

# **Tables of Molecular Vibrational Frequencies: Part 6**

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# Tables of Molecular Vibrational Frequencies

## Part 6

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The compilations of fundamental vibrational frequencies of molecules previously published in the NSRDS-NBS publication series and in this journal are here extended to 55 additional molecules. 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 ref. [1] plus tables for 52 additional molecules (a total of 223 molecules). A fifth set of tables, covering 58 molecules, was published in Volume 1 of this journal [3].

### 2. Molecules Selected

The present volume contains tables of fundamental vibrational frequencies for 55 additional 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 refs. [4], [5], and [6] 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.

A list of the molecules covered here is given at the beginning of the tables. The molecules are numbered starting with number 282, continuing the designations of Part 5 of the tables. In sum, these tables now offer data on nearly 340 molecules. To assist the reader in finding the information he needs, two indices are appended, covering the contents of the Consolidated Volume, plus Part 5 and the present material. The first index is ordered by structural and symmetry factors, and the second by empirical formula.

### 3. Description of 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 refs. [7] and [8].

#### 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 ref. [8], page 508.

#### 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

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

12–30 of ref. [8]. 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 ref. [8].

### 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 tradition. 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.

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
$C_s$	$A'$ , $A''$
$C_1$	$A_g$ , $A_u$
$C_{2v}$	$A_1$ , $A_2$ , $B_1$ , $B_2$
$C_{2h}$	$A_g$ , $A_u$ , $B_g$ , $B_u$
$D_2$	$A$ , $B_1$ , $B_2$ , $B_3$
$D_{2h}$	$A_g$ , $A_u$ , $B_{1g}$ , $B_{1u}$ , $B_{2g}$ , $B_{2u}$ , $B_{3g}$ , $B_{3u}$
$C_{3v}$	$A_1$ , $A_2$ , E
$D_3$	$A_1$ , $A_2$ , E
$C_{5v}$	$A_1$ , $A_2$ , $E_1$ , $E_2$
$C_{\infty v}$	$\Sigma^+$ , $\Sigma^-$ , $\pi$ , $\Delta$ , $\Phi$ , ...
$C_{4v}$ , $D_4$ , $D_{2d}$	$A_1$ , $A_2$ , $B_1$ , $B_2$ , E
$C_{6v}$ , $D_6$	$A_1$ , $A_2$ , $B_1$ , $B_2$ , $E_1$ , $E_2$
$D_{3d}$	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , $E_g$ , $E_u$
$D_{4d}$	$A_1$ , $A_2$ , $B_1$ , $B_2$ , $E_1$ , $E_2$ , $E_3$
$D_{3h}$	$A'_1$ , $A''_1$ , $A'_2$ , $A''_2$ , $E'_1$ , $E''_1$ , $E'_2$ , $E''_2$
$D_{5h}$	$A'_1$ , $A''_1$ , $A'_2$ , $A''_2$ , $E'_1$ , $E''_1$ , $E'_2$ , $E''_2$
$D_{4h}$	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , $B_{1g}$ , $B_{1u}$ , $B_{2g}$ , $B_{2u}$ , $E_g$ , $E_u$
$D_{6h}$	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , $B_{1g}$ , $B_{1u}$ , $B_{2g}$ , $B_{2u}$ , $E_{1g}$ , $E_{1u}$ , $E_{2g}$ , $E_{2u}$
$D_{\infty h}$	$\Sigma_g^+$ , $\Sigma_u^+$ , $\Sigma_g^-$ , $\Sigma_u^-$ , $\pi_g$ , $\pi_u$ , $\Delta_g$ , $\Delta_u$ , $\Phi_g$ , $\Phi_u$ , ...
$C_3$	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 <sub>1</sub> , F <sub>2</sub>
O <sub>h</sub>	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , E <sub>g</sub> , E <sub>u</sub> , F <sub>1g</sub> , F <sub>1u</sub> , F <sub>2g</sub> , F <sub>2u</sub>
T	A, E, F

### 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.

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

TABLE II. Definition of local symmetry coordinates

- (a) Local symmetry coordinates for the  $\text{CH}_3$  group (see fig. 1a)
  - $\text{CH}_3$  symmetrical stretching:  $(\Delta r_1 + \Delta r_2 + \Delta r_3) / \sqrt{3}$
  - $\text{CH}_3$  degenerate stretching:  $(2\Delta r_1 - \Delta r_2 - \Delta r_3) / \sqrt{6}$   
 $(\Delta r_2 - \Delta r_3) / \sqrt{2}$
  - $\text{CH}_3$  symmetrical deformation:  
 $(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12} - \Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3) / \sqrt{6}$
  - $\text{CH}_3$  degenerate deformation:  $(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12}) / \sqrt{6}$   
 $(\Delta\alpha_{31} - \Delta\alpha_{12}) / \sqrt{2}$
  - $\text{CH}_3$  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  $\text{CH}_2$  group (see fig. 1b)
  - $\text{CH}_2$  symmetrical stretching:  $(\Delta r_1 + \Delta r_2) / \sqrt{2}$
  - antisymmetrical stretching:  $(\Delta r_1 - \Delta r_2) / \sqrt{2}$
  - $\text{CH}_2$  scissors:  $(4\Delta\alpha - \Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y}) / \sqrt{20}$
  - $\text{CH}_2$  wagging:  $(\Delta\beta_{1X} + \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y}) / 2$
  - $\text{CH}_2$  twisting:  $(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y}) / 2$
  - $\text{CH}_2$  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:  $\Delta r_{\text{CH}}$
  - CH bending:  $(2\Delta\beta_{\text{HX}} - \Delta\beta_{\text{HY}} - \Delta\beta_{\text{HZ}}) / \sqrt{6}$   
 $(\Delta\beta_{\text{HY}} - \Delta\beta_{\text{HZ}}) / \sqrt{2}$
- (d) Local symmetry coordinates for the planar  $\text{CH}_2$  group (see fig. 1d)
  - $\text{CH}_2$  symmetrical stretching:  $(\Delta r_1 + \Delta r_2) / \sqrt{2}$
  - $\text{CH}_2$  antisymmetrical stretching:  $(\Delta r_1 - \Delta r_2) / \sqrt{2}$
  - $\text{CH}_2$  scissors:  $(2\Delta\alpha - \Delta\beta_1 - \Delta\beta_2) / \sqrt{6}$
  - $\text{CH}_2$  rocking:  $(\Delta\beta_1 - \Delta\beta_2) / \sqrt{2}$
  - $\text{CH}_2$  wagging:  $\Delta\theta \cdot \sin \alpha$ .
- (e) Local symmetry coordinates for the planar CH group (see fig. 1e)
  - CH stretching:  $\Delta r_{\text{CH}}$
  - in-plane CH bending:  $(\Delta\beta_{\text{HX}} - \Delta\beta_{\text{HY}}) / \sqrt{2}$
  - out-of-plane CH bending:  $\Delta\theta_{\text{H}} \cdot \sin \gamma_{\text{XY}}$ .

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  $\text{CX}_3$  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

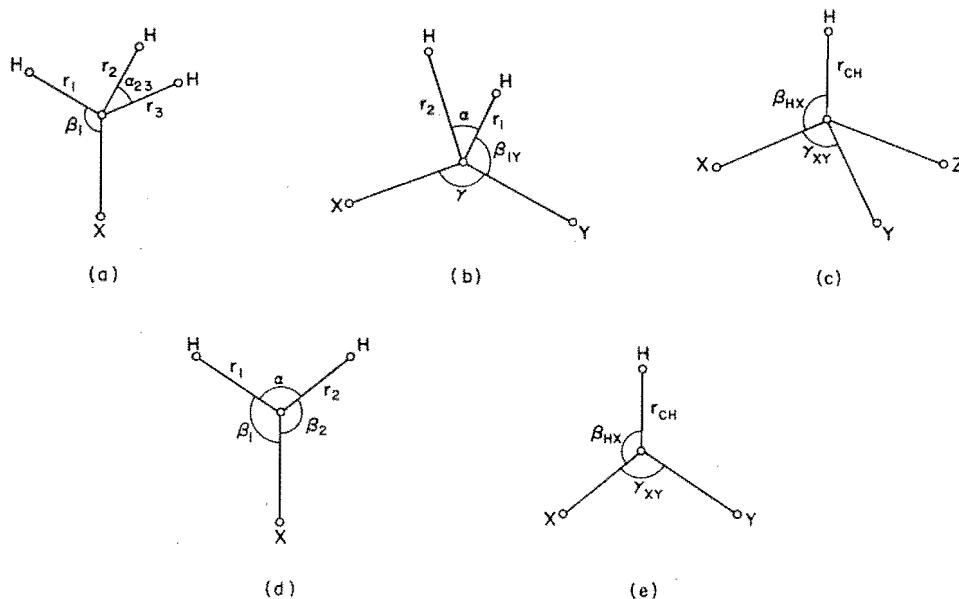


FIGURE 1. Parameters of methyl, methylene, and methin groups.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis*
A	$\text{cm}^{-1}$ 0 ~ 1	(i) Gas, grating spectrometer, rotational fine structure accurately analyzed. (ii) Gas, grating spectrometer, a sharp $Q$ branch.
B	1 ~ 3	(i) Gas, grating spectrometer, rotational fine structure partly analyzed. (ii) Gas, prism spectrometer, fairly high resolution (e.g., $700 \sim 1000 \text{ cm}^{-1}$ for NaCl prism).
C	3 ~ 6	(i) Gas, prism spectrometer, low resolution (e.g., $1000 \sim 2000 \text{ cm}^{-1}$ for NaCl prism). (ii) Solid, liquid or solution, accurate measurement.
D	6 ~ 15	(i) Gas, prism spectrometer, very low resolution (e.g., $> 2000 \text{ cm}^{-1}$ 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.

\*The uncertainty assigned here to each method of measurement is a typical value; greater accuracy is often achieved with some of the methods.

symmetry none of the normal vibrations are genuinely "symmetrical" or "degenerate" with respect to the three-fold symmetry axis of the  $\text{CX}_3$  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

The fundamental frequency  $\nu_i$  is defined as the difference between the term value  $G(\nu_i = 1, \text{all other } \nu_j = 0)$  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.

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 non-vibrational part  $A'\zeta^2$ , where  $A'$  is the rotational constant of the vibrational level and  $\zeta$  of the Coriolis coupling constant. This is in accord with the definition of  $\nu_0$  given in ref. [8], 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  $\text{cm}^{-1}$ ) 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 ref. [10] 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 will be found in ref. [9].

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 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 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.

### 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. Acknowledgements

I acknowledge the assistance of the members of my laboratory at the University of Tokyo in carrying out this project. I also express my sincere thanks to many members of the National Bureau of Standards, particularly to C. W. Beckett, D. R. Lide, Jr., E. L. Brady, and S. A. Rossmassler, who offered helpful suggestions in the planning of the tables, and to Carla Messina and J. H. Hilsenrath, who have provided invaluable guidance in automating the production and printing of these tables.

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## 6. List of Tables of Molecular Vibrational Frequencies

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**No. 282 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		
$b_1$	$\nu_3$	Anti. stretch.	3742 A	3741.58		

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**No. 283 Sulfur dioxide  $\text{S}^{18}\text{O}_2$** 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)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	1101 B	1100.65		
	$\nu_2$	Bend.	497 B	496.7		
$b_1$	$\nu_3$	Anti. stretch.	1318 B	1317.9		

**Reference**

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

**No. 284 Hypochlorous acid  $\text{HOCl}$** 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)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	OH stretch.	3609 A	3609 M		
	$\nu_2$	OCl stretch.	739 C	739 M		
	$\nu_3$	Bend.	1242 C	1242 S		

**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).

**No. 285 Hypochlorous acid-d DOCl**  
**Symmetry C<sub>s</sub>**

**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		
	$\nu_2$	OCl stretch.	739 C	739 M		
	$\nu_3$	Bend.	911 C	911 S		

**References**

See No. 284 (HOCl)

**No. 286 Thionitrosyl-S-fluoride NSF**  
**Symmetry C<sub>s</sub>**

**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		

**Reference**

[1] IR. H. Richert and O. Glemser, Z. Anorg. Allg. Chem. **307**, 328 (1961).

**No. 287 Thionitrosyl-S-chloride NSCl**  
**Symmetry C<sub>s</sub>**

**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. 288 trans-1,2-Difluorodiazine  $N_2F_2$ Symmetry  $C_{2h}$ Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (Gas)
$a_g$	$\nu_1$	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)	
$a_u$	$\nu_4$	Torsion	364 B	363.5 M	ia	
$b_u$	$\nu_5$	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. 289 Chlorine trifluoride  $ClF_3$ 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)	$cm^{-1}$ (Gas)
$a_1$	$\nu_1$	$ClF$ stretch.	752 C	751 S	752.1 S, p	
	$\nu_2$	$ClF_2$ s-stretch.	529 C	530 M	529.3 VS, p	
	$\nu_3$	$ClF_2$ ip-deform.	328 C	328 S	337 W, p	OV( $\nu_6$ ). 321
$b_1$	$\nu_4$	$ClF_2$ a-stretch.	702 C	702 VS		
	$\nu_5$	$ClF_2$ ip-deform.	442 C	442 W	431 W, dp	
$b_2$	$\nu_6$	$ClF_2$ op-deform.	328 D	328 S		OV( $\nu_3$ ).

## Reference

- [1] IR.R. H. Selig, H. H. Claassen, and J. H. Holloway, J. Chem. Phys. **52**, 3517 (1970).

No. 290      Bromine trifluoride       $\text{BrF}_3$   
 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)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	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	OV( $\nu_6$ ).
$b_1$	$\nu_4$	BrF <sub>2</sub> a-stretch.	614 C	614 VS	612 VW	
	$\nu_5$	$\text{BrF}_2$ ip-deform.	350 C	350 VW		
$b_2$	$\nu_6$	BrF <sub>2</sub> op-deform.	242 D	242 S		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).

No. 291      Ammonia-t<sub>3</sub>      NT<sub>3</sub>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)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	2014 A	2014.1		
	$\nu_2$	Sym. deform.	657 B	656.4 s <sup>a</sup> 657.2 a <sup>a</sup>		
$e$	$\nu_3$	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. 292      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. 293      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)	
$a$	$\nu_1$	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		
$b$	$\nu_5$	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. Winnewisser, *J. Mol. Spectry.* **36**, 414 (1970).

No. 294 Difluoro disulphane  $F_2S_2$   
Symmetry  $C_2$

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)	
<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. 295 Difluoroamine  $NF_2H$   
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)	$cm^{-1}$	
<i>a'</i>	$\nu_1$	NH stretch.	3193 C	3193 W		
	$\nu_2$	NH bend.	1307 B	1307 S		
	$\nu_3$	$NF_2$ s-stretch.	972 B	972 S		
	$\nu_4$	$NF_2$ scis.	500 C	500 M		
<i>a''</i>	$\nu_5$	NH bend.	1424 B	1424 S		
	$\nu_6$	$NF_2$ 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. 296 Ruthenium tetroxide RuO<sub>4</sub>**  
**Symmetry T<sub>d</sub>**
**Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	<i>v</i> <sub>1</sub>	Sym. stretch.	885 C	ia	885.3 S (Gas)	
<i>e</i>	<i>v</i> <sub>2</sub>	Deg. deform.	322 C	ia	322.4 M	
<i>f</i> <sub>2</sub>	<i>v</i> <sub>3</sub>	Deg. stretch.	921 C	921.0	912.9 W	
	<i>v</i> <sub>4</sub>	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. 297 Osmium tetroxide Os<sup>16</sup>O<sub>4</sub>**  
**Symmetry T<sub>d</sub>**
**Symmetry number σ = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Gas)	
<i>a</i> <sub>1</sub>	<i>v</i> <sub>1</sub>	Sym. stretch.	965 B	ia	965.2	
<i>e</i>	<i>v</i> <sub>2</sub>	Deg. deform.	333 B	ia	333.1	
<i>f</i> <sub>2</sub>	<i>v</i> <sub>3</sub>	Deg. stretch.	960 B	960.5	960.1	
	<i>v</i> <sub>4</sub>	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. **A1968**, 1663.  
 [6] R. G. 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. 298      Osmium tetroxide    Os<sup>18</sup>O<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
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (CCl <sub>4</sub> soln.)	
a <sub>1</sub>	$\nu_1$	Sym. stretch.	910 C	ia	909.7	
e	$\nu_2$	Deg. deform.	317 C	ia	316.6	
f <sub>2</sub>	$\nu_3$	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. 299      Dichlorosilane    SiH<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
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
a <sub>1</sub>	$\nu_1$	SiH <sub>2</sub> s-stretch.	2224 C	2224 S	2221 S, p	
	$\nu_2$	SiH <sub>2</sub> scis.	954 C	954 S	942 W, dp	
	$\nu_3$	SiCl <sub>2</sub> s-stretch.	527 C	527 W	514 S, p	
	$\nu_4$	SiCl <sub>2</sub> scis.	188 D		188 M, dp	
a <sub>2</sub>	$\nu_5$	SiH <sub>2</sub> twist.	710 D	ia	710 W, dp	
b <sub>1</sub>	$\nu_6$	SiH <sub>2</sub> a-stretch.	2237 B	2237 S		
	$\nu_7$	SiH <sub>2</sub> rock.	602 C	602 W		
b <sub>2</sub>	$\nu_8$	SiH <sub>2</sub> wag.	876 B	876 VS	868 VW, dp	
	$\nu_9$	SiCl <sub>2</sub> 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).

**MOLECULAR VIBRATIONAL FREQUENCIES**

**No. 300      Dichlorosilane-d<sub>2</sub>      SiD<sub>2</sub>Cl<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

**Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm<sup>-1</sup></i>	<i>cm<sup>-1</sup></i>	<i>cm<sup>-1</sup></i>	
				(Gas)		
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	SiD <sub>2</sub> s-stretch.	1608 C	1608 S		
	<i>ν</i> <sub>2</sub>	SiD <sub>2</sub> scis.	695 C	695 S		
	<i>ν</i> <sub>3</sub>	SiCl <sub>2</sub> s-stretch.	519 C	519 W		
	<i>ν</i> <sub>4</sub>	SiCl <sub>2</sub> scis.	187 D	187 W		
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>5</sub>	SiD <sub>2</sub> twist.	506 D	ia		CF.
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>6</sub>	SiD <sub>2</sub> a-stretch.	1637 C	1637 S		
	<i>ν</i> <sub>7</sub>	SiD <sub>2</sub> rock.	466 B	466 W		
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>8</sub>	SiD <sub>2</sub> wag.	663 B	663 VS		
	<i>ν</i> <sub>9</sub>	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. 301      Dibromosilane      SiH<sub>2</sub>Br<sub>2</sub>**  
**Symmetry C<sub>2v</sub>**

**Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm<sup>-1</sup></i>	<i>cm<sup>-1</sup></i>	<i>cm<sup>-1</sup></i>	
				(Gas)		
					(Liquid)	
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	SiH <sub>2</sub> s-stretch.	2206 D	2200 S	2206 S, p	
	<i>ν</i> <sub>2</sub>	SiH <sub>2</sub> scis.	942 C	942 VS	925 W, dp	
	<i>ν</i> <sub>3</sub>	SiBr <sub>2</sub> s-stretch.	407 C	407 M	393 S, p	
	<i>ν</i> <sub>4</sub>	SiBr <sub>2</sub> scis.	122 D		122 M, p	
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>5</sub>	SiH <sub>2</sub> twist.	688 D	ia	688 W, dp	
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>6</sub>	SiH <sub>2</sub> a-stretch.	2232 D	2200 S	2232 W, dp	
	<i>ν</i> <sub>7</sub>	SiH <sub>2</sub> rock.	556 C	556 S		
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>8</sub>	SiH <sub>2</sub> wag.	843 C	843 VS	828 VW, dp	
	<i>ν</i> <sub>9</sub>	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. 302 Phosphoryl fluorodichloride  $\text{OPFCl}_2$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	PO stretch.	1331 D		1331 p	
	$\nu_2$	PF stretch.	894 D		894 p	
	$\nu_3$	$\text{PCl}_2$ s-stretch.	547 D		547 p	
	$\nu_4$	PO ip-bend.	386 D		386 p	
	$\nu_5$	PF bend.	330 D		330 p	
	$\nu_6$	$\text{PCl}_2$ scis.	207 D		207 p	
	$\nu_7$	$\text{PCl}_2$ a-stretch.	620 D		620 dp	
	$\nu_8$	PO op-bend.	372 D		372 dp	
	$\nu_9$	$\text{PCl}_2$ rock.	254 D		254 dp	

## Reference

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

No. 303 Phosphoryl fluorodibromide  $\text{OPFBBr}_2$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	PO stretch.	1303 D		1303 p	
	$\nu_2$	PF stretch.	880 D		880 p	
	$\nu_3$	$\text{PBr}_2$ s-stretch.	466 D		466 p	
	$\nu_4$	PO ip-bend.	306 D		306 p	
	$\nu_5$	PF bend.	273 D		273 p	
	$\nu_6$	$\text{PBr}_2$ scis.	134 D		134 p	
	$\nu_7$	$\text{PBr}_2$ a-stretch.	538 D		538 dp	
	$\nu_8$	PO op-bend.	291 D		291 dp	
	$\nu_9$	$\text{PBr}_2$ rock.	220 D		220 dp	

## Reference

See No. 302 ( $\text{OPFCl}_2$ ).

No. 304 Phosphorus pentafluoride  $\text{PF}_5$   
Symmetry  $D_{3h}$

Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (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 (lsh) dp	
	$\nu_7$	PF bend.	174 C		174 (1b) dp	
$e''$	$\nu_8$	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. 305 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
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (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. 306 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. 307 Iridium(VI) fluoride  $\text{IrF}_6$**   
**Symmetry  $O_h$** 
**Symmetry number  $\sigma = 24$** 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_{1g}$	$\nu_1$	Sym. stretch.	702 B	ia	701.7 VS, p	
$e_g$	$\nu_2$	Deg. stretch.	645 C	ia	645 W, dp	
$f_{1u}$	$\nu_3$	Deg. stretch.	720 B	719.8 S	ia	
	$\nu_4$	Deg. deform.	276 B	276.0 S	ia	
$f_{2g}$	$\nu_5$	Deg. deform.	267 C	ia	267 W, dp	
$f_{2u}$	$\nu_6$	Deg. deform.	206 D	ia	ia	$\text{OC}(\nu_2 + \nu_6, \nu_2 - \nu_6, \nu_5 + \nu_6)$ . [1].

**References**

- [1] IR.R. B. Weinstock and G. L. Goodman, Advan. Chem. Phys. **9**, 169 (1966), and references cited there.  
 [2] R. H. 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. 308 Sulfur chloride pentafluoride $\text{SClF}_5$			Symmetry number $\sigma = 4$			
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)	
$a_1$	$\nu_1$	SF stretch.	855 B	854.6 VS	833 W, p	
	$\nu_2$	$\text{SF}_4$ s-stretch.	707 B	707.2 VS	704 S, p	
	$\nu_3$	$\text{SF}_4$ op-deform.	602 B	601.9 VS	603 W, p	
	$\nu_4$	SCl stretch.	402 B	401.7 VS	403 VS, p	
$b_1$	$\nu_5$	$\text{SF}_4$ a-stretch.	625 C	ia	625 M, dp	
	$\nu_6$	$\text{SF}_4$ op-deform.	271 C	ia	271 M, dp	
$b_2$	$\nu_7$	$\text{SF}_4$ ip-deform.	505 C	ia	505 W, dp	
$e$	$\nu_8$	$\text{SF}_4$ d-stretch.	909 B	909.0 VS	927 W, dp	
	$\nu_9$	SF bend.	579 B	579.0 M	584 VW, dp	
	$\nu_{10}$	$\text{SF}_4$ 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. 309 Tungsten chloride pentafluoride $\text{WClF}_5$			Symmetry number $\sigma = 4$			
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)	
$a_1$	$\nu_1$	WF stretch.	743 C	743 M	744 VS, p	
	$\nu_2$	$\text{WF}_4$ s-stretch.	703 C	703 VS	703 M, p	
	$\nu_3$	WCl stretch.	400 C	400 VS	407 S, p	
	$\nu_4$	$\text{WF}_4$ op-deform.	254 C	254 VS	257 W	
$b_1$	$\nu_5$	$\text{WF}_4$ a-stretch.	644 D	ia	644 W	
	$\nu_6$	$\text{WF}_4$ op-deform.	182 D	ia	182 W	
$b_2$	$\nu_7$	$\text{WF}_4$ ip-deform.	377 D	ia	377 M, dp	
$e$	$\nu_8$	$\text{WF}_4$ d-stretch.	671 C	671 S	661 M, dp	
	$\nu_9$	WF bend.	302 C	302 M	307 M, dp	
	$\nu_{10}$	$\text{WF}_4$ 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 1131 (1968).

**No. 310 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
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$\sigma^+$	$\nu_1$	CF stretch.	1077 A	1076.52		
$\pi$	$\nu_2$	Deform.	451 A	451.32		
$\sigma^+$	$\nu_3$	CN stretch.	2323 C	2323		

**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. 311 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
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$\sigma^+$	$\nu_1$	CI stretch.	486 C	485.8		
$\pi$	$\nu_2$	Deform.	305 C	304.5		
$\sigma^+$	$\nu_3$	CN stretch.	2188 C	2188.0		

**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. 312 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
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (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. Wolitz, 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. 313      Carbonyl chloride     $\text{COCl}_2$   
 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)	
$a_1$	$\nu_1$	CO stretch.	1827 B	1827 VS	1807 M	
	$\nu_2$	$\text{CCl}_2$ s-stretch.	567 C	567 M	573 VS	
	$\nu_3$	$\text{CCl}_2$ deform.	285 C	285 W	302 S	
$b_1$	$\nu_4$	$\text{CCl}_2$ a-stretch.	849 B	849 S	832 VW	
	$\nu_5$	CO deform.	440 C	440 M	442 M	
$b_2$	$\nu_6$	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. 314      Carbonyl bromide     $\text{COBr}_2$   
 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)	
$a_1$	$\nu_1$	CO stretch.	1828 B	1828 VS		
	$\nu_2$	$\text{CBr}_2$ s-stretch.	425 C	425 M	429 S	
	$\nu_3$	$\text{CBr}_2$ deform.	181 D		181 S	
$b_1$	$\nu_4$	$\text{CBr}_2$ a-stretch.	757 C	787 VS 747 VS		FR( $\nu_2 + \nu_5$ ).
	$\nu_5$	CO deform.	350 C	350 VW	350 M, b	
$b_2$	$\nu_6$	Op-deform.	512 B	512 M		

## 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. 315      Thiocarbonyl fluoride       $\text{SCF}_2$   
 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)	$\text{cm}^{-1}$
$a_1$	$\nu_1$	CS stretch.	1368 C	1368 VS		
	$\nu_2$	$\text{CF}_2$ s-stretch.	787 C	787 M		
	$\nu_3$	$\text{CF}_2$ scis.	526 C	526 M		
$b_1$	$\nu_4$	$\text{CF}_2$ a-stretch.	1189 C	1189 S		
	$\nu_5$	$\text{CF}_2$ rock.	417 C	417 VW		
$b_2$	$\nu_6$	$\text{CF}_2$ wag.	622 C	622 W		

## Reference

- [1] IR. A. J. Downs, Spectrochim. Acta **19**, 1165 (1963).

No. 316      Isocyanic acid       $\text{HNCO}$   
 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		

\* 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. 317 Isocyanic acid-d DNCO

Symmetry C<sub>2</sub>

Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a'</i>	<i>ν<sub>1</sub></i>	ND stretch.	2635 B	2634.9		
	<i>ν<sub>2</sub></i>	CO stretch.	2235 C	2235		
	<i>ν<sub>3</sub></i>	CN stretch.	1310 C	1310		
	<i>ν<sub>4</sub></i>	ND bend.	758 C <sup>a</sup>	766.8		
	<i>ν<sub>5</sub></i>	CNO deform.	458 C <sup>a</sup>	460		
<i>a''</i>	<i>ν<sub>6</sub></i>	CNO deform.	603 B <sup>a</sup>	602.9		

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

## Reference

[1] IR. R. A. Ashby and R. L. Werner, Spectrochim. Acta 22, 1345 (1966).

## No. 318 Carbonyl chlorofluoride COClF

Symmetry C<sub>2</sub>

Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a'</i>	<i>ν<sub>1</sub></i>	CO stretch.	1868 C	1876 VS 1847 VS	1858 M 1832 M	FR( <i>ν<sub>2</sub></i> + <i>ν<sub>3</sub></i> ).
	<i>ν<sub>2</sub></i>	CF stretch.	1095 B	1095 S	1085 VW	
	<i>ν<sub>3</sub></i>	CCl stretch.	776 C	776 M	765 VS	
	<i>ν<sub>4</sub></i>	CO deform.	501 C	501 W	506 S	
	<i>ν<sub>5</sub></i>	CClF deform.	415 C	415 VW	410 M	
<i>a''</i>	<i>ν<sub>6</sub></i>	Op-deform.	667 B	667 M	665 VW	

## References

See No. 312 (COF<sub>2</sub>).

No. 319      Carbonyl bromochloride COBrCl  
 Symmetry C<sub>s</sub>

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)	
<i>a'</i>	$\nu_1$	CO stretch.	1828 B	1828 VS		
	$\nu_2$	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	
<i>a''</i>	$\nu_6$	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. 320      Trifluoromethane-d CDF<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
				$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$
				(Gas)		
<i>a</i> <sub>1</sub>	$\nu_1$	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		
	$\nu_4$	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, 1377 (1971).

No. 321 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 (solid)		
	$\nu_2$	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		
	$\nu_5$	$\text{BH}_3$ 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. 322 Borine Carbonyl-d<sub>3</sub>  $^{10}\text{BD}_3\text{CO}$ 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 (solid)		
	$\nu_4$	BC stretch.	630 B	629.5 S		
	$\nu_5$	$\text{BD}_3$ 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. 321 ( $^{10}\text{BH}_3\text{CO}$ ).

No. 323 Borine Carbonyl  $^{11}\text{BH}_3\text{CO}$   
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)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{BH}_3$ s-stretch.	2380 C	2379 M (solid)	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. 324 Borine Carbonyl- $d_3$   $^{11}\text{BD}_3\text{CO}$   
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)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{BD}_3$ s-stretch.	1679 C	1679.0 M	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. 323 ( $^{11}\text{BH}_3\text{CO}$ ).

No. 325    Dichloroacetylene     $C_2Cl_2$   
 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)	$cm^{-1}$ (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. 326    Dibromoacetylene     $C_2Br_2$ 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)	$cm^{-1}$ ( $C_6H_6$ 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. 325 ( $C_2Cl_2$ ).

No. 327 Diiodoacetylene  $C_2I_2$   
Symmetry  $D_{\infty h}$

Symmetry number  $\sigma = 2$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$	$cm^{-1}$	
						(C <sub>6</sub> H <sub>6</sub> 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 <sub>2</sub> 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 <sub>6</sub> H <sub>6</sub> 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. 328 Bromochloroacetylene  $C_2ClBr$   
Symmetry  $C_\infty$

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) (C <sub>6</sub> H <sub>6</sub> 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 (CCl <sub>4</sub> soln.)	
$\pi$	$\nu_4$	CCCl deform.	326 D		326 VS, dp (CCl <sub>4</sub> soln.)	
	$\nu_5$	CCBr deform.	152 C	152 S	165 M	

## Reference

- [1] IR.R. P. Klaboe and E. Kloster-Jensen, Spectrochim. Acta **26A**, 1567 (1970).

**No. 329 Chloroiodoacetylene C<sub>2</sub>ClI****Symmetry C<sub>oo</sub>****Symmetry number σ = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (C <sub>6</sub> H <sub>6</sub> soln.)	
σ <sup>+</sup>	ν <sub>1</sub>	CC stretch.	2191 C	2191 VS	2178 VS, p	
	ν <sub>2</sub>	CCl stretch.	886 C	886 VS	880 VW	
	ν <sub>3</sub>	CI stretch.	276 D		276 M, p	
π	ν <sub>4</sub>	CCl deform.	325 D		325 VS, dp	
	ν <sub>5</sub>	CCI deform.	135 C	135 S	145 VW (CCl <sub>4</sub> soln.)	

**Reference**See No. 328 (C<sub>2</sub>ClBr).**No. 330 trans-1,2-Difluoroethylene CHFCHF****Symmetry C<sub>2h</sub>****Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			<i>cm</i> <sup>-1</sup>	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
a <sub>g</sub>	ν <sub>1</sub>	CH stretch.	3111 C	ia	3111 VS, p	
	ν <sub>2</sub>	CC stretch.	1694 C	ia	1694 VS, p	
	ν <sub>3</sub>	CH bend.	1286 C	ia	1286 S, p	
	ν <sub>4</sub>	CF stretch.	1123 C	ia	1123 M, p	
	ν <sub>5</sub>	CCF deform.	548 C	ia	548 S, p	
a <sub>u</sub>	ν <sub>6</sub>	CH bend.	875 B	875 S	ia	
	ν <sub>7</sub>	Torsion	329 D	333 M (Xe Matrix) 325 M (Xe Matrix)	ia	
b <sub>g</sub>	ν <sub>8</sub>	CH bend.	788 C	ia	788 S, dp	
b <sub>u</sub>	ν <sub>9</sub>	CH stretch.	3114 C	3114 M	ia	
	ν <sub>10</sub>	CH bend.	1274 C	1274 M	ia	
	ν <sub>11</sub>	CF stretch.	1159 C	1159 VS	ia	
	ν <sub>12</sub>	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. 331    trans-1,2-Difluoroethylene-d<sub>1</sub> CHFCDF  
 Symmetry C<sub>s</sub>

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
<i>a'</i>	$\nu_1$	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		
	$\nu_{10}$	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. 330 (CHFCHF).

No. 332    trans-1,2-Difluoroethylene-d<sub>2</sub> CDFCDF  
 Symmetry C<sub>2h</sub>

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)	
<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	
	$\nu_6$	CD bend.	651 B	651 S	ia	
<i>a<sub>u</sub></i>	$\nu_7$	Torsion	309 C	309 S	ia	
	$\nu_8$	CD bend.	685 C	ia	685 S, dp	
<i>b<sub>g</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] I.R.R. N. C. Craig and J. Overend, J. Chem. Phys. **51**, 1127 (1969).

No. 333 1,4-Dioxane C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>Symmetry C<sub>2h</sub>

Symmetry number σ = 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>	
				(Liquid)	(Liquid)	
<i>a<sub>g</sub></i>	<i>ν<sub>1</sub></i>	CH <sub>2</sub> a-stretch.	2966 C	ia	2966 (10)p	
	<i>ν<sub>2</sub></i>	CH <sub>2</sub> s-stretch.	2855 C	ia	2855 (8)p	
	<i>ν<sub>3</sub></i>	CH <sub>2</sub> scis.	1443 C	ia	1443 (8)p	
	<i>ν<sub>4</sub></i>	CH <sub>2</sub> wag.	1334 C	ia	1334 (2)p	
	<i>ν<sub>5</sub></i>	CH <sub>2</sub> twist.	1303 C	ia	1303 (8)p	
	<i>ν<sub>6</sub></i>	CH <sub>2</sub> rock.	1127 C	ia	1127 (3)p	
	<i>ν<sub>7</sub></i>	CC stretch.	1015 C	ia	1015 (6)p	
	<i>ν<sub>8</sub></i>	CO stretch.	834 C	ia	834 (8)p	
	<i>ν<sub>9</sub></i>	OCC deform.	503 E	ia		CF[2].
	<i>ν<sub>10</sub></i>	COC deform.	427 C	ia	433 (2)p	FR(2 <i>ν<sub>27</sub></i> ).
					422 (1)	
<i>a<sub>u</sub></i>	<i>ν<sub>11</sub></i>	CH <sub>2</sub> a-stretch.	2974 C	2974 M	ia	
	<i>ν<sub>12</sub></i>	CH <sub>2</sub> s-stretch.	2867 C	2867 S	ia	
	<i>ν<sub>13</sub></i>	CH <sub>2</sub> scis.	1457 C	1457 M	ia	
	<i>ν<sub>14</sub></i>	CH <sub>2</sub> wag.	1367 C	1367 W	ia	
	<i>ν<sub>15</sub></i>	CH <sub>2</sub> twist.	1264 C	1264 S	ia	
	<i>ν<sub>16</sub></i>	CO stretch.	1123 C	1123 VS	ia	
	<i>ν<sub>17</sub></i>	CH <sub>2</sub> rock.	1088 C	1088 M	ia	
	<i>ν<sub>18</sub></i>	CC stretch.	894 C	894 M	ia	
	<i>ν<sub>19</sub></i>	OCC deform.	224 C	224 VW	ia	
<i>b<sub>g</sub></i>	<i>ν<sub>20</sub></i>	CH <sub>2</sub> a-stretch.	2966 C	ia	2966 (10)p	SF( <i>ν<sub>1</sub></i> ).
	<i>ν<sub>21</sub></i>	CH <sub>2</sub> s-stretch.	2855 C	ia	2855 (8)p	SF( <i>ν<sub>2</sub></i> ).
	<i>ν<sub>22</sub></i>	CH <sub>2</sub> scis.	1461 C	ia	1461 (2)dp	
	<i>ν<sub>23</sub></i>	CH <sub>2</sub> wag.	1396 C	ia	1396 (1)	
	<i>ν<sub>24</sub></i>	CH <sub>2</sub> twist.	1216 C	ia	1216 (5)dp	
	<i>ν<sub>25</sub></i>	CO stretch.	1109 C	ia	1109 (3)dp	
	<i>ν<sub>26</sub></i>	CH <sub>2</sub> rock.	852 C	ia	852 (1)dp	
	<i>ν<sub>27</sub></i>	OCC deform.	486 C	ia	486 (4)dp	
<i>b<sub>u</sub></i>	<i>ν<sub>28</sub></i>	CH <sub>2</sub> a-stretch.	2974 C	2974 M	ia	SF( <i>ν<sub>19</sub></i> ).
	<i>ν<sub>29</sub></i>	CH <sub>2</sub> s-stretch.	2867 C	2867 S	ia	SF( <i>ν<sub>20</sub></i> ).
	<i>ν<sub>30</sub></i>	CH <sub>2</sub> scis.	1457 C	1457 M	ia	
	<i>ν<sub>31</sub></i>	CH <sub>2</sub> wag.	1377 C	1377 W	ia	
	<i>ν<sub>32</sub></i>	CH <sub>2</sub> twist.	1296 C	1296 M	ia	
	<i>ν<sub>33</sub></i>	CH <sub>2</sub> rock.	1052 C	1052 W	ia	
	<i>ν<sub>34</sub></i>	CO stretch.	871 C	871 S	ia	
	<i>ν<sub>35</sub></i>	OCC deform.	610 C	610 M	ia	
	<i>ν<sub>36</sub></i>	COC deform.	276 C	276 M	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).

No. 334      Hexacarbonylchromium(0)     $\text{Cr}^{(12\text{C})^6\text{O}}_6$   
 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	$\text{OC}(\nu_5 + \nu_7)$ .
$f_{1u}$	$\nu_6$	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.	533 D	ia	533.1 W (solid)	
	$\nu_{11}$	CCrC deform.	114 D	ia	114.2 S (solid)	
$f_{2u}$	$\nu_{12}$	CrCO bend.	511 D	ia	ia	$\text{OC}(\nu_{10} + \nu_{12},$ $\nu_5 + \nu_{12})$ .
	$\nu_{13}$	CCrC deform.	68 E	ia	ia	$\text{OC}(\nu_3 + \nu_{13})$ .

## 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).

No. 335 Hexacarbonylmolybdenum (0)  $\text{Mo}^{(12)\text{C}^{16}\text{O}}_6$ 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.	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	$\text{OC}(\nu_5 + \nu_7)$ .
$f_{1u}$	$\nu_6$	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	
$f_{2g}$	$\nu_9$	CMoC deform.	82 B	81.6 M	ia	
	$\nu_{10}$	MoCO bend.	477 D	ia	476.5 W (solid)	
	$\nu_{11}$	CMoC deform.	104 D	ia	103.7 S (solid)	
$f_{2u}$	$\nu_{12}$	MoCO bend.	507 D	ia	ia	$\text{OC}(\nu_5 + \nu_{12},$ $\nu_{10} + \nu_{12})$ .
[6]IR.R.Th.	$\nu_{13}$	CMoC deform.	60 E	ia	ia	$\text{OC}(\nu_3 + \nu_{13},$ $\nu_{10} + \nu_{13})$ .

## 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. 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).

**No. 336 Hexacarbonyltungsten(0) W( $^{12}\text{C}^{16}\text{O}$ )<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
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (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	$\text{OC}(\nu_5 + \nu_7)$ .
$f_{1u}$	$\nu_6$	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.	485 D	ia	485.0 W (solid)	
	$\nu_{11}$	CWC deform.	108 D	ia	107.6 S (solid)	
$f_{2u}$	$\nu_{12}$	WCO bend.	521 D	ia	ia	$\text{OC}(\nu_5 + \nu_7,$ $\nu_{10} + \nu_{12})$ .
	$\nu_{13}$	CWC deform.	61 E	ia	ia	$\text{OC}(\nu_3 + \nu_{13})$ .

**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).

## APPENDIX I

## A. Structure-Symmetry Index

This index and the one which follows cover the entire list of compounds analyzed so far under this project, and presented in the Tables of Molecular Vibrational Frequencies, Consolidated Volume [2], Part 5[3] and the present publication.

Here the 336 molecules are ordered by structural and symmetry factors, following the principles set forth in ref [2]. Name, chemical formula and Table Number are listed. Tables numbered 1 through 223 may be found in ref [2], tables numbered 224 through 281 in ref [3], and tables numbered 282 through 336 in the present increment.

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

Nitrous oxide	<sup>14</sup> N <sub>2</sub> O	1
Nitrous oxide	<sup>14</sup> N <sup>15</sup> NO	2
Nitrous oxide	<sup>15</sup> N <sub>2</sub> O	3
Nitrogen dioxide	<sup>14</sup> NO <sub>2</sub>	224
Nitrogen dioxide	<sup>15</sup> NO <sub>2</sub>	225
Water	H <sub>2</sub> O	4
Water	H <sub>2</sub> <sup>18</sup> O	282
Water-d <sub>1</sub>	HDO	5
Water-d <sub>2</sub>	D <sub>2</sub> O	6
Oxygen difluoride	F <sub>2</sub> O	7
Oxygen dichloride	Cl <sub>2</sub> O	8
Hydrogen sulfide	H <sub>2</sub> S	9
Deuterium sulfide	D <sub>2</sub> S	10
Sulfur dioxide	<sup>32</sup> S <sup>16</sup> O <sub>2</sub>	11
Sulfur dioxide	S <sup>18</sup> O <sub>2</sub>	283
Sulfur dichloride	SCl <sub>2</sub>	226
Hydrogen selenide	H <sub>2</sub> Se	12
Hydrogen deuterium selenide	HDSe	13
Nitrosyl fluoride	<sup>16</sup> O <sup>14</sup> NF	227
Nitrosyl fluoride	<sup>16</sup> O <sup>15</sup> NF	228
Nitrosyl fluoride	<sup>18</sup> O <sup>14</sup> NF	229
Nitrosyl fluoride	<sup>18</sup> O <sup>15</sup> NF	230
Nitrosyl chloride	<sup>16</sup> O <sup>14</sup> NCl	231
Nitrosyl chloride	<sup>16</sup> O <sup>15</sup> NCl	232
Nitrosyl chloride	<sup>18</sup> O <sup>14</sup> NCl	233
Nitrosyl chloride	<sup>18</sup> O <sup>15</sup> NCl	234
Nitrosyl bromide	<sup>16</sup> O <sup>14</sup> NBr	235
Nitrosyl bromide	<sup>16</sup> O <sup>15</sup> NBr	236
Nitrosyl bromide	<sup>18</sup> O <sup>15</sup> NBr	237
Hypochlorous acid	HOCl	284
Hypochlorous acid-d	DOCl	285
Thionitrosyl-S-fluoride	NSF	286
Thionitrosyl-S-chloride	NSCl	287

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

Boron trifluoride	<sup>10</sup> BF <sub>3</sub>	238
Boron trifluoride	<sup>11</sup> BF <sub>3</sub>	239
Sulfur trioxide	SO <sub>3</sub>	240

Ammonia	NH <sub>3</sub>	14
Ammonia-d <sub>3</sub>	ND <sub>3</sub>	15
Ammonia-t <sub>3</sub>	NT <sub>3</sub>	291
Nitrogen trifluoride	NF <sub>3</sub>	16
Phosphine	PH <sub>3</sub>	17
Phosphine-d <sub>3</sub>	PD <sub>3</sub>	18
Phosphorus trifluoride	PF <sub>3</sub>	19
Phosphorus trichloride	PCl <sub>3</sub>	20
Arsine	AsH <sub>3</sub>	21
Arsine-d <sub>3</sub>	AsD <sub>3</sub>	22
Arsenic trifluoride	AsF <sub>3</sub>	292
Stibine	SbH <sub>3</sub>	23
Stibine-d <sub>3</sub>	SbD <sub>3</sub>	24
Trans-1,2-Difluorodiazine	N <sub>2</sub> F <sub>2</sub>	288
Nitryl fluoride	F <sup>14</sup> NO <sub>2</sub>	241
Nitryl fluoride	F <sup>15</sup> NO <sub>2</sub>	242
Nitryl chloride	Cl <sup>14</sup> NO <sub>2</sub>	243
Nitryl chloride	Cl <sup>15</sup> NO <sub>2</sub>	244
Chlorine trifluoride	ClF <sub>3</sub>	289
Bromine trifluoride	BrF <sub>3</sub>	290
Hydrogen peroxide	H <sub>2</sub> O <sub>2</sub>	247
Hydrogen persulfide	H <sub>2</sub> S <sub>2</sub>	293
Difluoro disulfane	F <sub>2</sub> S <sub>2</sub>	294
Hydrazoic acid	HN <sub>3</sub>	245
Hydrazoic acid-d <sub>1</sub>	DN <sub>3</sub>	246
Difluoroamine	NF <sub>2</sub> H	295
C <sub>0</sub> -five-atomic molecules		
Thionyl fluoride	SOF <sub>2</sub>	248
Thionyl chloride	SOCl <sub>2</sub>	249
Thionyl bromide	SOBr <sub>2</sub>	250
Silane	SiH <sub>4</sub>	25
Silane-d <sub>2</sub>	SiH <sub>2</sub> D <sub>2</sub>	26
Silane-d <sub>3</sub>	SiHD <sub>3</sub>	27
Silane-d <sub>4</sub>	SiD <sub>4</sub>	28
Silicon tetrafluoride	SiF <sub>4</sub>	29
Silicon tetrachloride	SiCl <sub>4</sub>	30
Silicon tetrabromide	SiBr <sub>4</sub>	31
Silicon tetraiodide	SiI <sub>4</sub>	32
Germane	GeH <sub>4</sub>	33
Germane-d <sub>1</sub>	GeH <sub>3</sub> D	34
Germane-d <sub>2</sub>	GeH <sub>2</sub> D <sub>2</sub>	35
Germane-d <sub>3</sub>	GeHD <sub>3</sub>	36
Germane-d <sub>4</sub>	GeD <sub>4</sub>	37
Germanium tetrachloride	GeCl <sub>4</sub>	38
Germanium tetrabromide	GeBr <sub>4</sub>	39
Tin (IV) chloride	SnCl <sub>4</sub>	40
Tin (IV) bromide	SnBr <sub>4</sub>	41
Ruthenium tetroxide	RuO <sub>4</sub>	296
Osmium tetroxide	Os <sup>16</sup> O <sub>4</sub>	297
Osmium tetroxide	Os <sup>18</sup> O <sub>4</sub>	298
Silyl fluoride	SiH <sub>3</sub> F	42
Silyl chloride	SiH <sub>3</sub> Cl	43
Silyl bromide	SiH <sub>3</sub> Br	44
Trifluorosilane	SiHF <sub>3</sub>	251
Trifluorosilane-d	SiDF <sub>3</sub>	252
Trichlorosilane	SiHCl <sub>3</sub>	253

Trichlorosilane-d	$\text{SiDCl}_3$	254	Carbon disulfide	$\text{CS}_2$	60
Tribromosilane	$\text{SiHBr}_3$	255	Hydrogen cyanide	$\text{HCN}$	62
Bromotrichlorosilane	$\text{SiBrCl}_3$	45	Deuterium cyanide	$\text{DCN}$	63
Trichloroiodosilane	$\text{SiCl}_3\text{I}$	46	Cyanogen fluoride	$\text{FCN}$	310
Tribromochlorosilane	$\text{SiBr}_3\text{Cl}$	47	Cyanogen chloride	$^{35}\text{CICN}$	64
Chlorotriiodosilane	$\text{SiClI}_3$	48	Cyanogen chloride	$^{37}\text{CICN}$	65
Phosphoryl fluoride	$\text{POF}_3$	256	Cyanogen bromide	$^{79}\text{BrCN}$	66
Phosphoryl chloride	$\text{POCl}_3$	257	Cyanogen bromide	$^{81}\text{BrCN}$	67
Phosphoryl bromide	$\text{POBr}_3$	258	Cyanogen iodide	$\text{ICN}$	311
Germyl fluoride	$\text{GeH}_3\text{F}$	259	Carbonyl sulfide	$\text{COS}$	61
Germyl fluoride-d <sub>3</sub>	$\text{GeD}_3\text{F}$	260			
Germyl chloride	$\text{GeH}_3\text{Cl}$	261			
Germyl chloride-d <sub>3</sub>	$\text{GeD}_3\text{Cl}$	262			
Germyl bromide	$\text{GeH}_3\text{Br}$	263	Formaldehyde	$\text{H}_2\text{CO}$	68
Germyl bromide-d <sub>3</sub>	$\text{GeD}_3\text{Br}$	264	Formaldehyde-d <sub>1</sub>	$\text{HDCO}$	69
Germyl iodide	$\text{GeH}_3\text{I}$	265	Formaldehyde-d <sub>2</sub>	$\text{D}_2\text{CO}$	70
Germyl iodide-d <sub>3</sub>	$\text{GeD}_3\text{I}$	266	Carbonyl fluoride	$\text{COF}_2$	312
Trichlorogermane	$\text{GeHCl}_3$	267	Carbonyl chloride	$\text{COCl}_2$	313
Tribromogermane	$\text{GeHBr}_3$	268	Carbonyl bromide	$\text{COBr}_2$	314
Sulfuryl fluoride	$\text{SO}_2\text{F}_2$	269	Thiocarbonyl fluoride	$\text{SCF}_2$	315
Sulfuryl chloride	$\text{SO}_2\text{Cl}_2$	270	Isocyanic acid	$\text{HNCO}$	316
Dichlorosilane	$\text{SiH}_2\text{Cl}_2$	299	Isocyanic acid-d	$\text{DNCO}$	317
Dichlorosilane-d <sub>2</sub>	$\text{SiD}_2\text{Cl}_2$	300	Carbonyl chlorofluoride	$\text{COClF}$	318
Dibromosilane	$\text{SiH}_2\text{Br}_2$	301	Carbonyl bromochloride	$\text{COBrCl}$	319
Dibromodichlorosilane	$\text{SiBr}_2\text{Cl}_2$	49			
Selenium dioxide difluoride	$\text{SeO}_2\text{F}_2$	271			
Phosphoryl fluorodichloride	$\text{OPFCl}_2$	302			
Phosphoryl fluorodibromide	$\text{OPFBr}_2$	303			
<b>C<sub>0</sub>-six-atomic molecules</b>					
Phosphorus pentafluoride	$\text{PF}_5$	304	Methane	$\text{CH}_4$	71
Vanadium pentafluoride	$\text{VF}_5$	305	Methane-d <sub>1</sub>	$\text{CH}_3\text{D}$	72
Arsenic pentafluoride	$\text{AsF}_5$	306	Methane-d <sub>2</sub>	$\text{CH}_2\text{D}_2$	73
			Methane-d <sub>3</sub>	$\text{CHD}_3$	74
			Methane-d <sub>4</sub>	$\text{CD}_4$	75
			Carbon tetrafluoride	$\text{CF}_4$	76
			Carbon tetrachloride	$\text{CCl}_4$	77
			Carbon tetrabromide	$\text{CBr}_4$	78
			Carbon tetraiodide	$\text{CI}_4$	79
			Methyl fluoride	$\text{CH}_3\text{F}$	80
			Methyl fluoride-d <sub>3</sub>	$\text{CD}_3\text{F}$	81
			Methyl chloride	$\text{CH}_3\text{Cl}$	82
			Methyl chloride-d <sub>3</sub>	$\text{CD}_3\text{Cl}$	83
			Methyl bromide	$\text{CH}_3\text{Br}$	84
			Methyl bromide-d <sub>3</sub>	$\text{CD}_3\text{Br}$	85
			Methyl iodide	$\text{CH}_3\text{I}$	86
			Methyl iodide-d <sub>3</sub>	$\text{CD}_3\text{I}$	87
			Trifluoromethane	$\text{CHF}_3$	88
			Trifluoromethane-d	$\text{CDF}_3$	320
			Trichloromethane	$\text{CHCl}_3$	89
			Trichloromethane-d <sub>1</sub>	$\text{CDCl}_3$	90
			Tribromomethane	$\text{CHBr}_3$	91
Digermane	$\text{GeH}_3\text{GeH}_3$	273	Tribromomethane-d <sub>1</sub>	$\text{CDBr}_3$	92
Digermane-d <sub>6</sub>	$\text{GeD}_3\text{GeD}_3$	274	Bromotrichloromethane	$\text{CBrCl}_3$	93
Diborane	<sup>10</sup> $\text{B}_2\text{H}_6$	55	Tribromochloromethane	$\text{CBr}_3\text{Cl}$	94
Diborane	<sup>11</sup> $\text{B}_2\text{H}_6$	56	Dichloromethane	$\text{CH}_2\text{Cl}_2$	95
Diborane	<sup>10</sup> $\text{B}_2\text{D}_6$	57	Dichloromethane-d <sub>1</sub>	$\text{CHDCl}_2$	96
			Dichloromethane-d <sub>2</sub>	$\text{CD}_2\text{Cl}_2$	97
<b>C<sub>1</sub>-triatomic molecules</b>					
Carbon dioxide	<sup>12</sup> $\text{CO}_2$	58	Dibromomethane	$\text{CH}_2\text{Br}_2$	98
Carbon dioxide	<sup>13</sup> $\text{CO}_2$	59	Dibromomethane-d <sub>2</sub>	$\text{CHDBr}_2$	99
			Dibromodichloromethane	$\text{CD}_2\text{Br}_2$	100
				$\text{CBr}_2\text{Cl}_2$	101

Bromochloromethane	$\text{CH}_2\text{BrCl}$	102	Ethylene-d <sub>4</sub>	$\text{C}_2\text{D}_4$	125			
Bromochloromethane-d <sub>1</sub>	$\text{CHDBrCl}$	103	Tetrafluoroethylene	$\text{CF}_2\text{CF}_2$	126			
Bromochloromethane-d <sub>2</sub>	$\text{CD}_2\text{BrCl}$	104	Tetrachloroethylene	$\text{CCl}_2\text{CCl}_2$	127			
Formic acid	$\text{HCOOH}$	105	Tetrabromoethylene	$\text{CBr}_2\text{CBr}_2$	128			
Formic acid-d <sub>2</sub>	DCOOD	106	Trans-1,2-Difluoroethylene	$\text{CHFCHF}$	330			
<b>C<sub>1</sub>-six-atomic molecules</b>								
Borine carbonyl	<sup>10</sup> $\text{BH}_3\text{CO}$	321	Trans-1,2-Dichloroethylene-d <sub>1</sub>	$\text{CHClCDCl}$	133			
Borine carbonyl-d <sub>3</sub>	<sup>10</sup> $\text{BD}_3\text{CO}$	322	Trans-1,2-Dichloroethylene-d <sub>2</sub>	$\text{CDCICDCI}$	134			
Borine carbonyl	<sup>11</sup> $\text{BH}_3\text{CO}$	323	Trans-1,2-Dichloro-1,2-Difluoroethylene					
Borine carbonyl-d <sub>3</sub>	<sup>11</sup> $\text{BD}_3\text{CO}$	324		$\text{CFCICFCI}$	138			
Methanol	$\text{CH}_3\text{OH}$ (Gas)	107	Cis-1,2-Difluoroethylene	$\text{CHFCHF}$	129			
Methanol	$\text{CH}_3\text{OH}$ (Liquid)	108	Cis-1,2-Difluoroethylene-d <sub>1</sub>	$\text{CHFCDF}$	130			
Methanol-d <sub>1</sub>	$\text{CH}_3\text{OD}$ (Gas)	109	Cis-1,2-Dichloroethylene	$\text{CHClCHCl}$	135			
Methanol-d <sub>1</sub>	$\text{CH}_3\text{OD}$ (Liquid)	110	Cis-1,2-Dichloroethylene-d <sub>1</sub>	$\text{CHClCDCl}$	136			
Methanol-d <sub>3</sub>	$\text{CD}_3\text{OH}$ (Gas)	111	1,1-Dichloroethylene	$\text{CH}_2\text{CCl}_2$	139			
Methanol-d <sub>3</sub>	$\text{CD}_3\text{OH}$ (Liquid)	112	1,1-Dichloroethylene-d <sub>1</sub>	$\text{CHDCCl}_2$	140			
Methanol-d <sub>4</sub>	$\text{CD}_3\text{OD}$ (Gas)	113	1,1-Dichloro-2,2-Difluoroethylene	$\text{CF}_2\text{CCl}_2$	142			
<b>C<sub>1</sub>-seven-atomic molecules</b>								
Methylamine	$\text{CH}_3\text{NH}_2$	114	Silylacetylene	$\text{SiH}_3\text{CCH}$	148			
Methylamine-d <sub>2</sub>	$\text{CH}_3\text{ND}_2$	115	Ethylene oxide	$\text{C}_2\text{H}_4\text{O}$	149			
Methylamine-d <sub>3</sub>	$\text{CD}_3\text{NH}_2$	116	Ethylene oxide-d <sub>4</sub>	$\text{C}_2\text{D}_4\text{O}$	150			
Methylamine-d <sub>5</sub>	$\text{CD}_3\text{ND}_2$	117	1,2,5-Oxadiazole	$\text{C}_2\text{H}_2\text{N}_2\text{O}$	147			
<b>C<sub>1</sub>-eight-atomic molecules</b>								
Methylsilane	$\text{CH}_3\text{SiH}_3$	275	Acetaldehyde	$\text{CH}_3\text{CHO}$	151			
Methylsilane-d <sub>3</sub>	$\text{CH}_3\text{SiD}_3$	276	Acetaldehyde-d <sub>1</sub>	$\text{CH}_3\text{CDO}$	152			
Methylgermane	$\text{CH}_3\text{GeH}_3$	277	Acetaldehyde-d <sub>4</sub>	$\text{CD}_3\text{CDO}$	153			
Methyl-d <sub>3</sub> -germane	$\text{CD}_3\text{GeH}_3$	278	<b>C<sub>2</sub>-eight-atomic molecules</b>					
<b>C<sub>2</sub>-four-atomic molecules</b>								
Acetylene	$\text{C}_2\text{H}_2$	118	Ethane	$\text{CH}_3\text{CH}_3$	154			
Acetylene-d <sub>1</sub>	$\text{C}_2\text{HD}$	119	Ethane-d <sub>3</sub>	$\text{CH}_3\text{CD}_3$	155			
Acetylene-d <sub>2</sub>	$\text{C}_2\text{D}_2$	120	Ethane-d <sub>6</sub>	$\text{CD}_3\text{CD}_3$	156			
Cyanogen	$\text{C}_2\text{N}_2$	279	Hexafluoroethane	$\text{CF}_3\text{CF}_3$	157			
Dichloroacetylene	$\text{C}_2\text{Cl}_2$	325	Hexachloroethane	$\text{CCl}_3\text{CCl}_3$	158			
Dibromoacetylene	$\text{C}_2\text{Br}_2$	326	Hexabromoethane	$\text{CBr}_3\text{CBr}_3$	159			
Diiodoacetylene	$\text{C}_2\text{I}_2$	327	1,2-Dichloroethane, trans form	$\text{CH}_2\text{ClCH}_2\text{Cl}$	160			
Fluoroacetylene	$\text{CHCF}$	121	1,2-Dichloroethane, gauche form	$\text{CH}_2\text{ClCH}_2\text{Cl}$	161			
Chloroacetylene	$\text{CHCCl}$	122	1,2-Dibromoethane, trans form	$\text{CH}_2\text{BrCH}_2\text{Br}$	162			
Bromoacetylene	$\text{CHCBr}$	123	1,2-Dibromoethane, gauche form	$\text{CH}_2\text{BrCH}_2\text{Br}$	163			
Bromochloroacetylene	$\text{C}_2\text{ClBr}$	328	1-Bromo-2-chloroethane,	$\text{CH}_2\text{ClCH}_2\text{Br}$	164			
Chloroiodoacetylene	$\text{C}_2\text{ClI}$	329	trans form					
<b>C<sub>2</sub>-six-atomic molecules</b>								
Methyl cyanide	$\text{CH}_3\text{CN}$	143	1-Bromo-2-chloroethane, trans form	$\text{CH}_2\text{ClCH}_2\text{Br}$	165			
Methyl cyanide-d <sub>3</sub>	$\text{CD}_3\text{CN}$	144	Fluoroethane	$\text{CH}_3\text{CH}_2\text{F}$	166			
Methyl isocyanide	$\text{CH}_3\text{NC}$	145	Chloroethane	$\text{CH}_3\text{CH}_2\text{Cl}$	167			
Methyl isocyanide-d <sub>3</sub>	$\text{CD}_3\text{NC}$	146	Bromoethane	$\text{CH}_3\text{CH}_2\text{Br}$	168			
Ethylene	$\text{C}_2\text{H}_4$	124	Ethylene imine	$\text{C}_2\text{H}_5\text{N}$	169			
			Methyl formate	$\text{HCOOCH}_3$	170			

**C<sub>2</sub>-nine-atomic molecules**

Dimethylether	CH <sub>3</sub> OCH <sub>3</sub>	176
Dimethylether-d <sub>3</sub>	CH <sub>3</sub> OCD <sub>3</sub>	177

**C<sub>3</sub>-five-atomic molecules**

Carbon suboxide	C <sub>3</sub> O <sub>2</sub>	280
Carbon subsulfide	C <sub>3</sub> S <sub>2</sub>	281

**C<sub>3</sub>-seven-atomic molecules**

Allene	CH <sub>2</sub> CCH <sub>2</sub>	178
Methylacetylene	CH <sub>3</sub> CCH	179
Methylacetylene-d <sub>1</sub>	CH <sub>3</sub> CCD	180
Methylacetylene-d <sub>3</sub>	CD <sub>3</sub> CCH	181
Methylacetylene-d <sub>4</sub>	CD <sub>3</sub> CCD	182
Malononitrile	NCCH <sub>2</sub> CN	183
Malononitrile-d <sub>2</sub>	NCCD <sub>2</sub> CN	184

**C<sub>3</sub>-eight-atomic molecules**

Propenal	C <sub>3</sub> H <sub>4</sub> O	185
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**C<sub>3</sub>-nine-atomic molecules**

Cyclopropane	C <sub>3</sub> H <sub>6</sub>	186
Cyclopropane-d <sub>6</sub>	C <sub>3</sub> D <sub>6</sub>	187
Ethylcyanide	CH <sub>3</sub> CH <sub>2</sub> CN	188

**C<sub>3</sub>-ten-atomic molecules**

Acetone	CH <sub>3</sub> COCH <sub>3</sub>	189
Acetone-d <sub>3</sub>	CH <sub>3</sub> COCD <sub>3</sub>	190
Acetone-d <sub>6</sub>	CD <sub>3</sub> COCD <sub>3</sub>	191

**C<sub>3</sub>-eleven-atomic molecules**

Propane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	192
Propane-d <sub>2</sub>	CH <sub>3</sub> CD <sub>2</sub> CH <sub>3</sub>	193
Propane-d <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> CD <sub>3</sub>	194
Propane-d <sub>6</sub>	CD <sub>3</sub> CH <sub>2</sub> CD <sub>3</sub>	195
Propane-d <sub>8</sub>	CD <sub>3</sub> CD <sub>2</sub> CD <sub>3</sub>	196
Methyl acetate	CH <sub>3</sub> COOCH <sub>3</sub>	197
Methyl acetate-d <sub>3</sub>	CD <sub>3</sub> COOCH <sub>3</sub>	198
Methyl-d <sub>3</sub> -acetate	CH <sub>3</sub> COOCD <sub>3</sub>	199
Methyl acetate-d <sub>6</sub>	CD <sub>3</sub> COOCD <sub>3</sub>	200

**C<sub>4</sub>-six-atomic molecules**

Butadiyne	HCCCCH	201
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**C<sub>4</sub>-nine-atomic molecules**

Furan	C <sub>4</sub> H <sub>4</sub> O	202
Thiophene	C <sub>4</sub> H <sub>4</sub> S	203
Thiophene-d <sub>4</sub>	C <sub>4</sub> D <sub>4</sub> S	204

**T. SHIMANOUCHI****C<sub>4</sub>-ten-atomic molecules**

1,3-Butadiene	CH <sub>2</sub> CHCHCH <sub>2</sub>	205
1,3-Butadiene-d <sub>1</sub> , trans	CH <sub>2</sub> CHCHCHD	206
1,3-Butadiene-1,1,2-d <sub>3</sub>	CH <sub>2</sub> CHCDCD <sub>2</sub>	207
1,3-Butadiene-1,1,4-d <sub>4</sub>	CD <sub>2</sub> CHCHCD <sub>2</sub>	208
1,3-Butadiene-d <sub>6</sub>	CD <sub>2</sub> CDCDCD <sub>2</sub>	209
2-Butyne	CH <sub>3</sub> CCCH <sub>3</sub>	210

**C<sub>4</sub>-12-atomic molecules**

Cyclobutane	C <sub>4</sub> H <sub>8</sub>	211
Cyclobutane-d <sub>8</sub>	C <sub>4</sub> D <sub>8</sub>	212
2-Methylpropene	(CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub>	213
2-Methyl-d <sub>3</sub> -propene-3,3,3-d <sub>3</sub>	CD <sub>3</sub> CCH <sub>2</sub>	214

**C<sub>4</sub>-13-atomic molecules**

2-Butanone, trans form	CH <sub>3</sub> COCH <sub>2</sub> CH <sub>3</sub>	215
1,4-Dioxane	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	333
n-Butane, trans form	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	216
n-Butane, gauche form	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	217

**C<sub>6</sub>-12-atomic molecules**

Benzene	C <sub>6</sub> H <sub>6</sub>	218
Benzene-d <sub>6</sub>	C <sub>6</sub> D <sub>6</sub>	219

**C<sub>6</sub>-13-atomic molecules**

Hexacarbonylchromium	Cr( <sup>12</sup> C <sup>16</sup> O) <sub>6</sub>	334
Hexacarbonylmolybdenum	Mo( <sup>12</sup> C <sup>16</sup> O) <sub>6</sub>	335
Hexacarbonyltungsten	W( <sup>12</sup> C <sup>16</sup> O) <sub>6</sub>	336

**C<sub>6</sub>-18-atomic molecules**

Cyclohexane	C <sub>6</sub> H <sub>12</sub>	220
Cyclohexane-d <sub>12</sub>	C <sub>6</sub> D <sub>12</sub>	221

**Polymer**

Poly-(methylene)	-(CH <sub>2</sub> )n-	222
Poly-(methylene-d <sub>2</sub> )	-(CD <sub>2</sub> )n-	223

**B. Empirical Formula Index**

In this index molecules are divided into two groups: (a) those containing no carbon atoms, for which the formulas are arranged with the elemental symbols 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.

<b>Compounds Not Containing Carbon</b>				
AsF <sub>3</sub>	Arsenic trifluoride	292	Cl <sub>4</sub> Ge	Germanium tetrachloride
AsF <sub>5</sub>	Arsenic pentafluoride	306	Cl <sub>4</sub> Si	Silicon tetrachloride
AsH <sub>3</sub>	Arsine	21	Cl <sub>4</sub> Sn	Tin (IV) chloride
AsH <sub>3</sub>	Arsine-d <sub>3</sub>	22	FGeH <sub>3</sub>	Germyl fluoride
BF <sub>3</sub>	Boron trifluoride- <sup>10</sup> BF <sub>3</sub>	238	FGeH <sub>3</sub>	Germyl fluoride-d <sub>3</sub>
BF <sub>3</sub>	Boron trifluoride- <sup>11</sup> BF <sub>3</sub>	239	FNO	Silyl fluoride
B <sub>2</sub> H <sub>6</sub>	Diborane- <sup>11</sup> B <sub>2</sub> H <sub>6</sub>	55	FNO	Nitrosyl fluoride- <sup>16</sup> O <sup>14</sup> NF
B <sub>2</sub> H <sub>6</sub>	Diborane- <sup>10</sup> B <sub>2</sub> D <sub>6</sub>	56	FNO <sub>2</sub>	Nitrosyl fluoride- <sup>16</sup> O <sup>15</sup> NF
BrCl <sub>3</sub> Si	Bromotrichlorosilane	45	FNO <sub>2</sub>	Nitrosyl fluoride- <sup>18</sup> O <sup>14</sup> NF
BrF <sub>3</sub>	Bromine trifluoride	290	FNS	Nitrosyl fluoride- <sup>18</sup> O <sup>15</sup> NF
BrGeH <sub>3</sub>	Germyl bromide	263	F <sub>2</sub> HN	Nitryl fluoride-F <sup>14</sup> NO <sub>2</sub>
BrGeH <sub>3</sub>	Germyl bromide-d <sub>3</sub>	264	F <sub>2</sub> N <sub>2</sub>	Nitryl fluoride-F <sup>15</sup> NO <sub>2</sub>
BrH <sub>3</sub> Si	Silyl bromide	44	F <sub>2</sub>	Thionitrosyl-S-fluoride
BrNO	Nitrosyl bromide- <sup>16</sup> O <sup>14</sup> NBr	235	F <sub>2</sub> OS	Difluoroamine
BrNO	Nitrosyl bromide- <sup>16</sup> O <sup>15</sup> NBr	236	F <sub>2</sub> O <sub>2</sub> S	Trans-1,2-Difluorodiazine
BrNO	Nitrosyl bromide- <sup>18</sup> O <sup>15</sup> NBr	237	F <sub>2</sub> O <sub>2</sub> Se	Oxygen difluoride
Br <sub>2</sub> Cl <sub>2</sub> Si	Dibromodichlorosilane	49	F <sub>2</sub> S <sub>2</sub>	Thionyl fluoride
Br <sub>2</sub> FOP	Phosphoryl fluorodibromide	303	F <sub>3</sub> HSi	Sulfuryl fluoride
Br <sub>2</sub> H <sub>2</sub> Si	Dibromosilane	301	F <sub>3</sub> HSi	Selenium dioxide difluoride
Br <sub>2</sub> OS	Thionyl bromide	250	F <sub>3</sub> N	Difluoro disulfane
Br <sub>3</sub> ClSi	Tribromochlorosilane	47	F <sub>3</sub> OP	Trifluorosilane
Br <sub>3</sub> GeH	Tribromogermane	268	F <sub>3</sub> P	Trifluorosilane-d
Br <sub>3</sub> HSi	Tribromosilane	255	F <sub>4</sub> Si	Nitrogen trifluoride
Br <sub>3</sub> OP	Phosphoryl bromide	258	F <sub>5</sub>	Phosphorus trifluoride
Br <sub>4</sub> Ge	Germanium tetrabromide	39	F <sub>5</sub> V	Silicon tetrafluoride
Br <sub>4</sub> Si	Silicon tetrabromide	31	F <sub>6</sub> Ir	Phosphorus pentafluoride
Br <sub>4</sub> Sn	Tin (IV) bromide	41	F <sub>6</sub> Mo	Vanadium pentafluoride
ClF <sub>3</sub>	Chlorine trifluoride	289	F <sub>6</sub> S	Iridium fluoride
ClF <sub>5</sub> S	Sulfur chloride pentafluoride	308	F <sub>6</sub> Se	Molybdenum (IV) fluoride
ClF <sub>5</sub> W	Tungsten chloride pentafluoride	309	F <sub>6</sub> Te	Sulfur hexafluoride
ClGeH <sub>3</sub>	Germyl chloride	261	F <sub>6</sub> U	Selenium hexafluoride
ClGeH <sub>3</sub> -d <sub>3</sub>	Germyl chloride-d <sub>3</sub>	262	F <sub>6</sub> W	Tellurium hexafluoride
CIHO	Hypochlorous acid	284	GeH <sub>3</sub> I	Uranium (IV) fluoride
CIHO	Hypochlorous acid-d	2855	GeH <sub>3</sub> I	Tungsten (IV) fluoride
CIH <sub>3</sub> Si	Silyl chloride	43	GeH <sub>4</sub>	Germyl iodide
CII <sub>3</sub> Si	Chlorotriiodosilane	48	GeH <sub>4</sub>	Germyl iodide-d <sub>3</sub>
CINO	Nitrosyl chloride- <sup>16</sup> O <sup>14</sup> NO	231	GeH <sub>4</sub>	Germane
CINO	Nitrosyl chloride- <sup>16</sup> O <sup>15</sup> NCl	232	GeH <sub>4</sub>	Germane-d <sub>1</sub>
CINO	Nitrosyl chloride- <sup>18</sup> O <sup>14</sup> NCl	233	GeH <sub>4</sub>	Germane-d <sub>2</sub>
CINO	Nitrosyl chloride- <sup>18</sup> O <sup>15</sup> NCl	234	Ge <sub>2</sub> H <sub>6</sub>	Germane-d <sub>3</sub>
CINO <sub>2</sub>	Nitryl chloride-Cl <sup>14</sup> NO <sub>2</sub>	235	Ge <sub>2</sub> H <sub>6</sub>	Germane-d <sub>4</sub>
CINO <sub>2</sub>	Nitryl chloride-Cl <sup>15</sup> NO <sub>2</sub>	244	HN <sub>3</sub>	Digermane
CINS	Thionitrosyl-S-chloride	287	HN <sub>3</sub>	Digermane-d <sub>6</sub>
Cl <sub>2</sub> FOP	Phosphoryl fluorodichloride	302	H <sub>2</sub> O	Hydrazoic acid
Cl <sub>2</sub> H <sub>2</sub> Si	Dichlorosilane	299	H <sub>2</sub> O	Hydrazoic acid-d <sub>1</sub>
Cl <sub>2</sub> H <sub>2</sub> Si	Dichlorosilane-d <sub>2</sub>	300	H <sub>2</sub> O	Water
Cl <sub>2</sub> O	Oxygen dichloride	8	H <sub>2</sub> O	Water-d <sub>1</sub>
Cl <sub>2</sub> OS	Thionyl chloride	249	H <sub>2</sub> O <sub>2</sub>	Water-d <sub>2</sub>
Cl <sub>2</sub> O <sub>2</sub> S	Sulfuryl chloride	270	H <sub>2</sub> S	Hydrogen peroxide
Cl <sub>2</sub> S	Sulfur dichloride	226	H <sub>2</sub> S	Hydrogen sulfide
Cl <sub>3</sub> GeH	Trichlorogermane	267	H <sub>2</sub> S <sub>2</sub>	Deuterium sulfide
Cl <sub>3</sub> HSi	Trichlorosilane	253	H <sub>2</sub> Se	Hydrogen persulfide
Cl <sub>3</sub> HSi	Trichlorosilane-d	254	H <sub>2</sub> Se	Hydrogen selenide
Cl <sub>3</sub> ISi	Trichloroiodosilane	46	H <sub>3</sub> N	Hydrogen deuterium selenide
Cl <sub>3</sub> OP	Phosphoryl chloride	257	H <sub>3</sub> N	Ammonia
Cl <sub>3</sub> P	Phosphorus trichloride	20	H <sub>3</sub> N	Ammonia-d <sub>3</sub>
				Ammonia-t <sub>3</sub>

H <sub>3</sub> P	Phosphine	17	CH <sub>2</sub> Br <sub>2</sub>	Dibromomethane	98
H <sub>3</sub> P	Phosphine-d <sub>3</sub>	18	CH <sub>2</sub> Br <sub>2</sub>	Dibromomethane-d <sub>1</sub>	99
H <sub>3</sub> Sb	Stibine	23	CH <sub>2</sub> Br <sub>2</sub>	Dibromomethane-d <sub>2</sub>	100
H <sub>3</sub> Sb	Stibine-d <sub>3</sub>	24	CH <sub>2</sub> Cl <sub>2</sub>	Dichloromethane	95
H <sub>4</sub> Si	Silane	25	CH <sub>2</sub> Cl <sub>2</sub>	Dichloromethane-d <sub>1</sub>	96
H <sub>4</sub> Si	Silane-d <sub>2</sub>	26	CH <sub>2</sub> Cl <sub>2</sub>	Dichloromethane-d <sub>2</sub>	97
H <sub>4</sub> Si	Silane-d <sub>3</sub>	27	CH <sub>2</sub> O	Formaldehyde	68
H <sub>4</sub> Si	Silane-d <sub>4</sub>	28	CH <sub>2</sub> O	Formaldehyde-d <sub>1</sub>	69
I <sub>4</sub> Si	Silicon tetraiodide	32	CH <sub>2</sub> O	Formaldehyde-d <sub>2</sub>	70
NO <sub>2</sub>	Nitrogen dioxide- <sup>14</sup> NO <sub>2</sub>	224	CH <sub>2</sub> O <sub>2</sub>	Formic acid	105
NO <sub>2</sub>	Nitrogen dioxide- <sup>15</sup> NO <sub>2</sub>	225	CH <sub>2</sub> O <sub>2</sub>	Formic acid-d <sub>2</sub>	106
N <sub>2</sub> O	Nitrous oxide	1	CH <sub>3</sub> BO	Borine carbonyl- <sup>10</sup> BH <sub>3</sub> CO	321
N <sub>2</sub> O	Nitrous oxide- <sup>14</sup> N <sup>15</sup> NO	2	CH <sub>3</sub> BO	Borine carbonyl-d <sub>3</sub> <sup>10</sup> BD <sub>3</sub> CO	322
N <sub>2</sub> O	Nitrous oxide- <sup>15</sup> N <sub>2</sub> O	3	CH <sub>3</sub> BO	Borine carbonyl- <sup>11</sup> BH <sub>3</sub> CO	323
O <sub>2</sub> S	Sulfur dioxide	11	CH <sub>3</sub> BO	Borine carbonyl-d <sub>3</sub> <sup>11</sup> BD <sub>3</sub> CO	324
O <sub>2</sub> S	Sulfur dioxide-S <sup>18</sup> O <sub>2</sub>	283	CH <sub>3</sub> Br	Methyl bromide	84
O <sub>3</sub> S	Sulfur trioxide	240	CH <sub>3</sub> Br	Methyl bromide-d <sub>3</sub>	85
O <sub>4</sub> Os	Osmium tetroxide-Os <sup>16</sup> O <sub>4</sub>	297	CH <sub>3</sub> Cl	Methyl chloride	82
O <sub>4</sub> Os	Osmium tetroxide-Os <sup>18</sup> O <sub>4</sub>	298	CH <sub>3</sub> Cl	Methyl chloride-d <sub>3</sub>	83
O <sub>4</sub> Ru	Ruthenium tetroxide	296	CH <sub>3</sub> F	Methyl fluoride	80
			CH <sub>3</sub> F	Methyl fluoride-d <sub>3</sub>	81
			CH <sub>3</sub> I	Methyl iodide	86
			CH <sub>3</sub> I	Methyl iodide-d <sub>3</sub>	87
CBrClO	Carbonyl bromochloride	319	CH <sub>4</sub>	Methane	71
CBrCl <sub>3</sub>	Bromotrichloromethane	93	CH <sub>4</sub>	Methane-d <sub>1</sub>	72
CBrN	Cyanogen bromide- <sup>79</sup> BrCN	66	CH <sub>4</sub>	Methane-d <sub>2</sub>	73
CBrN	Cyanogen bromide- <sup>81</sup> BrCN	67	CH <sub>4</sub>	Methane-d <sub>3</sub>	74
CBr <sub>2</sub> Cl <sub>2</sub>	Dibromodichloromethane	101	CH <sub>4</sub>	Methane-d <sub>4</sub>	75
CBr <sub>2</sub> O	Carbonyl bromide	314	CH <sub>4</sub> O (Gas)	Methanol	107
CBr <sub>3</sub> Cl	Tribromochloromethane	94	CH <sub>4</sub> O	Methanol	108
CBr <sub>4</sub>	Carbon tetrabromide	78	(Liquid)		
CClFO	Carbonyl chlorofluoride	318	CH <sub>4</sub> O (Gas)	Methanol-d <sub>1</sub>	109
CCIN	Cyanogen chloride- <sup>35</sup> ClCN	64	CH <sub>4</sub> O	Methanol-d <sub>1</sub>	110
CCIN	Cyanogen chloride- <sup>37</sup> ClCN	65	(Liquid)		
CCl <sub>2</sub> O	Carbonyl chloride	313	CH <sub>4</sub> O (Gas)	Methanol-d <sub>3</sub>	111
CCl <sub>4</sub>	Carbon tetrachloride	77	CH <sub>4</sub> O	Methanol-d <sub>3</sub>	112
CFN	Cyanogen fluoride	310	(Liquid)		
CF <sub>2</sub> O	Carbonyl fluoride	312	CH <sub>4</sub> O (Gas)	Methanol-d <sub>4</sub>	113
CF <sub>2</sub> S	Thiocarbonyl fluoride	315	CH <sub>5</sub> N	Methylamine	114
CF <sub>4</sub>	Carbon tetrafluoride	76	CH <sub>5</sub> N	Methylamine-d <sub>2</sub>	115
CIN	Cyanogen iodide	311	CH <sub>5</sub> N	Methylamine-d <sub>3</sub>	116
Cl <sub>4</sub>	Carbon tetraiodide	79	CH <sub>5</sub> N	Methylamine-d <sub>5</sub>	117
COS	Carbonyl sulfide	61	CH <sub>6</sub> Ge	Methylgermane	277
CO <sub>2</sub>	Carbon dioxide	58	CH <sub>6</sub> Ge	Methyl-d <sub>3</sub> -germane	278
CO <sub>2</sub>	Carbon dioxide- <sup>13</sup> CO <sub>2</sub>	59	CH <sub>6</sub> Si	Methylsilane	275
CS <sub>2</sub>	Carbon disulfide	60	CH <sub>6</sub> Si	Methylsilane-d <sub>3</sub>	276
CHBr <sub>3</sub>	Tribromomethane	91	C <sub>2</sub> BrCl	Bromoacetylene	328
CHBr <sub>3</sub>	Tribromomethane-d <sub>1</sub>	92	C <sub>2</sub> Br <sub>2</sub>	Dibromoacetylene	326
CHCl <sub>3</sub>	Trichloromethane	89	C <sub>2</sub> Br <sub>4</sub>	Tetrabromoethylene	128
CHCl <sub>3</sub>	Trichloromethane-d <sub>1</sub>	90	C <sub>2</sub> Br <sub>6</sub>	Hexabromoethane	159
CHF <sub>3</sub>	Trifluoromethane	88	C <sub>2</sub> ClI	Chloroiodoacetylene	329
CHF <sub>3</sub>	Trifluoromethane-d	320	C <sub>2</sub> Cl <sub>2</sub>	Dichloroacetylene	325
CHN	Hydrogen cyanide	62	C <sub>2</sub> Cl <sub>2</sub> F <sub>2</sub>	trans-1,2-Dichloro-	
CHN	Deuterium cyanide	63		1,2-difluoroethylene	138
CHNO	Isocyanic acid	316	C <sub>2</sub> Cl <sub>2</sub> F <sub>2</sub>	1,1-Dichloro-2,2-difluoroethylene	142
CHNO	Isocyanic acid-d	317	C <sub>2</sub> Cl <sub>4</sub>	Tetrachloroethylene	127
CH <sub>2</sub> BrCl	Bromochloromethane	102	C <sub>2</sub> Cl <sub>6</sub>	Hexachloroethane	158
CH <sub>2</sub> BrCl	Bromochloromethane-d <sub>1</sub>	103	C <sub>2</sub> F <sub>4</sub>	Tetrafluoroethylene	126
CH <sub>2</sub> BrCl	Bromochloromethane-d <sub>2</sub>	104	C <sub>2</sub> F <sub>6</sub>	Hexafluoroethane	157

C <sub>2</sub> I <sub>2</sub>	Diiodoacetylene	327	C <sub>2</sub> H <sub>6</sub> O	Dimethylether	176
C <sub>2</sub> N <sub>2</sub>	Cyanogen	279	C <sub>2</sub> H <sub>6</sub> O	Dimethylether-d <sub>3</sub>	177
C <sub>2</sub> HBr	Bromoacetylene	123	C <sub>3</sub> O <sub>2</sub>	Carbon suboxide	280
C <sub>2</sub> HCl	Chloroacetylene	122	C <sub>3</sub> S <sub>2</sub>	Carbon subsulfide	281
C <sub>2</sub> HF	Fluoroacetylene	121	C <sub>3</sub> H <sub>2</sub> N <sub>2</sub>	Malononitrile	183
C <sub>2</sub> H <sub>2</sub>	Acetylene	118	C <sub>3</sub> H <sub>2</sub> N <sub>2</sub>	Malononitrile-d <sub>2</sub>	184
C <sub>2</sub> H <sub>2</sub>	Acetylene-d <sub>1</sub>	119	C <sub>3</sub> H <sub>4</sub>	Allene	178
C <sub>2</sub> H <sub>2</sub>	Acetylene-d <sub>2</sub>	120	C <sub>3</sub> H <sub>4</sub>	Methylacetylene	179
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	trans-1,2-Dichloroethylene	132	C <sub>3</sub> H <sub>4</sub>	Methylacetylene-d <sub>1</sub>	180
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	trans-1,2-Dichloroethylene-d <sub>1</sub>	133	C <sub>3</sub> H <sub>4</sub>	Methylacetylene-d <sub>3</sub>	181
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	trans-1,2-Dichloroethylene-d <sub>2</sub>	134	C <sub>3</sub> H <sub>4</sub>	Methylacetylene-d <sub>4</sub>	182
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	cis-1,2-Dichloroethylene	135	C <sub>3</sub> H <sub>4</sub> O	Propenal	185
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	cis-1,2-Dichloroethylene-d <sub>1</sub>	136	C <sub>3</sub> H <sub>5</sub> N	Ethylcyanide	188
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	cis-1,2-dichloroethylene-d <sub>2</sub>	137	C <sub>3</sub> H <sub>6</sub>	Cyclopropane	186
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	1,1-Dichloroethylene	139	C <sub>3</sub> H <sub>6</sub>	Cyclopropane-d <sub>6</sub>	187
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	1,1-Dichloroethylene-d <sub>1</sub>	140	C <sub>3</sub> H <sub>6</sub> O	Acetone	189
C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub>	1,1-Dichloroethylene-d <sub>2</sub>	141	C <sub>3</sub> H <sub>6</sub> O	Acetone-d <sub>3</sub>	190
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	cis-1,2-Difluoroethylene	129	C <sub>3</sub> H <sub>6</sub> O	Acetone-d <sub>6</sub>	191
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	cis-1,2-Difluoroethylene-d <sub>1</sub>	130	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	Methyl acetate	197
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	cis-1,2-Difluoroethylene-d <sub>2</sub>	131	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	Methyl-d <sub>3</sub> -acetate	198
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	trans-1,2-Difluoroethylene	330	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	Methyl acetate-d <sub>3</sub>	199
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	trans-1,2-Difluoroethylene-d <sub>1</sub>	331	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	Methyl acetate-d <sub>6</sub>	200
C <sub>2</sub> H <sub>2</sub> F <sub>2</sub>	trans-1,2-Difluoroethylene-d <sub>2</sub>	332	C <sub>3</sub> H <sub>8</sub>	Propane	192
C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> O	1,2,5-Oxadiazole	147	C <sub>3</sub> H <sub>8</sub>	Propane-d <sub>3</sub>	193
C <sub>2</sub> H <sub>3</sub> N	Methyl cyanide	143	C <sub>3</sub> H <sub>8</sub>	Propane-d <sub>2</sub>	194
C <sub>2</sub> H <sub>3</sub> N	Methyl cyanide-d <sub>3</sub>	144	C <sub>3</sub> H <sub>8</sub>	Propane-d <sub>6</sub>	195
C <sub>2</sub> H <sub>3</sub> N	Methyl isocyanide	145	C <sub>3</sub> H <sub>8</sub>	Propane-d <sub>8</sub>	196
C <sub>2</sub> H <sub>3</sub> N	Methyl isocyanide-d <sub>3</sub>	146	C <sub>4</sub> H <sub>2</sub>	Butadiyne	201
C <sub>2</sub> H <sub>4</sub>	Ethylene	124	C <sub>4</sub> H <sub>4</sub> O	Furan	202
C <sub>2</sub> H <sub>4</sub>	Ethylene-d <sub>4</sub>	125	C <sub>4</sub> H <sub>4</sub> S	Thiophene	203
C <sub>2</sub> H <sub>4</sub> BrCl	1-Bromo-2-chloroethane, trans form	164	C <sub>4</sub> H <sub>4</sub> S	Thiophene-d <sub>4</sub>	204
C <sub>2</sub> H <sub>4</sub> BrCl	1-Bromo-2-chloroethane, trans form	165	C <sub>4</sub> H <sub>6</sub>	1,3-Butadiene	205
C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>	1,2-Dibromoethane, trans form	162	C <sub>4</sub> H <sub>6</sub>	1,3-Butadiene-d <sub>1</sub> , trans	206
C <sub>2</sub> H <sub>4</sub> Br <sub>2</sub>	1,2-Dibromoethane, gauche form	163	C <sub>4</sub> H <sub>6</sub>	1,3-Butadiene-1,1,2-d <sub>3</sub>	207
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	1,2-Dichloroethane, trans form	160	C <sub>4</sub> H <sub>6</sub>	1,3-Butadiene-1,1,4,4-d <sub>4</sub>	208
C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub>	1,2-dichloroethane, gauche form	161	C <sub>4</sub> H <sub>6</sub>	1,3-Butadiene-d <sub>6</sub>	209
C <sub>2</sub> H <sub>4</sub> O	Ethylene oxide	149	C <sub>4</sub> H <sub>6</sub>	2-Butyne	210
C <sub>2</sub> H <sub>4</sub> O	Ethylene oxide-d <sub>4</sub>	150	C <sub>4</sub> H <sub>8</sub>	Cyclobutane	211
C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde	151	C <sub>4</sub> H <sub>8</sub>	Cyclobutane-d <sub>8</sub>	212
C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde-d <sub>1</sub>	152	C <sub>4</sub> H <sub>8</sub>	2-Methylpropene	213
C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde-d <sub>4</sub>	153	C <sub>4</sub> H <sub>8</sub>	2-Methyl-d <sub>3</sub> -propene-3,3,3-d <sub>3</sub>	214
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate	170	C <sub>4</sub> H <sub>8</sub> O	2-Butanone, trans form	215
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate-d <sub>1</sub>	171	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	1,4-Dioxane	333
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate-d <sub>3</sub>	172	C <sub>4</sub> H <sub>10</sub>	n-Butane, trans form	216
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate-d <sub>4</sub>	173	C <sub>4</sub> H <sub>10</sub>	n-Butane, gauche form	217
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Acetic acid	174	C <sub>6</sub> CrO <sub>6</sub>	Hexacarbonylchromium	334
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Acetic acid-d <sub>1</sub>	175	C <sub>6</sub> MoO <sub>6</sub>	Hexacarbonylmolybdenum	335
C <sub>2</sub> H <sub>4</sub> Si	Silylacetylene	148	C <sub>6</sub> O <sub>6</sub> W	Hexacarbonyltungsten	336
C <sub>2</sub> H <sub>5</sub> Br	Bromoethane	168	C <sub>6</sub> H <sub>6</sub>	Benzene	218
C <sub>2</sub> H <sub>5</sub> Cl	Chloroethane	167	C <sub>6</sub> H <sub>6</sub>	Benzene-d <sub>6</sub>	219
C <sub>2</sub> H <sub>5</sub> F	Fluoroethane	166	C <sub>6</sub> H <sub>12</sub>	Cyclohexane	220
C <sub>2</sub> H <sub>5</sub> N	Ethylene imine	169	C <sub>6</sub> H <sub>12</sub>	Cyclohexane-d <sub>12</sub>	221
C <sub>2</sub> H <sub>6</sub>	Ethane	154	-(CH <sub>2</sub> )n-	Poly- (methylene)	222
C <sub>2</sub> H <sub>6</sub>	Ethane-d <sub>3</sub>	155	-(CH <sub>2</sub> )n-	Poly- (methylene-d <sub>2</sub> )	223
C <sub>2</sub> H <sub>6</sub>	Ethane-d <sub>6</sub>	156			