

# **Tables of Molecular Vibrational Frequencies: Part 7**

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# Tables of Molecular Vibrational Frequencies

## Part 7

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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 50 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, and a sixth set, covering 55 molecules, have appeared in earlier issues of this journal [3, 4].

### 2. Molecules Selected

The present volume contains tables of fundamental vibrational frequencies for 50 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. [5], [6], and [7] 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 337, continuing the designations of Part 6 of the tables.

### 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. [8] and [9].

#### 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. [9], 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 12-30 of ref. [9]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be

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

defined uniquely. In such cases we generally follow the notation adopted in ref. [9].

### 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
$C_{6v}$	$A_1$ , $A_2$ , $E_1$ , $E_2$
$C_{\infty v}$	$\Sigma^+$ , $\Sigma^-$ , $\pi$ , $\Delta$ , $\Phi$ , ...
$C_{4v}$ , $D_4$ , $D_{2d}$	$A_1$ , $A_2$ , $B_1$ , $B_2$ , E
$C_{6v}$ , $D_6$	$A_1$ , $A_2$ , $B_1$ , $B_2$ , $E_1$ , $E_2$
$D_{3d}$	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , $E_g$ , $E_u$
$D_{4d}$	$A_1$ , $A_2$ , $B_1$ , $B_2$ , $E_1$ , $E_2$ , $E_3$
$D_{3h}$	$A_1'$ , $A_1''$ , $A_2'$ , $A_2''$ , $E'$ , $E''$
$D_{5h}$	$A_1'$ , $A_1''$ , $A_2'$ , $A_2''$ , $E_1'$ , $E_1''$ , $E_2'$ , $E_2''$
$D_{4h}$	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , $B_{1g}$ , $B_{1u}$ , $B_{2g}$ , $B_{2u}$ , $E_g$ , $E_u$
$D_{6h}$	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , $B_{1g}$ , $B_{1u}$ , $B_{2g}$ , $B_{2u}$ , $E_{1g}$ , $E_{1u}$ , $E_{2g}$ , $E_{2u}$
$D_{\infty h}$	$\Sigma_g^+$ , $\Sigma_u^+$ , $\Sigma_g^-$ , $\Sigma_u^-$ , $\pi_g$ , $\pi_u$ , $\Delta_g$ , $\Delta_u$ , $\Phi_g$ , $\Phi_u$ , ...
$C_3$	A, E
$C_6$	A, B, $E_1$ , $E_2$
$S_6$	$A_g$ , $A_u$ , $E_g$ , $E_u$
$C_{3h}$	$A'$ , $A''$ , $E'$ , $E''$
$C_{4h}$	$A_g$ , $A_u$ , $B_g$ , $B_u$ , $E_g$ , $E_u$
$C_{6h}$	$A_g$ , $A_u$ , $B_g$ , $B_u$ , $E_{1g}$ , $E_{1u}$ , $E_{2g}$ , $E_{2u}$
$T_d$ , O	$A_1$ , $A_2$ , E, $F_1$ , $F_2$
$O_h$	$A_{1g}$ , $A_{1u}$ , $A_{2g}$ , $A_{2u}$ , $E_g$ , $E_u$ , $F_{1g}$ , $F_{1u}$ , $F_{2g}$ , $F_{2u}$
T	A, E, F

### 3.5. 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  $CH_3$  group (see fig. 1a)  
 $CH_3$  symmetrical stretching:  $(\Delta r_1 + \Delta r_2 + \Delta r_3) / \sqrt{3}$   
 $CH_3$  degenerate stretching:  $(2\Delta r_1 - \Delta r_2 - \Delta r_3) / \sqrt{6}$   
 $(\Delta r_2 - \Delta r_3) / \sqrt{2}$   
 $CH_3$  symmetrical deformation:  
 $(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12} - \Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3) / \sqrt{6}$   
 $CH_3$  degenerate deformation:  $(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12}) / \sqrt{6}$   
 $(\Delta\alpha_{31} - \Delta\alpha_{12}) / \sqrt{2}$   
 $CH_3$  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  $CH_2$  group (see fig. 1b)  
 $CH_2$  symmetrical stretching:  $(\Delta r_1 + \Delta r_2) / \sqrt{2}$   
 $CH_2$  antisymmetrical stretching:  $(\Delta r_1 - \Delta r_2) / \sqrt{2}$   
 $CH_2$  scissors:  $(4\Delta\alpha - \Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y}) / \sqrt{20}$   
 $CH_2$  wagging:  $(\Delta\beta_{1X} + \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y}) / 2$   
 $CH_2$  twisting:  $(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y}) / 2$   
 $CH_2$  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:  $\Delta r_{CH}$   
 $CH$  bending:  $(2\Delta\beta_{HX} - \Delta\beta_{HY} - \Delta\beta_{HZ}) / \sqrt{6}$   
 $(\Delta\beta_{HY} - \Delta\beta_{HZ}) / \sqrt{2}$
- (d) Local symmetry coordinates for the planar  $CH_2$  group (see fig. 1d)  
 $CH_2$  symmetrical stretching:  $(\Delta r_1 + \Delta r_2) / \sqrt{2}$   
 $CH_2$  antisymmetrical stretching:  $(\Delta r_1 - \Delta r_2) / \sqrt{2}$   
 $CH_2$  scissors:  $(2\Delta\alpha - \Delta\beta_1 - \Delta\beta_2) / \sqrt{6}$   
 $CH_2$  rocking:  $(\Delta\beta_1 - \Delta\beta_2) / \sqrt{2}$   
 $CH_2$  wagging:  $\Delta\theta \cdot \sin\alpha$ .
- (e) Local symmetry coordinates for the planar CH group (see fig. 1e)  
 $CH$  stretching:  $\Delta r_{CH}$   
in-plane CH bending:  $(\Delta\beta_{HX} - \Delta\beta_{HY}) / \sqrt{2}$   
out-of-plane CH bending:  $\Delta\theta_H \cdot \sin\gamma_{XY}$ .

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

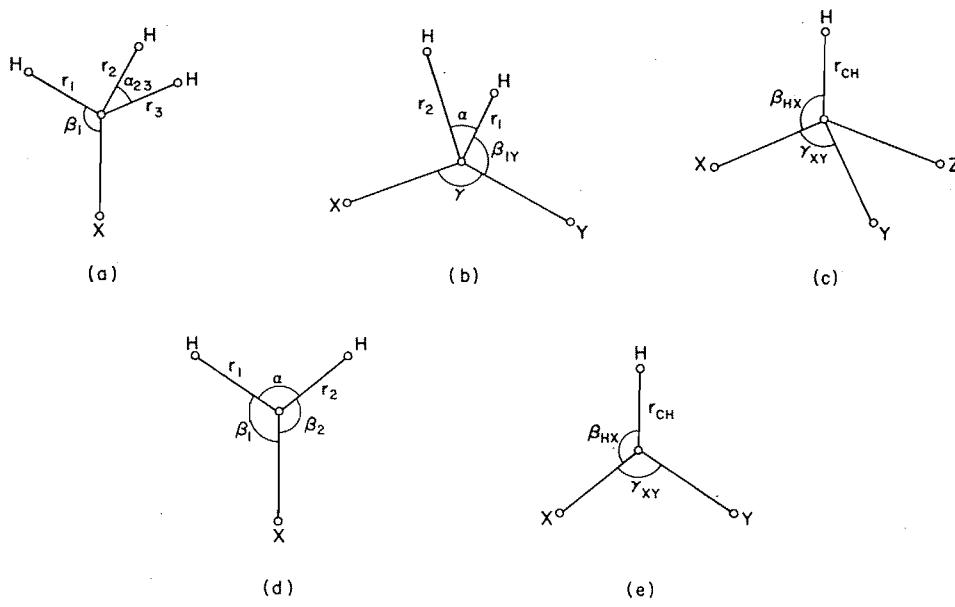


FIGURE 1. Parameters of methyl, methylene, and methin groups.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis*
A	cm <sup>-1</sup> 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 ~ 1000 cm <sup>-1</sup> for NaCl prism).
C	3 ~ 6	(i) Gas, prism spectrometer, low resolution (e.g., 1000 ~ 2000 cm <sup>-1</sup> for NaCl prism). (ii) Solid, liquid or solution, accurate measurement.
D	6 ~ 15	(i) Gas, prism spectrometer, very low resolution (e.g., > 2000 cm <sup>-1</sup> for NaCl prism). (ii) Solid, liquid or solution, inaccurate measurement.
E	15 ~ 30	(i) Value estimated from Fermi resonance doublet. (ii) Value estimated from overtone or combination tone. (iii) Calculated frequency.

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

indicating the correspondence between similar modes in large and small molecules.

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

The fundamental frequency  $\nu_i$  is defined as the difference between the term value  $G(\nu_i = 1, \text{all other } \nu_j = 0)$  and  $G(\nu_i = 0, \text{and other } \nu_j = 0)$  expressed in cm<sup>-1</sup>. 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 cm<sup>-1</sup>.

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 cm<sup>-1</sup> 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

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

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. [9], 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. [11] 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. [10].

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

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358	Chloronitrate ClO <sup>14</sup> NO <sub>2</sub> .....	240	383	Chlorodiacylene C1CCCC.....	255
359	Chloronitrate ClO <sup>15</sup> NO <sub>2</sub> .....	241	384	Bromodiacylene BrCCCC.....	255
360	Thiophosphoryl chlorodifluoride PSF <sub>2</sub> Cl.....	241	385	Iododiacylene ICCCCH.....	256
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No. 337 Krypton difluoride KrF<sub>2</sub>Symmetry D<sub>∞h</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> (Gas)	cm <sup>-1</sup> (Gas)
σ <sub>g</sub> <sup>+</sup>	ν <sub>1</sub>	Sym. stretch.	449 B	ia	449	
σ <sub>u</sub> <sup>+</sup>	ν <sub>2</sub>	Antisym. stretch.	590 A	589.89 VS	ia	
π <sub>u</sub>	ν <sub>3</sub>	Bend.	233 B	232.6 S	ia	

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J. Amer. Chem. Soc. **90**, 5690 (1968).

## No. 338 Hypofluorous acid HOF

Symmetry C<sub>s</sub>

Symmetry number σ = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup>	cm <sup>-1</sup> (Nitrogen matrix)	cm <sup>-1</sup>
a'	ν <sub>1</sub>	OH stretch.	3537 C	3537.1		
	ν <sub>2</sub>	OF stretch.	1393 C	1393.0		
	ν <sub>3</sub>	Bend.	886 C	886.0		

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No. 339    Nitrogen trifluoride     $^{15}\text{NF}_3$   
 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)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.	1009 A	1008.93		
	$\nu_2$	Sym. deform.	645 B	644.84		
$e$	$\nu_3$	Deg. stretch.	886 A	886.34		
	$\nu_4$	Deg. deform.	492 B	492.02		

## References

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

No. 340    Phosphorus triiodide     $\text{PI}_3$   
 Symmetry  $\text{C}_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ ( $\text{CS}_2, \text{C}_6\text{H}_6,$ $\text{CH}_2\text{Cl}_2$ soln.)	$\text{cm}^{-1}$ $\text{C}_6\text{H}_6,$ $\text{CCl}_4$ soln.)	
$a_1$	$\nu_1$	$\text{PI}_3$ s-stretch.	303 D	306 M	303 (3) p	
	$\nu_2$	$\text{PI}_3$ s-deform.	111 D	112 VW	111 (7) p	
$e$	$\nu_3$	$\text{PI}_3$ d-stretch.	325 D	328 VS	325 (1b) dp	
	$\nu_4$	$\text{PI}_3$ d-deform.	79 D	80 VW, b	79 (10) dp	

## References

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

No. 341      Arsenic triiodide       $\text{AsI}_3$   
 Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Solid)	$\text{cm}^{-1}$ ( $\text{CHBr}_3, \text{CS}_2$ soln.)	
$a_1$	$\nu_1$	$\text{AsI}_3$ s-stretch.	219 C	225.7	218.5 p	
	$\nu_2$	$\text{AsI}_3$ s-deform.	94 C	101.6	94 p	
$e$	$\nu_3$	$\text{AsI}_3$ d-stretch.	224 C	201.2 VVS,b	223.5 dp	
	$\nu_4$	$\text{AsI}_3$ d-deform.	71 C	73.6	71 dp	

## References

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

No. 342      Chlorodifluoroammonia  $\text{NClF}_2$   
 Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	$\text{NF}_2$ s-stretch.	930 C	930.2		
	$\nu_2$	$\text{NCl}$ stretch.	697 C	696.9		
	$\nu_3$	$\text{NF}_2$ deform.	556 C	555.5		
	$\nu_4$	$\text{NClF}$ s-deform.	377 C	377		
$a''$	$\nu_5$	$\text{NF}_2$ a-stretch.	855 C	855.4		
	$\nu_6$	$\text{NClF}$ a-deform.	382 D	382*		

\* An average of two splitting bands.

## References

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

**No. 343      Dichlorofluoroammonia  $\text{NCl}_2\text{F}$**   
**Symmetry  $\text{C}_s$** 
**Symmetry number  $\sigma = 1$** 

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

**References**

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

**No. 344      Thionitrosyl trifluoride       $\text{NSF}_3$**   
**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)	
$a_1$	$\nu_1$	NS stretch.	1515 B	1515	1512 p	
	$\nu_2$	$\text{NF}_3$ s-stretch.	775 B	775	768 p	
	$\nu_3$	$\text{NF}_3$ s-deform.	521 B	521	520 dp	
$e$	$\nu_4$	$\text{NF}_3$ d-stretch.	811 B	811	812 dp	
	$\nu_5$	$\text{NF}_3$ d-deform.	429 B	429	430 dp	
	$\nu_6$	$\text{NF}_3$ rock.	342 B	342	340 dp	

**References**

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

No. 345      Thiophosphoryl trifluoride       $\text{PSF}_3$   
 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)	
$a_1$	$\nu_1$	$\text{PF}_3$ s-stretch.	981 B	981 VS	969 (4.5) p	
	$\nu_2$	PS stretch.	695 B	695 M	696 (100) p	
	$\nu_3$	$\text{PF}_3$ s-deform.	440 B	440 M	441 (20) p	
$e$	$\nu_4$	$\text{PF}_3$ d-stretch.	945 B	945 VS	937 (6.0) dp	
	$\nu_5$	$\text{PF}_3$ d-deform.	402 C	402 M	404 (13) dp	
	$\nu_6$	$\text{PF}_3$ rock.	275 B	275 W	276 (37) dp	

## References

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

No. 346      Thiophosphoryl trichloride       $\text{PSCl}_3$   
 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)	
$a_1$	$\nu_1$	PS stretch.	770 B	770	750 (8) p	
	$\nu_2$	$\text{PCl}_3$ s-stretch.	431 B	431	435 (100) p	
	$\nu_3$	$\text{PCl}_3$ s-deform.	252 E	252	250 (56) dp	OV( $\nu_5$ ).
$e$	$\nu_4$	$\text{PCl}_3$ d-stretch.	547 B	547	539 (8) dp	
	$\nu_5$	$\text{PCl}_3$ d-deform.	252 D	252	250 (56) dp	OV( $\nu_3$ ).
	$\nu_6$	$\text{PCl}_3$ rock.	174 D	174	174 (49) dp	
				(liquid)		

## References

- [1] IR. G. Cilento, D. A. Ramsay, and R. N. Jones J. Amer. Chem. Soc. **71**, 2753 (1949).
- [2] IR.R. J. R. Durig and J. W. Clark, J. Chem. Phys. **46**, 3057 (1967).

**No. 347 Perchlorylfluoride  $^{35}\text{ClO}_3\text{F}$**   
**Symmetry  $\text{C}_{3v}$**

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{ClO}_3$ s-stretch.	1063 B	1061 S	1062.8 VS	
	$\nu_2$	ClF stretch.	717 B	714 S	716.8 S	
	$\nu_3$	$\text{ClO}_3$ s-deform.	549 B	549 W	548.8 M	
$e$	$\nu_4$	$\text{ClO}_3$ d-stretch.	1314 B	1315 VS	1314 W	
	$\nu_5$	$\text{ClO}_3$ d-deform.	573 B	590.55 M	573 W	
	$\nu_6$	$\text{ClO}_3$ rock.	414 B	405 W	414 W	

**References**

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

**No. 348 Vanadyl(V) chloride  $\text{VOCl}_3$**   
**Symmetry  $\text{C}_{3v}$**

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	VO stretch.	1042 C	1035 VS	1042 (1.8) p	
	$\nu_2$	$\text{VCl}_3$ s-stretch.	408 C	408 S	408 (10.0) p	
	$\nu_3$	$\text{VCl}_3$ s-deform.	125 C		125 (3.8) p	
$e$	$\nu_4$	$\text{VCl}_3$ d-stretch.	502 D	502 VS	502 (2.0) dp	
	$\nu_5$	$\text{VCl}_3$ d-deform.	249 C		249 (1.5) dp	
	$\nu_6$	$\text{VCl}_3$ rock.	164 C		164 (0.8) dp	

**References**

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

No. 349      Permanganyl fluoride     $\text{MnO}_3\text{F}$   
 Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

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

## Reference

- [1] IR.      M. J. Reisfeld, L. B. Asprey, and N. A. Matuiyoff, Spectrochim. Acta **27A**, 765 (1971).

No. 350      Rhenium (VII) oxide chloride     $\text{ReO}_3\text{Cl}$   
 Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

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

## References

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

**No. 351 Rhenium (VII) oxide bromide  $\text{ReO}_3\text{Br}$** **Symmetry  $C_3v$** **Symmetry number  $\sigma = 3$** 

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

**References**

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

**No. 352 Nitric acid  $\text{H}^{14}\text{NO}_3$** **Symmetry  $C_s$** **Symmetry number  $\sigma = 1$** 

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

**Reference**

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

No. 353 Nitric acid-d  $D^{14}NO_3$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 354 Nitric acid  $H^{15}NO_3$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 355      Nitric acid-d       $D^{15}NO_3$   
 Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 356      Fluoronitrate       $FO^{14}NO_2$   
 Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## References

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

No. 357      Fluoronitrate       $\text{FO}^{15}\text{NO}_2$   
 Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	NO a-stretch.	1720 C	1719.8 VS		
	$\nu_2$	$\text{NO}_2$ s-stretch.	1291 B	1290.5 VS		
	$\nu_3$	OF stretch.	928 B	927.5 S		
	$\nu_4$	$\text{NO}_2$ scis.	792 B	791.8 S		
	$\nu_5$	NO stretch.	632 B	631.5 VW		
	$\nu_6$	$\text{NO}_2$ rock.	455 B	454.4 MS		
	$\nu_7$	OF bend.	302 B	301.6 VW		
$a''$	$\nu_8$	$\text{NO}_2$ wag.	690 C	690.2 M		
	$\nu_9$	OF torsion	151 D	151.2		$\text{OC}(\nu_1 + \nu_9, \nu_1 - \nu_9,$ $\nu_3 + \nu_9).$

## References

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

No. 358      Chloronitrate       $\text{ClO}^{14}\text{NO}_2$   
 Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	$\text{NO}_2$ a-stretch.	1735 B	1735.4 VS		
	$\nu_2$	$\text{NO}_2$ s-stretch.	1292 B	1291.9 VS		
	$\nu_3$	OCl stretch.	809 C	809.3 S		
	$\nu_4$	$\text{NO}_2$ scis.	780 C	780.2 MS		
	$\nu_5$	NO stretch.	560 B	560.0 S		
	$\nu_6$	$\text{NO}_2$ rock.	434 B	434.1 M		
	$\nu_7$	OCl bend.	270 C	270    VVV		
$a''$	$\nu_8$	$\text{NO}_2$ wag.	711 B	710.8 W		
	$\nu_9$	OCl torsion	121 E	121		$\text{OC}(\nu_5 + \nu_7 - \nu_9).$

## References

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

No. 359 Chloronitrate  $\text{ClO}^{15}\text{NO}_2$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	$\text{NO}_2$ a-stretch.	1694 B	1694.0 VS		
	$\nu_2$	$\text{NO}_2$ s-stretch.	1280 B	1280.2 VS		
	$\nu_3$	OCl stretch.	805 C	804.7 MS		
	$\nu_4$	$\text{NO}_2$ scis.	773 C	772.9 S		
	$\nu_5$	NO stretch.	557 B	556.8 S		
	$\nu_6$	$\text{NO}_2$ rock.	432 B	432.2 M		
	$\nu_7$	OCl bend.	263 D	263		$\text{OC}(\nu_5 + \nu_7)$ .
$a''$	$\nu_8$	$\text{NO}_2$ wag.	694 B	693.7 W		
	$\nu_9$	OCl torsion	122 E	122		$\text{OC}(\nu_5 + \nu_7 - \nu_9)$ .

## References

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

No. 360 Thiophosphoryl chlorodifluoride  $\text{PSF}_2\text{Cl}$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	$\text{PF}_2$ s-stretch.	946 B	946 VS	939 (3.7) p	
	$\nu_2$	PS stretch.	738 B	738 VS	727 (50) p	
	$\nu_3$	$\text{PCl}$ stretch.	541 B	541 S	536 (100) p	
	$\nu_4$	$\text{PCl}$ bend.	395 B	395 M	394 (31) p	
	$\nu_5$	$\text{PF}_2$ scis.	361 B	361 M	359 (38) p	
	$\nu_6$	PS ip-bend.	207 C	198	207 (65) p	
$a''$	$\nu_7$	$\text{PF}_2$ s-stretch.	920 B	920 VS	913 (6.5) dp	
	$\nu_8$	$\text{PF}_2$ rock.	317 B	317 M	314 (14) dp	
	$\nu_9$	PS op-bend.	251 C		251 (14) dp	

## Reference

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

**No. 361      Thiophosphoryl dichlorofluoride  $\text{PSFCl}_2$**   
**Symmetry  $C_s$**

**Symmetry number  $\sigma = 1$**

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

**Reference**

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

**No. 362      Phosphorus difluoride trichloride  $\text{PCl}_3\text{F}_2$**   
**Symmetry  $D_{3h}$**

**Symmetry number  $\sigma = 6$**

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

**References**

- [1] IR.R. J. E. Griffiths, R. P. Carter, Jr., and R. R. Holmes, J. Chem. Phys. **41**, 863 (964).  
[2] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8**, 2612 (1969).  
[3] Th. I. R. Beattie, K. M. S. Livingston, and D. J. Reynolds, J. Chem. Phys. **51**, 4269 (1969).

No. 363 Phosphorus pentachloride  $\text{PCl}_5$   
Symmetry  $D_{3h}$

Symmetry number  $\sigma = 6$ 

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

## References

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

No. 364 Antimony pentachloride  $SbCl_5$   
Symmetry  $D_{3h}$

Symmetry number  $\sigma = 6$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$cm^{-1}$	$cm^{-1}$	$cm^{-1}$
				(Gas)	(Liquid)	
$a_1'$	$\nu_1$	$SbCl_3$ s-stretch.	357 C		357 (10) p	
	$\nu_2$	$SbCl_2$ s-stretch.	307 C	306 W (liquid)	307 (4) dp	
$a_2''$	$\nu_3$	$SbCl_2$ a-stretch.	384 C	384 VS		
	$\nu_4$	$SbCl_3$ op-deform.	154 D	154 ( $CCl_4$ soln.)		
$e'$	$\nu_5$	$SbCl_3$ d-stretch.	398 C	398 VS	397 (2)	
	$\nu_6$	$SbCl_3$ d-deform.	177 C	172 S ( $CCl_4$ soln.)	177 (4) dp	
$e''$	$\nu_7$	SbCl bend.	72 D		72 dp	
	$\nu_8$	SbCl bend.	165 C		165 (2) dp	

## References

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

No. 365 Methylmercuric iodide  $CH_3HgI$   
Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$cm^{-1}$	$cm^{-1}$	$cm^{-1}$
				(Solid)	( $CH_3NO_2$ soln.)	
$a_1$	$\nu_1$	$CH_3$ s-stretch.	2920 D	2920 M	2914 (Solid)	
	$\nu_2$	$CH_3$ s-deform.	1180 D	1180 M	1182 p	
	$\nu_3$	CHg stretch.	531 D	531 M	538 p	
	$\nu_4$	HgI stretch.	184 D	184 M	180 p	
$e$	$\nu_5$	$CH_3$ d-stretch.	3008 D	3008 M		
	$\nu_6$	$CH_3$ d-deform.	1400 D	1400 W		
	$\nu_7$	$CH_3$ rock.	781 D	781 S		
	$\nu_8$	CHgI bend.	64 D	64 M		

## References

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

No. 366 Methyltriiodogermane  $\text{CH}_3\text{GeI}_3$   
Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch.	2911 C	2911 M	2909 W	
	$\nu_2$	$\text{CH}_3$ s-deform.	1225 C	1225 M	1222 W	
	$\nu_3$	CGe stretch.	597 C	597 S	596 M	
	$\nu_4$	$\text{GeI}_3$ s-stretch.	195 C	196 M (Solid)	195 S	
	$\nu_5$	$\text{GeI}_3$ s-deform.	92 C	96 M (Solid)	92 S	
$a_2$	$\nu_6$	Torsion	123 D	123 VW (Solid)	123 VW	
$e$	$\nu_7$	$\text{CH}_3$ d-stretch.	2999 C	2999 M	2996 W	
	$\nu_8$	$\text{CH}_3$ d-deform.	1392 C	1392 S	1394 (Solid)	
	$\nu_9$	$\text{CH}_3$ rock.	810 C	810 S	809 (Solid)	
	$\nu_{10}$	$\text{GeI}_3$ d-stretch.	252 C	252 S	251 M	
	$\nu_{11}$	$\text{GeI}_3$ rock.	147 C		147 M	
	$\nu_{12}$	$\text{GeI}_3$ d-deform.	67 C		67 S	

## References

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

No. 367 Methylstannane  $\text{CH}_3\text{SnH}_3$   
Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

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

## References

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

No. 368 Methylstannane-d<sub>3</sub>, CH<sub>3</sub>SnD<sub>3</sub>  
Symmetry C<sub>3v</sub>

Symmetry number σ = 3

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> <sub>1</sub>	<i>v</i> <sub>1</sub>	CH <sub>3</sub> s-stretch.	2930 D	2930 M		
	<i>v</i> <sub>2</sub>	SnD <sub>3</sub> s-stretch.	1352 D	1352.0 S		OV( <i>v</i> <sub>9</sub> ).
	<i>v</i> <sub>3</sub>	CH <sub>3</sub> s-deform.	1205 C	1204.5 S		
	<i>v</i> <sub>4</sub>	SnC stretch.	509 C	509.1 M		
	<i>v</i> <sub>5</sub>	SnD <sub>3</sub> s-deform.	493 C	493.0 S		
<i>a</i> <sub>2</sub>	<i>v</i> <sub>6</sub>	Torsion	101 C			MW[1].
<i>e</i>	<i>v</i> <sub>7</sub>	CH <sub>3</sub> d-stretch.	3000 D	3000 W		
	<i>v</i> <sub>8</sub>	CH <sub>3</sub> d-deform.	1400 D	1400 W		
	<i>v</i> <sub>9</sub>	SnD <sub>3</sub> d-stretch.	1352 C	1352.0 S		OV( <i>v</i> <sub>2</sub> ).
	<i>v</i> <sub>10</sub>	CH <sub>3</sub> rock.	765 D	765 W		
	<i>v</i> <sub>11</sub>	SnD <sub>3</sub> d-deform.	503 C	502.5 S		
	<i>v</i> <sub>12</sub>	SnD <sub>3</sub> rock.	317 D	316.6 M		

## References

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

No. 369 Methyl-d<sub>3</sub>-stannane CD<sub>3</sub>SnH<sub>3</sub>  
Symmetry C<sub>3v</sub>

Symmetry number σ = 3

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> <sub>1</sub>	<i>v</i> <sub>1</sub>	CD <sub>3</sub> s-stretch.	2144 B	2144.3 M		
	<i>v</i> <sub>2</sub>	SnH <sub>3</sub> s-stretch.	1889 D	1889.0 S		OV( <i>v</i> <sub>8</sub> ).
	<i>v</i> <sub>3</sub>	CD <sub>3</sub> s-deform.	920 B	920.2 M		
	<i>v</i> <sub>4</sub>	SnH <sub>3</sub> s-deform.	704 B	703.5 S		
	<i>v</i> <sub>5</sub>	SnC stretch.	478 B	478.0 M		
<i>a</i> <sub>2</sub>	<i>v</i> <sub>6</sub>	Torsion	88 C			MW[1].
<i>e</i>	<i>v</i> <sub>7</sub>	CD <sub>3</sub> d-stretch.	2255 C	2254.5 M		
	<i>v</i> <sub>8</sub>	SnH <sub>3</sub> d-stretch.	1889 B	1889.0 S		OV( <i>v</i> <sub>2</sub> ).
	<i>v</i> <sub>9</sub>	CD <sub>3</sub> d-deform.	1017 C	1017.1 W		
	<i>v</i> <sub>10</sub>	SnH <sub>3</sub> d-deform.	738 B	738.1 M		
	<i>v</i> <sub>11</sub>	CD <sub>3</sub> rock.	628 B	628.4 S		
	<i>v</i> <sub>12</sub>	SnH <sub>3</sub> rock.	392 C	392.4 W		

## References

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

No. 370 Trifluoroacetonitrile  $\text{CF}_3\text{CN}$   
Symmetry  $\text{C}_{3v}$

Symmetry number  $\sigma = 3$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$	$\text{cm}^{-1}$	$\text{cm}^{-1}$
				(Gas)	(Liquid)	
$a_1$	$\nu_1$	CN stretch.	2278 B	2278.3	2274 S, p	
	$\nu_2$	$\text{CF}_3$ s-stretch.	1227 B	1227.2	1222 VW	
	$\nu_3$	CC stretch.	802 B	801.7	818 M, p	
	$\nu_4$	$\text{CF}_3$ s-deform.	522 B	521.8	521 M, p	
$e$	$\nu_5$	$\text{CF}_3$ d-stretch.	1214 B	1214.3	1192 W	
	$\nu_6$	$\text{CF}_3$ d-deform.	618 B	618.3	620 W, dp	
	$\nu_7$	$\text{CF}_3$ rock.	463 B	462.7	463 W, dp	
	$\nu_8$	CCN deform.	196 B	196.0	192 S, dp	

## References

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

No. 371 Chloro cyanoacetylene C<sub>2</sub>CCCN  
Symmetry  $\text{C}_{\infty v}$

Symmetry number  $\sigma = 1$ 

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

## References

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

**No. 372      Bromo cyanoacetylene BrCCCN**  
**Symmetry  $C_{\infty v}$**

**Symmetry number  $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ ( $C_6H_6$ soln.)	
$\sigma^+$	$\nu_1$	CN stretch.	2292 C	2292 VS	2276 VS, p	
	$\nu_2$	$C \equiv C$ stretch.	2150 C	2150 S	2123 W	
	$\nu_3$	C-C stretch.	1054 B	1054 VW	1052 W	
	$\nu_4$	$CBr$ stretch.	419 B	419 W	418 M, p	
$\pi^+$	$\nu_5$	CCN bend.	485 B	485 S	489 S	
	$\nu_6$	CCC bend.	312 B	312 M	317 S	
	$\nu_7$	$CCBr$ bend.	142 D		142 VW	

**References**

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

**No. 373      Iodo cyanoacetylene ICCCCN**  
**Symmetry  $C_{\infty v}$**

**Symmetry number  $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1} \downarrow$ (Gas)	$cm^{-1}$ ( $C_6H_6$ soln.)	
$\sigma^+$	$\nu_1$	CN stretch.	2270 C	2270 S	2265 VS, p	
	$\nu_2$	$C \equiv C$ stretch.	2131 C	2131 M	2125 M, p	
	$\nu_3$	C-C stretch.	1031 C	1031 S	1034 W, p	
	$\nu_4$	CI stretch.	364 B	364 W	356 M	
$\pi^+$	$\nu_5$	CCN bend.	496 B	496 M	497 S, dp	
	$\nu_6$	CCC bend.	309 C	309 W	315 M, dp	
	$\nu_7$	CCI bend.	130 D		130 VW	

**References**

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

No. 374 Chloropropadiene  $\text{CH}_2\text{CCHCl}$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 375 Bromopropadiene  $\text{CH}_2\text{CCHBr}$

Symmetry  $C_s$ Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 376 Iodopropadiene  $\text{CH}_2\text{CCHI}$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 377 Trifluoropropyne  $\text{CF}_3\text{CCH}$   
Symmetry  $C_{3v}$

Symmetry number  $\sigma = 3$ 

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

## References

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

No. 378 Trifluoropropyne-d  $\text{CF}_3\text{CCD}$   
Symmetry  $\text{C}_{3v}$

Symmetry number  $\sigma = 3$ 

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

## References

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

No. 379 Propargyl fluoride  $\text{CHCCH}_2\text{F}$   
Symmetry  $\text{C}_s$

Symmetry number  $\sigma = 1$ 

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)
$a'$	$\nu_1$	CH stretch.	3338 C	3338 S	3330 (4), p	
	$\nu_2$	$\text{CH}_2$ s-stretch.	2955 C	2955 M	2960 (22), p	
	$\nu_3$	$\text{C}\equiv\text{C}$ stretch.	2150 C	2150 W	2135 (43), p	
	$\nu_4$	$\text{CH}_2$ scis.	1465 C	1465 VW	1458 (3), dp	
	$\nu_5$	$\text{CH}_2$ wag.	1381 C	1381 S	1374 (3), dp	
	$\nu_6$	CF stretch.	1039 C	1039 VS		
	$\nu_7$	C-C stretch.	940 C	940 M	935 (6), p	
	$\nu_8$	CH bend.	675 C	675 S	692 (1), dp	
				(CS <sub>2</sub> soln.)		
	$\nu_9$	CCF deform.	539 C	539 W	544 (3), p	
	$\nu_{10}$	CCC deform.	211 C		211 (10), dp	
$a''$	$\nu_{11}$	$\text{CH}_2$ a-stretch.	2972 C	2972 M	2986 (7), dp	
	$\nu_{12}$	$\text{CH}_2$ twist.	1242 D	1240 VW	1242 (1), dp	
	$\nu_{13}$	$\text{CH}_2$ rock.	1018 D	1018 W	1012 (3b), p	
	$\nu_{14}$	CH bend.	635 C	635 S	646 (1b), dp	
	$\nu_{15}$	CCC deform.	310 C		310 (4), dp	

## Reference

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

No. 380      Propargyl chloride       $\text{CHCCH}_2\text{Cl}$   
 Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 381 Propargyl bromide  $\text{CHCCH}_2\text{Br}$   
Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 382 Propargyl iodide  $\text{CHCCH}_2\text{I}$   
 Symmetry  $C_s$

Symmetry number  $\sigma = 1$ 

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

\* Estimated from the corresponding frequencies of other propargyl halides.

## Reference

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

No. 383 Chlorodiacetylene CICCCCH  
Symmetry  $C_{\infty h}$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 384 Bromodiacetylene BrCCCCH  
Symmetry  $C_{\infty h}$

Symmetry number  $\sigma = 1$ 

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

## Reference

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

No. 385 Iododiacetylene		ICCCCH		Symmetry number $\sigma = 1$		
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$	
$\sigma^+$	$\nu_1$	CH stretch.	3332 C	3332 VS		
	$\nu_2$	C≡C a-stretch.	2211 C	2211 S		
	$\nu_3$	C≡C s-stretch.	2060 C	2060 VW		
	$\nu_4$	C-C stretch.	1025 D	1025 VW (CS <sub>2</sub> soln.)		
$\pi$	$\nu_5$	CI stretch.	362 C	362 M		
	$\nu_6$	CH bend.	623 B	623 VS		
	$\nu_7$	CCCC a-bend.	473 B	473 M		
	$\nu_8$	CCCC s-bend.	357 C	357 W		
	$\nu_9$	CCI bend.	110 E	110		OC( $\nu_8 + \nu_9, \nu_7 + \nu_9$ ).

**Reference**

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

No. 386 Dicyanodiacetylene		NCCCCCCN		Symmetry number $\sigma = 2$		
Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			$cm^{-1}$	$cm^{-1}$ (Gas)	$cm^{-1}$ (CCl <sub>4</sub> soln.)	
$\sigma_g^+$	$\nu_1$	CN s-stretch.	2235 C	ia	2235 VS, p	
	$\nu_2$	C≡C s-stretch.	2183 C	ia	2183 M, p	
	$\nu_3$	C-C s-stretch.	1288 C	ia	1287.5 W, p	
	$\nu_4$	C-C stretch.	571	ia	571 W, dp	
$\sigma_u^+$	$\nu_5$	CN a-stretch.	2266 B	2266 S	ia	
	$\nu_6$	C≡C a-stretch.	2097 B	2097 M	ia	
	$\nu_7$	C-C a-stretch.	717 B	717 S	ia	
$\pi_g$	$\nu_8$	Bend.	501 C	ia	501 M, dp	
	$\nu_9$	Bend.	455 C	ia	455 W, dp	
					(C <sub>6</sub> H <sub>14</sub> soln.)	
$\pi_u$	$\nu_{10}$	Bend.	170 D	ia	170 W, b, dp	
	$\nu_{11}$	Bend.	491 B	490.5 VS	ia	
	$\nu_{12}$	Bend.	276 B	276 VS	ia	
	$\nu_{13}$	Bend.	62 B	61.5 VS	ia	

**Reference**

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