (1960).  
 [3] Th. A. Müller, B. Krebs, and W. Hölte, *Spectrochim. Acta* **23A**, 2753 (1967).

**No. 95 Rhenium (VII) oxide bromide  $\text{ReO}_3\text{Br}$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ ( $\text{CCl}_4$ soln.)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{ReO}_3$ s-stretch.	997 C	997 S		
	$\nu_2$	$\text{ReO}_3$ s-deform.	350 C	350 M		
	$\nu_3$	ReBr stretch.	195 C	195 M		
$e$	$\nu_4$	$\text{ReO}_3$ d-stretch.	963 C	963 VS		
	$\nu_5$	$\text{ReO}_3$ d-deform.	332 C	332 S		
	$\nu_6$	ReBr bend.	168 C	168 M		

**References**

- [1] IR.R. F. A. Miller and G. L. Carlson, *Spectrochim. Acta* **16**, 1148 (1960).  
 [2] Th. A. Müller, B. Krebs, and W. Hölting, *Spectrochim. Acta* **23A**, 2753 (1967).

**No. 96 Sulfuryl fluoride  $\text{SO}_2\text{F}_2$** Symmetry  $C_{2v}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ $\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ $\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{SO}_2$ s-stretch.	1269 C	1269 S	1270 M	
	$\nu_2$	$\text{SF}_2$ s-stretch.	848 C	848 S	847 S	
	$\nu_3$	$\text{SO}_2$ scis.	544 D	544.3 M	543 M	
	$\nu_4$	$\text{SF}_2$ scis.	385 D	384.5 VW		
$a_2$	$\nu_5$	$\text{SF}_2$ twist.	388 C	ia	388 W	
$b_1$	$\nu_6$	$\text{SO}_2$ a-stretch.	1502 C	1502 S	1502 VW	
	$\nu_7$	$\text{SO}_2$ rock.	553 D	552.8 M		
	$\nu_8$	$\text{SF}_2$ a-stretch.	885 C	885 S	883 VW	
	$\nu_9$	$\text{SO}_2$ wag.	539 D	539.4 M		

**References**

- [1] IR. W. D. Perkins and M. K. Wilson, *J. Chem. Phys.* **20**, 1791 (1952).  
 [2] R. P. Bender and J. M. Wood, Jr., *J. Chem. Phys.* **23**, 1316 (1955).  
 [3] Th. G. R. Hunt and M. K. Wilson, *Spectrochim. Acta* **18**, 959 (1962).  
 [4] IR. D. R. Lide, Jr., D. E. Mann, and J. J. Comeford, *Spectrochim. Acta* **21**, 497 (1965).  
 [5] Th. H. Toyuki and K. Shimizu, *Bull. Chem. Soc. Japan*, **39**, 2364 (1966).  
 [6] IR. A. J. Sumodi and E. L. Pace, *Spectrochim. Acta* **28A**, 1129 (1972).

**No. 97      Sulfuryl chloride       $\text{SO}_2\text{Cl}_2$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{SO}_2$ s-stretch.	1205 C	1205 S	1182 S, p	
	$\nu_2$	$\text{SO}_2$ scis.	577 D	577 VS	560 VS, p	
	$\nu_3$	$\text{SO}_2$ s-stretch.	408 D		408 VS, p	
	$\nu_4$	$\text{SO}_2$ scis.	218 D		218 VS, p	
$a_2$	$\nu_5$	$\text{SO}_2$ twist.	282 D	ia	282 S, dp	
$b_1$	$\nu_6$	$\text{SO}_2$ a-stretch.	1434 C	1434 S	1414 M, dp	
	$\nu_7$	$\text{SO}_2$ rock.	388 D		388 S, dp	
$b_2$	$\nu_8$	$\text{SO}_2$ a-stretch.	586 D	586 VS	580 VW, dp	
	$\nu_9$	$\text{SO}_2$ wag.	362 D		362 sh, dp	

**References**

- [1] R. R. Vogel-Hogler, *Acta. Phys. Austriaca*, **1**, 323 (1948).  
 [2] IR. D. E. Martz and R. T. Lagemann, *J. Chem. Phys.* **22**, 1193 (1954).  
 [3] R. R. J. Gillespie and E. A. Robinson, *Can. J. Chem. Phys.* **39**, 2171 (1961).  
 [4] Th. G. R. Hunt and M. K. Wilson, *Spectrochim. Acta* **18**, 959 (1962).  
 [5] Th. H. Toyuki and K. Shimizu, *Bull. Chem. Soc. Japan* **39**, 2364 (1966).

**No. 98      Dichlorosilane       $\text{SiH}_2\text{Cl}_2$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{SiH}_2$ s-stretch.	2224 C	2224 S	2221 S, p	
	$\nu_2$	$\text{SiH}_2$ scis.	954 C	954 S	942 W, dp	
	$\nu_3$	$\text{SiCl}_2$ s-stretch.	527 C	527 W	514 S, p	
	$\nu_4$	$\text{SiCl}_2$ scis.	188 D		188 M, dp	
$a_2$	$\nu_5$	$\text{SiH}_2$ twist.	710 D	ia	710 W, dp	
$b_1$	$\nu_6$	$\text{SiH}_2$ a-stretch.	2237 B	2237 S		
	$\nu_7$	$\text{SiH}_2$ rock.	602 C	602 W		
$b_2$	$\nu_8$	$\text{SiH}_2$ wag.	876 B	876 VS	868 VW, dp	
	$\nu_9$	$\text{SiCl}_2$ a-stretch.	590 C	590 S	566 VW, dp	

**References**

- [1] IR.R. J. A. Hawkins and M. K. Wilson, *J. Chem. Phys.* **21**, 360 (1953).  
 [2] IR. J. A. Hawkins, S. R. Polo, and M. K. Wilson, *J. Chem. Phys.* **21**, 1122 (1953).  
 [3] IR. D. H. Christensen and O. F. Nielsen, *J. Mol. Spectry.* **27**, 489 (1968).  
 [4] Th. D. H. Christensen and O. F. Nielsen, *J. Mol. Spectry.* **33**, 425 (1970).

**No. 99      Dichlorosilane-d<sub>2</sub>      SiD<sub>2</sub>Cl<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	SiD <sub>2</sub> s-stretch.	1608 C	1608 S		
	$\nu_2$	SiD <sub>2</sub> scis.	695 C	695 S		
	$\nu_3$	SiCl <sub>2</sub> s-stretch.	519 C	519 W		
	$\nu_4$	SiCl <sub>2</sub> scis.	187 D	187 W		
<i>a</i> <sub>2</sub>	$\nu_5$	SiD <sub>2</sub> twist.	506 D	ia		CF.
<i>b</i> <sub>1</sub>	$\nu_6$	SiD <sub>2</sub> a-stretch.	1637 C	1637 S		
	$\nu_7$	SiD <sub>2</sub> rock.	466 B	466 W		
<i>b</i> <sub>2</sub>	$\nu_8$	SiD <sub>2</sub> wag.	663 B	663 VS		
	$\nu_9$	SiCl <sub>2</sub> a-stretch.	566 C	566 W		

**References**

- [1] IR.      D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **27**, 489 (1968).  
 [2] Th.      D. H. Christensen and O. F. Nielsen, J. Mol. Spectry. **33**, 425 (1970).

**No. 100      Dibromosilane      SiH<sub>2</sub>Br<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	SiH <sub>2</sub> s-stretch.	2206 D	2200 S	2206 S, p	
	$\nu_2$	SiH <sub>2</sub> scis.	942 C	942 VS	925 W, dp	
	$\nu_3$	SiBr <sub>2</sub> s-stretch.	407 C	407 M	393 S, p	
	$\nu_4$	SiBr <sub>2</sub> scis.	122 D		122 M, p	
<i>a</i> <sub>2</sub>	$\nu_5$	SiH <sub>2</sub> twist.	688 D	ia	688 W, dp	
<i>b</i> <sub>1</sub>	$\nu_6$	SiH <sub>2</sub> a-stretch.	2232 D	2200 S	2232 W, dp	
	$\nu_7$	SiH <sub>2</sub> rock.	556 C	556 S		
<i>b</i> <sub>2</sub>	$\nu_8$	SiH <sub>2</sub> wag.	843 C	843 VS	828 VW, dp	
	$\nu_9$	SiBr <sub>2</sub> a-stretch.	471 C	471 S	456 W, dp	

**References**

- [1] R.      F. François and M. Buisset, Comptes Rendus **230**, 1946 (1950).  
 [2] IR.      D. W. Mayo, H. E. Opitz, and J. S. Peake, J. Chem. Phys. **23**, 1344 (1955).

**No. 101 Selenium dioxide difluoride  $\text{SeO}_2\text{F}_2$** Symmetry  $C_{2v}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1$	$\nu_1$	$\text{SeO}_2$ s-stretch.	973 C	973 S	969 S, p	
	$\nu_2$	$\text{SeF}_2$ s-stretch.	700 C	700 S	702 S, p	
	$\nu_3$	$\text{SeO}_2$ scis.	360 C	360 S	357 M	
	$\nu_4$	$\text{SeF}_2$ scis.	284 C	284 W	280 M	
$a_2$	$\nu_5$	$\text{SeF}_2$ twist.	272 E			OV( $2\nu_5$ ).
$b_1$	$\nu_6$	$\text{SeO}_2$ a-stretch.	1059 C	1059 S	1059 W	
	$\nu_7$	$\text{SeO}_2$ rock.	335 D	335 S	334 M	OV( $\nu_9$ ).
$b_2$	$\nu_8$	$\text{SeF}_2$ s-stretch.	756 C	756 W		
	$\nu_9$	$\text{SeO}_2$ wag.	335 D	335 S	334 M	OV( $\nu_7$ ).

**References**

- [1] R. Paetzold and K. H. Ziegenbalg, Z. Chem. **4**, 461 (1964).  
 [2] IR.R. T. Birchall and R. J. Gillespie, Spectrochim. Acta **22**, 681 (1966).

**No. 102 Nitric acid  $\text{H}^{14}\text{NO}_3$** Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)		
$a'$	$\nu_1$	OH stretch.	3550 B	3550.0 M		
	$\nu_2$	$\text{NO}_2$ a-stretch.	1708 B	1708.2 VS		
	$\nu_3$	OH bend.	1331 B	1330.7 S		
	$\nu_4$	$\text{NO}_2$ s-stretch.	1325 B	1324.9 VS		
	$\nu_5$	$\text{NO}_2$ scis.	879 B	878.6 S		
	$\nu_6$	NO stretch.	647 B	646.6 W		
	$\nu_7$	$\text{NO}_2$ rock.	579 B	579.0 W		
$a''$	$\nu_8$	$\text{NO}_2$ wag.	762 B	762.2 S		
	$\nu_9$	Torsion	456 B	455.8 M		

**Reference**

- [1] IR. G. E. McGraw, D. L. Bernitt, and I. C. Hisatsune, J. Chem. Phys. **42**, 237 (1965).

**No. 103 Nitric acid-d  $D^{14}NO_3$**   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$a'$	$\nu_1$	OD stretch.	2622 B	2621.5 M		
	$\nu_2$	$NO_2$ a-stretch.	1687 B	1687.0 VS		
	$\nu_3$	$NO_2$ s-stretch.	1308 B	1308.4 VS		
	$\nu_4$	OD bend.	1014 B	1013.6 M		
	$\nu_5$	$NO_2$ scis.	888 B	888.0 S		
	$\nu_6$	NO stretch.	641 B	641.0 S		
	$\nu_7$	$NO_2$ rock.	541 B	541.0 W		
$a''$	$\nu_8$	$NO_2$ wag.	763 B	762.8 S		
	$\nu_9$	Torsion	342 B	342.0 M		

**Reference**See No. 102( $H^{14}NO_3$ ).

**No. 104 Nitric acid  $H^{15}NO_3$**   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$a'$	$\nu_1$	OH stretch.	3550 B	3550.0 M		
	$\nu_2$	$NO_2$ a-stretch.	1672 B	1672.0 VS		
	$\nu_3$	OH bend.	1327 B	1327.0 S		
	$\nu_4$	$NO_2$ s-stretch.	1321 B	1320.6 S		
	$\nu_5$	$NO_2$ scis.	871 B	870.8 S		
	$\nu_6$	NO stretch.	647 B	646.6 W		
	$\nu_7$	$NO_2$ rock.	578 B	578.0 W		
$a''$	$\nu_8$	$NO_2$ wag.	744 B	743.6 S		
	$\nu_9$	Torsion	456 B	455.9 M		

**Reference**See No. 102( $H^{14}NO_3$ ).



**No. 105 Nitric acid-d  $D^{15}NO_3$** Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				(Gas)		
			$cm^{-1}$	$cm^{-1}$	$cm^{-1}$	
$a'$	$\nu_1$	OD stretch.	2622 B	2621.9 M		
	$\nu_2$	$NO_2$ a-stretch.	1656 B	1655.5 VS		
	$\nu_3$	$NO_2$ s-stretch.	1291 B	1290.7 S		
	$\nu_4$	OD bend.	1012 B	1011.5 M		
	$\nu_5$	$NO_2$ scis.	876 B	876.3 S		
	$\nu_6$	NO stretch.	641 B	640.9 S		
	$\nu_7$	$NO_2$ rock.	541 B	541.0 VW		
$a''$	$\nu_8$	$NO_2$ wag.	743 B	743.4 S		
	$\nu_9$	Torsion	345 D			OV( $\nu_7 + \nu_9$ , $\nu_8 + \nu_9$ ).

**Reference**See No. 102( $H^{14}NO_3$ ).**No. 106 Fluoronitrate  $FO^{14}NO_2$** Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$	$cm^{-1}$	
				(Gas)		
$a'$	$\nu_1$	$NO_2$ a-stretch.	1759 C	1759.1 VS		
	$\nu_2$	$NO_2$ s-stretch.	1301 B	1300.9 VS		
	$\nu_3$	OF stretch.	928 B	927.7 S		
	$\nu_4$	$NO_2$ scis.	804 B	803.7 S		
	$\nu_5$	NO stretch.	633 B	633.0 VW		
	$\nu_6$	$NO_2$ rock.	455 B	454.5 MS		
	$\nu_7$	OF bend.	303 B	302.6 VW		
$a''$	$\nu_8$	$NO_2$ wag.	709 C	708.5 M		
	$\nu_9$	OF torsion	152 B	151.6 VVW		

**References**

- [2] IR. A. J. Arvia, L. F. R. Cafferata, and H. J. Schumacher, Chem. Ber. **96**, 1187 (1963).  
 [2] IR. R. H. Miller, P. L. Bernitt, and I. C. Hisatsune, Spectrochim. Acta **23A**, 223 (1967).

No. 107		Fluoronitrate	FO <sup>15</sup> NO <sub>2</sub>	Symmetry number $\sigma = 1$		
Symmetry C <sub>s</sub>						
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a'	$\nu_1$	NO a-stretch.	1720 C	1719.8 VS		
	$\nu_2$	NO <sub>2</sub> s-stretch.	1291 B	1290.5 VS		
	$\nu_3$	OF stretch.	928 B	927.5 S		
	$\nu_4$	NO <sub>2</sub> scis.	792 B	791.8 S		
	$\nu_5$	NO stretch.	632 B	631.5 VW		
	$\nu_6$	NO <sub>2</sub> rock.	455 B	454.4 MS		
	$\nu_7$	OF bend.	302 B	301.6 VW		
a''	$\nu_8$	NO <sub>2</sub> wag.	690 C	690.2 M		
	$\nu_9$	OF torsion	151 D	151.2		OC( $\nu_1 + \nu_9$ , $\nu_1 - \nu_9$ , $\nu_3 + \nu_9$ ).

## References

See No. 106(FO<sup>14</sup>NO<sub>2</sub>).

No. 108		Chloronitrate	ClO <sup>14</sup> NO <sub>2</sub>	Symmetry number $\sigma = 1$		
Symmetry C <sub>s</sub>						
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a'	$\nu_1$	NO <sub>2</sub> a-stretch.	1735 B	1735.4 VS		
	$\nu_2$	NO <sub>2</sub> s-stretch.	1292 B	1291.9 VS		
	$\nu_3$	OCl stretch.	809 C	809.3 S		
	$\nu_4$	NO <sub>2</sub> scis.	780 C	780.2 MS		
	$\nu_5$	NO stretch.	560 B	560.0 S		
	$\nu_6$	NO <sub>2</sub> rock.	434 B	434.1 M		
	$\nu_7$	OCl bend.	270 C	270 VVW		
a''	$\nu_8$	NO <sub>2</sub> wag.	711 B	710.8 W		
	$\nu_9$	OCl torsion	121 E	121		OC( $\nu_5 + \nu_7 - \nu_9$ ).

## References

- [1] IR. K. Brandle, M. Schmeisser, and W. Luttke, Chem. Ber. **93**, 2300 (1960).  
 [2] IR. A. J. Arvia, L. F. R. Cafferata, and H. J. Schumacher, Chem. Ber. **96**, 1187 (1963).  
 [3] IR. R. H. Miller, P. L. Bernitt, and I. C. Hisatsune, Spectrochim. Acta **23A**, 223 (1967).

No. 109		Chloronitrate	ClO <sup>15</sup> NO <sub>2</sub>		Symmetry number $\sigma = 1$	
Symmetry C <sub>s</sub>						
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a'	$\nu_1$	NO <sub>2</sub> a-stretch.	1694 B	1694.0 VS		
	$\nu_2$	NO <sub>2</sub> s-stretch.	1280 B	1280.2 VS		
	$\nu_3$	OCl stretch.	805 C	804.7 MS		
	$\nu_4$	NO <sub>2</sub> scis.	773 C	772.9 S		
	$\nu_5$	NO stretch.	557 B	556.8 S		
	$\nu_6$	NO <sub>2</sub> rock.	432 B	432.2 M		
a''	$\nu_7$	OCl bend.	263 D	263		OC( $\nu_5 + \nu_7$ ).
	$\nu_8$	NO <sub>2</sub> wag.	694 B	693.7 W		
	$\nu_9$	OCl torsion	122 E	122		OC( $\nu_5 + \nu_7 - \nu_9$ ).

## References

- [1] IR. K. Brandle, M. Schmeisser, and W. Luttke, Chem. Ber. **93**, 2300 (1960).  
 [2] IR. A. J. Arvia, L. F. R. Cafferata, and H. J. Schumacher, Chem. Ber. **96**, 1187 (1963).  
 [3] IR. R. H. Miller, P. L. Bernitt, and I. C. Hisatsune, Spectrochim. Acta **23A**, 223 (1967).

No. 110		Phosphoryl dichlorofluoride		POCl <sub>2</sub> F		Symmetry C <sub>s</sub>		Symmetry number σ = 1	
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments			
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>				
					(Liquid)				
a'	ν <sub>1</sub>	PO stretch.	1331 D		1331 p				
	ν <sub>2</sub>	PF stretch.	894 D		894 p				
	ν <sub>3</sub>	PCl <sub>2</sub> s-stretch.	547 D		547 p				
	ν <sub>4</sub>	PO ip-bend.	386 D		386 p				
	ν <sub>5</sub>	PF bend.	330 D		330 p				
	ν <sub>6</sub>	PCl <sub>2</sub> scis.	207 D		207 p				
a''	ν <sub>7</sub>	PCl <sub>2</sub> a-stretch.	620 D		620 dp				
	ν <sub>8</sub>	PO op-bend.	372 D		372 dp				
	ν <sub>9</sub>	PCl <sub>2</sub> rock.	254 D		254 dp				

## Reference

- [1] R. M. L. Delwaulle and F. François, Comptes Rendus **222**, 550 (1946).

**No. 111 Phosphoryl dibromofluoride POBr<sub>2</sub>F**Symmetry C<sub>s</sub>Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
<i>a'</i>	$\nu_1$	PO stretch.	1303 D		(Liquid) 1303 p	
	$\nu_2$	PF stretch.	880 D		880 p	
	$\nu_3$	PBr <sub>2</sub> s-stretch.	466 D		466 p	
	$\nu_4$	PO ip-bend.	306 D		306 p	
	$\nu_5$	PF bend.	273 D		273 p	
	$\nu_6$	PBr <sub>2</sub> scis.	134 D		134 p	
<i>a''</i>	$\nu_7$	PBr <sub>2</sub> a-stretch.	538 D		538 dp	
	$\nu_8$	PO op-bend.	291 D		291 dp	
	$\nu_9$	PBr <sub>2</sub> rock.	220 D		220 dp	

**Reference**See No. 110(POCl<sub>2</sub>F).**No. 112 Thiophosphoryl chlorodifluoride PSClF<sub>2</sub>**Symmetry C<sub>s</sub>Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
<i>a'</i>	$\nu_1$	PF <sub>2</sub> s-stretch.	946 B	(Gas) 946 VS	(Liquid) 939 (3.7) p	
	$\nu_2$	PS stretch.	738 B	738 VS	727 (50) p	
	$\nu_3$	PCl stretch.	541 B	541 S	536 (100) p	
	$\nu_4$	PCl bend.	395 B	395 M	394 (31) p	
	$\nu_5$	PF <sub>2</sub> scis.	361 B	361 M	359 (38) p	
	$\nu_6$	PS ip-bend.	207 C	198	207 (65) p	
<i>a''</i>	$\nu_7$	PF <sub>2</sub> s-stretch.	920 B	920 VS	913 (6.5) dp	
	$\nu_8$	PF <sub>2</sub> rock.	317 B	317 M	314 (14) dp	
	$\nu_9$	PS op-bend.	251 C		251 (14) dp	

**Reference**[1] IR.R. J. R. Durig and J. W. Clark, J. Chem. Phys. **46**, 3057 (1967).

**No. 113 Thiophosphoryl dichlorofluoride  $\text{PSCl}_2\text{F}$** Symmetry  $\text{C}_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	PF stretch.	912 B	912 VS	902 (2) p	
	$\nu_2$	PS stretch.	753 B	753 VS	737 (17) p	
	$\nu_3$	$\text{PCl}_2$ s-stretch.	478 B	478 S	474 (100) p	
	$\nu_4$	PF bend.	331 B	331 M	327 (13) dp	
	$\nu_5$	PS ip-bend.	268 B	268 M	267 (32) p	
	$\nu_6$	$\text{PCl}_2$ scis.	192 D	192 W	193 (65) dp	OV( $\nu_9$ ).
$a''$	$\nu_7$	$\text{PCl}_2$ a-stretch.	575 C	575 S	567 (6) dp	
	$\nu_8$	PS op-bend.	319 B	319 M	317 (19) dp	
	$\nu_9$	$\text{PCl}_2$ rock.	192 D	192 W	193 (65) dp	OV( $\nu_6$ ).

**Reference**See No. 112( $\text{PSClF}_2$ ).**No. 114 Phosphorus pentafluoride  $\text{PF}_5$** Symmetry  $\text{D}_{3h}$ Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1'$	$\nu_1$	$\text{PF}_3$ s-stretch.	816 B		816 (10) p	
	$\nu_2$	$\text{PF}_2$ s-stretch.	648 C		648 (1b) p	
$a_2''$	$\nu_3$	$\text{PF}_2$ a-stretch.	947 B	946.6 VS		
	$\nu_4$	$\text{PF}_3$ op-deform.	575 B	575.1 M		
$e'$	$\nu_5$	$\text{PF}_3$ d-stretch.	1024 B	1024 VS	1029 (1b)	
	$\nu_6$	$\text{PF}_3$ d-deform.	533 B	532.5 M	535 (1sh) dp	
$e''$	$\nu_7$	PF bend.	174 C		174 (1b) dp	
	$\nu_8$	PF bend.	520 C		520 (1b) dp	

**References**

- [1] IR. J. E. Griffiths, R. P. Carter, and R. R. Holmes, J. Chem. Phys. **41**, 863 (1964).
- [2] IR. L. C. Hoskins, J. Chem. Phys. **42**, 2631 (1965).
- [3] IR. J. E. Griffiths, J. Chem. Phys. **42**, 2632 (1965).
- [4] IR.R. L. C. Hoskins and R. C. Lord, J. Chem. Phys. **46**, 2402 (1967).
- [5] IR. R. M. Deiters and R. R. Holmes, J. Chem. Phys. **48**, 4796 (1968).
- [6] R. I. W. Levin, J. Chem. Phys. **50**, 1031 (1969).
- [7] Th. I. W. Levin, J. Mol. Spectry. **33**, 61 (1970).
- [8] R. F. A. Miller and R. J. Capwell, Spectrochim. Acta **27A**, 125 (1971).

**No. 115 Phosphorus trichloride difluoride  $\text{PCl}_3\text{F}_2$**   
**Symmetry  $D_{3h}$**

Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1'$	$\nu_1$	$\text{PF}_2$ s-stretch.	633 C		633 M, p	
	$\nu_2$	$\text{PCl}_3$ s-stretch.	387 C		387 S, p	
$a_2''$	$\nu_3$	$\text{PF}_2$ a-stretch.	867 C	867 VS		
	$\nu_4$	$\text{PCl}_3$ op-deform.	328 C	328 M		
$e'$	$\nu_5$	$\text{PCl}_3$ d-stretch.	625 C	625 VS	609 VW, dp	
	$\nu_6$	$\text{PCl}_3$ d-deform.	404 C	404 VS	408 M, dp	
	$\nu_7$	PF bend.	122 C		122 S, dp	
$e''$	$\nu_8$	PF bend.	357 C		357 W, dp	

**References**

- [1] IR.R. J. E. Griffiths, R. P. Carter, Jr., and R. R. Holmes, J. Chem. Phys. **41**, 863 (1964).  
 [2] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8**, 2612 (1969).  
 [3] Th. I. R. Beattie, K. M. S. Livingston, and D. J. Reynolds, J. Chem. Phys. **51**, 4269 (1969).

**No. 116 Phosphorus pentachloride  $\text{PCl}_5$**   
**Symmetry  $D_{3h}$**

Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ ( $\text{C}_6\text{H}_6$ or $\text{CS}_2$ soln.)	
$a_1'$	$\nu_1$	$\text{PCl}_3$ s-stretch.	395 D		395 VS, p	
	$\nu_2$	$\text{PCl}_2$ s-stretch.	370 D		370 VW	
$a_2''$	$\nu_3$	$\text{PCl}_2$ a-stretch.	465 C	465 VS	441 VW	
	$\nu_4$	$\text{PCl}_3$ op-deform.	299 D	299 S ( $\text{CS}_2$ soln.)	301	
$e'$	$\nu_5$	$\text{PCl}_3$ d-stretch.	592 C	592 VS	581 W, p	
	$\nu_6$	$\text{PCl}_3$ d-deform.	273 D	273 S ( $\text{CS}_2$ soln.)	281 W, dp	
	$\nu_7$	PCl bend.	100 C	100 W	100 M, dp	
$e''$	$\nu_8$	PCl bend.	261 D		261 W, dp	

**References**

- [1] R. H. Moureu, P. Sue, and M. Magat, Contribution a l' étude de la structure moleculaire. Vol. commém. Victor Hérni, p.125 Maison Desoerg, Liege (1947/48).  
 [2] IR.R. J. K. Wilmschurst and H. J. Bernstein, J. Chem. Phys. **27**, 661 (1957).  
 [3] IR.R. G. L. Carlson, Spectrochim. Acta **19**, 1291 (1963).  
 [4] R. M. J. Taylor and L. A. Woodward, J. Chem. Soc. **1963**, 4670 (1963).  
 [5] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8**, 2612 (1969).  
 [6] Th. R. R. Holmes and R. M. Deiters, J. Chem. Phys. **51**, 4043 (1969).

**No. 117 Vanadium pentafluoride  $\text{VF}_5$**   
**Symmetry  $D_{3h}$** 
Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1'$	$\nu_1$	$\text{VF}_3$ s-stretch.	718 B		718 VS	
	$\nu_2$	$\text{VF}_2$ s-stretch.	608 B		608 M	
$a_2''$	$\nu_3$	$\text{VF}_2$ a-stretch.	784 B	784 S		
	$\nu_4$	$\text{VF}_3$ op-deform.	331 B	331 W		
$e'$	$\nu_5$	$\text{VF}_3$ d-stretch.	810 C	810 M	812 W	
	$\nu_6$	$\text{VF}_3$ d-deform.	282 C	282 M	286 VW	
	$\nu_7$	VF bend.	110 D	109.5 M	99 W	
$e''$	$\nu_8$	VF bend.	336 B		336 M	

**References**

- [1] IR. R. G. Cavell and H. C. Clark, *Inorg. Chem.* **3**, 1789 (1964).  
 [2] IR.R. H. H. Claassen and H. Selig, *J. Chem. Phys.* **44**, 4039 (1966).  
 [3] IR.R. I. R. Beattie, K. M. S. Livingston, G. A. Ozin, and D. J. Reynolds, *J. Chem. Soc. A* **1969**, 958.  
 [4] IR.R. H. Selig, J. H. Holloway, J. Tyson, and H. H. Claassen, *J. Chem. Phys.* **53**, 2559 (1970).

**No. 118 Arsenic pentafluoride  $\text{AsF}_5$**   
**Symmetry  $D_{3h}$** 
Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1'$	$\nu_1$	$\text{AsF}_3$ s-stretch.	734 C		734.3 VS, p	
	$\nu_2$	$\text{AsF}_2$ s-stretch.	644 C		644 M, p?	
$a_2''$	$\nu_3$	$\text{AsF}_2$ a-stretch.	787 B	787.4 VS		
	$\nu_4$	$\text{AsF}_3$ op-deform.	400 B	400.4 S		
$e'$	$\nu_5$	$\text{AsF}_3$ d-stretch.	811 B	811.4 VS	813 M, dp	
	$\nu_6$	$\text{AsF}_3$ d-deform.	372 C	372 S	366	
					(Liquid)	
	$\nu_7$	AsF bend.	123 C	123 W	130 M, dp	
$e''$	$\nu_8$	AsF bend.	386 C		386 M, dp	

**References**

- [1] IR.R. L. C. Hoskins and R. C. Lord, *J. Chem. Phys.* **46**, 2402 (1967).  
 [2] Th. I. W. Levin, *J. Mol. Spectry.* **33**, 61 (1970).  
 [3] R. H. Selig, J. H. Holloway, J. Tyson, and H. H. Claassen, *J. Chem. Phys.* **53**, 2559 (1970).  
 [4] IR. L. C. Hoskins and C. N. Perng, *J. Chem. Phys.* **55**, 5063 (1971).

**No. 119 Antimony pentachloride  $\text{SbCl}_5$** Symmetry  $D_{3h}$ Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1'$	$\nu_1$	$\text{SbCl}_3$ s-stretch.	357 C		357 (10) p	
	$\nu_2$	$\text{SbCl}_2$ s-stretch.	307 C	306 W	307 (4) dp	
				(liquid)		
$a_2''$	$\nu_3$	$\text{SbCl}_2$ a-stretch.	384 C	384 VS		
	$\nu_4$	$\text{SbCl}_3$ op-deform.	154 D	154		
				( $\text{CCl}_4$ soln.)		
$e'$	$\nu_5$	$\text{SbCl}_3$ d-stretch.	398 C	398 VS	397 (2)	
	$\nu_6$	$\text{SbCl}_3$ d-deform.	177 C	172 S	177 (4) dp	
				( $\text{CCl}_4$ soln.)		
	$\nu_7$	$\text{SbCl}$ bend.	72 D		72 dp	
$e''$	$\nu_8$	$\text{SbCl}$ bend.	165 C		165 (2) dp	

**References**

- [1] IR. J. K. Wilmschurst, J. Mol. Spectry. **5**, 343 (1960).  
 [2] IR.R. G. L. Carlson, Spectrochim. Acta **19**, 1291 (1963).  
 [3] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8**, 2612 (1969).  
 [4] Th. R. R. Holmes and R. M. Deiters, J. Chem. Phys. **51**, 4043 (1969).

**No. 120 Tellurium hexafluoride  $\text{TeF}_6$** Symmetry  $O_h$ Symmetry number  $\sigma = 24$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Gas)	
$a_{2g}$	$\nu_1$	Sym. stretch.	697 B	ia	697.1 VS	
$e_g$	$\nu_2$	Deg. stretch.	670 C	ia	670.3 W	
$f_{1u}$	$\nu_3$	Deg. stretch.	751 C	751.0	ia	
	$\nu_4$	Deg. deform.	327 C	326.5	ia	
$f_{2g}$	$\nu_5$	Deg. deform.	314 C	ia	314 W	
$f_{2u}$	$\nu_6$	Deg. deform.	197 E	ia	ia	OC( $2\nu_6$ ) [3].

**References**

- [1] IR.R. B. Weinstock and Goodman, Advan. Chem. Phys. **9**, 169 (1966), and references cited there.  
 [2] IR. S. Abramowitz and I. W. Levin, J. Chem. Phys. **44**, 3353 (1966).  
 [3] R. H. H. Claassen, G. L. Goodman, J. H. Holloway, and H. Selig, J. Chem. Phys. **53**, 341 (1970).



**No. 121 Iridium(VI)fluoride IrF<sub>6</sub>**  
 Symmetry O<sub>h</sub>
Symmetry number  $\sigma = 24$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Gas)	
<i>a<sub>1g</sub></i>	$\nu_1$	Sym. stretch.	702 B	ia	701.7 VS, p	
<i>e<sub>g</sub></i>	$\nu_2$	Deg. stretch.	645 C	ia	645 W, dp	
<i>f<sub>1u</sub></i>	$\nu_3$	Deg. stretch.	720 B	719.8 S	ia	
	$\nu_4$	Deg. deform.	276 B	276.0 S	ia	
<i>f<sub>2g</sub></i>	$\nu_5$	Deg. deform.	267 C	ia	267 W, dp	
<i>f<sub>2u</sub></i>	$\nu_6$	Deg. deform.	206 D	ia	ia	OC( $\nu_2 + \nu_6$ , $\nu_2 - \nu_6$ , $\nu_5 + \nu_6$ ). [1].

**References**

- [1] IR.R. B. Weinstock and G. L. Goodman, *Advan. Chem. Phys.* **9**, 169 (1966), and references cited there.  
 [2] R. H. H. Claassen and H. Selig, *Israel J. Chem.* **7**, 449 (1969).  
 [3] IR. H. Kim, P. A. Souder, and H. H. Claassen, *J. Mol. Spectry.* **26**, 46 (1968).

**No. 122 Sulfur chloride pentafluoride SClF<sub>5</sub>**  
 Symmetry C<sub>4v</sub>
Symmetry number  $\sigma = 4$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
<i>a<sub>1</sub></i>	$\nu_1$	SF stretch.	855 B	854.6 VS	833 W, p	
	$\nu_2$	SF <sub>4</sub> s-stretch.	707 B	707.2 VS	704 S, p	
	$\nu_3$	SF <sub>4</sub> op-deform.	602 B	601.9 VS	603 W, p	
	$\nu_4$	SCl stretch.	402 B	401.7 VS	403 VS, p	
<i>b<sub>1</sub></i>	$\nu_5$	SF <sub>4</sub> a-stretch.	625 C	ia	625 M, dp	
	$\nu_6$	SF <sub>4</sub> op-deform.	271 C	ia	271 M, dp	
<i>b<sub>2</sub></i>	$\nu_7$	SF <sub>4</sub> ip-deform.	505 C	ia	505 W, dp	
<i>e</i>	$\nu_8$	SF <sub>4</sub> d-stretch.	909 B	909.0 VS	927 W, dp	
	$\nu_9$	SF bend.	579 B	579.0 M	584 VW, dp	
	$\nu_{10}$	SF <sub>4</sub> ip-deform.	441 B	441.0 S	442 M, dp	
	$\nu_{11}$	SCl bend.	397 B	396.5 S	396 S, dp	

**References**

- [1] IR.R. L. H. Cross, H. L. Roberts, P. Goggin, and L. A. Woodward, *Trans. Faraday Soc.* **56**, 945 (1960).  
 [2] IR.R. J. E. Griffiths, *Spectrochim. Acta* **23A**, 2145 (1967).

**No. 123 Tungsten chloride pentafluoride  $\text{WClF}_5$**   
**Symmetry  $C_{4v}$**

Symmetry number  $\sigma = 4$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1$	$\nu_1$	WF stretch.	743 C	743 M	744 VS, p	
	$\nu_2$	WF <sub>4</sub> s-stretch.	703 C	703 VS	703 M, p	
	$\nu_3$	WCl stretch.	400 C	400 VS	407 S, p	
	$\nu_4$	WF <sub>4</sub> op-deform.	254 C	254 VS	257 W	
$b_1$	$\nu_5$	WF <sub>4</sub> a-stretch.	644 D	ia	644 W	
	$\nu_6$	WF <sub>4</sub> op-deform.	182 D	ia	182 W	
$b_2$	$\nu_7$	WF <sub>4</sub> ip-deform.	377 D	ia	377 M, dp	
$e$	$\nu_8$	WF <sub>4</sub> d-stretch.	671 C	671 S	661 M, dp	
	$\nu_9$	WF bend.	302 C	302 M	307 M, dp	
	$\nu_{10}$	WF <sub>4</sub> ip-deform.	278 C	278 S	290 W	
	$\nu_{11}$	WCl bend.	228 C	228 S	227 W	

**Reference**

- [1] IR.R. D. M. Adams, G. W. Fraser, D. M. Morris, and R. D. Peacock, J. Chem. Soc. A **1968**, 1131.

**No. 124 Iodine heptafluoride  $\text{IF}_7$**   
**Symmetry  $D_{5h}$**

Symmetry number  $\sigma = 10$ 

Sym. class	No.	Approximate type of mode <sup>a</sup>	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Gas)	
$a_1'$	$\nu_1$	IF <sub>ax</sub> s-stretch.	676 C	ia	676 W, p	
	$\nu_2$	IF <sub>eq</sub> s-stretch.	635 C	ia	635 S, p	
$a_2''$	$\nu_3$	IF <sub>ax</sub> a-stretch.	672 C	672 VS	ia	
	$\nu_4$	F <sub>eq</sub> IF <sub>ax</sub> deform.	257 C	257 W	ia	
$e_1'$	$\nu_5$	IF <sub>eq</sub> a-stretch.	746 C	746 S, b	ia	
	$\nu_6$	F <sub>eq</sub> IF <sub>eq</sub> deform.	425 C	425 VS	ia	
	$\nu_7$	F <sub>ax</sub> IF <sub>ax</sub> deform.	363 C	363 S	ia	
$e_1''$	$\nu_8$	F <sub>eq</sub> IF <sub>ax</sub> deform.	310 C	ia	310 W, dp	
$e_2'$	$\nu_9$	IF <sub>eq</sub> a-stretch.	510 C	ia	510 W, dp	
	$\nu_{10}$	F <sub>eq</sub> IF <sub>eq</sub> deform.	352 C	ia	352 W, dp	
$e_2''$	$\nu_{11}$	F <sub>eq</sub> IF <sub>ax</sub> deform.	200 D	ia	ia	CF[2]. OC( $\nu_2 + \nu_{11}$ , $\nu_5 + \nu_{11}$ ).

<sup>a</sup> F<sub>ax</sub> and F<sub>eq</sub> represent the axial and equatorial fluorine atoms, respectively.

**References**

- [1] IR.R. H. H. Claassen, E. L. Gasner, and H. Salig, J. Chem. Phys. **49**, 1803 (1968).  
 [2] IR.R.Th. H. H. Eysel and K. Seppelt, J. Chem. Phys. **56**, 5081 (1972).  
 [3] Th. E. Wendling and S. Rahmondi, Bull. Soc. Chim. (France) **1**, 33 (1972).

No. 125 Digermane  $\text{GeH}_3\text{GeH}_3$ Symmetry  $D_{3d}$ Symmetry number  $\sigma = 6$ 

-sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_{1g}$	$\nu_1$	$\text{GeH}_3$ s-stretch.	2068 C	ia	2068 S, p	
	$\nu_2$	$\text{GeH}_3$ s-deform.	832 C	ia	832 VW, p	
	$\nu_3$	GeGe stretch.	268 C	ia	268.4 S, p	
$a_{1u}$	$\nu_4$	Torsion	146 E <sup>a</sup>	ia	ia	
$a_{2u}$	$\nu_5$	$\text{GeH}_3$ s-stretch.	2077 B	2077.0 VS	ia	
	$\nu_6$	$\text{GeH}_3$ s-deform.	756 B	756.0 VS	ia	
$e_u$	$\nu_7$	$\text{GeH}_3$ d-stretch.	2091 B	2090.7 S	ia	
	$\nu_8$	$\text{GeH}_3$ d-deform.	879 B	879.0 S	ia	
	$\nu_9$	$\text{GeH}_3$ rock.	370 B	370.3 M	ia	
$e_g$	$\nu_{10}$	$\text{GeH}_3$ d-stretch.	2081 E	ia		CF[4].
	$\nu_{11}$	$\text{GeH}_3$ d-deform.	880 C	ia	879.6 M, dp	
	$\nu_{12}$	$\text{GeH}_3$ rock.	567 C	ia	566.6 W, dp	

<sup>a</sup> Estimated from combination bands.

## References

- [1] IR. D. A. Dows and R. M. Hexter, J. Chem. Phys. **24**, 1029 (1956).  
 [2] IR.R. V. A. Crawford, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **37**, 2377 (1962).  
 [3] IR.R. J. E. Griffiths and G. E. Walraffen, J. Chem. Phys. **40**, 321 (1964).  
 [4] Th. E. A. Clark and A. Weber, J. Chem. Phys. **45**, 1759 (1966).

No. 126 Digermane- $d_6$   $\text{GeD}_3\text{GeD}_3$ Symmetry  $D_{3d}$ Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_{1g}$	$\nu_1$	$\text{GeD}_3$ s-stretch.	1484 C	ia	1483.7 S, p	
	$\nu_2$	$\text{GeD}_3$ s-deform.	600 C	ia	600 VW, p	
	$\nu_3$	GeGe stretch.	264 C	ia	264 S, p	CF[3].
$a_{1u}$	$\nu_4$	Torsion	106 E <sup>a</sup>	ia	ia	
$a_{2u}$	$\nu_5$	$\text{GeD}_3$ s-stretch.	1490 B	1489.9 VS	ia	
	$\nu_6$	$\text{GeD}_3$ s-deform.	546 C	546.2 S	ia	
	$\nu_8$	$\text{GeD}_3$ d-deform.	630 B	629.7 M	ia	
$e_u$	$\nu_7$	$\text{GeD}_3$ d-stretch.	1511 C	1511 S	ia	
	$\nu_9$	$\text{GeD}_3$ rock.	262 C	262 S	ia	
$e_g$	$\nu_{10}$	$\text{GeD}_3$ d-stretch.	1501 B	ia	1501	
	$\nu_{11}$	$\text{GeD}_3$ d-deform.	626 C	ia	626.1 M, dp	
	$\nu_{12}$	$\text{GeD}_3$ rock.	412 C	ia	412.0 W, dp	

<sup>a</sup> From the product rule.

## References

- [1] IR.R. V. A. Crawford, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **37**, 2377 (1962).  
 [2] IR.R. J. E. Griffiths and G. E. Walraffen, J. Chem. Phys. **40**, 321 (1964).  
 [3] Th. E. A. Clark and A. Weber, J. Chem. Phys. **45**, 1759 (1966).

**No. 127 Cyanogen fluoride FCN**  
Symmetry  $C_{\infty v}$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$\sigma^+$	$\nu_1$	CN stretch.	2323 C	2323		
$\pi$	$\nu_2$	Deform.	451 A	451.32		
$\sigma^+$	$\nu_3$	CF stretch.	1077 A	1076.52		

**References**

- [1] IR. R. E. Dodd and R. Little, *Spectrochim. Acta* **16**, 1083 (1960).  
 [2] IR. A. R. H. Cole, L. Isaacson, and R. C. Lord, *Spectrochim. Acta* **23**, 86 (1967).  
 [3] Th. A. Ruoff, *Spectrochim. Acta* **26A**, 545 (1970).

**No. 128 Cyanogen iodide ICN**  
Symmetry  $C_{\infty v}$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$\sigma^+$	$\nu_1$	CN stretch.	2188 C	2188.0		
$\pi$	$\nu_2$	Deform.	305 C	304.5		
$\sigma^+$	$\nu_3$	CI stretch.	486 C	485.8		

**References**

- [1] IR. S. Hemple and E. R. Nixon, *J. Chem. Phys.* **47**, 4273 (1967).  
 [2] Th. A. Ruoff, *Spectrochim. Acta* **26A**, 545 (1970).

**No. 129 Carbonyl fluoride COF<sub>2</sub>**  
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	CO stretch.	1928 C	1928 VS	1944 VW	
	$\nu_2$	CF <sub>2</sub> s-stretch.	965 B	965 VS	965 VS	
	$\nu_3$	CF <sub>2</sub> deform.	584 C	584 M	571 W	
$b_1$	$\nu_4$	CF <sub>2</sub> a-stretch.	1249 B	1249 VS	1238 VW	
	$\nu_5$	CO deform.	626 C	626 M	620 M	
$b_2$	$\nu_6$	Op-deform.	774 B	774 M	771 VW	

**References**

- [1] IR.R. A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, *J. Chem. Phys.* **20**, 596 (1952).  
 [2] Th. J. Overend and J. R. Scherer, *J. Chem. Phys.* **32**, 1296 (1960).

**No. 130 Carbonyl chloride COCl<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	CO stretch.	1827 B	1827 VS	1807 M	
	$\nu_2$	CCl <sub>2</sub> s-stretch.	567 C	567 M	573 VS	
	$\nu_3$	CCl <sub>2</sub> deform.	285 C	285 W	302 S	
<i>b</i> <sub>1</sub>	$\nu_4$	CCl <sub>2</sub> a-stretch.	849 B	849 S	832 VW	
	$\nu_5$	CO deform.	440 C	440 M	442 M	
<i>b</i> <sub>2</sub>	$\nu_6$	Op-deform.	580 C	580 M		

**References**

- [1] IR.R. A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, J. Chem. Phys. **20**, 596 (1952).  
 [2] IR. E. Catalano and K. S. Pitzer, J. Amer. Chem. Soc. **80**, 1054 (1958).  
 [3] IR.R. J. Overend and J. C. Evans, Trans. Faraday Soc. **55**, 1817 (1959).  
 [4] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

**No. 131 Carbonyl bromide COBr<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	CO stretch.	1828 B	1828 VS		
	$\nu_2$	CBr <sub>2</sub> s-stretch.	425 C	425 M	429 S	
	$\nu_3$	CBr <sub>2</sub> deform.	181 D		181 S	
<i>b</i> <sub>1</sub>	$\nu_4$	CBr <sub>2</sub> a-stretch.	757 C	787 VS		
				747 VS		
	$\nu_5$	CO deform.	350 C	350 VW	350 M, b	FR( $\nu_2 + \nu_5$ ).
<i>b</i> <sub>2</sub>	$\nu_6$	Op-deform.	512 B	512 M		

**References**

- [1] IR R J. Overend and J. C. Evans, Trans. Faraday Soc. **15**, 1817 (1959).  
 [2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

**No. 132 Thiocarbonyl fluoride SCF<sub>2</sub>**Symmetry C<sub>2v</sub>Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	CS stretch.	1368 C	1368 VS		
	$\nu_2$	CF <sub>2</sub> s-stretch.	787 C	787 M		
	$\nu_3$	CF <sub>2</sub> scis.	526 C	526 M		
<i>b</i> <sub>1</sub>	$\nu_4$	CF <sub>2</sub> a-stretch.	1189 C	1189 S		
	$\nu_5$	CF <sub>2</sub> rock.	417 C	417 VW		
<i>b</i> <sub>2</sub>	$\nu_6$	CF <sub>2</sub> wag.	622 C	622 W		

**References**

- [1] IR. A. J. Downs, Spectrochim. Acta **19**, 1165 (1963).  
 [2] IR. M. J. Hopper, J. W. Russel, and J. Overend, Spectrochim. Acta **28A**, 1215 (1972).

**No. 133 Thiocarbonyl chloride CSCI<sub>2</sub>**Symmetry C<sub>2v</sub>Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	CS stretch.	1137 C	1137 VS	1121 (10)	
	$\nu_2$	CCl <sub>2</sub> s-stretch.	505 C	505 M	496 (5)	
	$\nu_3$	CCl <sub>2</sub> scis.	220 D	220 VW, b	200 (1)	
<i>b</i> <sub>1</sub>	$\nu_4$	CCl <sub>2</sub> a-stretch.	816 C	816 VS		
	$\nu_5$	CS deform.	294 C	294	287 (3)	
<i>b</i> <sub>2</sub>	$\nu_6$	op-Bend.	473 C	473 W		

**References**

- [1] R. H. W. Thompson, J. Chem. Phys. **6**, 748 (1938).  
 [2] IR. A. J. Downs, Spectrochim. Acta **19**, 1165 (1963).  
 [3] IR. M. J. Hopper, J. W. Russell, and J. Overend, Spectrochim. Acta **28A**, 1215 (1972).

**No. 134      Isocyanic acid      HNCO**Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	NH stretch.	3531 C	3531 S	3410	
	$\nu_2$	CO stretch.	2274 C	2274 VS		
	$\nu_3$	CN stretch.	1327 C	1327 W	1318	
	$\nu_4$	NH bend.	762 B <sup>a</sup>	777.1 S		
	$\nu_5$	NCO deform.	643 B <sup>a</sup>	659.8 M		
$a''$	$\nu_6$	NCO deform.	610 B <sup>a</sup>	577.5 M		

<sup>a</sup> Three fundamentals,  $\nu_4$ ,  $\nu_5$ , and  $\nu_6$ , are strongly coupled through Coriolis interaction.

The unperturbed frequencies are given in this column [3].

**References**

- [1] R. G. Herzberg and C. Reid, Disc. Faraday Soc. **9**, 92 (1950).  
 [2] IR. C. Reid, J. Chem. Phys. **18**, 1544 (1954).  
 [3] IR. R. A. Ashby and R. L. Werner, J. Mol. Spectry. **18**, 184 (1965).

**No. 135      Isocyanic acid-d      DNCO**Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	ND stretch.	2621 B	2620.7		
	$\nu_2$	CO stretch.	2235 C	2235		
	$\nu_3$	CN stretch.	1310 C	1310		
	$\nu_4$	ND bend.	758 C <sup>a</sup>	766.8		
	$\nu_5$	CNO deform.	458 C <sup>a</sup>	460		
$a''$	$\nu_6$	CNO deform.	603 B <sup>a</sup>	602.9		

<sup>a</sup> See footnote of HNCO.**References**

- [1] IR. R. A. Ashby and R. L. Werner, Spectrochim. Acta **22**, 1345 (1966).  
 [2] IR. W. D. Sheasley, C. W. Mithews, E. L. Ferretti, K. N. Rao, J. Mol. Spectry. **37**, 377 (1971).

**No. 136 Carbonyl chlorofluoride COClF**Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
$a'$	$\nu_1$	CO stretch.	1868 C	1876 VS (Gas) 1847 VS	1858 M (Liquid) 1832 M	FR( $\nu_2 + \nu_3$ ).
	$\nu_2$	CF stretch.	1095 B	1095 S	1085 VW	
	$\nu_3$	CCl stretch.	776 C	776 M	765 VS	
	$\nu_4$	CO deform.	501 C	501 W	506 S	
	$\nu_5$	CClF deform.	415 C	415 VW	410 M	
$a''$	$\nu_6$	Op-deform.	667 B	667 M	665 VW	

**References**

- [1] IR.R. A. H. Nielsen, T. G. Burke, P. J. H. Woltz, and E. A. Jones, J. Chem. Phys. **20**, 596 (1952).  
 [2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).

**No. 137 Carbonyl bromochloride COBrCl**Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
$a'$	$\nu_1$	CO stretch.	1828 B	1828 VS (Gas)	(Liquid)	
	$\nu_2$	CCl stretch.	806 C	806 VS		
	$\nu_3$	CBr stretch.	517 C	517 M	518 M	
	$\nu_4$	CO deform.	374 C	374 W	372 M	
	$\nu_5$	CBrCl deform.	240 D		240 S	
$a''$	$\nu_6$	Op-deform.	547 B	547 W		

**References**

- [1] IR.R. J. Overend and J. C. Evans, Trans. Faraday Soc. **55**, 1817 (1959).  
 [2] Th. J. Overend and J. R. Scherer, J. Chem. Phys. **32**, 1296 (1960).



**No. 138 Thiocarbonyl bromochloride CSBrCl****Symmetry  $C_s$** **Symmetry number  $\sigma = 1$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a'$	$\nu_1$	CS stretch.	1130 C	1130 S	1125 W, p	
	$\nu_2$	CCl stretch.	764 C	764 S	761 W	
	$\nu_3$	CBr stretch.	438 C	438 M	437 S, p	
	$\nu_4$	CBrCl deform.	256 D	256 W	257 M, p	
	$\nu_5$	CS deform.	222 D	(liquid) 222 VW	222 M, p	
$a''$	$\nu_6$	op-Bend.	405 E	(liquid)		CF [1].

**Reference**[1] IR.R.Th. J. L. Brema and D. C. Moule, Spectrochim. Acta **28A**, 809 (1972).**No. 139 Trifluoromethane-d CDF<sub>3</sub>****Symmetry  $C_{3v}$** **Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)		
$a_1$	$\nu_1$	CD stretch.	2261 B	2261.0 S		
	$\nu_2$	CF <sub>3</sub> s-stretch.	1111 B	1110.6 M		
	$\nu_3$	CF <sub>3</sub> s-deform.	694 B	694.2 M		
$e$	$\nu_4$	CD bend.	1202 D	1202.2 M		FR( $\nu_3 + \nu_6$ ).
	$\nu_5$	CF <sub>3</sub> d-stretch.	975 B	975.1 S		
	$\nu_6$	CF <sub>3</sub> d-deform.	502 B	502.4 M		

**References**

- [1] IR. S. R. Polo and M. K. Wilson, J. Chem. Phys. **21**, 1129 (1953).  
 [2] IR. C. C. Costain, J. Mol. Spectry. **9**, 317 (1962).  
 [3] IR.Th. A. Ruoff, H. Bürger, and S. Biedermann, Spectrochim. Acta **27A**, 1359 (1971).

**No. 140 Chlorotrifluoromethane  $\text{CClF}_3$**   
**Symmetry  $C_{3v}$** 
Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{CF}_3$ s-stretch.	1105 C	1105 VS	1106 W, p	
	$\nu_2$	CCl stretch.	781 C	781 S	781.7 VS, p	
	$\nu_3$	$\text{CF}_3$ s-deform.	476 C		475.8 S, p	
$e$	$\nu_4$	$\text{CF}_3$ d-stretch.	1212 C	1212 VS	1217 W, dp	
	$\nu_5$	$\text{CF}_3$ d-deform.	563 C	563 M	560 W, dp	
	$\nu_6$	CCl bend.	350 C		350 M, dp	

**References**

- [1] IR. H. W. Thompson and R. B. Temple, J. Chem. Soc. **1948**, 1422.  
 [2] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47**, 202 (1951).  
 [3] R. H. H. Claassen, J. Chem. Phys. **22**, 50 (1954).  
 [4] R. W. Holzer and H. Moser, J. Mol. Spectry. **20**, 188 (1966).  
 [5] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

**No. 141 Bromotrifluoromethane  $\text{CBrF}_3$**   
**Symmetry  $C_{3v}$** 
Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{CF}_3$ s-stretch.	1089 C	1089 VS	1082 (8) p	
	$\nu_2$	$\text{CF}_3$ s-deform.	760 C	760 VS	761 (9) p	
	$\nu_3$	CBr stretch.	349 C	350*	349 (7) p	
$e$	$\nu_4$	$\text{CF}_3$ d-stretch.	1210 C	1210 VS	1207 (8) dp	
	$\nu_5$	$\text{CF}_3$ d-deform.	547 C	547 M	541 (2) dp	
	$\nu_6$	CBr bend.	306 C	297*	306 (2) dp	

\* Estimated from overtone and combination bands.

**References**

- [1] IR.R. W. F. Edgell and C. E. May, J. Chem. Phys. **20**, 1822 (1952).  
 [2] IR. E. K. Plyler and N. Acquista, J. Res. NBS **48**, 92 (1952).  
 [3] IR. P. R. McGee, F. F. Cleveland, A. G. Meister, C. E. Decker, and S. I. Miller, J. Chem. Phys. **21**, 242 (1953).  
 [4] R. W. Holzer, J. Mol. Spectry. **25**, 123 (1968).  
 [5] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

**No. 142 Trifluoroiodomethane CF<sub>3</sub>I**Symmetry C<sub>3v</sub>Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	CF <sub>3</sub> s-stretch.	1080 C	1080 VS	1056	
	$\nu_2$	CF <sub>3</sub> s-deform.	742 C	742 VS	741	
	$\nu_3$	CI stretch.	286 E	286 <sup>a</sup>	284 <sup>a</sup>	
<i>e</i>	$\nu_4$	CF <sub>3</sub> d-stretch.	1187 C	1187 VS	1168	
	$\nu_5$	CF <sub>3</sub> d-deform.	537 C	537	537	
	$\nu_6$	CI bend.	260 E	260 <sup>a</sup>	260 <sup>a</sup>	

<sup>a</sup> Estimated from overtone and combination bands.**References**

- [1] IR.R. W. F. Edgell and C. E. May, J. Chem. Phys. **20**, 1822 (1952).  
 [2] IR. E. K. Plyler and N. Acquista, J. Res. NBS **48**, 92 (1952).  
 [3] IR. P. R. McGee, F. F. Cleveland, A. G. Meister, C. E. Decker, and S. I. Miller, J. Chem. Phys. **21**, 242 (1953).  
 [4] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

**No. 143 Trichlorofluoromethane CCl<sub>3</sub>F**Symmetry C<sub>3v</sub>Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Gas)	
<i>a</i> <sub>1</sub>	$\nu_1$	CF stretch.	1085 C	1085 S	1090 VW, p	
	$\nu_2$	CCl <sub>3</sub> s-stretch.	535 C	535 M	535 VS, p	
	$\nu_3$	CCl <sub>3</sub> s-deform.	350 C	350 VS	349.5 S, p	
<i>e</i>	$\nu_4$	CCl <sub>3</sub> d-deform.	847 C	847 VS	847 M, dp	
	$\nu_5$	CF bend.	394 C	401 VW	394 S, dp	
	$\nu_6$	CCl <sub>3</sub> d-deform.	241 C		241 S, dp	

**References**

- [1] IR. H. W. Thompson and R. B. Temple, J. Chem. Soc. **1948**, 1422.  
 [2] R. J. P. Zietlow, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **18**, 1076 (1950).  
 [3] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47**, 202 (1951).  
 [4] IR. J. P. Zietlow and F. F. Cleveland, J. Chem. Phys. **21**, 1778 (1951).  
 [5] R. H. H. Claassen, J. Chem. Phys. **22**, 50 (1954).  
 [6] R. W. Holzer and H. Moser, J. Mol. Spectry. **20**, 188 (1966).  
 [7] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 144 Trichloriodomethane  $\text{CCl}_3\text{I}$ Symmetry  $\text{C}_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Liquid)	(Liquid)	
$a_1$	$\nu_1$	$\text{CCl}_3$ s-stretch.	684 D	684 VS	687 W, b, p	
	$\nu_2$	CI stretch.	390 D	390 M	405 W, p	
	$\nu_3$	$\text{CCl}_3$ s-deform.	224 D	224 W	224 W	
$e$	$\nu_4$	$\text{CCl}_3$ d-stretch.	755 D	755 VS		
	$\nu_5$	$\text{CCl}_3$ d-deform.	284 D	284 W	288 W, dp	
	$\nu_6$	CI bend.	188 D	188 M		

## Reference

[1] IR.R. R. H. Mann and P. M. Manis, J. Mol. Spectry. **45**, 65 (1973).No. 145 Tribromofluoromethane  $\text{CBr}_3\text{F}$ Symmetry  $\text{C}_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
					(Liquid)	
$a_1$	$\nu_1$	CF stretch.	1069 D		1069 p	
	$\nu_2$	$\text{CBr}_3$ s-stretch.	398 D		398 p	
	$\nu_3$	$\text{CBr}_3$ s-deform.	218 D		218 p	
$e$	$\nu_4$	$\text{CBr}_3$ d-stretch.	743 D		743 dp	
	$\nu_5$	CF bend.	306 D		306 dp	
	$\nu_6$	$\text{CBr}_3$ d-deform.	150 D		150 dp	

## References

- [1] R. M. L. Delwaulle and M. F. Francois, Comptes Rendus **214**, 828 (1942).  
 [2] R. M. L. Delwaulle and M. F. Francois, J. Phys. (Paris) **7**, 15 (1946).  
 [3] Th. A. G. Meister, S. E. Rosson, and F. F. Cleveland, J. Chem. Phys. **18**, 346 (1950).  
 [4] Th. L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

**No. 146** Dichlorodifluoromethane  $\text{CCl}_2\text{F}_2$ Symmetry  $\text{C}_{2v}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{CF}_2$ s-stretch.	1101 C	1101 S	1098 M	
	$\nu_2$	$\text{CCl}_2$ s-stretch.	667 C	667 S	667.2 S, p	
	$\nu_3$	$\text{CF}_2$ scis.	458 D		457.5 S	
	$\nu_4$	$\text{CCl}_2$ scis.	262 C		261.5 S, dp	
$a_2$	$\nu_5$	$\text{CF}_2$ twist.	322 C	ia	322 W, dp	
$b_1$	$\nu_6$	$\text{CF}_2$ a-stretch.	1159 C	1159 S	1167 W, dp	
	$\nu_7$	$\text{CF}_2$ rock.	446 C	446 W		
$b_2$	$\nu_8$	$\text{CCl}_2$ a-stretch.	902 E	922 VS	923 W, dp	
				882 VS		FR( $\nu_3 + \nu_9$ ).
	$\nu_9$	$\text{CF}_2$ wag.	437 C	437 W	433 M	

**References**See No. 143( $\text{CCl}_3\text{F}$ ).**No. 147** Dibromodifluoromethane  $\text{CBr}_2\text{F}_2$ Symmetry  $\text{C}_{2v}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CF}_2$ s-stretch.	1090 C	1090	1077 W, p	
	$\nu_2$	$\text{CF}_2$ scis.	623 C	623	624 W, p	
	$\nu_3$	$\text{CBr}_2$ s-stretch.	340 D		340 S, p	
	$\nu_4$	$\text{CBr}_2$ scis.	168 D		168 M, p	
$a_2$	$\nu_5$	$\text{CF}_2$ twist.	281 D	ia	281 W, dp	
$b_1$	$\nu_6$	$\text{CF}_2$ a-stretch.	1153 C	1153 VS	1141 VW, dp	
	$\nu_7$	$\text{CF}_2$ rock.	369 D		369 VW, dp	
$b_2$	$\nu_8$	$\text{CBr}_2$ a-stretch.	831 C	831 VS	816 W, dp	
	$\nu_9$	$\text{CF}_2$ wag.	325 D		325 VW, dp	

**References**

- [1] R. G. Glockler and G. R. Leader, *J. Chem. Phys.* **7**, 553 (1939).  
 [2] IR. E. K. Plyler and N. Acquista, *J. Res. NBS* **48**, 92 (1952).  
 [3] IR. C. E. Decker and F. F. Cleveland, *J. Chem. Phys.* **21**, 189 (1953).  
 [4] IR.R. C. E. Decker, A. G. Meister, F. F. Cleveland, and R. B. Bernstein, *J. Chem. Phys.* **21**, 1781 (1953).  
 [5] Th. L. H. Ngai and R. H. Mann, *J. Mol. Spectry.* **38**, 322 (1971).

**No. 148 Bromodichlorofluoromethane CBrCl<sub>2</sub>F**Symmetry C<sub>s</sub>Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a'</i>	$\nu_1$	CF stretch.	1080 C	1080 VS	1070 (3) p	
	$\nu_2$	CCl <sub>2</sub> s-stretch.	796 C	796 VS	783 (12) p	
	$\nu_3$	CBr stretch.	502 C	502 M	504 (100) p	
				(liquid)		
	$\nu_4$	CCl <sub>2</sub> scis.	339 D		339 (14) p	
	$\nu_5$	CBrF scis.	306 D		306 (98) p	
	$\nu_6$	CCl <sub>2</sub> wag.	218 D		218 (53) p	
<i>a''</i>	$\nu_7$	CCl <sub>2</sub> a-stretch.	838 C	838 VS	831 (5) dp	
	$\nu_8$	CCl <sub>2</sub> twist.	392 D		392 (10) dp	
	$\nu_9$	CCl <sub>2</sub> rock.	204 D		204 (34) dp	

**References**

- [1] R. M. L. Delwaulle and F. François, *Comptes Rendus* **214**, 828 (1942).  
 [2] IR.R. R. L. Gilbert, E. A. Piotrowski, J. M. Dowing, and F. F. Cleveland, *J. Chem. Phys.* **31**, 1633 (1959).  
 [3] Th. L. H. Ngai and R. H. Mann, *J. Mol. Spectry.* **38**, 322 (1971).

**No. 149 Dibromochlorofluoromethane CBr<sub>2</sub>ClF**Symmetry C<sub>s</sub>Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a'</i>	$\nu_1$	CF stretch.	1075 C	1075 VS	1059 (2) p	
	$\nu_2$	CCl stretch.	806 E	795 VS	793 (4) p	
	$\nu_3$	CBr <sub>2</sub> s-stretch.	460 C	814 VS 460 W (liquid)	815 (5) p 464 (58) p	FR( $\nu_3 + \nu_4$ ).
	$\nu_4$	CClF scis.	341 D		341 (17) p	
	$\nu_5$	CBr <sub>2</sub> scis.	268 D		268 (100) p	
	$\nu_6$	CBr <sub>2</sub> wag.	162 D		162 (50) p	
<i>a''</i>	$\nu_7$	CBr <sub>2</sub> a-stretch.	754 C	754 VS	742 (11) dp	
	$\nu_8$	CBr <sub>2</sub> twist.	308 D		308 (6) dp	
	$\nu_9$	CBr <sub>2</sub> rock.	196 D		196 (20) dp	

**References**See No. 148(CBrCl<sub>2</sub>F).

**No. 150**      **Borine Carbonyl**  $^{10}\text{BH}_3\text{CO}$   
**Symmetry**  $\text{C}_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{BH}_3$ s-stretch.	2387 D	2387 M		
	$\nu_2$	CO stretch.	2166 D	2166.0 VS		
	$\nu_3$	$\text{BH}_3$ s-deform.	1083 C	1083.1 S		
	$\nu_4$	BC stretch.	707 B	707.0 S		
$e$	$\nu_5$	$\text{BH}_3$ d-stretch.	2456 D	2456 VS		
	$\nu_6$	$\text{BH}_3$ d-deform.	1115 E	1114.8 S		
	$\nu_7$	$\text{BH}_3$ rock.	819 B	818.8 M		
	$\nu_8$	BCO bend.	314 B	313.7 S		

**References**

- [1] IR. R. D. Cowan, J. Chem. Phys. **18**, 1101 (1950).  
 [2] IR.Th. G. W. Bethke and M. K. Wilson, J. Chem. Phys. **26**, 1118 (1957).

**No. 151**      **Borine Carbonyl- $\text{d}_3$**   $^{10}\text{BD}_3\text{CO}$   
**Symmetry**  $\text{C}_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{BD}_3$ s-stretch.	1695 C	1694.8 M		
	$\nu_2$	CO stretch.	2169 D	2169.0 VS		
	$\nu_3$	$\text{BD}_3$ s-deform.	888 D	888.4 W		
	$\nu_4$	BC stretch.	630 B	629.5 S		
$e$	$\nu_5$	$\text{BD}_3$ d-stretch.	1852 C	1852 S		
	$\nu_6$	$\text{BD}_3$ d-deform.	802 B	801.5 W		
	$\nu_7$	$\text{BD}_3$ rock.	718 B	718.0 S		
	$\nu_8$	BCO bend.	266 B	266.0 S		

**References**

See No. 150( $^{10}\text{BH}_3\text{CO}$ ).

**No. 152 Borine Carbonyl  $^{11}\text{BH}_3\text{CO}$**   
**Symmetry  $C_{3v}$** 
Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{BH}_3$ s-stretch.	2380 C	(Gas) 2379 M (solid)	(Liquid) 2380 S, p	
	$\nu_2$	CO stretch.	2165 D	2164.7 VS	2169 S, p	
	$\nu_3$	$\text{BH}_3$ s-deform.	1073 C	1073.4 S	1073 S, p	
	$\nu_4$	BC stretch.	691 B	691.4 S	692 W, p	
$e$	$\nu_5$	$\text{BH}_3$ d-stretch.	2444 D	2444 VS	2434 S	
	$\nu_6$	$\text{BH}_3$ d-deform.	1106 E	1105.8 S	1101 M	
	$\nu_7$	$\text{BH}_3$ rock.	809 B	809.3 M	816 W	
	$\nu_8$	BCO bend.	313 B	313.2 S	317 M	

**References**

- [1] IR. R. D. Cowan, J. Chem. Phys. **18**, 1101 (1950).  
 [2] IR.Th. G. W. Bethke and M. K. Wilson, J. Chem. Phys. **26**, 1118 (1957).  
 [3] R.Th. R. C. Taylor, J. Chem. Phys. **26**, 1131 (1957).

**No. 153 Borine Carbonyl- $\text{d}_3$   $^{11}\text{BD}_3\text{CO}$**   
**Symmetry  $C_{3v}$** 
Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{BD}_3$ s-stretch.	1679 C	(Gas) 1679.0 M	(Liquid) 1678 S	
	$\nu_2$	CO stretch.	2169 D	2168.5 VS	2169 S	
	$\nu_3$	$\text{BD}_3$ s-deform.	860 C	867.7 W (solid)	860 M	
	$\nu_4$	BC stretch.	625 B	624.8 S	619 M	
$e$	$\nu_5$	$\text{BD}_3$ d-stretch.	1840 C	1840 S	1825 S	
	$\nu_6$	$\text{BD}_3$ d-deform.	801 B	801.3 W	808 M	
	$\nu_7$	$\text{BD}_3$ rock.	709 B	709.3 S	706 W	
	$\nu_8$	BCO bend.	266 B	266.0 S	264 W	

**References**See No. 152( $^{11}\text{BH}_3\text{CO}$ ).



**No. 154 Methylmercuric iodide  $\text{CH}_3\text{HgI}$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected frequency value of	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Solid)	$\text{cm}^{-1}$ ( $\text{CH}_3\text{NO}_2$ soln.)	
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch.	2920 D	2920 M	2914 (Solid)	
	$\nu_2$	$\text{CH}_3$ s-deform.	1180 D	1180 M	1182 p	
	$\nu_3$	$\text{CHg}$ stretch.	531 D	531 M	538 p	
	$\nu_4$	$\text{HgI}$ stretch.	184 D	184 M	180 p	
$e$	$\nu_5$	$\text{CH}_3$ d-stretch.	3008 D	3008 M		
	$\nu_6$	$\text{CH}_3$ d-deform.	1400 D	1400 W		
	$\nu_7$	$\text{CH}_3$ rock.	781 D	781 S		
	$\nu_8$	$\text{CHgI}$ bend.	64 D	64 M		

**References**

- [1] R. F. Fehér, W. Kolb and L. Leverenz, Z. Naturforsch., A **2**, 454 (1947).  
 [2] IR.R. P. L. Goggin and L. A. Woodward, Trans. Faraday Soc. **62**, 1423 (1966).  
 [3] IR.Th. J. H. S. Green, Spectrochim. Acta **24A**, 863 (1968).

**No. 155 Methylsilane  $\text{CH}_3\text{SiH}_3$** Symmetry  $C_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch.	2898 E	2928.8 M		FR( $\nu_2 + \nu_5$ ).
	$\nu_2$	$\text{SiH}_3$ s-stretch.	2169 C	2867.4 M		
	$\nu_3$	$\text{CH}_3$ s-deform.	1260 C	2169 S		
	$\nu_4$	$\text{SiH}_3$ s-deform.	940 C	1260 M		
	$\nu_5$	$\text{CSi}$ stretch.	700 C	940 VS		
$a_2$	$\nu_6$	Torsion	187 D	700 S		187.6(A). MW. 186.9(E).
$e$	$\nu_7$	$\text{CH}_3$ d-stretch.	2982 A	ia		
	$\nu_8$	$\text{SiH}_3$ d-stretch.	2166 A	2981.6 M		
	$\nu_9$	$\text{CH}_3$ d-deform.	1403 C	2965.7 S		
	$\nu_{10}$	$\text{SiH}_3$ d-deform.	980 D	1403 M		
	$\nu_{11}$	$\text{CH}_3$ rock.	868 B	980 <sup>a</sup>		
	$\nu_{12}$	$\text{SiH}_3$ rock.	540 C	867.5 S		

<sup>a</sup> The band origin is not determined clearly.**References**

- [1] IR. S. Kaye and S. Tannenbaum, J. Org. Chem. **18**, 1750 (1953).  
 [2] IR. D. F. Ball, P. L. Goggin, D. C. McKean, and L. A. Woodward, Spectrochim. Acta **16**, 1358 (1960).  
 [3] IR. R. E. Wilde, J. Mol. Spectry. **8**, 427 (1962).  
 [4] IR. M. Randie, Spectrochim. Acta **18**, 115 (1962).  
 [5] Th. E. A. Clark and A. Weber, J. Chem. Phys. **45**, 1759 (1966).

**No. 156 Methylsilane-d<sub>3</sub> CH<sub>3</sub>SiD<sub>3</sub>**  
**Symmetry C<sub>3v</sub>**

**Symmetry number  $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	CH <sub>3</sub> s-stretch.	2923 A	2923.4 M		
	$\nu_2$	SiD <sub>3</sub> s-stretch.	1558 C	1558 M		
	$\nu_3$	CH <sub>3</sub> s-deform.	1262 C	1262 S		
	$\nu_4$	CSi stretch.	741 C	741 VS		
	$\nu_5$	SiD <sub>3</sub> s-deform.	652 C	652 S		
<i>a</i> <sub>2</sub>	$\nu_6$	Torsion	172 D	ia		172.1(A) MW. 171.9(E)
<i>e</i>	$\nu_7$	CH <sub>3</sub> d-stretch.	2982 A	2981.8 M		
	$\nu_8$	SiD <sub>3</sub> d-stretch.	1577 C	1577 VS		
	$\nu_9$	CH <sub>3</sub> d-deform.	1401 C	1401 M		
	$\nu_{10}$	CH <sub>3</sub> rock.	825 C	825 S		
	$\nu_{11}$	SiD <sub>3</sub> d-deform.	668 C	668 S		
	$\nu_{12}$	SiD <sub>3</sub> rock.	433 C	433		

**References**

- [1] IR. D. E. Ball, P. L. Goggin, D. C. McKean, and L. A. Woodward, *Spectrochim. Acta* **16**, 1358 (1960).  
 [2] IR. R. E. Wilde, *J. Mol. Spectry* **8**, 427 (1962).  
 [3] Th. E. A. Clark and A. Weber, *J. Chem. Phys.* **45**, 1759 (1966).

**No. 157 Methylgermane CH<sub>3</sub>GeH<sub>3</sub>**  
**Symmetry C<sub>3v</sub>**

**Symmetry number  $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	CH <sub>3</sub> s-stretch.	2938 B	2937.8 S		
	$\nu_2$	GeH <sub>3</sub> s-stretch.	2085 B	2084.8 S		
	$\nu_3$	CH <sub>3</sub> s-deform.	1254 B	1254.1 M		
	$\nu_4$	GeH <sub>3</sub> s-deform.	843 B	842.5 VS		
	$\nu_5$	CGe stretch.	602 B	601.6 VS		
<i>a</i> <sub>2</sub>	$\nu_6$	Torsion	157 D	ia		158.1(A) MW. 156.1(E)
<i>e</i>	$\nu_7$	CH <sub>3</sub> d-stretch.	2997 B	2997.2 S		
	$\nu_8$	GeH <sub>3</sub> d-stretch.	2084 B	2084.3 S		
	$\nu_9$	CH <sub>3</sub> d-deform.	1428 C	1427.7 W		
	$\nu_{10}$	GeH <sub>3</sub> d-deform.	900 C	900.4 S		
	$\nu_{11}$	CH <sub>3</sub> rock.	848 C	847.5 S		
	$\nu_{12}$	GeH <sub>3</sub> rock.	506 C	505.9 S		

**References**

- [1] IR. J. E. Griffiths, *J. Chem. Phys.* **38**, 2879 (1963).  
 [2] Th. E. A. Clark and A. Weber, *J. Chem. Phys.* **45**, 1759 (1966).

**No. 158 Methyl-d<sub>3</sub>-germane CD<sub>3</sub>GeH<sub>3</sub>**Symmetry C<sub>3v</sub>Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	CD <sub>3</sub> s-stretch.	2090 C	2091.0 S		
	$\nu_2$	GeH <sub>3</sub> s-stretch.	2073 C	2073 S		
	$\nu_3$	CD <sub>3</sub> s-deform.	978 C	977.5 S		
	$\nu_4$	GeH <sub>3</sub> s-deform.	844 C	844.3 S		
	$\nu_5$	CGe stretch.	550 B	549.6 S		
<i>a</i> <sub>2</sub>	$\nu_6$	Torsion	132 D	ia		131.7(A) MW. 131.5(E)
<i>e</i>	$\nu_7$	CD <sub>3</sub> d-stretch.	2248 B	2247.5 S		
	$\nu_8$	GeH <sub>3</sub> d-stretch.	2089 B	2089.0 S		
	$\nu_9$	CD <sub>3</sub> d-deform.	1032 B	1032.0 M		
	$\nu_{10}$	GeH <sub>3</sub> d-deform.	904 B	903.9 S		
	$\nu_{11}$	CD <sub>3</sub> rock.	713 C	713 S		
	$\nu_{12}$	GeH <sub>3</sub> rock.	452 B	451.8 S		

**References**See No. 157(CH<sub>3</sub>GeH<sub>3</sub>).**No. 159 Methyltriiodogermane CH<sub>3</sub>GeI<sub>3</sub>**Symmetry C<sub>3v</sub>Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Liquid)	cm <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	CH <sub>3</sub> s-stretch.	2911 C	2911 M	2909 W	
	$\nu_2$	CH <sub>3</sub> s-deform.	1225 C	1225 M	1222 W	
	$\nu_3$	CGe stretch.	597 C	597 S	596 M	
	$\nu_4$	GeI <sub>3</sub> s-stretch.	195 C	196 M	195 S	
	$\nu_5$	GeI <sub>3</sub> s-deform.	92 C	96 M (Solid)	92 S	
<i>a</i> <sub>2</sub>	$\nu_6$	Torsion	123 D	123 Vw (Solid)	123 Vw	
<i>e</i>	$\nu_7$	CH <sub>3</sub> d-stretch.	2999 C	2999 M	2996 W	
	$\nu_8$	CH <sub>3</sub> d-deform.	1392 C	1392 S	1394 (Solid)	
	$\nu_9$	CH <sub>3</sub> rock.	810 C	810 S	809 (Solid)	
	$\nu_{10}$	GeI <sub>3</sub> d-stretch.	252 C	252 S	251 M	
	$\nu_{11}$	GeI <sub>3</sub> rock.	147 C		147 M	
	$\nu_{12}$	GeI <sub>3</sub> d-deform.	67 C		67 S	

**References**

- [1] IR. R. J. Cross and F. Glockling, J. Organometal. Chem. **3**, 146 (1965).  
 [2] IR.R.Th. J. R. Durig, C. F. Jumper, and J. N. Willis, Jr., J. Mol. Spectry. **37**, 260 (1971).

**No. 160      Methylstannane    $\text{CH}_3\text{SnH}_3$**   
**Symmetry  $C_{3v}$**

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch.	2933 B	2932.5 W		
	$\nu_3$	$\text{CH}_3$ s-deform.	1209 B	1209.3 W		
	$\nu_2$	$\text{SnH}_3$ s-stretch.	1875 D	1874.5 S		OV( $\nu_8$ ).
	$\nu_4$	$\text{SnH}_3$ s-deform.	695 B	694.5 S		
	$\nu_5$	SnC stretch.	527 B	526.9 M		
$a_2$	$\nu_6$	Torsion	109 C			MW[1].
$e$	$\nu_7$	$\text{CH}_3$ d-stretch.	3005 B	3005.4 W		
	$\nu_8$	$\text{SnH}_3$ d-stretch.	1875 B	1874.5 S		OV( $\nu_2$ ).
	$\nu_9$	$\text{CH}_3$ d-deform.	1417 B	1417.0 W		
	$\nu_{10}$	$\text{CH}_3$ rock.	774 C	774.1 M		
	$\nu_{11}$	$\text{SnH}_3$ d-deform.	741 C	741.3 M		
	$\nu_{12}$	$\text{SnH}_3$ rock.	416 B	416.3 M		

**References**

- [1] MW. P. Cahill and S. Butcher, J. Chem. Phys. **35**, 2255 (1961).  
 [2] IR. H. Kimmel and C. R. Dillard, Spectrochim. Acta **24A**, 909 (1968).

**No. 161      Methylstannane- $d_3$     $\text{CH}_3\text{SnD}_3$**   
**Symmetry  $C_{3v}$**

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch.	2930 D	2930 M		
	$\nu_2$	$\text{SnD}_3$ s-stretch.	1352 D	1352.0 S		OV( $\nu_9$ ).
	$\nu_3$	$\text{CH}_3$ s-deform.	1205 C	1204.5 S		
	$\nu_4$	SnC stretch.	509 C	509.1 M		
	$\nu_5$	$\text{SnD}_3$ s-deform.	493 C	493.0 S		
$a_2$	$\nu_6$	Torsion	101 C			MW[1].
$e$	$\nu_7$	$\text{CH}_3$ d-stretch.	3000 D	3000 W		
	$\nu_8$	$\text{CH}_3$ d-deform.	1400 D	1400 W		
	$\nu_9$	$\text{SnD}_3$ d-stretch.	1352 C	1352.0 S		OV( $\nu_2$ ).
	$\nu_{10}$	$\text{CH}_3$ rock.	765 D	765 W		
	$\nu_{11}$	$\text{SnD}_3$ d-deform.	503 C	502.5 S		
	$\nu_{12}$	$\text{SnD}_3$ rock.	317 D	316.6 M		

**References**See No. 160( $\text{CH}_3\text{SnH}_3$ ).

**No. 162 Methyl-d<sub>3</sub>-stannane CD<sub>3</sub>SnH<sub>3</sub>****Symmetry C<sub>3v</sub>****Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	CD <sub>3</sub> s-stretch.	2144 B	2144.3 M		OV( $\nu_8$ ).
	$\nu_2$	SnH <sub>3</sub> s-stretch.	1889 D	1889.0 S		
	$\nu_3$	CD <sub>3</sub> s-deform.	920 B	920.2 M		
	$\nu_4$	SnH <sub>3</sub> s-deform.	704 B	703.5 S		
	$\nu_5$	SnC stretch.	478 B	478.0 M		
<i>a</i> <sub>2</sub>	$\nu_6$	Torsion	88 C			MW[1].
<i>e</i>	$\nu_7$	CD <sub>3</sub> d-stretch.	2255 C	2254.5 M		OV( $\nu_2$ ).
	$\nu_8$	SnH <sub>3</sub> d-stretch.	1889 B	1889.0 S		
	$\nu_9$	CD <sub>3</sub> d-deform.	1017 C	1017.1 W		
	$\nu_{10}$	SnH <sub>3</sub> d-deform.	738 B	738.1 M		
	$\nu_{11}$	CD <sub>3</sub> rock.	628 B	628.4 S		
	$\nu_{12}$	SnH <sub>3</sub> rock.	392 C	392.4 W		

**References**See No. 160(CH<sub>3</sub>SnH<sub>3</sub>).**No. 163 Cyanogen C<sub>2</sub>N<sub>2</sub>****Symmetry D<sub>∞h</sub>****Symmetry number  $\sigma = 2$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Gas)	
$\sigma_g^+$	$\nu_1$	CN s-stretch.	2330 B	2339.9 <sup>a</sup>	2330.5	
	$\nu_2$	NN stretch.	846 C	ia	845.5	
$\sigma_u^+$	$\nu_3$	CN a-stretch.	2158 A	2157.83	ia	
$\pi_g$	$\nu_4$	CCN bend.	503 C	ia	502.8	
$\pi_u$	$\nu_5$	CCN bend.	234 B	233.1 <sup>a</sup>	233.7	

<sup>a</sup> Determined from difference bands[3].**References**

- [1] R. A. Langseth and C. K. Moller, Acta Chem. Scand. **4**, 725 (1950).
- [2] IR. G. D. Craine and H. W. Thompson, Trans. Faraday Soc. **49**, 1273 (1953).
- [3] IR. A. G. Maki, J. Chem. Phys. **43**, 3193 (1965).
- [4] Th. W. Sawodnt and A. Ruoff, J. Mol. Spectry. **34**, 173 (1970).
- [5] R.IR.Th. L. J. Jones, J. Mol. Spectry. **45**, 55 (1973).
- [6] IR. M. A. Picard, Spectrochim. Acta **29**, 423 (1973).
- [7] R.Th. L. H. Jones, J. Mol. Spectry. **49**, 82 (1974).

**No. 164 Dichloroacetylene  $C_2Cl_2$**   
**Symmetry  $D_{2h}$** 
Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
$\sigma_g^+$	$\nu_1$	CC stretch.	2234 D	ia	2234 S, p	
	$\nu_2$	CCl stretch.	477 D	ia	477 M, p	
$\sigma_u^+$	$\nu_3$	CCl stretch.	988 C	988 VS	ia	
$\pi_g$	$\nu_4$	CCCl deform.	333 D	ia	333 VS, dp	
$\pi_u$	$\nu_5$	CCCl deform.	172 C	172 S	ia	

**Reference**[1] IR.R. P. Klaboe and E. Kloster-Jensen, *Spectrochim. Acta* **26A**, 1567 (1970).
**No. 165 Dibromoacetylene  $C_2Br_2$**   
**Symmetry  $D_{2h}$** 
Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ ( $C_6H_6$ soln.)	
$\sigma_g^+$	$\nu_1$	CC stretch.	2185 D	ia	2185 VS, p	
	$\nu_2$	CBr stretch.	267 D	ia	267 M, p	
$\sigma_u^+$	$\nu_3$	CBr stretch.	832 C	832 VS	ia	
$\pi_g$	$\nu_4$	CCBr deform.	311 D	ia	311 VS, dp	
$\pi_u$	$\nu_5$	CCBr deform.	137 C	137 S	ia	

**Reference**See No. 164( $C_2Cl_2$ ).
**No. 166 Diiodoacetylene  $C_2I_2$**   
**Symmetry  $D_{2h}$** 
Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$	$cm^{-1}$ ( $C_6H_6$ soln.)	
$\sigma_g^+$	$\nu_1$	CC stretch.	2118 D	ia	2118 VS, p	
	$\nu_2$	CI stretch.	190 D	ia	190 S, p	
$\sigma_u^+$	$\nu_3$	CI stretch.	720 D	720 VS ( $CS_2$ soln.)	ia	
$\pi_g$	$\nu_4$	CCI deform.	296 D	ia	296 VS, dp	
$\pi_u$	$\nu_5$	CCI deform.	132 D	132 M ( $C_6H_6$ soln.)	ia	

**References**

- [1] IR.R. A. G. Meister and F. F. Cleveland, *J. Chem. Phys.* **17**, 212 (1949).  
 [2] IR.R. P. Klaboe and E. Kloster-Jensen, *Spectrochim. Acta* **26A**, 1567 (1970).

**No. 167 Bromochloroacetylene  $C_2BrCl$** Symmetry  $C_{\infty v}$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ ( $C_6H_6$ soln.)	
$\sigma^+$	$\nu_1$	CC stretch.	2223 C	2223 VS	2205 M, p	
	$\nu_2$	CCl stretch.	923 C	923 VS	917 VS	
	$\nu_3$	CBr stretch.	389 C	389 VW	388 S, p	
$\pi$	$\nu_4$	CCCl deform.	326 D		( $CCl_4$ soln.) 326 VS, dp	
	$\nu_5$	CCBr deform.	152 C	152 S	( $CCl_4$ soln.) 165 M	

**Reference**See No. 164( $C_2Cl_2$ ).**No. 168 Chloriodoacetylene  $C_2ClI$** Symmetry  $C_{\infty v}$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ ( $C_6H_6$ soln.)	
$\sigma^+$	$\nu_1$	CC stretch.	2191 C	2191 VS	2178 VS, p	
	$\nu_2$	CCl stretch.	886 C	886 VS	880 VW	
	$\nu_3$	CI stretch.	276 D		276 M, p	
$\pi$	$\nu_4$	CCCl deform.	325 D		325 VS, dp	
	$\nu_5$	CCI deform.	135 C	135 S	145 VW ( $CCl_4$ soln.)	

**Reference**See No. 167( $C_2ClBr$ ).

**No. 169 Bromoindiacetylene  $C_2BrI$**   
**Symmetry  $C_{2v}$**

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ ( $CS_2$ soln.)	
$\sigma^+$	$\nu_1$	CC stretch.	2166 B	2166 S	2153 VS	
	$\nu_2$	CBr stretch.	782 C	782 M	775 VW	
	$\nu_3$	CI stretch.	222 D		222 M, p	
$\pi$	$\nu_4$	CBr bend.	304 D		304 VS, dp	
	$\nu_5$	CI bend.	122 B	122 S		

**Reference**

- [1] IR.R. D. H. Christensen, T. Stroger-Hansen, P. Klaboe, E. Kloster-Jensen, and E. E. Tucker, *Spectrochim. Acta* **28A**, 939 (1972).

**No. 170 Trifluoroacetonitrile  $CF_3CN$**   
**Symmetry  $C_{3v}$**

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
$a_1$	$\nu_1$	CN stretch.	2275 B	2275.0	2274 S, p	
	$\nu_2$	$CF_3$ s-stretch.	1227 B	1227.2	1222 VW	
	$\nu_3$	CC stretch.	802 B	801.7	818 M, p	
	$\nu_4$	$CF_3$ s-deform.	522 B	521.8	521 M, p	
$e$	$\nu_5$	$CF_3$ d-stretch.	1214 B	1214.3	1192 W	
	$\nu_6$	$CF_3$ d-deform.	618 B	618.3	620 W, dp	
	$\nu_7$	$CF_3$ rock.	463 B	462.7	463 W, dp	
	$\nu_8$	CCN deform.	196 B	196.0	192 S, dp	

**References**

- [1] IR.R. W. F. Edgell and R. M. Potter, *J. Chem. Phys.* **24**, 80 (1956).  
 [2] IR. J. A. Faniran and H. F. Shurvell, *Spectrochim. Acta* **26A**, 1459 (1970).  
 [3] IR.Th. J. A. Faniran and H. F. Shurvell, *Spectrochim. Acta* **27A**, 1945 (1971).



**No. 171**      **trans-1,2-Difluoroethylene**   **CHFCHF**Symmetry  $C_{2h}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_g$	$\nu_1$	CH stretch.	3111 C	ia	3111 VS, p	
	$\nu_2$	CC stretch.	1694 C	ia	1694 VS, p	
	$\nu_3$	CH bend.	1286 C	ia	1286 S, p	
	$\nu_4$	CF stretch.	1123 C	ia	1123 M, p	
	$\nu_5$	CCF deform.	548 C	ia	548 S, p	
$a_u$	$\nu_6$	CH bend.	875 B	875 S	ia	
	$\nu_7$	Torsion	329 D	333 M (Xe Matrix) 325 M	ia	
				(Xe Matrix)		
$b_g$	$\nu_8$	CH bend.	788 C	ia	788 S, dp	
$b_u$	$\nu_9$	CH stretch.	3114 C	3114 M	ia	
	$\nu_{10}$	CH bend.	1274 C	1274 M	ia	
	$\nu_{11}$	CF stretch.	1159 C	1159 VS	ia	
	$\nu_{12}$	CCF deform.	341 D	341 M (Xe Matrix)	ia	

**Reference**[1] IR.R.      N. C. Craig and J. Overend, J. Chem. Phys. **51**, 1127 (1969).**No. 172**      **trans-1,2-Difluoroethylene- $d_1$**    **CHFCD $F$** Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	CH stretch.	3110 C	3110 M	3112 S, p	
	$\nu_2$	CD stretch.	2335 C	2335 M	2333 M, p	
	$\nu_3$	CC stretch.	1674 C		1674 S, p	
	$\nu_4$	CH bend.	1274 C	1274 M	1274 M, p	
	$\nu_5$	CF stretch.	1166 C	1166 VS	1155 VW	
	$\nu_6$	CF stretch.	1138 C	1138 M	1119 M, p	
	$\nu_7$	CD bend.	940 C	940 M	941 M, dp	
	$\nu_8$	CCF deform.	542 C		542 S, p	
	$\nu_9$	CCF deform.	332 D	332 M		
$a''$	$\nu_{10}$	CH bend.	828 B	828 S	829 M, dp	
	$\nu_{11}$	CD bend.	673 B	673 M	673 M, dp	
	$\nu_{12}$	Torsion	316 C	316 S		

**Reference**

See No. 171(CHFCHF).

No. 173 trans-1,2-Difluoroethylene-d<sub>2</sub> CDFCDFSymmetry C<sub>2h</sub>Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a<sub>g</sub></i>	$\nu_1$	CD stretch.	2355 C	ia	2355 S, p	
	$\nu_2$	CC stretch.	1642 C	ia	1642 VS, p	
	$\nu_3$	CF stretch.	1109 C	ia	1109 S, p	
	$\nu_4$	CD bend.	935 C	ia	935 M, dp	
	$\nu_5$	CCF deform.	538 C	ia	538 S, p	
<i>a<sub>u</sub></i>	$\nu_6$	CD bend.	651 B	651 S	ia	
	$\nu_7$	Torsion	309 C	309 S	ia	
<i>b<sub>g</sub></i>	$\nu_8$	CD bend.	685 C	ia	685 S, dp	
<i>b<sub>u</sub></i>	$\nu_9$	CD stretch.	2312 C	2312 M	ia	
	$\nu_{10}$	CF stretch.	1173 C	1173 VS	ia	
	$\nu_{11}$	CD bend.	942 C	942 M	ia	
	$\nu_{12}$	CCF deform.	324 D	324 M	ia	

## References

- [1] R. N. C. Craig and J. Overend, *Spectrochim. Acta* **20**, 1561 (1964).  
 [2] IR.R. N. C. Craig and J. Overend, *J. Chem. Phys.* **51**, 1127 (1969).

No. 174 Glyoxal C<sub>2</sub>H<sub>2</sub>O<sub>2</sub>Symmetry C<sub>2h</sub>Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)		
<i>a<sub>g</sub></i>	$\nu_1$	CH stretch.	2843 B	ia		EL[4].
	$\nu_2$	CO stretch.	1745 B	ia		EL[4].
	$\nu_3$	CH bend.	1338 D	ia		OC[1].
	$\nu_4$	CC stretch.	1065 B	ia		EL[4].
	$\nu_5$	CCO deform.	551 B	ia		EL[3].
<i>a<sub>u</sub></i>	$\nu_6$	CH bend.	801 B	801.36 M		
	$\nu_7$	Torsion	127 B	126.5 W		EL[3].
<i>b<sub>g</sub></i>	$\nu_8$	CH bend.	1048 B	ia		[5].
<i>b<sub>u</sub></i>	$\nu_9$	CH stretch.	2835 B	2835.07 VS		
	$\nu_{10}$	CO stretch.	1732 C	1732 VS		
	$\nu_{11}$	CH bend.	1312 B	1312.38 S		
	$\nu_{12}$	CCO deform.	339 B	338.55 S		

## References

- [1] IR.R. R. K. Harris, *Spectrochim. Acta* **20**, 1129 (1964).  
 [2] IR. A. R. H. Cole and G. A. Osborne, *J. Mol. Spectry.* **36**, 276 (1970).  
 [3] EL. F. W. Birss, J. M. Brown, A. R. H. Cole, A. Loftus, S. L. N. G. Krishnamachari, G. A. Osborne, J. Puldus, D. A. Ramsay, and L. Watmann, *Can. J. Phys.* **48**, 1230 (1970).  
 [4] EL. W. Holzer and D. A. Ramsay, *Can. J. Phys.* **48**, 1759 (1970).  
 [5] IR. A. R. H. Cole and G. A. Osborne, *Spectrochim. Acta* **27A**, 2461 (1971).

**No. 175 Glyoxal-d<sub>1</sub> C<sub>2</sub>HDO<sub>2</sub>**Symmetry C<sub>s</sub>Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a'	$\nu_1$	CH stretch.	2835 B	3835.2 S		
	$\nu_2$	CD stretch.	2130 B	2130.2 S		
	$\nu_3$	CO s-stretch.	1735 D	1735 M		
	$\nu_4$	CO a-stretch.	1717 C	1717 VS		
	$\nu_5$	CH bend.	1335 B	1335.0 W		
	$\nu_6$	CC stretch.	1104 E			CF[1].
	$\nu_7$	CD bend.	972 B	971.6 M		
a''	$\nu_8$	CCO s-deform.	542 D	542 <sup>a</sup>		EL[2].
	$\nu_9$	CCO a-deform.	323 B	323.7 S		
	$\nu_{10}$	CH bend.	999 D	999 W		
	$\nu_{11}$	CO bend.	688 D			CF. <sup>b</sup>
	$\nu_{12}$	Torsion	124 B	123.9 W		

<sup>a</sup> From the analyses of electronic transitions.<sup>b</sup> From the product rule.**References**

- [1] Th. T. Fukuyama, Ph. D. Thesis (University of Tokyo, 1970).  
 [2] IR. A. R. H. Cole and G. A. Osborne, *Spectrochim. Acta* **27A**, 2461 (1971).

**No. 176 Glyoxal-d<sub>2</sub> C<sub>2</sub>D<sub>2</sub>O<sub>2</sub>**Symmetry C<sub>2h</sub>Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a <sub>g</sub>	$\nu_1$	CD stretch.	2138 D	ia		OC[5].
	$\nu_2$	CO stretch.	1722 C	ia		OC[5].
	$\nu_3$	CD bend.	1130 D	ia		OC[5].
	$\nu_4$	CC stretch.	915 E	ia		CF[3].
	$\nu_5$	CCO deform.	537 B	ia		EL[2].
a <sub>u</sub>	$\nu_6$	CD bend.	630 D			CF[1]. <sup>a</sup>
	$\nu_7$	Torsion	118 B	118.2 W		EL[2].
b <sub>g</sub>	$\nu_8$	CD bend.	911 D	ia		CF[1]. <sup>a</sup>
b <sub>u</sub>	$\nu_9$	CD stretch.	2130 C	2130 S		
	$\nu_{10}$	CO stretch.	1710 C	1710 VS		
	$\nu_{11}$	CH bend.	1010 B	1010.12 M		
	$\nu_{12}$	CCO deform.	311 B	311.05 M		

<sup>a</sup> From the product rule**References**

- [1] IR. J. C. D. Brand and G. J. Minkoff, *J. Chem. Soc.* **1954**, 2970.  
 [2] EL. J. C. D. Brand, *Trans. Faraday Soc.* **50**, 431 (1954).  
 [3] Th. T. Fukuyama, K. Kuchitsu, and Y. Morino, *Bull. Chem. Soc. Japan*, **41**, 3019 (1968).  
 [4] EL. D. M. Agar, E. J. Bair, F. W. Birss, P. Bovrell, P. C. Chen, C. N. Gurrie, A. J. McHugh, B. J. Orr, D. A. Ramsay, and J. Y. Roncin, *Can. J. Phys.* **49**, 323 (1971).  
 [5] IR. A. R. H. Cole and G. A. Osborne, *Spectrochim. Acta* **27A**, 2461 (1971).

**No. 177 Acetyl fluoride CH<sub>3</sub>COF**  
**Symmetry C<sub>s</sub>**
Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a'</i>	$\nu_1$	CH <sub>3</sub> d-stretch.	3043 C	3043 W	3043 VW	
	$\nu_2$	CH <sub>3</sub> s-stretch.	2955 C	2955 VW	2952 S	
	$\nu_3$	C=O stretch.	1870 C	1870 VS	1847 S	
	$\nu_4$	CH <sub>3</sub> d-deform.	1440 C	1440 W	1440 W	
	$\nu_5$	CH <sub>3</sub> s-deform.	1378 C	1378 M	1379 W	
	$\nu_6$	CF stretch.	1188 C	1188 VS	1178 VW	
	$\nu_7$	CH <sub>3</sub> rock.	1000 C	1000 M	1003 M	
	$\nu_8$	CC stretch.	826 C	826 S	822 S	
	$\nu_9$	OCF deform.	598 C	598 W	602 M	
	$\nu_{10}$	OCF deform.	420 D	420 VW	428 W	
<i>a''</i>	$\nu_{11}$	CH <sub>3</sub> d-stretch.	3004 C	3004 W	3004 VW	
	$\nu_{12}$	CH <sub>3</sub> d-deform.	1437 D	1437 W	1440 W	
	$\nu_{13}$	CH <sub>3</sub> rock.	1054 C	1054 M		
	$\nu_{14}$	C=O op-bend.	567 C	567 W	573 W	
	$\nu_{15}$	CH <sub>3</sub> torsion	123 E			CF[1].

**References**

- [1] MW. L. Pierce and L. C. Krisher, J. Chem. Phys. **31**, 875 (1959).  
 [2] R. H. Seewan-Albert and L. Kahovec, Acta Phys. Austriaca **1**, 352 (1948).  
 [3] IR. J. A. Ramsey and J. A. Ladd, J. Chem. Soc. **B1968**, 118.  
 [4] IR.R. C. V. Berney and A. D. Cormier, Spectrochim. Acta **28A**, 1813 (1972).

**No. 178 Acetyl fluoride-d<sub>3</sub> CD<sub>3</sub>COF**  
**Symmetry C<sub>s</sub>**
Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a'</i>	$\nu_1$	CD <sub>3</sub> d-stretch.	2274 D	2286 M	2272 W	
				2263 M		
	$\nu_2$	CD <sub>3</sub> s-stretch.	2144 C	2144 W	2140 S	
	$\nu_3$	C=O stretch.	1869 C	1869 VS	1849 M	
	$\nu_4$	CF stretch.	1204 C	1204 VS	1196 VW	
	$\nu_5$	CD <sub>3</sub> s-deform.	1149 C	1149 W		
	$\nu_6$	CD <sub>3</sub> d-deform.	1030 C	1030 S	1030 W	
	$\nu_7$	CD <sub>3</sub> rock.	839 C	839 M	845 M	
	$\nu_8$	CC stretch.	778 C	778 S	774 M	
	$\nu_9$	OCF deform.	575 C	575 M	578 M	
<i>a''</i>	$\nu_{10}$	OCF deform.	395 D	395 VW	378 W	
	$\nu_{11}$	CD <sub>3</sub> d-stretch.	2242 C	2242 W	2250 W	
	$\nu_{12}$	CD <sub>3</sub> d-deform.	1057 C	1057 M	1053 W	
	$\nu_{13}$	CD <sub>3</sub> rock.	915 C	915 M		
	$\nu_{14}$	C=O op-bend.	491 C	491 M	495 W	
	$\nu_{15}$	CD <sub>3</sub> torsion	93 E			CF[1].

**References**

- [1] MW. L. Pierce and L. C. Krisher, J. Chem. Phys. **31**, 875 (1959).  
 [2] IR. C. V. Berney, R. L. Redington and K. C. Lin, J. Chem. Phys. **53**, 1713 (1970).  
 [3] IR.R. C. V. Berney and A. D. Cormier, Spectrochim. Acta **28A**, 1813 (1972).

**No. 179      Dimethylzinc       $\text{CH}_3\text{ZnCH}_3$** **Symmetry  $D_{3h}(G^+_{36})^a$** **Symmetry number  $\sigma = 6$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1'$	$\nu_1$	$\text{CH}_3$ s-stretch.	2900 C	ia	2900 S, p	
	$\nu_2$	$\text{CH}_3$ s-deform.	1157 C	ia	1157 S, p	
	$\nu_3$	CZn s-stretch.	503 C	ia	503 VS, p	
$a_1''$	$\nu_4$	Torsion		ia	ia	
$a_2''$	$\nu_5$	$\text{CH}_3$ s-stretch.	2915 C	2915 S	ia	
	$\nu_6$	$\text{CH}_3$ s-deform.	1183 C	1183 M	ia	
	$\nu_7$	CZn a-stretch.	613 C	613	ia	
$e'$	$\nu_8$	$\text{CH}_3$ d stretch.	2966 C	2966 S	2947	
	$\nu_9$	$\text{CH}_3$ d-deform.	1301 C	1301 M	1302 W	
	$\nu_{10}$	$\text{CH}_3$ rock.	704 C	704 S		
$e''$	$\nu_{11}$	CZnC deform.	134 D		134 sh	
	$\nu_{12}$	$\text{CH}_3$ d-stretch.	2843 C	2843	2830	
	$\nu_{13}$	$\text{CH}_3$ d-deform.	1434 C		1434 W	
	$\nu_{14}$	$\text{CH}_3$ rock.	620 C		620 M	

<sup>a</sup> Free rotation [3,5].**References**

- [1] IR.R. H. S. Gutowsky, J. Chem. Phys. **17**, 128 (1949).  
 [2] Th.IR. D. R. J. Boyd, R. L. Williams, and H. W. Thompson, Nature **167**, 766 (1951).  
 [3] IR.R. J.-L. Bribes, Ph. D. Thesis, (Universite des Sciences et Techniques du Languedoc 1971).  
 [4] Th. A. M. W. Bakke, J. Mol. Spectry. **41**, 1 (1972).  
 [5] IR.R. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

**No. 180      Dimethylzinc- $d_6$        $\text{CD}_3\text{ZnCD}_3$** **Symmetry  $D_{3h}(G^+_{36})^a$** **Symmetry number  $\sigma = 6$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1'$	$\nu_1$	$\text{CD}_3$ s-stretch.	2109 C	ia	2109 S, p	
	$\nu_2$	$\text{CD}_3$ s-deform.	898 C	ia	898 S, p	
	$\nu_3$	CZn s-stretch.	458 C	ia	458 S, p	
$a_1''$	$\nu_4$	Torsion		ia	ia	
$a_2''$	$\nu_5$	$\text{CD}_3$ s-stretch.	2117 C	2117 M	ia	
	$\nu_6$	$\text{CD}_3$ s-deform.	934 C	934 M	ia	
	$\nu_7$	CZn a-stretch.	554 C	554 S	ia	
$e'$	$\nu_8$	$\text{CD}_3$ d-stretch.	2219 C	2219 M	2206 M	
	$\nu_9$	$\text{CD}_3$ d-deform.	960 C	960 W		
	$\nu_{10}$	$\text{CD}_3$ rock.	585 D	585 sh		
$e''$	$\nu_{11}$	CZnC deform.	96 D		96 sh	
	$\nu_{12}$	$\text{CD}_3$ d-stretch.	2073 C	2073 W	2075 sh	
	$\nu_{13}$	$\text{CD}_3$ d-deform.	1006 C	1006 W		
	$\nu_{14}$	$\text{CD}_3$ rock.	495 C		495 W, p	

<sup>a</sup> Free rotation [1].**Reference**

- [1] IR.R. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

No. 181 Dimethylcadmium  $\text{CH}_3\text{CdCH}_3$ Symmetry  $D_{3h}(G_{36})^a$ Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1'$	$\nu_1$	$\text{CH}_3$ s-stretch.	2903 C	ia	2903 S, p	
	$\nu_2$	$\text{CH}_3$ s-deform.	1127 C	ia	1127 S, p	
	$\nu_3$	$\text{CCd}$ s-stretch.	459 C	ia	459 S, p	
$a_1''$	$\nu_4$	Torsion		ia	ia	
$a_2''$	$\nu_5$	$\text{CH}_3$ s-stretch.	2923 C	2923 S	ia	
	$\nu_6$	$\text{CH}_3$ s-deform.	1136 C	1136 M	ia	
	$\nu_7$	$\text{CCd}$ a-stretch.	535 C	535 S	ia	
$e'$	$\nu_8$	$\text{CH}_3$ d-stretch.	2980 C	2980 VS		
	$\nu_9$	$\text{CH}_3$ d-deform.	1315 C	1315	1324	
	$\nu_{10}$	$\text{CH}_3$ rock.	700 C	700 S		
	$\nu_{11}$	$\text{CCdC}$ deform.	124 C	124 W	120 W, b	
$e''$	$\nu_{12}$	$\text{CH}_3$ d-stretch.	2859 C	2859	2834 M	
	$\nu_{13}$	$\text{CH}_3$ d-deform.	1427 C		1427 W	
	$\nu_{14}$	$\text{CH}_3$ rock.	634 C		634 M, dp	

<sup>a</sup> Free rotation [3,5].

## References

- [1] R. F. Fehér, W. Kolb, and L. Leverenz, *Z. Naturforsch.* **2a**, 454 (1947).  
 [2] IR. H. S. Gutowsky, *J. Amer. Soc.* **71**, 3194 (1949).  
 [3] IR.R. J.-L. Briber, Ph. D. Thesis, (Universite des Sciences et Techniques du Languedoc 1971).  
 [4] Th. A. M. W. Bakke, *J. Mol. Spectry.* **41**, 1 (1972).  
 [5] IR.R. J. R. Durig and S. C. Brown, *J. Mol. Spectry.* **45**, 338 (1973).

No. 182 Dimethylcadmium- $d_6$   $\text{CD}_3\text{CdCD}_3$ Symmetry  $D_{3h}(G_{36})^a$ Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1'$	$\nu_1$	$\text{CD}_3$ s-stretch.	2112 C	ia	2112 S, p	
	$\nu_2$	$\text{CD}_3$ s-deform.	873 C	ia	873 S, p	
	$\nu_3$	$\text{CCd}$ s-stretch.	419 C	ia	419 S, p	
$a_1''$	$\nu_4$	Torsion		ia	ia	
$a_2''$	$\nu_5$	$\text{CD}_3$ s-stretch.	2120 C	2120 S	ia	
	$\nu_6$	$\text{CD}_3$ s-deform.	900 C	900 W	ia	
	$\nu_7$	$\text{CCd}$ a-stretch.	492 C	492 S	ia	
$e'$	$\nu_8$	$\text{CD}_3$ d-stretch.	2229 C	2229 S	2214 M, dp	
	$\nu_9$	$\text{CD}_3$ d-deform.	1047 D		1047 W	
	$\nu_{10}$	$\text{CD}_3$ rock.	538 C	538 S		
	$\nu_{11}$	$\text{CCdC}$ deform.	109 D		109 sh	
$e''$	$\nu_{12}$	$\text{CD}_3$ d-stretch.	2080 D	2080	2086 sh	
	$\nu_{13}$	$\text{CD}_3$ d-deform.	1126 C		1126	
	$\nu_{14}$	$\text{CD}_3$ rock.	476 C		476 M, dp	

<sup>a</sup> Free rotation [1].

## Reference

See No. 180( $\text{CD}_3\text{ZnCD}_3$ ).

No. 183 Dimethylmercury  $\text{CH}_3\text{HgCH}_3$ Symmetry  $D_{3h}(G^+_{3h})^a$ Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1'$	$\nu_1$	$\text{CH}_3$ s-stretch.	2911 C	ia	2911 VS, p	
	$\nu_2$	$\text{CH}_3$ s-deform.	1182 C	ia	1182 VS, p	
	$\nu_3$	$\text{CHg}$ s-stretch.	515 C	ia	515 VS, p	
$a_1''$	$\nu_4$	Torsion		ia	ia	
$a_2''$	$\nu_5$	$\text{CH}_3$ s-stretch.	2925 D	2925 b	ia	
	$\nu_6$	$\text{CH}_3$ s-deform.	1191 C	1191 M	ia	
	$\nu_7$	$\text{CHg}$ a-stretch.	540 C	540 VS	ia	
$e'$	$\nu_8$	$\text{CH}_3$ d-stretch.	2962 C	2962 S		
	$\nu_9$	$\text{CH}_3$ d-deform.	1397 C		1397 W, dp	
	$\nu_{10}$	$\text{CH}_3$ rock.	780 C	780 VS	779 VW, dp	
	$\nu_{11}$	$\text{CHgC}$ deform.	161 C		161 M, dp	
$e''$	$\nu_{12}$	$\text{CH}_3$ d-stretch.	2874 C		2874 S, p	
	$\nu_{13}$	$\text{CH}_3$ d-deform.	1442 C		1442 W, dp	
	$\nu_{14}$	$\text{CH}_3$ rock.	699 C	700 sh	699 M, dp	

<sup>a</sup> Free rotation [3,6].

## References

- [1] IR.R. H. S. Gutowsky, J. Chem. Phys. **17**, 128 (1949).
- [2] Th.IR. D. R. J. Boyd, R. L. Williams and H. W. Thompson, Nature **167**, 766 (1951).
- [3] IR.R. J.-L. Bribes et R. Gaufres, J. Chim. Phys. **67**, 1168 (1970).
- [4] Th. J.-L. Bribes et R. Gaufres, J. Mol. Structure **9**, 423 (1971).
- [5] Th. A. M. W. Bakke, J. Mol. Spectry. **41**, 1 (1972).
- [6] Th. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

No. 184 Dimethylmercury-d<sub>6</sub> CD<sub>3</sub>HgCD<sub>3</sub>Symmetry D<sub>3h</sub>'(G<sup>+</sup><sub>36</sub>)<sup>a</sup>Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a</i> <sub>1</sub> '	$\nu_1$	CD <sub>3</sub> s-stretch.	2111 C	ia	2111 M, p	
	$\nu_2$	CD <sub>3</sub> s-deform.	909 C	ia	909 VS, p	
	$\nu_3$	CHg s-stretch.	471 C	ia	471	
<i>a</i> <sub>1</sub> "	$\nu_4$	Torsion		ia	ia	
<i>a</i> <sub>2</sub> "	$\nu_5$	CD <sub>3</sub> s-stretch.	2114 C	2114 S	ia	
	$\nu_6$	CD <sub>3</sub> s-deform.	931 C	931 M	ia	
	$\nu_7$	CHg a-stretch.	491 C	491 VS	ia	
<i>e</i> '	$\nu_8$	CD <sub>3</sub> d-stretch.	2224 C	2224	2224 S, dp	
	$\nu_9$	CD <sub>3</sub> d-deform.	1030 C	1030 M	1030 W, dp	
	$\nu_{10}$	CD <sub>3</sub> rock.	598 C	598 VS		
	$\nu_{11}$	CHgC deform.	141 C		141 S, dp	
<i>e</i> "	$\nu_{12}$	CD <sub>3</sub> d-stretch.	2039 C	2039	2044 M, p	
	$\nu_{13}$	CD <sub>3</sub> d-deform.	1050 C		1050 VW, p	
	$\nu_{14}$	CD <sub>3</sub> rock.	525 C		525 M, sh, dp	

<sup>a</sup> Free rotation [2,4].

## References

- [1] IR.R. J.-L. Briber et R. Gaufres, J. Chim. Phys. **67**, 1168 (1970).
- [2] Th. J.-L. Briber et R. Gaufres, J. Mol. Structure **9**, 423 (1971).
- [3] Th. A. M. W. Bakke, J. Mol. Spectry. **41**, 1 (1972).
- [4] Th. J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).



No. 185 Azomethane  $\text{CH}_3\text{NNCH}_3$ Symmetry  $\text{C}_{2h}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_g$	$\nu_1$	$\text{CH}_3$ d-stretch.	2977 C	ia	2977 M, dp	
	$\nu_2$	$\text{CH}_3$ s-stretch.	2916 C	ia	2916 S, p	
	$\nu_3$	NN stretch.	1580 C	ia	1580 VW, p	
	$\nu_4$	$\text{CH}_3$ d-deform.	1434 C	ia	1434 M	
	$\nu_5$	$\text{CH}_3$ s-deform.	1380 C	ia	1380 W	
	$\nu_6$	CN stretch.	1176 C	ia	1176 VW	
	$\nu_7$	$\text{CH}_3$ rock.	916 C	ia	916 M	
	$\nu_8$	CCN bend.	589 C	ia	589 VS, p	
$a_u$	$\nu_9$	$\text{CH}_3$ d-stretch.	2966 D	2966 W, sh (solid)	ia	
	$\nu_{10}$	$\text{CH}_3$ d-deform.	1438 C	1438	ia	
	$\nu_{11}$	$\text{CH}_3$ rock.	1109 C	1109 W	ia	
	$\nu_{12}$	CCN bend.	312 D	312 S (solid)	ia	
$b_g$	$\nu_{13}$	$\text{CH}_3$ torsion	222 D	222 VW	ia	
	$\nu_{14}$	$\text{CH}_3$ d-stretch.	2982 D	ia	2982 VS (solid)	
	$\nu_{15}$	$\text{CH}_3$ d-deform.	1447 D	ia	1447 S (solid)	
	$\nu_{16}$	$\text{CH}_3$ rock.	1010 D	ia	1010 VW	
	$\nu_{17}$	$\text{CH}_3$ torsion	223 D	ia	223 W (solid)	
$b_u$	$\nu_{18}$	$\text{CH}_3$ d-stretch.	2982 C	2982 VS	ia	
	$\nu_{19}$	$\text{CH}_3$ s-stretch.	2926 C	2926 VS	ia	
	$\nu_{20}$	$\text{CH}_3$ d-deform.	1445 C	1445 S	ia	
	$\nu_{21}$	$\text{CH}_3$ s-deform.	1393 C	1393 M	ia	
	$\nu_{22}$	CN stretch.	1300 C	1300 VW	ia	
	$\nu_{23}$	$\text{CH}_3$ rock.	1009 C	1009 W	ia	
	$\nu_{24}$	CCN bend.	352 C	352 M	ia	

## References

- [1] IR.R. J. R. Durig, C. B. Pate, and W. C. Harris, J. Chem. Phys. **56**, 5652 (1972).  
 [2] R.Th. R. A. R. Pearce, I. W. Lewin, and W. C. Harris, J. Chem. Phys. **59**, 1209 (1973).

No. 186 Azomethane-d<sub>6</sub> CD<sub>3</sub>NNCD<sub>3</sub>Symmetry C<sub>2h</sub>Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
<i>a<sub>g</sub></i>	$\nu_1$	CD <sub>3</sub> d-stretch.	2227 C	(Gas) ia	(Liquid) 2227 M	
	$\nu_2$	CD <sub>3</sub> s-stretch.	2117 C	ia	2117 S, p	
	$\nu_3$	NN stretch.	1563 C	ia	1563 VW, dp	
	$\nu_4$	CN stretch.	1125 C	ia	1125 W, p	
	$\nu_5$	CD <sub>3</sub> d-deform.	1042 C	ia	1042 M	
	$\nu_6$	CD <sub>3</sub> s-deform.	1035 D	ia	1035 (solid)	
	$\nu_7$	CD <sub>3</sub> rock.	764 C	ia	764 M, p	
	$\nu_8$	CNN bend.	524 C	ia	524 VS, p	
<i>a<sub>u</sub></i>	$\nu_9$	CD <sub>3</sub> d-stretch.	2178 C	2178 VW	ia	
	$\nu_{10}$	CD <sub>3</sub> d-deform.	1043 D	1043 S (solid)	ia	
	$\nu_{11}$	CD <sub>3</sub> rock.	894 D	894 S, b	ia	OV( $\nu_{23}$ ).
	$\nu_{12}$	CCN bend.	273 C	273 M	ia	
	$\nu_{13}$	CD <sub>3</sub> torsion	166 D	166 VW (solid)	ia	
<i>b<sub>g</sub></i>	$\nu_{14}$	CD <sub>3</sub> d-stretch.	2250 C	ia	2250 M	
	$\nu_{15}$	CD <sub>3</sub> d-deform.	1057 C	ia	1057 M (solid)	
	$\nu_{16}$	CD <sub>3</sub> rock.	792 D	ia	792 W	
	$\nu_{17}$	CD <sub>3</sub> torsion	183 D	ia	183 W (solid)	
<i>b<sub>u</sub></i>	$\nu_{18}$	CD <sub>3</sub> d-stretch.	2239 C	2239 VS	ia	
	$\nu_{19}$	CD <sub>3</sub> s-stretch.	2111 C	2111 M	ia	
	$\nu_{20}$	CN stretch.	1116 D	1116 VW (solid)	ia	
	$\nu_{21}$	CD <sub>3</sub> d-deform.	1047 C	1047 M	ia	
	$\nu_{22}$	CD <sub>3</sub> s-deform.	1029 C	1029 sh	ia	
	$\nu_{23}$	CD <sub>3</sub> rock.	894 D	894 S, b	ia	OV( $\nu_{11}$ ).
	$\nu_{24}$	CNN bend.	304 C	304 M	ia	

## References

See No. 185(CH<sub>3</sub>NNCH<sub>3</sub>)

**No. 187 Carbon suboxide  $C_3O_2$** Symmetry  $D_{\infty h}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (Gas)	
$\sigma_g^+$	$\nu_1$	CO s-stretch.	2196 B	ia	2196.5 W	
	$\nu_2$	CC s-stretch.	786 B	ia	786.1 W, p	
$\sigma_u^+$	$\nu_3$	CO a-stretch.	2258 B	2258 S		
	$\nu_4$	CC a-stretch.	1573 B	1573 S		
$\pi_g$	$\nu_5$	CCO bend.	573 C	ia	573.0 W	
$\pi_u$	$\nu_6$	CCO bend.	550 B	550 S		
	$\nu_7$	CCC bend,	61 B	61		

**References**

- [1] IR.R. D. A. Long, F. S. Murfin, and R. L. Williams, Proc. Roy. Soc. (London) **A223**, 251 (1984).  
 [2] IR. F. A. Miller and W. G. Fateley, Spectrochim. Acta **20**, 253 (1964).  
 [3] IR. W. J. Lafferty, A. G. Maki, and E. K. Plyler, J. Chem. Phys. **40**, 224 (1964).  
 [4] IR. F. A. Miller, D. H. Lemmon, and R. E. Witowski, Spectrochim. Acta **21**, 1709 (1965).  
 [5] IR. W. H. Smith and G. E. Leroi, J. Chem. Phys. **45**, 1767 (1966).  
 [6] Th. R. L. Redington, Spectrochim. Acta **23A**, 1863 (1967).  
 [7] R. W. H. Smith and J. J. Barrett, J. Chem. Phys. **51**, 1475 (1969).  
 [8] Th. K. Ramaswamy and K. Spinivasan, J. Mol. Structure **3**, 473 (1969).  
 [9] R.IR.Th. L. A. Carreira, R. O. Carter, J. R. Durig, R. C. Lord, and C. C. Milionis, J. Chem. Phys. **59**, 1028 (1973).

**No. 188 Carbon subsulfide  $C_3S_2$** Symmetry  $D_{\infty h}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ ( $CS_2$ soln.)	
$\sigma_g^+$	$\nu_1$	CC s-stretch.	1663 D	ia	1663 S	
	$\nu_2$	CS s-stretch.	485 D	ia	485 S, p	
$\sigma_u^+$	$\nu_3$	CC a-stretch.	2089 B	2088.5 VS	ia	
	$\nu_4$	CS a-stretch.	1030 B	1029.8 S	ia	
$\pi_g$	$\nu_5$	CCS bend.	470 D	ia	470 M	
$\pi_u$	$\nu_6$	CCS bend.	502 C	502 VW	ia	
	$\nu_7$	CCC bend.	94 C	94 W	ia	

**References**

- [1] IR.R. W. H. Smith and G. E. Leroi, J. Chem. Phys. **45**, 1778 (1966).  
 [2] Th. W. H. Smith and G. E. Leroi, J. Chem. Phys. **45**, 1784 (1966).  
 [3] Th. K. Ramaswamy and K. Spinivasan, J. Mol. Structure **31**, 473 (1969).

**No. 189 Chloro cyanoacetylene ClCCCN**Symmetry  $C_{2v}$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ ( $\text{C}_6\text{H}_6$ soln.)	
$\sigma^+$	$\nu_1$	CN stretch.	2297 C	2297 VS	2290 VS, p	
	$\nu_2$	$\text{C}\equiv\text{C}$ stretch.	2194 B	2194 W	2196 M, p	
	$\nu_3$	C-C stretch.	1093 C	1093 S	1103 W, p	
	$\nu_4$	CCl stretch.	527 B	527 M	530 M, p	
$\pi$	$\nu_5$	CCN bend.	483 B	483 S	487 S	
	$\nu_6$	CCC bend.	333 C	333 M	338 M	
	$\nu_7$	CCCl bend.	145 D		145 VW	

**References**

- [1] IR. S. J. Cyvin, E. Kloster-Jensen, and P. Klaboe, *Acta Chem. Scand.* **19**, 903 (1965).  
 [2] IR.R. P. Klaboe and E. Kloster-Jensen, *Spectrochim. Acta* **23A**, 1981 (1967).

**No. 190 Bromo cyanoacetylene BrCCCN**Symmetry  $C_{2v}$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ ( $\text{C}_6\text{H}_6$ soln.)	
$\sigma^+$	$\nu_1$	CN stretch.	2292 C	2292 VS	2276 VS, p	
	$\nu_2$	$\text{C}\equiv\text{C}$ stretch.	2150 C	2150 S	2123 W	
	$\nu_3$	C-C stretch.	1054 B	1054 VW	1052 W	
	$\nu_4$	CBr stretch.	419 B	419 W	418 M, p	
$\pi$	$\nu_5$	CCN bend.	485 B	485 S	489 S	
	$\nu_6$	CCC bend.	312 B	312 M	317 S	
	$\nu_7$	CCBr bend.	142 D		142 VW	

**References**

See No. 189(ClCCCN).

**No. 191 Iodo cyanoacetylene ICCCN**Symmetry  $C_{\infty v}$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ ( $\text{C}_6\text{H}_6$ soln.)	
$\sigma^+$	$\nu_1$	CN stretch.	2270 C	2270 S	2265 VS, p	
	$\nu_2$	$\text{C}\equiv\text{C}$ stretch.	2131 C	2131 M	2125 M, p	
	$\nu_3$	C-C stretch.	1031 C	1031 S	1034 W, p	
	$\nu_4$	CI stretch.	364 B	364 W	356 M	
$\pi$	$\nu_5$	CCN bend.	496 B	496 M	497 S, dp	
	$\nu_6$	CCC bend.	309 C	309 W	315 M, dp	
	$\nu_7$	CCI bend.	130 D		130 VW	

**References**

See No. 189(CICCCN).

**No. 192 Chloropropadiene  $\text{CH}_2\text{CCHCl}$** Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	CH stretch.	3079 C	3079 S	3062 S, p	OV( $\nu_{11}$ ).
	$\nu_2$	$\text{CH}_2$ s-stretch.	3009 C	3009 M	2990 S, p	
	$\nu_3$	CCC a-stretch.	1963 C	1963 M	1951 W, dp	
	$\nu_4$	$\text{CH}_2$ scis.	1435 C	1435 S	1419 S, p	
	$\nu_5$	CH bend.	1256 C	1256 VS	1244 W, p	
	$\nu_6$	CCC s-stretch.	1101 C	1101 S	1095 VS, p	
	$\nu_7$	$\text{CH}_2$ wag.	875 C	875 VS	877 W, dp	
	$\nu_8$	CCl stretch.	767 C	767 VS	751 W, dp	
	$\nu_9$	CCC deform.	592 C	592 W		
	$\nu_{10}$	CCCl deform.	494 C	494 M	490 VS, p	
$a''$	$\nu_{11}$	$\text{CH}_2$ a-stretch.	3079 C	3079 S	3062 S, p	OV( $\nu_1$ ).
	$\nu_{12}$	$\text{CH}_2$ rock.	999 B	999 W	995 W, dp	
	$\nu_{13}$	CH bend.	822 B	822 S	815 W, dp	
	$\nu_{14}$	CCC deform.	548 B	548 M	546 W, dp	
	$\nu_{15}$	CCCl deform.	184 C		184 S, dp	

**Reference**[1] IR.R. R. A. Nyquist, Y. S. Lo, and J. C. Evans, Spectrochim. Acta **20**, 619 (1964).

**No. 193 Bromopropadiene  $\text{CH}_2\text{CCHBr}$**   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a'$	$\nu_1$	CH stretch.	3080 C	3080 M	3060 (46), p	OV( $\nu_{11}$ ).
	$\nu_2$	$\text{CH}_2$ s-stretch.	3005 C	3005 M	2985 (63), p	
	$\nu_3$	CCC a-stretch.	1961 C	1961 W	1954 (19), p	
	$\nu_4$	$\text{CH}_2$ scis.	1432 B	1432 S	1422	
	$\nu_5$	CH bend.	1217 C	1217 VS	1209 (12)	
	$\nu_6$	CCC s-stretch.	1078 C	1078 W	1086 (29), p	
	$\nu_7$	$\text{CH}_2$ wag.	862 C	862 VS	873 (3), dp	
	$\nu_8$	CBr stretch.	681 C	681 VS	667 (31), p	
	$\nu_9$	CCC deform.	603 C	603 W		
	$\nu_{10}$	CCBr deform.	423 C	423 VW	426 (33), p	
				( $\text{CS}_2$ soln.)		
$a''$	$\nu_{11}$	$\text{CH}_2$ a-stretch.	3080 C	3080 M	3060 (46), p	OV( $\nu_1$ ).
	$\nu_{12}$	$\text{CH}_2$ rock.	1000 B	1000 W		
	$\nu_{13}$	CH bend.	812 B	812 S	806 (3), dp	
	$\nu_{14}$	CCC deform.	519 B	519 M		
	$\nu_{15}$	CCCl deform.	169 C		169 (43b), dp	

**Reference**See No. 192( $\text{CH}_2\text{CCHCl}$ ).

**No. 194 Iodopropadiene  $\text{CH}_2\text{CCHI}$**   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a'$	$\nu_1$	CH stretch.	3070 C	3070 M	3057 M	OV( $\nu_{11}$ ).
	$\nu_3$	CCC a-stretch.	1953 C	1953 M	1947 VS	
	$\nu_2$	$\text{CH}_2$ s-stretch.	3004 C	3004 W	2978 VS	
	$\nu_4$	$\text{CH}_2$ scis.	1425 B	1425 M	1412 VS	
	$\nu_5$	CH bend.	1178 C	1178 VS	1174 S, p	
	$\nu_6$	CCC s-stretch.	1076 C	1076 M	1076 VS, p	
	$\nu_7$	$\text{CH}_2$ wag.	854 C	854 S		
	$\nu_8$	CCC deform.	625 C	625 S	635 W	
	$\nu_9$	CI stretch.	609 C	609 S		
	$\nu_{10}$	CCI deform.	387 C		387 S, p	
$a''$	$\nu_{11}$	$\text{CH}_2$ a-stretch.	3070 C	3070 M	3057 M	OV( $\nu_1$ ).
	$\nu_{12}$	$\text{CH}_2$ rock.	995 B	995 W		
	$\nu_{13}$	CH bend.	807 B	807 S		
	$\nu_{14}$	CCC deform.	485 B	485 W		
	$\nu_{15}$	CCI deform.	154 C		154 W	

**Reference**See No. 192( $\text{CH}_2\text{CCHCl}$ ).

**No. 195 Trifluoropropyne  $\text{CF}_3\text{CCH}$** **Symmetry  $\text{C}_{3v}$** **Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	CH stretch.	3327 B	3327.3 S	3316 (9) p	FR( $\nu_4 + \nu_6 + \nu_{10}$ ).
	$\nu_2$	$\text{C}\equiv\text{C}$ stretch.	2165 C	2165.4 S	2156 (80) p	
	$\nu_3$	$\text{CF}_3$ s-stretch.	1253 B	1253.2 VS	1250 (1b)	
	$\nu_4$	C-C stretch.	812 B	811.9 W	810 (50) p	
	$\nu_5$	$\text{CF}_3$ s-deform.	536 B	536.1 M	537 (11) p	
$e$	$\nu_6$	$\text{CF}_3$ d-stretch.	1179 B	1179.2 VS	1155 (5b) dp	
	$\nu_7$	CH bend.	686 B	685.5 S	696 (6) dp	
	$\nu_8$	$\text{CF}_3$ d-deform.	612 B	611.9 M	606 (4) dp	
	$\nu_9$	$\text{CF}_3$ rock.	453 B	453.0 M	445 (6) dp	
	$\nu_{10}$	CCC bend.	171 B	171 M	170 (100) dp	

**References**

- [1] IR.R. C. V. Berney, L. R. Cousins, and F. A. Miller, *Spectrochim. Acta* **19**, 2019 (1963).  
 [2] IR. R. H. Sanborn, *Spectrochim. Acta* **23A**, 1999 (1967).

**No. 196 Trifluoropropyne-d  $\text{CF}_3\text{CCD}$** **Symmetry  $\text{C}_{3v}$** **Symmetry number  $\sigma = 3$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	CD stretch.	2626 B	2626.0 M		
	$\nu_2$	$\text{C}\equiv\text{C}$ stretch.	2014 B	2013.9 S		
	$\nu_3$	$\text{CF}_3$ s-stretch.	1250 B	1249.7 VS		
	$\nu_4$	C-C stretch.	808 B	808.4 W		
	$\nu_5$	$\text{CF}_3$ s-deform.	529 B	528.9 M		
$e$	$\nu_6$	$\text{CF}_3$ d-stretch.	1179 B	1179.0 VS		
	$\nu_8$	$\text{CF}_3$ d-deform.	611 B	611.3 M		
	$\nu_7$	CD bend.	539 B	538.5 S		
	$\nu_9$	$\text{CF}_3$ rock.	456 B	455.5 M		
	$\nu_{10}$	CCC bend.	163 B	163 M		

**References**

- [1] IR.R. C. V. Berney, L. R. Cousins, and F. A. Miller, *Spectrochim. Acta* **19**, 2019 (1963).  
 [2] IR. R. H. Sanborn, *Spectrochim. Acta* **23A**, 1999 (1967).

**No. 197**      **1-Chloro-3,3,3-trifluoropropyne**  $\text{CF}_3\text{CCCl}$   
**Symmetry**  $\text{C}_{3v}$

**Symmetry number**  $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{C}\equiv\text{C}$ stretch.	2270 C	2270 VS	2266 S, p	
	$\nu_2$	$\text{CF}_3$ s-stretch.	1276 C	1276 VS	1272 W	
	$\nu_3$	$\text{C}-\text{C}$ stretch.	937 C	937 S	933 S, p	
	$\nu_4$	$\text{CCl}$ stretch.	723 C	723 S	723 S, p	
	$\nu_5$	$\text{CF}_3$ s-deform.	377 C	377 W	374 S, p	
$e$	$\nu_6$	$\text{CF}_3$ d-stretch.	1174 C	1174 VS	1153 W, b	
	$\nu_7$	$\text{CF}_3$ d-deform.	606 C	606 M	603 W	
	$\nu_8$	$\text{CF}_3$ rock.	448 D		448 M, dp	
	$\nu_9$	$\text{CCCCl}$ deform.	311 C	311 W	316 VS, dp	
	$\nu_{10}$	$\text{CCCCl}$ deform.	97 D		97 VS, dp	

**Reference**

- [1] IR.R.      E. Augdahl, E. Kloster-Jensen, V. Devarajan and S. J. Cyvin, *Spectrochim. Acta* **29A**, 1329 (1973).

**No. 198**      **1-Bromo-3,3,3-trifluoropropyne**  $\text{CF}_3\text{CCBr}$   
**Symmetry**  $\text{C}_{3v}$

**Symmetry number**  $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{C}\equiv\text{C}$ stretch.	2243 C	2243 S	2236 M, p	
	$\nu_2$	$\text{CF}_3$ s-stretch.	1275 C	1275 VS	1267 W	
	$\nu_3$	$\text{C}-\text{C}$ stretch.	883 C	883 S	879 S, p	
	$\nu_4$	$\text{CBr}$ stretch.	687 C	687 S	684 M, p	
	$\nu_5$	$\text{CF}_3$ s-deform.	285 D	285 M	292 VS	
$e$	$\nu_6$	$\text{CF}_3$ d-stretch.	1176 C	1176 VS	1155 W, b	
	$\nu_7$	$\text{CF}_3$ d-deform.	607 C	607 M	606 W	
	$\nu_8$	$\text{CF}_3$ rock.	455 D	455 VW	452 S	
	$\nu_9$	$\text{CCCBBr}$ deform.	278 D	278 VW, sh		
	$\nu_{10}$	$\text{CCCBBr}$ deform.	90 D		90 VS, dp	

**Reference**

See No. 197( $\text{CF}_3\text{CCCl}$ ).



**No. 199** 1-Iodo-3,3,3-trifluoropropyne  $\text{CF}_3\text{CCI}$ Symmetry  $\text{C}_{3v}$ Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a_1$	$\nu_1$	$\text{C}\equiv\text{C}$ stretch.	2218 C	2218 S	2207 S, p	
	$\nu_2$	$\text{CF}_3$ s-stretch.	1264 C	1264 VS	1253 W	
	$\nu_3$	$\text{C}-\text{C}$ stretch.	857 C	857 M	857 S, p	
	$\nu_4$	$\text{CI}$ stretch.	661 C	661 S	658 M	
	$\nu_5$	$\text{CF}_3$ s-deform.	250 D	250 W, sh	254 VS, p	
$e$	$\nu_6$	$\text{CF}_3$ d-stretch.	1174 C	1174 VS	1150 W, b	
	$\nu_7$	$\text{CF}_3$ d-deform.	608 C	608 W	605 W	
	$\nu_8$	$\text{CF}_3$ rock.	450 C	450 W	449 M, dp	
	$\nu_9$	CCCI deform.	263 C	263 M	267 VS, dp	
	$\nu_{10}$	CCCI deform.	85 D		85 VS, dp	

**Reference**See No. 197( $\text{CF}_3\text{CCCl}$ ).**No. 200** Propargyl fluoride  $\text{CHCCH}_2\text{F}$ Symmetry  $\text{C}_s$ Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a'$	$\nu_1$	$\text{CH}$ stretch.	3338 C	3338 S	3330 (4), p	
	$\nu_2$	$\text{CH}_2$ s-stretch.	2955 C	2955 M	2960 (22), p	
	$\nu_3$	$\text{C}=\text{C}$ stretch.	2150 C	2150 W	2135 (43), p	
	$\nu_4$	$\text{CH}_2$ scis.	1465 C	1465 VW	1458 (3), dp	
	$\nu_5$	$\text{CH}_2$ wag.	1381 C	1381 S	1374 (3), dp	
	$\nu_6$	$\text{CF}$ stretch.	1039 C	1039 VS		
	$\nu_7$	$\text{C}-\text{C}$ stretch.	940 C	940 M	935 (6), p	
	$\nu_8$	$\text{CH}$ bend.	675 C	675 S	692 (1), dp	
	$\nu_9$	CCF deform.	539 C	539 W	544 (3), p	
	$\nu_{10}$	CCC deform.	211 C		211 (10), dp	
$a''$	$\nu_{11}$	$\text{CH}_2$ a-stretch.	2972 C	2972 M	2986 (7), dp	
	$\nu_{12}$	$\text{CH}_2$ twist.	1242 D	1240 VW	1242 (1), dp	
	$\nu_{13}$	$\text{CH}_2$ rock.	1018 D	1018 W	1012 (3b), p	
	$\nu_{14}$	$\text{CH}$ bend.	635 C	635 S	646 (1b), dp	
	$\nu_{15}$	CCC deform.	310 C		310 (4), dp	

**Reference**[1] IR.R. J. C. Evans and R. A. Nyquist, *Spectrochim. Acta* **19**, 1153 (1963).

**No. 201 Propargyl chloride  $\text{CHCCH}_2\text{Cl}$**   
 Symmetry  $C_s$ 
Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a'$	$\nu_1$	CH stretch.	3335 C	3335 VS	3305 (2), p	
	$\nu_2$	$\text{CH}_2$ s-stretch.	2968 C	2968 M	2957 (29), p	
	$\nu_3$	$\text{C}\equiv\text{C}$ stretch.	2147 C	2147 W	2130 (35), p	
	$\nu_4$	$\text{CH}_2$ scis.	1441 C	1441 M	1432 (2), p	
	$\nu_5$	$\text{CH}_2$ wag.	1271 C	1271 VS	1267 (5), p	
	$\nu_6$	C-C stretch.	960 C	960 S	961 (2), dp	
	$\nu_7$	CCl stretch.	725 C	725 VS	713 (12), p	
	$\nu_8$	CH bend.	650 D	650 S	650 (2b)	
				( $\text{CS}_2$ soln.)		
	$\nu_9$	CCCl deform.	451 C	451	452 (5), p	
	$\nu_{10}$	CCC deform.	186 D		186 (10), dp	
$a''$	$\nu_{11}$	$\text{CH}_2$ a-stretch.	3002 C	3002 M	2995 (4), dp	
	$\nu_{12}$	$\text{CH}_2$ twist.	1179 B	1179 W	1174 (1), dp	
	$\nu_{13}$	$\text{CH}_2$ rock.	908 D		908 (1), dp	
	$\nu_{14}$	CH bend.	637 D	637 M	650 (2b), dp	
	$\nu_{15}$	CCC deform.	311 C		311 (4), dp	

**Reference**See No. 200( $\text{CHCCH}_2\text{F}$ ).
**No. 202 Propargyl bromide  $\text{CHCCH}_2\text{Br}$**   
 Symmetry  $C_s$ 
Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$	
				(Gas)	(Liquid)	
$a'$	$\nu_1$	CH stretch.	3335 C	3335 S	3305 (2), p	
	$\nu_2$	$\text{CH}_2$ s-stretch.	2976 C	2976 W	2958 (20), p	
	$\nu_3$	$\text{C}\equiv\text{C}$ stretch.	2138 D	2138 VW	2125 (36), p	
	$\nu_4$	$\text{CH}_2$ scis.	1431 C	1431 W	1425 (2), dp	
	$\nu_5$	$\text{CH}_2$ wag.	1218 C	1218 S	1214 (9), p	
	$\nu_6$	C-C stretch.	961 C	961 M	962 (3), p	
	$\nu_7$	CH bend.	652 C	652 VS		
				( $\text{CS}_2$ soln.)		
	$\nu_8$	CBr stretch.	621 C	621 S	618 (22), p	
	$\nu_9$	CCBr deform.	399 C	399	399 (9), p	
				( $\text{CS}_2$ soln.)		
	$\nu_{10}$	CCC deform.	168 C		168 (10), p	
$a''$	$\nu_{11}$	$\text{CH}_2$ a-stretch.	3006 C	3006	3008 (4), p	
				( $\text{CS}_2$ soln.)		
	$\nu_{12}$	$\text{CH}_2$ twist.	1152 D	1152 VW	1146 (1)	
	$\nu_{13}$	$\text{CH}_2$ rock.	866 D		866 (1), dp	
	$\nu_{14}$	CH bend.	637 C	637 S		
	$\nu_{15}$	CCC deform.	314 C		314 (3), dp	

**Reference**See No. 200( $\text{CHCCH}_2\text{F}$ ).

**No. 203 Propargyl iodide  $\text{CHCCH}_2\text{I}$**   
**Symmetry  $\text{C}_s$**

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency $\text{cm}^{-1}$	Infrared $\text{cm}^{-1}$	Raman $\text{cm}^{-1}$	Comments
				(Gas)	(Liquid)	
$a'$	$\nu_1$	CH stretch.	3335 C	3335 S		
	$\nu_2$	$\text{CH}_2$ s-stretch.	2958 C	2958	2957 VS	
				( $\text{CS}_2$ soln.)		
	$\nu_3$	$\text{C}\equiv\text{C}$ stretch.	2130 C	2130 C	2128 VS	
				( $\text{CCl}_4$ soln.)		
	$\nu_4$	$\text{CH}_2$ scis.	1423 C	1423 W	1414	
	$\nu_5$	$\text{CH}_2$ wag.	1160 C	1160 M	1160 VS	
	$\nu_6$	C-C stretch.	959 C	959 W	964 S	
	$\nu_7$	CH bend.	640 C	640 S	650 VW, b	OV( $\nu_{14}$ ).
	$\nu_8$	CI stretch.	570 C	570 W	567 VS	
$a''$	$\nu_9$	CCI deform.	364 C		364 S	
	$\nu_{10}$	CCC deform.	157 C		157 M	
	$\nu_{11}$	$\text{CH}_2$ a-stretch.	3008 D	3008	2990 b	
				( $\text{CS}_2$ soln.)		
	$\nu_{12}$	$\text{CH}_2$ twist.	1116 D	1116		
				( $\text{CS}_2$ soln.)		
	$\nu_{13}$	$\text{CH}_2$ rock.	810 E <sup>a</sup>			
	$\nu_{14}$	CH bend.	640 D	640 S	650 VW, b	OV( $\nu_7$ ).
	$\nu_{15}$	CCC deform.	314 C		314 VW	

<sup>a</sup> Estimated from the corresponding frequencies of other propargyl halides.**Reference**See No. 200( $\text{CHCCH}_2\text{F}$ ).

**No. 204 Chlorodiacetylene  $\text{ClCCCCCH}$**   
**Symmetry  $\text{C}_{2v}$**

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency $\text{cm}^{-1}$	Infrared $\text{cm}^{-1}$	Raman $\text{cm}^{-1}$	Comments
				(Gas)		
$\sigma^-$	$\nu_1$	CH stretch.	3327 C	3327 VS		
	$\nu_2$	$\text{C}\equiv\text{C}$ a-stretch.	2252 C	2252 VS		
	$\nu_3$	$\text{C}\equiv\text{C}$ s-stretch.	2071 C	2071 M		
	$\nu_4$	C-C stretch.	1093 C	1093 S		
	$\nu_5$	CCl stretch.	525 C	525 S		
$\pi$	$\nu_6$	CH bend.	621 B	621 VS		
	$\nu_7$	CCCC a-bend.	463 B	463 S		
	$\nu_8$	CCCC s-bend.	335 C	335 M		
	$\nu_9$	CCCl bend.	133 E	133		OC( $\nu_1 + \nu_9$ , $\nu_6 + \nu_9$ , $\nu_7 + \nu_9$ ).

**Reference**[1] IR. P. Klaboe and E. Kloster-Jensen, Spectrochim. Acta **23A**, 2733 (1967).

**No. 205 Bromodiacetylene BrCCCCH**  
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$\sigma^+$	$\nu_1$	CH stretch.	3335 C	3335 VS		
	$\nu_2$	$\text{C}\equiv\text{C}$ a-stretch.	2237 C	2237 S		
	$\nu_3$	$\text{C}\equiv\text{C}$ s-stretch.	2095 C	2095 W		
	$\nu_4$	C-C stretch.	1046 C	1046 M		
	$\nu_5$	CBr stretch.	425 C	425 M		
$\pi$	$\nu_6$	CH bend.	623 C	623 VS		
	$\nu_7$	CCCC a-bend.	470 B	470 S		
	$\nu_8$	CCCC s-bend.	355 B	355 M		
	$\nu_9$	CCBr bend.	118 E			$\text{OC}(\nu_1+\nu_9, \nu_7+\nu_9).$

**Reference**

See No. 204(CICCCCH).

**No. 206 Iododiacetylene ICCCH**  
Symmetry  $C_{2v}$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$\sigma^-$	$\nu_1$	CH stretch.	3332 C	3332 VS		
	$\nu_2$	$\text{C}\equiv\text{C}$ a-stretch.	2211 C	2211 S		
	$\nu_3$	$\text{C}\equiv\text{C}$ s-stretch.	2060 C	2060 VW		
	$\nu_4$	C-C stretch.	1025 D	1025 VW ( $\text{CS}_2$ soln.)		
$\pi$	$\nu_5$	CI stretch.	362 C	362 M		
	$\nu_6$	CH bend.	623 B	623 VS		
	$\nu_7$	CCCC a-bend.	473 B	473 M		
	$\nu_8$	CCCC s-bend.	357 C	357 W		
	$\nu_9$	CCI bend.	110 E	110		$\text{OC}(\nu_8+\nu_9, \nu_7+\nu_9).$

**Reference**

See No. 204(CICCCCH).

No. 207 1,4-Dioxane  $C_4H_8O_2$ Symmetry  $C_{2h}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$	$cm^{-1}$	
				(Gas)	(Liquid)	
$a_g$	$\nu_1$	$CH_2$ a-stretch.	2968 C	ia	2968 S, p	
	$\nu_2$	$CH_2$ s-stretch.	2856 C	ia	2856 S, p	
	$\nu_3$	$CH_2$ scis.	1444 C	ia	1444 M, p	
	$\nu_4$	$CH_2$ wag.	1397 C	ia	1397 W, p	
	$\nu_5$	$CH_2$ twist.	1305 C	ia	1305 S, p	
	$\nu_6$	$CH_2$ rock.	1128 C	ia	1128 M, p	
	$\nu_7$	CC stretch.	1015 C	ia	1015 S, p	
	$\nu_8$	CO stretch.	837 C	ia	837 VS, p	
	$\nu_9$	OCC deform.	435 C	ia	435 M	
	$\nu_{10}$	COC deform.	424 C	ia	424 M, p	
$a_u$	$\nu_{11}$	$CH_2$ a-stretch.	2970 C	2970 M	ia	
	$\nu_{12}$	$CH_2$ s-stretch.	2863 C	2863 VS	ia	
	$\nu_{13}$	$CH_2$ scis.	1449 C	1449 S	ia	
	$\nu_{14}$	$CH_2$ wag.	1369 C	1369 S	ia	
	$\nu_{15}$	$CH_2$ twist.	1256 C	1256 S	ia	
	$\nu_{16}$	CO stretch.	1136 C	1136 VS	ia	
	$\nu_{17}$	$CH_2$ rock.	1086 C	1086 S	ia	
	$\nu_{18}$	CC stretch.	881 C	881 S	ia	
	$\nu_{19}$	OCC deform.	288 C	288 W,sh	ia	
	$\nu_{20}$	$CH_2$ a-stretch.	2968 C	ia	2968 S, p	SF( $\nu_1$ ).
$b_g$	$\nu_{21}$	$CH_2$ s-stretch.	2856 C	ia	2856 S, p	SF( $\nu_2$ ).
	$\nu_{22}$	$CH_2$ scis.	1459 C	ia	1459 M, dp	
	$\nu_{23}$	$CH_2$ wag.	1335 C	ia	1335 W	
	$\nu_{24}$	$CH_2$ twist.	1217 C	ia	1217 M, dp	
	$\nu_{25}$	CO stretch.	1110 C	ia	1110 M, dp	
	$\nu_{26}$	$CH_2$ rock.	853 C	ia	853 M,sh, dp	
	$\nu_{27}$	OCC deform.	490 C	ia	490 M, dp	
	$\nu_{28}$	$CH_2$ a-stretch.	2970 C	2970 M	ia	SF( $\nu_{11}$ ).
$b_u$	$\nu_{29}$	$CH_2$ a-stretch.	2863 C	2863 VS	ia	SF( $\nu_{12}$ ).
	$\nu_{30}$	$CH_2$ scis.	1457 C	1457 S	ia	
	$\nu_{31}$	$CH_2$ wag.	1378 C	1378 M	ia	
	$\nu_{32}$	$CH_2$ twist.	1291 C	1291 S	ia	
	$\nu_{33}$	$CH_2$ rock.	1052 C	1052 S	ia	
	$\nu_{34}$	CO stretch.	889 C	889 S	ia	
	$\nu_{35}$	OCC deform.	610 C	610 S	ia	
	$\nu_{36}$	COC deform.	274 C	274 S	ia	

## References

- [1] IR.R. F. E. Malherbe and H. J. Bernstein, J. Amer. Chem. Soc. **74**, 4408 (1952), and references cited there.
- [2] IR.Th. R. G. Snyder and G. Zerbi, Spectrochim. Acta **23A**, 391 (1967).
- [3] IR.R.Th. O. H. Ellested and P. Klaboe, Spectrochim. Acta **27A**, 1025 (1971).

**No. 208 Diethynyl ketone (HC≡C)<sub>2</sub>CO**  
**Symmetry C<sub>2v</sub>**
Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	CH stretch.	3325 C	3325 S	3275 W, b	OV( $\nu_{13}$ ).
	$\nu_2$	C≡C stretch.	2097 C	2098 VS, sh	2097 VS, p	
				(liquid)		
	$\nu_3$	CO stretch.	1669 C	1669 S	1636 S, p	
	$\nu_4$	C-C stretch.	739 C	739 VW	749 M, p	
	$\nu_5$	CH bend.	648 C	648 S		
<i>a</i> <sub>2</sub>	$\nu_6$	C-C-C deform.	571 C		571 W	
	$\nu_7$	C≡C-C deform.	122 C	122 VW		
	$\nu_8$	CH bend.	712 C	ia	712 VW, dp	
<i>b</i> <sub>1</sub>	$\nu_9$	C≡C-C deform.	268 C	ia	268 M	
	$\nu_{10}$	CH bend.	729 C	729 S	733 VW	
<i>b</i> <sub>2</sub>					(solid)	
	$\nu_{11}$	CO op-bend.	688 C	688 S	689 VW	
	$\nu_{12}$	C≡C-C deform.	190 C	190 VW	200 W	
	$\nu_{13}$	CH stretch.	3325 C	3325 S	3275 VW, b	OV( $\nu_1$ ).
	$\nu_{14}$	C≡C stretch.	2115 C	2115 S	2107 M	
	$\nu_{15}$	C-C stretch.	1144 C	1144 VS		
	$\nu_{16}$	CH bend.	682 C	682 M		
	$\nu_{17}$	CO ip-bend.	548 C	548 M		
	$\nu_{18}$	C≡C-C deform.	229 C	229 VW	239 M	

**Reference**[1] IR.R. F. A. Miller, B. M. Harney, and J. Tyrrell, Spectrochim. Acta **27A**, 1003 (1971).
**No. 209 Dicyanodiacetylene NCCCCCN**  
**Symmetry D<sub>2h</sub>**
Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup>	cm <sup>-1</sup>	
				(Gas)	(CCl <sub>4</sub> soln.)	
$\sigma_g^+$	$\nu_1$	CN s-stretch.	2235 C	ia	2235 VS, p	
	$\nu_2$	C≡C s-stretch.	2183 C	ia	2183 M, p	
	$\nu_3$	C-C s-stretch.	1288 C	ia	1287.5 W, p	
	$\nu_4$	C-C stretch.	571	ia	571 W, dp	
$\sigma_u^+$	$\nu_5$	CN a-stretch.	2266 B	2266 S	ia	
	$\nu_6$	C=C a-stretch.	2097 B	2097 M	ia	
	$\nu_7$	C-C a-stretch.	717 B	717 S	ia	
$\pi_g$	$\nu_8$	Bend.	501 C	ia	501 M, dp	
	$\nu_9$	Bend.	455 C	ia	455 W, dp	
$\pi_u$					(C <sub>6</sub> H <sub>14</sub> soln.)	
	$\nu_{10}$	Bend.	170 D	ia	170 W, b, dp	
	$\nu_{11}$	Bend.	491 B	490.5 VS	ia	
	$\nu_{12}$	Bend.	276 B	276 VS	ia	
	$\nu_{13}$	Bend.	62 B	61.5 VS	ia	

**Reference**[1] IR.R. F. A. Miller and D. H. Lemmon, Spectrochim. Acta **23A**, 1415 (1967).

No. 210 Hexacarbonylchromium(0)  $\text{Cr}(^{12}\text{C}^{16}\text{O})_6$ Symmetry  $\text{O}_h$ Symmetry number  $\sigma = 24$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ ( $\text{CCl}_4$ soln.)	
$a_{1g}$	$\nu_1$	CO stretch.	2112 C	ia	2112.4 M	
	$\nu_2$	CrC stretch.	381 C	ia	381.2 S	
$e_g$	$\nu_3$	CO stretch.	2018 C	ia	2018.4 M	
	$\nu_4$	CrC stretch.	394 D	ia	394 W	
$f_{1g}$	$\nu_5$	CrCO bend.	364 D	ia	ia	OC( $\nu_5 + \nu_7$ ).
$f_{1u}$	$\nu_6$	CO stretch.	2000 B	2000.4 VS	ia	
	$\nu_7$	CrC stretch.	668 B	668.1 VS	ia	
	$\nu_8$	CrCO bend.	441 B	440.5 S	ia	
	$\nu_9$	CCrC deform.	98 B	97.8 M	ia	
$f_{2g}$	$\nu_{10}$	CrCO bend.	436 D	ia	436.4 (liquid)	
	$\nu_{11}$	CCrC deform.	95 D	ia	94.8 S (liquid)	
$f_{2u}$	$\nu_{12}$	CrCO bend.	511 D	ia	ia	OC( $\nu_{10} + \nu_{12}$ , $\nu_5 + \nu_{12}$ ).
	$\nu_{13}$	CCrC deform.	68 E	ia	ia	OC( $\nu_3 + \nu_{13}$ ).

## References

- [1] IR. N. J. Hawkins, H. C. Mattraw, W. W. Sabol, and D. R. Carpenter, J. Chem. Phys. **23**, 2422 (1955).  
 [2] Th. H. Murata and K. Kawai, J. Chem. Phys. **27**, 605 (1957).  
 [3] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).  
 [4] IR.Th. J. M. Smith and L. H. Jones, J. Mol. Spectry. **20**, 248 (1966).  
 [5] IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).  
 [6] R.Th. R. Pince et R. Poilblanc, Spectrochim. Acta **28A**, 907 (1972).

**No. 211 Hexacarbonylmolybdenum(0) Mo(<sup>12</sup>C<sup>16</sup>O)<sub>6</sub>**  
**Symmetry O<sub>h</sub>**

Symmetry number  $\sigma = 24$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm <sup>-1</sup>	cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (CCl <sub>4</sub> soln.)	
$a_{1g}$	$\nu_1$	CO stretch.	2117 C	ia	2116.7 M	
	$\nu_2$	MoC stretch.	402 C	ia	402.2 S	
$e_g$	$\nu_3$	CO stretch.	2019 C	ia	2018.8 M	
	$\nu_4$	MoC stretch.	392 C	ia	392 W	
$f_{1g}$	$\nu_5$	MoCO bend.	342 D	ia	ia	OC( $\nu_5 + \nu_7$ ).
$f_{1u}$	$\nu_6$	CO stretch.	2003 B	2003.0 VS	ia	
	$\nu_7$	MoC stretch.	596 B	595.6 VS	ia	
	$\nu_8$	MoCO bend.	367 B	367.2 S	ia	
	$\nu_9$	CMoC deform.	82 B	81.6 M	ia	
$f_{2g}$	$\nu_{10}$	MoCO bend.	448 D	ia	448.3	
					(liquid)	
	$\nu_{11}$	CMoC deform.	86 D	ia	86.0 S	
					(liquid)	
$f_{2u}$	$\nu_{12}$	MoCO bend.	507 D	ia	ia	OC( $\nu_5 + \nu_{12}$ , $\nu_{10} + \nu_{12}$ )
	$\nu_{13}$	CMoC deform.	60 E	ia	ia	OC( $\nu_3 + \nu_{13}$ , $\nu_{10} + \nu_{13}$ ).

**References**

- [1] IR. N. J. Hawkins, H. C. Matraw, W. W. Sabol, and D. R. Carpenter, J. Chem. Phys. **23**, 2422 (1955).  
 [2] Th. H. Murata and K. Kawai, J. Chem. Phys. **27**, 605 (1957).  
 [3] IR. L. H. Jones, J. Chem. Phys. **36**, 2375 (1962).  
 [4] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).  
 [5] IR.Th. J. M. Smith and L. H. Jones, J. Mol. Spectry. **20**, 248 (1966).  
 [6] IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).  
 [7] R.Th. R. Pince et R. Poilblanc, Spectrochim. Acta **28A**, 907 (1972).



No. 212 Hexacarbonyltungsten(0)  $\text{W}(^{12}\text{C}^{16}\text{O})_6$ Symmetry  $\text{O}_h$ Symmetry number  $\sigma = 24$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ ( $\text{CS}_2$ soln.)	
$a_{1g}$	$\nu_1$	CO stretch.	2117 C	ia	2116.6 M	
	$\nu_2$	WC stretch.	427 C	ia	427.1 S	
$e_g$	$\nu_3$	CO stretch.	2010 C	ia	2009.8 M	
	$\nu_4$	WC stretch.	412 C	ia	412 W	
$f_{1g}$	$\nu_5$	WCO bend.	362 D	ia	ia	OC( $\nu_5 + \nu_7$ ).
$f_{1u}$	$\nu_6$	CO stretch.	1998 B	1997.6 VS	ia	
	$\nu_7$	WC stretch.	587 B	586.6 VS	ia	
	$\nu_8$	WCO bend.	374 B	374.4 S	ia	
	$\nu_9$	CWC deform.	82 C	82.0 M	ia	
$f_{2g}$	$\nu_{10}$	WCO bend.	458 D	ia	458.3 (liquid)	
	$\nu_{11}$	CWC deform.	88 D	ia	88.3 S (liquid)	
$f_{2u}$	$\nu_{12}$	WCO bend.	521 D	ia	ia	OC( $\nu_5 + \nu_7$ , $\nu_{10} + \nu_{12}$ ).
	$\nu_{13}$	CWC deform.	61 E	ia	ia	

## References

- [1] IR.Th. L. H. Jones, Spectrochim. Acta **19**, 329 (1963).  
 [2] IR.Th. J. M. Smith and L. H. Jones, J. Mol. Spectry. **20**, 248 (1966).  
 [3] IR.R.Th. L. H. Jones, R. S. McDowell, and M. Goldblatt, Inorg. Chem. **8**, 2349 (1969).  
 [4] R.Th. R. Pince et R. Poilblanc, Spectrochim. Acta **28A**, 907 (1972).

### Empirical Formula Index for Consolidated Volumes I and II

In this index molecules are divided into two groups: (a) those containing no carbon atoms, which are arranged with the elemental symbols of the empirical formulas in alphabetical order and are listed alphabetically, and in ascending order of the empirical formula subscripts; (b) molecules containing carbon, which are ordered in the same way except that carbon is listed first and hydrogen second. No distinction is made for isotopic species in the empirical formula; thus deuterium is listed as H.

As an assistance to users of these data, this Index identifies the molecules treated in the present Consolidated Volume II and also those in the earlier Consolidated Volume I, which is available as part of a previous publication series, the NSRDS-NBS series distributed by the U.S. Government Printing Office. It can be ordered as Tables of Molecular Vibrational Frequencies, Consolidated Volume I, (SD Catalog No. C13.48:39), stock number 003-003-00845-1, price \$5.10, from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

#### Compounds Not Containing Carbon

Empirical Formula	Name	Volume and Number	Empirical Formula	Name	Volume and Number
AlCl <sub>3</sub>	Aluminum trichloride	II-36	Br <sub>3</sub> ClSi	Tribromochlorosilane	I-47
AsF <sub>3</sub>	Arsenic trifluoride	II-38	Br <sub>3</sub> GeH	Tribromogermane	II-93
AsF <sub>5</sub>	Arsenic pentafluoride	II-118	Br <sub>3</sub> HSi	Tribromosilane	II-75
AsH <sub>3</sub>	Arsine	I-21	Br <sub>3</sub> OP	Phosphoryl bromide	II-78
AsH <sub>3</sub>	Arsine-d <sub>3</sub>	I-22	Br <sub>4</sub> Ge	Germanium tetrabromide	I-39
AsI <sub>3</sub>	Arsenic triiodide	II-39	Br <sub>4</sub> Hf	Hafnium tetrabromide	II-66
BF <sub>3</sub>	Boron trifluoride- <sup>10</sup> BF <sub>3</sub>	II-31	Br <sub>4</sub> Si	Silicon tetrabromide	I-31
BF <sub>3</sub>	Boron trifluoride- <sup>11</sup> BF <sub>3</sub>	II-22	Br <sub>4</sub> Sn	Tin (IV) bromide	I-41
B <sub>2</sub> H <sub>6</sub>	Diborane- <sup>10</sup> B <sub>2</sub> H <sub>6</sub>	I-55	Br <sub>4</sub> Ti	Titanium tetrabromide	II-59
B <sub>2</sub> H <sub>6</sub>	Diborane- <sup>11</sup> B <sub>2</sub> D <sub>6</sub>	I-56	Br <sub>4</sub> Zn	Zirconium tetrabromide	II-62
BrCl <sub>3</sub> Si	Bromotrichlorosilane	I-45	ClFO <sub>3</sub>	Perchloryl fluoride	II 81
BrF <sub>3</sub>	Bromine trifluoride	II-46	ClF <sub>2</sub> N	Chlorodifluoroammonia	II-53
BrGeH <sub>3</sub>	Germyl bromide	II-88	ClF <sub>2</sub> PS	Thiophosphoryl chlorodifluoride	II-112
BrGeH <sub>3</sub>	Germyl bromide-d <sub>3</sub>	II-89	ClF <sub>3</sub>	Chlorine trifluoride	II-45
BrH <sub>3</sub> Si	Silyl bromide	I-44	ClF <sub>5</sub> S	Sulfur chloride pentafluoride	II-122
BrNO	Nitrosyl bromide- <sup>16</sup> O <sup>14</sup> NBr	II-23	ClF <sub>5</sub> W	Tungsten chloride pentafluoride	II-123
BrNO	Nitrosyl bromide- <sup>16</sup> O <sup>15</sup> NBr	II-24	ClGeH <sub>3</sub>	Germyl chloride	II-86
BrNO	Nitrosyl bromide- <sup>18</sup> O <sup>15</sup> NBr	II-25	ClGeH <sub>3</sub> -d <sub>3</sub>	Germyl chloride-d <sub>3</sub>	II-87
BrO <sub>3</sub> Re	Rhenium (VII) oxide bromide	II-95	ClHO	Hypochlorous acid	II-27
Br <sub>2</sub> Cl <sub>2</sub> Si	Dibromodichlorosilane	I-49	ClHO	Hypochlorous acid-d	II-28
Br <sub>2</sub> FOP	Phosphoryl dibromofluoride	II-111	ClH <sub>3</sub> Si	Silyl chloride	I-43
Br <sub>2</sub> H <sub>2</sub> Si	Dibromosilane	II-100	ClI <sub>3</sub> Si	Chlorotriiodosilane	I-48
Br <sub>2</sub> OS	Thionyl bromide	II-57	ClNO	Nitrosyl chloride- <sup>16</sup> O <sup>14</sup> NO	II-19
Br <sub>2</sub> Sn	Tin (II) bromide	II-12	ClNO	Nitrosyl chloride- <sup>16</sup> O <sup>15</sup> NCl	II-20
			ClNO	Nitrosyl chloride- <sup>18</sup> O <sup>14</sup> NCl	II-21
			ClNO	Nitrosyl chloride- <sup>18</sup> O <sup>15</sup> NCl	II-22
			ClNO <sub>2</sub>	Nitryl chloride-Cl <sup>14</sup> NO <sub>2</sub>	II-43
			ClNO <sub>2</sub>	Nitryl chloride-Cl <sup>15</sup> NO <sub>2</sub>	II-44
			ClNO <sub>3</sub>	Chloronitrate-ClO <sup>14</sup> NO <sub>2</sub>	II-108
			ClNO <sub>3</sub>	Chloronitrate-ClO <sup>15</sup> NO <sub>2</sub>	II-109
			ClNS	Thionitrosyl-S-chloride	II-30
			ClO <sub>3</sub> Re	Rhenium (VII) oxide chloride	II-94
			Cl <sub>2</sub> FN	Dichlorofluoroammonia	II-54
			Cl <sub>2</sub> FOP	Phosphoryl dichlorofluoride	II-110
			Cl <sub>2</sub> FPS	Thiophosphoryl dichlorofluoride	II-113
			Cl <sub>2</sub> Ge	Germanium (II) chloride	II-9
			Cl <sub>2</sub> H <sub>2</sub> Si	Dichlorosilane	II-98
			Cl <sub>2</sub> H <sub>2</sub> Si	Dichlorosilane-d <sub>2</sub>	II 99
			Cl <sub>2</sub> O	Oxygen dichloride	I-8
			Cl <sub>2</sub> OS	Thionyl chloride	II-56
			Cl <sub>2</sub> O <sub>2</sub> S	Sulfuryl chloride	II-97
			Cl <sub>2</sub> Pb	Lead (II) chloride	II-14
			Cl <sub>2</sub> S	Sulfur dichloride	II-8
			Cl <sub>2</sub> Sn	Tin (II) chloride	II-11
			Cl <sub>3</sub> F <sub>2</sub> P	Phosphorus trichloride difluoride	II-115
			Cl <sub>3</sub> GeH	Trichlorogermane	II-92
			Cl <sub>3</sub> HSi	Trichlorosilane	II-73
			Cl <sub>3</sub> HSi	Trichlorosilane-d	II-74
			Cl <sub>3</sub> ISi	Trichloroiodosilane	I-46
			Cl <sub>3</sub> OP	Phosphoryl chloride	II-77
			Cl <sub>3</sub> OV	Vanadyl (V) chloride	II-82

Empirical Formula	Name	Volume and Number	Empirical Formula	Name	Volume and Number
Cl <sub>3</sub> P	Phosphorus trichloride	I-20	F <sub>6</sub> Te	Tellurium hexafluoride	II-120
Cl <sub>3</sub> PS	Thiophosphoryl trichloride	II-80	F <sub>6</sub> U	Uranium (VI) fluoride	I-54
			F <sub>6</sub> W	Tungsten (VI) fluoride	I-53
Cl <sub>4</sub> Ge	Germanium tetrachloride	I-38	GeH <sub>3</sub> I	Germyl iodide	II-90
Cl <sub>4</sub> Hf	Hafnium tetrachloride	II-65	GeH <sub>3</sub> I	Germyl iodide-d <sub>3</sub>	II-91
Cl <sub>4</sub> Si	Silicon tetrachloride	I-30	GeH <sub>4</sub>	Germane	I-33
Cl <sub>4</sub> Sn	Tin (IV) chloride	I-40	GeH <sub>4</sub>	Germane-d <sub>1</sub>	I-34
Cl <sub>4</sub> Ti	Titanium tetrachloride	II-58	GeH <sub>4</sub>	Germane-d <sub>2</sub>	I-35
Cl <sub>4</sub> Zn	Zirconium tetrachloride	II-61	GeH <sub>4</sub>	Germane-d <sub>3</sub>	I-36
			GeH <sub>4</sub>	Germane-d <sub>4</sub>	I-37
Cl <sub>5</sub> P	Phosphorus pentachloride	II-116	Ge <sub>2</sub> H <sub>6</sub>	Digermene	II-125
Cl <sub>5</sub> Sb	Antimony pentachloride	II-119	Ge <sub>2</sub> H <sub>6</sub>	Digermene-d <sub>6</sub>	II-126
FGeH <sub>3</sub>	Germyl fluoride	II-84			
FGeH <sub>3</sub>	Germyl fluoride-d <sub>3</sub>	II-85			
FHO	Hypofluorous acid	II-26	HNO <sub>3</sub>	Nitric acid-H <sup>14</sup> NO <sub>3</sub>	II-102
FH <sub>3</sub> Si	Silyl fluoride	I-42	HNO <sub>3</sub>	Nitric acid-d-D <sup>14</sup> NO <sub>3</sub>	II-103
FMnO <sub>3</sub>	Permanganyl fluoride	II-83	HNO <sub>3</sub>	Nitric acid-H <sup>15</sup> NO <sub>3</sub>	II-104
FNO	Nitrosyl fluoride- <sup>16</sup> O <sup>14</sup> NF	II-15	HNO <sub>3</sub>	Nitric acid-d-D <sup>15</sup> NO <sub>3</sub>	II-105
FNO	Nitrosyl fluoride- <sup>16</sup> O <sup>15</sup> NF	II-16	HN <sub>3</sub>	Hydrazoic acid	II-50
FNO	Nitrosyl fluoride- <sup>18</sup> O <sup>14</sup> NF	II-17	HN <sub>3</sub>	Hydrazoic acid-d	II-51
FNO	Nitrosyl fluoride- <sup>18</sup> O <sup>15</sup> NF	II-18			
FNO <sub>2</sub>	Nitryl fluoride-F <sup>14</sup> NO <sub>2</sub>	II-41	H <sub>2</sub> O	Water	I-4
FNO <sub>2</sub>	Nitryl fluoride-F <sup>15</sup> NO <sub>2</sub>	II-42	H <sub>2</sub> O	Water-H <sub>2</sub> <sup>18</sup> O	II-6
FNO <sub>3</sub>	Fluoronitrate-FO <sup>14</sup> NO <sub>2</sub>	II-106	H <sub>2</sub> O	Water-d <sub>1</sub>	I-5
FNO <sub>3</sub>	Fluoronitrate-FO <sup>15</sup> NO <sub>2</sub>	II-107	H <sub>2</sub> O	Water-d <sub>2</sub>	I-6
FNS	Thionitrosyl-S-fluoride	II-29	H <sub>2</sub> O <sub>2</sub>	Hydrogen peroxide	II-47
F <sub>2</sub> HN	Diffuoroamine	II-52	H <sub>2</sub> S	Hydrogen sulfide	I-9
F <sub>2</sub> N <sub>2</sub>	trans-1,2-Difluorodiazine	II-40	H <sub>2</sub> S	Hydrogen sulfide-d <sub>2</sub>	I-10
F <sub>2</sub> O	Oxygen difluoride	I-7	H <sub>2</sub> S <sub>2</sub>	Hydrogen persulfide	II-48
F <sub>2</sub> Kr	Krypton difluoride	II-1	H <sub>2</sub> Se	Hydrogen selenide	I-12
F <sub>2</sub> OS	Thionyl fluoride	II-55	H <sub>2</sub> Se	Hydrogen selenide-d <sub>1</sub>	I-13
F <sub>2</sub> O <sub>2</sub> S	Sulfuryl fluoride	II-96			
F <sub>2</sub> O <sub>2</sub> Se	Selenium dioxide difluoride	II-101	H <sub>3</sub> N	Ammonia	I-14
F <sub>2</sub> Pb	Lead (II) fluoride	II-13	H <sub>3</sub> N	Ammonia-d <sub>3</sub>	I-15
F <sub>2</sub> S <sub>2</sub>	Diffuoro disulfane	II-49	H <sub>3</sub> N	Ammonia-t <sub>3</sub>	II-34
F <sub>2</sub> Sn	Tin (II) fluoride	II-10	H <sub>3</sub> P	Phosphine	I-17
			H <sub>3</sub> P	Phosphine-d <sub>3</sub>	I-18
F <sub>3</sub> HSi	Trifluorosilane	II-71	H <sub>3</sub> Sb	Stibine	I-23
F <sub>3</sub> HSi	Trifluorosilane-d	II-72	H <sub>3</sub> Sb	Stibine-d <sub>3</sub>	I-24
F <sub>3</sub> N	Nitrogen trifluoride- <sup>14</sup> NF <sub>3</sub>	I-16			
F <sub>3</sub> N	Nitrogen trifluoride- <sup>15</sup> NF <sub>3</sub>	II-35	H <sub>4</sub> Si	Silane	I-25
F <sub>3</sub> NS	Thionitrosyl trifluoride	II-70	H <sub>4</sub> Si	Silane-d <sub>2</sub>	I-26
F <sub>3</sub> OP	Phosphoryl fluoride	II-76	H <sub>4</sub> Si	Silane-d <sub>3</sub>	I-27
F <sub>3</sub> P	Phosphorus trifluoride	I-19	H <sub>4</sub> Si	Silane-d <sub>4</sub>	I-28
F <sub>3</sub> PS	Thiophosphoryl trifluoride	II-79			
			IF <sub>7</sub>	Iodine heptafluoride	II-124
F <sub>4</sub> Si	Silicon tetrafluoride	I-29	I <sub>3</sub> P	Phosphorus triiodide	II-37
F <sub>5</sub> P	Phosphorus pentafluoride	II-114			
F <sub>5</sub> V	Vanadium pentafluoride	II-117	I <sub>4</sub> Hf	Hafnium tetraiodide	II-67
			I <sub>4</sub> Si	Silicon tetraiodide	I-32
F <sub>6</sub> Ir	Iridium (VI) fluoride	II-121	I <sub>4</sub> Ti	Titanium tetraiodide	II-60
F <sub>6</sub> Mo	Molybdenum (VI) fluoride	I-52	I <sub>4</sub> Zr	Zirconium tetraiodide	II-63
F <sub>6</sub> S	Sulfur hexafluoride	I-50			
F <sub>6</sub> Se	Selenium hexafluoride	I-51	NO <sub>2</sub>	Nitrogen dioxide- <sup>14</sup> NO <sub>2</sub>	II-2

Empirical Formula	Name	Volume and Number	Empirical Formula	Name	Volume and Number
NO <sub>2</sub>	Nitrogen dioxide- <sup>15</sup> NO <sub>2</sub>	II-3	CHCl <sub>3</sub>	Trichloromethane	I-89
N <sub>2</sub> O	Nitrous oxide	I-1	CHCl <sub>3</sub>	Trichloromethane-d <sub>1</sub>	I-90
N <sub>2</sub> O	Nitrous oxide- <sup>14</sup> N <sup>15</sup> NO	I-2	ClIF <sub>3</sub>	Trifluoromethane	I-88
N <sub>2</sub> O	Nitrous oxide- <sup>15</sup> N <sub>2</sub> O	I-3	CHF <sub>3</sub>	Trifluoromethane-d	II-139
O <sub>2</sub> S	Sulfur dioxide	I-11	CHN	Hydrogen cyanide	I-62
O <sub>2</sub> S	Sulfur dioxide-S <sup>18</sup> O <sub>2</sub>	II-7	CHN	Hydrogen cyanide-d <sub>1</sub>	I-63
O <sub>3</sub>	Ozone- <sup>16</sup> O <sub>3</sub>	II-4	CHNO	Isocyanic acid	II-134
O <sub>3</sub>	Ozone- <sup>18</sup> O <sub>3</sub>	II-5	CHNO	Isocyanic acid-d	II-135
O <sub>3</sub> S	Sulfur trioxide	II-33	CH <sub>2</sub> BrCl	Bromochloromethane	I-102
O <sub>4</sub> Os	Osmium tetroxide-Os <sup>16</sup> O <sub>4</sub>	II-68	CH <sub>2</sub> BrCl	Bromochloromethane-d <sub>1</sub>	I-103
O <sub>4</sub> Os	Osmium tetroxide-Os <sup>18</sup> O <sub>4</sub>	II-69	CH <sub>2</sub> BrCl	Bromochloromethane-d <sub>2</sub>	I-104
O <sub>4</sub> Ru	Ruthenium tetroxide	II-64	CH <sub>2</sub> Br <sub>2</sub>	Dibromomethane	I-98
<b>Compounds Containing Carbon</b>			CH <sub>2</sub> Br <sub>2</sub>	Dibromomethane-d <sub>1</sub>	I-99
CBrClO	Carbonyl bromochloride	II-137	CH <sub>2</sub> Br <sub>2</sub>	Dibromomethane-d <sub>2</sub>	I-100
CBrClS	Thiocarbonyl bromochloride	II-138	CH <sub>2</sub> Cl <sub>2</sub>	Dichloromethane	I-95
CBrCl <sub>2</sub> F	Bromodichlorofluoromethane	II-148	CH <sub>2</sub> Cl <sub>2</sub>	Dichloromethane-d <sub>1</sub>	I-96
CBrCl <sub>3</sub>	Bromotrichloromethane	I-93	CH <sub>2</sub> Cl <sub>2</sub>	Dichloromethane-d <sub>2</sub>	I-97
CBrF <sub>3</sub>	Bromotrifluoromethane	II-141	CH <sub>2</sub> O	Formaldehyde	I-68
CBrN	Cyanogen bromide- <sup>79</sup> BrCN	I-66	CH <sub>2</sub> O	Formaldehyde-d <sub>1</sub>	I-69
CBrN	Cyanogen bromide- <sup>81</sup> BrCN	I-67	CH <sub>2</sub> O	Formaldehyde-d <sub>2</sub>	I-70
CBr <sub>2</sub> ClF	Dibromochlorofluoromethane	II-149	CH <sub>2</sub> O <sub>2</sub>	Formic acid	I-105
CBr <sub>2</sub> Cl <sub>2</sub>	Dibromodichloromethane	I-101	CH <sub>2</sub> O <sub>2</sub>	Formic acid-d <sub>2</sub>	I-106
CBr <sub>2</sub> F <sub>2</sub>	Dibromodifluoromethane	II-147	CH <sub>3</sub> BO	Borine carbonyl- <sup>10</sup> BH <sub>3</sub> CO	II-150
CBr <sub>2</sub> O	Carbonyl bromide	II-131	CH <sub>3</sub> BO	Borine carbonyl-d <sub>3</sub> <sup>10</sup> BD <sub>3</sub> CO	II-151
CBr <sub>3</sub> Cl	Tribromochloromethane	I-94	CH <sub>3</sub> BO	Borine carbonyl- <sup>11</sup> BH <sub>3</sub> CO	II-152
CBr <sub>3</sub> F	Tribromofluoromethane	II-145	CH <sub>3</sub> BO	Borine carbonyl-d <sub>3</sub> <sup>11</sup> BD <sub>3</sub> CO	II-153
CBr <sub>4</sub>	Carbon tetrabromide	I-78	CH <sub>3</sub> Br	Methylbromide	I-84
CClFO	Carbonyl chlorofluoride	II-136	CH <sub>3</sub> Br	Methylbromide-d <sub>3</sub>	I-85
CClF <sub>3</sub>	Chlorotrifluoromethane	II-140	CH <sub>3</sub> Cl	Methylchloride	I-82
CClN	Cyanogen chloride- <sup>35</sup> ClCN	I-64	CH <sub>3</sub> Cl	Methylchloride-d <sub>3</sub>	I-83
CClN	Cyanogen chloride- <sup>37</sup> ClCN	I-65	CH <sub>3</sub> F	Methylfluoride	I-80
CCl <sub>2</sub> F <sub>2</sub>	Dichlorodifluoromethane	II-146	CH <sub>3</sub> F	Methylfluoride-d <sub>3</sub>	I-81
CCl <sub>2</sub> O	Carbonyl chloride	II-130	CH <sub>3</sub> GeI <sub>3</sub>	Methyltriiodogermane	II-159
CCl <sub>2</sub> S	Thiocarbonyl chloride	II-133	CH <sub>3</sub> HgI	Methylmercuric iodide	II-154
CCl <sub>3</sub> F	Trichlorofluoromethane	II-143	CH <sub>3</sub> I	Methyliodide	I-86
CCl <sub>3</sub> I	Trichloriodomethane	II-144	CH <sub>3</sub> I	Methyliodide-d <sub>3</sub>	I-87
CCl <sub>4</sub>	Carbon tetrachloride	I-77	CH <sub>4</sub>	Methane	I-71
CFN	Cyanogen fluoride	II-127	CH <sub>4</sub>	Methane-d <sub>1</sub>	I-72
CF <sub>2</sub> O	Carbonyl fluoride	II-129	CH <sub>4</sub>	Methane-d <sub>2</sub>	I-73
CF <sub>2</sub> S	Thiocarbonyl fluoride	II-132	CH <sub>4</sub>	Methane-d <sub>3</sub>	I-74
CF <sub>3</sub> I	Trifluoroiodomethane	II-142	CH <sub>4</sub>	Methane-d <sub>4</sub>	I-75
CF <sub>4</sub>	Carbon tetrafluoride	I-76	CH <sub>4</sub> O	Methanol (Gas)	I-107
CIN	Cyanogen iodide	II-128	CH <sub>4</sub> O	Methanol (Liquid)	I-108
Cl <sub>4</sub>	Carbon tetraiodide	I-79	CH <sub>4</sub> O	Methanol-d <sub>1</sub> (Gas)	I-109
COS	Carbonyl sulfide	I-61	CH <sub>4</sub> O	Methanol-d <sub>1</sub> (Liquid)	I-110
CO <sub>2</sub>	Carbon dioxide	I-58	CH <sub>4</sub> O	Methanol-d <sub>3</sub> (Gas)	I-111
CO <sub>2</sub>	Carbon dioxide- <sup>13</sup> CO <sub>2</sub>	I-59	CH <sub>4</sub> O	Methanol-d <sub>3</sub> (Liquid)	I-112
CS <sub>2</sub>	Carbon disulfide	I-60	CH <sub>4</sub> O	Methanol-d <sub>4</sub> (Gas)	I-113
CHBr <sub>3</sub>	Tribromomethane	I-91	CH <sub>5</sub> N	Methylamine	I-114
CHBr <sub>3</sub>	Tribromomethane-d <sub>1</sub>	I-92	CH <sub>5</sub> N	Methylamine-d <sub>2</sub>	I-115
			CH <sub>5</sub> N	Methylamine-d <sub>3</sub>	I-116
			CH <sub>5</sub> N	Methylamine-d <sub>5</sub>	I-117
			CH <sub>6</sub> Ge	Methylgermane	II-157
			CH <sub>6</sub> Ge	Methyl-d <sub>3</sub> -germane	II-158
			CH <sub>4</sub> Si	Methylsilane	II-155
			CH <sub>6</sub> Si	Methylsilane-d <sub>3</sub>	II-156

Empirica Formula	Name	Volume and Number	Empirica Formula	Name	Volume and Number
CH <sub>3</sub> Sn	Methylstannane	II-160	C <sub>2</sub> H <sub>4</sub> BrCl	1-Bromo-2-chloroethane (gauche form)	I-161
CH <sub>3</sub> Sn	Methylstannane-d <sub>3</sub>	II-161	C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>	1,2-Dibromoethane (trans form)	I-161
CH <sub>3</sub> Sn	Methyl-d <sub>3</sub> -stannane	II-162	C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>	1,2-Dibromoethane (gauche form)	I-161
C <sub>2</sub> BrCl	Bromochloroacetylene	II-167	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	1,2-Dichloroethane (trans form)	I-161
C <sub>2</sub> BrI	Bromoiodoacetylene	II-169	C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	1,2-Dichloroethane (gauche form)	I-161
C <sub>2</sub> Br <sub>2</sub>	Dibromoacetylene	II-165	C <sub>2</sub> H <sub>4</sub> O	Ethylene oxide	I-149
C <sub>2</sub> Br <sub>4</sub>	Tetrabromoethylene	I-128	C <sub>2</sub> H <sub>4</sub> O	Ethylene oxide-d <sub>4</sub>	I-150
C <sub>2</sub> Br <sub>6</sub>	Hexabromoethane	I-159	C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde	I-151
C <sub>2</sub> ClI	Chloroiodoacetylene	II-168	C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde-d <sub>1</sub>	I-152
C <sub>2</sub> Cl <sub>2</sub>	Dichloroacetylene	II-164	C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde-d <sub>4</sub>	I-153
C <sub>2</sub> Cl <sub>2</sub> F <sub>2</sub>	trans-1,2-Dichloro- 1,2-difluoroethylene	I-138	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate	I-170
C <sub>2</sub> Cl <sub>2</sub> F <sub>2</sub>	1,1-Dichloro-2,2-difluoroethylene	I-142	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate-d <sub>1</sub>	I-171
C <sub>2</sub> Cl <sub>4</sub>	Tetrachloroethylene	I-127	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate-d <sub>3</sub>	I-172
C <sub>2</sub> Cl <sub>6</sub>	Hexachloroethane	I-158	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate-d <sub>4</sub>	I-173
C <sub>2</sub> F <sub>3</sub> N	Trifluoroacetonitrile	II-170	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Acetic acid	I-174
C <sub>2</sub> F <sub>4</sub>	Tetrafluoroethylene	I-126	C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Acetic acid-d <sub>1</sub>	I-175
C <sub>2</sub> F <sub>6</sub>	Hexafluoroethane	I-157	C <sub>2</sub> H <sub>4</sub> Si	Silylacetylene	I-148
C <sub>2</sub> I <sub>2</sub>	Diiodoacetylene	II-166	C <sub>2</sub> H <sub>5</sub> Br	Bromoethane	I-168
C <sub>2</sub> N <sub>2</sub>	Cyanogen	II-163	C <sub>2</sub> H <sub>5</sub> Cl	Chloroethane	I-167
C <sub>2</sub> HBr	Bromoacetylene	I-123	C <sub>2</sub> H <sub>5</sub> F	Fluoroethane	I-166
C <sub>2</sub> HCl	Chloroacetylene	I-122	C <sub>2</sub> H <sub>5</sub> N	Ethylene imine	I-169
C <sub>2</sub> HF	Fluoroacetylene	I-121	C <sub>2</sub> H <sub>6</sub>	Ethane	I-154
C <sub>2</sub> H <sub>2</sub>	Acetylene	I-118	C <sub>2</sub> H <sub>6</sub>	Ethane-d <sub>3</sub>	I-155
C <sub>2</sub> H <sub>2</sub>	Acetylene-d <sub>1</sub>	I-119	C <sub>2</sub> H <sub>6</sub>	Ethane-d <sub>6</sub>	I-156
C <sub>2</sub> H <sub>2</sub>	Acetylene-d <sub>2</sub>	I-120	C <sub>2</sub> H <sub>6</sub> Cd	Dimethylcadmium	II-181
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	trans-1,2-Dichloroethylene	I-132	C <sub>2</sub> H <sub>6</sub> Cd	Dimethylcadmium-d <sub>6</sub>	II-182
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	trans-1,2-Dichloroethylene-d <sub>1</sub>	I-133	C <sub>2</sub> H <sub>6</sub> Hg	Dimethylmercury	II-183
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	trans-1,2-Dichloroethylene-d <sub>2</sub>	I-134	C <sub>2</sub> H <sub>6</sub> Hg	Dimethylmercury-d <sub>6</sub>	II-184
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	cis-1,2-Dichloroethylene	I-135	C <sub>2</sub> H <sub>6</sub> N <sub>2</sub>	Azomethane	II-185
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	cis-1,2-Dichloroethylene-d <sub>1</sub>	I-136	C <sub>2</sub> H <sub>6</sub> N <sub>2</sub>	Azomethane-d <sub>6</sub>	II-186
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	cis-1,2-Dichloroethylene-d <sub>2</sub>	I-137	C <sub>2</sub> H <sub>6</sub> O	Dimethylether	I-176
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	1,1-Dichloroethylene	I-139	C <sub>2</sub> H <sub>6</sub> O	Dimethylether-d <sub>3</sub>	I-177
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	1,1-Dichloroethylene-d <sub>1</sub>	I-140	C <sub>2</sub> H <sub>6</sub> Zn	Dimethylzinc	II-179
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	1,1-Dichloroethylene-d <sub>2</sub>	I-141	C <sub>2</sub> H <sub>6</sub> Zn	Dimethylzinc-d <sub>6</sub>	II-180
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	cis-1,2-Difluoroethylene	I-129	C <sub>3</sub> BrF <sub>3</sub>	1-Bromo-3,3,3-trifluoropropyne	II-198
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	cis-1,2-Difluoroethylene-d <sub>1</sub>	I-130	C <sub>3</sub> BrN	Bromo cyanoacetylene	II-190
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	cis-1,2-Difluoroethylene-d <sub>2</sub>	I-131	C <sub>3</sub> ClF <sub>3</sub>	1-Chloro-3-3-3-trifluoropropyne	II-197
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	trans-1,2-Difluoroethylene	II-171	C <sub>3</sub> ClN	Chloro cyanoacetylene	II-189
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	trans-1,2-Difluoroethylene-d <sub>1</sub>	II-172	C <sub>3</sub> F <sub>3</sub> I	1-Iodo-3-3-3-trifluoropropyne	II-199
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	trans-1,2-Difluoroethylene-d <sub>2</sub>	II-173	C <sub>3</sub> IN	Iodo cyanoacetylene	II-191
C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> O	1,2,5-Oxadiazole	I-147	C <sub>3</sub> O <sub>2</sub>	Carbon suboxide	II-187
C <sub>2</sub> H <sub>2</sub> O	Glyoxal	II-174	C <sub>3</sub> S <sub>2</sub>	Carbon subsulfide	II-188
C <sub>2</sub> H <sub>2</sub> O	Glyoxal-d <sub>1</sub>	II-175	C <sub>3</sub> HF <sub>3</sub>	Trifluoropropyne	II-195
C <sub>2</sub> H <sub>2</sub> O	Glyoxal-d <sub>2</sub>	II-176	C <sub>3</sub> HF <sub>3</sub>	Trifluoropropyne-d	II-196
C <sub>2</sub> H <sub>3</sub> N	Methylcyanide	I-143	C <sub>3</sub> H <sub>2</sub> N <sub>2</sub>	Malononitrile	I-183
C <sub>2</sub> H <sub>3</sub> N	Methylcyanide-d <sub>3</sub>	I-144	C <sub>3</sub> H <sub>2</sub> N <sub>2</sub>	Malononitrile-d <sub>2</sub>	I-184
C <sub>2</sub> H <sub>3</sub> N	Methyl isocyanide	I-145	C <sub>3</sub> H <sub>3</sub> Br	Bromopropadiene	II-193
C <sub>2</sub> H <sub>3</sub> N	Methyl isocyanide-d <sub>3</sub>	I-146	C <sub>3</sub> H <sub>3</sub> Br	Propargyl bromide	II-202
C <sub>2</sub> H <sub>3</sub> OF	Acetyl fluoride	II-177	C <sub>3</sub> H <sub>3</sub> Cl	Chloropropadiene	II-192
C <sub>2</sub> H <sub>3</sub> OF	Acetyl fluoride-d <sub>3</sub>	II-178	C <sub>3</sub> H <sub>3</sub> Cl	Propargyl chloride	II-201
C <sub>2</sub> H <sub>4</sub>	Ethylene	I-124	C <sub>3</sub> H <sub>3</sub> F	Propargyl fluoride	II-200
C <sub>2</sub> H <sub>4</sub>	Ethylene-d <sub>4</sub>	I-125	C <sub>3</sub> H <sub>3</sub> I	Iodopropadiene	II-194
C <sub>2</sub> H <sub>4</sub> BrCl	1-Bromo-2-chloroethane (trans form)	I-164	C <sub>3</sub> H <sub>3</sub> I	Propargyl iodide	II-203
			C <sub>3</sub> H <sub>4</sub>	Allene	I-178

Empirical Formula	Name	Volume and Number	Empirical Formula	Name	Volume and Number
$C_3H_4$	Methylacetylene	I-179	$C_4H_6$	1,3-Butadiene	I-205
$C_3H_4$	Methylacetylene- $d_1$	I-180	$C_4H_6$	1,3-Butadiene-1- $d_1$ , trans	I-206
$C_3H_4$	Methyl- $d_3$ -acetylene	I-181	$C_4H_6$	1,3-Butadiene-1,1,2- $d_3$	I-207
$C_3H_4$	Methylacetylene- $d_4$	I-182	$C_4H_6$	1,3-Butadiene-1,1,4,4- $d_4$	I-208
$C_3H_4O$	Propenal	I-185	$C_4H_6$	1,3-Butadiene- $d_6$	I-209
$C_3H_5N$	Ethylcyanide	I-188	$C_4H_6$	2-Butyne	I-210
$C_3H_6$	Cyclopropane	I-186	$C_4H_8$	Cyclobutane	I-211
$C_3H_6$	Cyclopropane- $d_6$	I-187	$C_4H_8$	Cyclobutane- $d_8$	I-212
$C_3H_6O$	Acetone	I-189	$C_4H_8$	2-Methylpropene	I-213
$C_3H_6O$	Acetone- $d_3$	I-190	$C_4H_8$	2-Methyl- $d_3$ -propene-3,3,3- $d_3$	I-214
$C_3H_6O$	Acetone- $d_6$	I-191	$C_4H_8O$	2-Butanone (trans form)	I-215
$C_3H_6O_2$	Methyl acetate	I-197	$C_4H_8O_2$	1,4-Dioxane	II-207
$C_3H_6O_2$	Methyl acetate- $d_3$	I-198	$C_4H_{10}$	n-Butane (trans form)	I-216
$C_3H_6O_2$	Methyl- $d_3$ -acetate	I-199	$C_4H_{10}$	n-Butane (gauche form)	I-217
$C_3H_6O_2$	Methyl acetate- $d_6$	I-200			
$C_3H_8$	Propane	I-192	$C_5H_2O$	Diethynyl ketone	II-208
$C_3H_8$	Propane- $d_2$	I-193			
$C_3H_8$	Propane- $d_3$	I-194	$C_6CrO_6$	Hexacarbonylchromium	II-210
$C_3H_8$	Propane- $d_6$	I-195	$C_6MoO_6$	Hexacarbonylmolybdenum	II-211
$C_3H_8$	Propane- $d_8$	I-196	$C_6N_2$	Dicyanodiacetylene	II-209
$C_4HBr$	Bromodiacetylene	II-205	$C_6O_6W$	Hexacarbonyltungsten	II-212
$C_4HCl$	Chlorodiacetylene	II-204	$C_6H_6$	Benzene	I-218
$C_4HI$	Iododiacetylene	II-206	$C_6H_6$	Benzene- $d_6$	I-219
$C_4H_2$	Butadiyne	I-201	$C_6H_{12}$	Cyclohexane	I-220
$C_4H_4O$	Furan	I-202	$C_6H_{12}$	Cyclohexane- $d_{12}$	I-221
$C_4H_4S$	Thiophene	I-203	$-(CH_2)_n-$	Poly-(methylene) $_n$	I-222
$C_4H_4S$	Thiophene- $d_4$	I-204	$-(CH_2)_n-$	Poly-(methylene- $d_2$ ) $_n$	I-223