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].[1] 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, σ, 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

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[1] 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 ν_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 ν_2, following the widely accepted tradition. For some deuterated compounds the frequencies are arranged so that the same ν_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_i	A_g, A_u
C_{2v}	A_1, A_2, B_1, B_2
C_{2h}	A_g, A_u, B_g, B_u
D_2	A, B_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
$C_{\infty v}$	$\Sigma^+, \Sigma^-, \pi, \Delta, \Phi, \ldots$
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}	$A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_{1g}, E_{1u}\ E_{2g}, E_{2u}$
$D_{\infty h}$	$\Sigma_g^+, \Sigma_u^+, \Sigma_g^-, \Sigma_u^-, \pi_g, \pi_u, \Delta_g, \Delta_u, \Phi_g, \Phi_u, \ldots$
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: $(\Delta r_1+\Delta r_2)\ /\ \sqrt{2}$
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. 2.
(c) Local symmetry coordinates for the CH group (see fig. 1c)
CH stretching: Δr_{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: Δr_{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

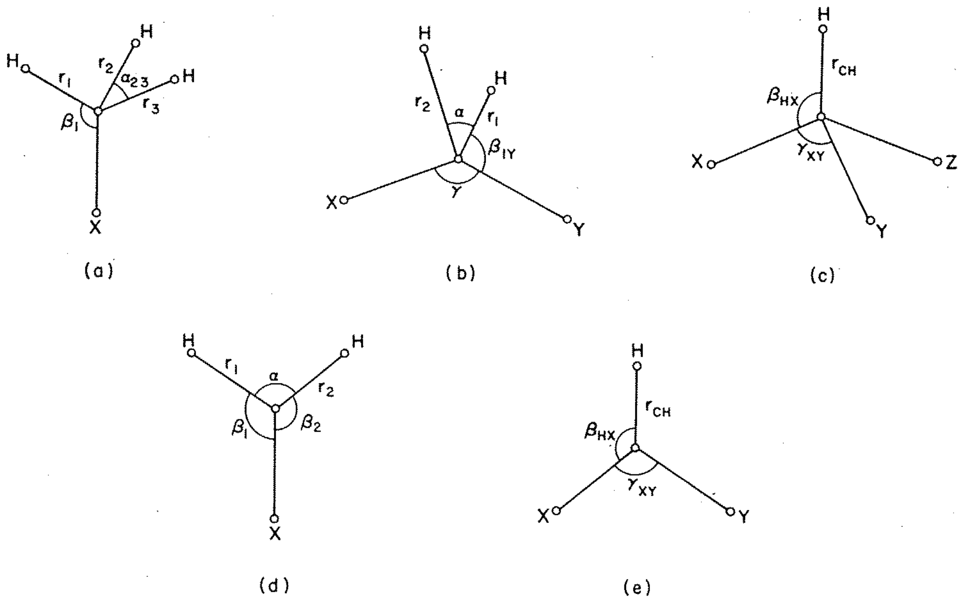

FIGURE 1. Parameters of methyl, methylene, and methin groups.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis*
	cm^{-1}	
A	$0 \sim 1$	(i) Gas, grating spectrometer, rotational fine structure accurately analyzed. (ii) Gas, grating spectrometer, a sharp Q branch.
B	$1 \sim 3$	(i) Gas, grating spectrometer, rotational fine structure partly analyzed. (ii) Gas, prism spectrometer, fairly high resolution (e.g., $700 \sim 1000$ cm^{-1} for NaCl prism).
C	$3 \sim 6$	(i) Gas, prism spectrometer, low resolution (e.g., $1000 \sim 2000$ cm^{-1} for NaCl prism). (ii) Solid, liquid or solution, accurate measurement.
D	$6 \sim 15$	(i) Gas, prism spectrometer, very low resolution (e.g., > 2000 cm^{-1} for NaCl prism). (ii) Solid, liquid or solution, inaccurate measurement.
E	$15 \sim 30$	(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[2]

The fundamental frequency ν_i is defined as the difference between the term value $G(v_i = 1$, all other $v_j = 0)$ and $G(v_i = 0$, and other $v_j = 0)$ expressed in cm^{-1}. Fundamental frequencies rather than harmonic frequencies (ω_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^{-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 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 ν_0 is chosen as the fundamental frequency and given the uncertainty code A (see below). For a well-analyzed perpendicular band of a symmetric

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

top molecule, the frequency listed contains the nonvibrational part $A'\zeta^2$, where A' is the rotational constant of the vibrational level and ζ of the Coriolis coupling constant. This is in accord with the definition of ν_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 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

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.

5. References

[1] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 6, Part 1, 56 pages (March 1967); Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 11, Part 2, 38 pages (October 1967); Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 17, Part 3, 39 pages (March 1968).

[2] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Consolidated Volume, Nat. Stand. Ref. Data. Ser., Nat. Bur. Stand. (U.S.), 39, 160 pages (June 1972).

[3] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 5, J. Phys. Chem. Ref. Data 1, 189 (1972).

[4] Shimanouchi, T., Tables of Molecular Vibrational Frequencies, Part 6, J. Phys. Chem. Ref. Data **2**, 121 (1973).

[5] Herzberg, G., Electronic Spectra of Polyatomic Molecules (D. Van Nostrand, Inc., New York, 1950).

[6] Herzberg, G., Electronic Spectra of Polyatomic Molecules (D. Van Nostrand, Inc., New York, 1966).

[7] Rosen, B., Ed., Selected Constants, Spectroscopic Data Relative to Diatomic Molecules (Pergamon Press, New York, 1955).

[8] Wilson, E. Bright, Jr., Decius, J. C., Cross, Paul C., Molecular Vibrations (McGraw-Hill Book Co., New York, 1955).

[9] Herzberg, G., Infrared and Raman Spectra of Polyatomic Molecules (D. Van Nostrand, Inc., New York, 1945).

[10] Shimanouchi, T., The Molecular Force Field, Chapter in Physical Chemistry, An Adv. Treatise, Vol. 4. Molecular Properties, pp. 233–306, D. Henderson, Ed. (Academic Press, New York, 1970).

[11] Starck, B., Landolt-Bornstein Numerical Data and Functional Relationships in Science and Technology, New Series, Group II, Vol. 4 (Springer-Verlag, Berlin, 1967).

6. List of Tables of Molecular Vibrational Frequencies

No. 337 Krypton difluoride KrF_2
Symmetry $D_{\infty h}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$ (Gas)	
σ_g^+	ν_1	Sym. stretch.	449 B	ia	449	
σ_u^+	ν_2	Antisym. stretch.	590 A	589.89 VS	ia	
π_u	ν_3	Bend.	233 B	232.6 S	ia	

References

[1] IR.R. H. H. Classen, G. L. Goodman, J. G. Malm, and F. Schreiner, J. Chem. Phys. **42,** 1229 (1965).

[2] IR. C. Murchison, S. Reichman, D. Anderson, J. Overend, and F. Schreiner, J. Amer. Chem. Soc. **90,** 5690 (1968).

No. 338 Hypofluorous acid HOF
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Nitrogen matrix)	*cm*$^{-1}$	
a'	ν_1	OH stretch.	3537 C	3537.1		
	ν_2	OF stretch.	1393 C	1393.0		
	ν_3	Bend.	886 C	886.0		

References

[1] IR. P. N. Noble and G. C. Pimentel, Spectrochim. Acta **24A,** 797 (1968).

[2] IR. J. A. Golb, H. H. Claassen, M. H. Studier, and E. H. Appklman, Spectrochim. Acta **28A,** 65 (1972).

No. 339 Nitrogen trifluoride $^{15}NF_3$

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1009 A	1008.93		
	ν_2	Sym. deform.	645 B	644.84		
e	ν_3	Deg. stretch.	886 A	886.34		
	ν_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 PI_3

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} (CS_2, C_6H_6, CH_2Cl_2 soln.)	cm^{-1} C_6H_6, CCl_4 soln.)	
a_1	ν_1	PI_3 s–stretch.	303 D	306 M	303 (3) p	
	ν_2	PI_3 s–deform.	111 D	112 VW	111 (7) p	
e	ν_3	PI_3 d–stretch.	325 D	328 VS	325 (1b) dp	
	ν_4	PI_3 d–deform.	79 D	80 VW, b	79 (10) dp	

References

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

No. 341 Arsenic triiodide AsI_3

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} (Solid)	cm^{-1} ($CHBr_3$,CS_2 soln.)	
a_1	ν_1	AsI_3 s–stretch.	219 C	225.7	218.5 p	
	ν_2	AsI_3 s–deform.	94 C	101.6	94 p	
e	ν_3	AsI_3 d–stretch.	224 C	201.2 VVS,b	223.5 dp	
	ν_4	AsI_3 d–deform.	71 C	73.6	71 dp	

References

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

No. 342 Chlorodifluoroammonia $NClF_2$

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'	ν_1	NF_2 s–stretch.	930 C	930.2		
	ν_2	NCl stretch.	697 C	696.9		
	ν_3	NF_2 deform.	556 C	555.5		
	ν_4	NClF s–deform.	377 C	377		
a''	ν_5	NF_2 a–stretch.	855 C	855.4		
	ν_6	NClF a–deform.	382 D	382[a]		

[a] 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 NCl_2F

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'	ν_1	NF stretch.	825 C	825 S		
	ν_2	NCl_2 s–stretch.	615 C	615 M		
	ν_3	NFCl s–deform.	409 C	409 W		
	ν_4	NCl_2 deform.	274 C	274 W		
a''	ν_5	NCl_2 a–stretch.	692 C	692 S		
	ν_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 NSF_3

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	NS stretch.	1515 B	1515	1512 p	
	ν_2	NF_3 s–stretch.	775 B	775	768 p	
	ν_3	NF_3 s–deform.	521 B	521	520 dp	
e	ν_4	NF_3 d–stretch.	811 B	811	812 dp	
	ν_5	NF_3 d–deform.	429 B	429	430 dp	
	ν_6	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 PSF_3

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$ (Liquid)	
a_1	ν_1	PF_3 s–stretch.	981 B	981 VS	969 (4.5) p	
	ν_2	PS stretch.	695 B	695 M	696 (100) p	
	ν_3	PF_3 s–deform.	440 B	440 M	441 (20) p	
e	ν_4	PF_3 d–stretch.	945 B	945 VS	937 (6.0) dp	
	ν_5	PF_3 d–deform.	402 C	402 M	404 (13) dp	
	ν_6	PF_3 rock.	275 B	275 W	276 (37) dp	

References

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

No. 346 Thiophosphoryl trichloride $PSCl_3$

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$ (Liquid)	
a_1	ν_1	PS stretch.	770 B	770	750 (8) p	
	ν_2	PCl_3 s–stretch.	431 B	431	435 (100) p	
	ν_3	PCl_3 s–deform.	252 E	252	250 (56) dp	OV(ν_5).
e	ν_4	PCl_3 d–stretch.	547 B	547	539 (8) dp	
	ν_5	PCl_3 d–deform.	252 D	252	250 (56) dp	OV(ν_3).
	ν_6	PCl_3 rock.	174 D	174 (liquid)	174 (49) dp	

References

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

No. 347 Perchlorylfluoride $^{35}ClO_3F$
Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	ClO_3 s–stretch.	1063 B	1061 S	1062.8 VS	
	ν_2	ClF stretch.	717 B	714 S	716.8 S	
	ν_3	ClO_3 s–deform.	549 B	549 W	548.8 M	
e	ν_4	ClO_3 d–stretch.	1314 B	1315 VS	1314 W	
	ν_5	ClO_3 d–deform.	573 B	590.55 M	573 W	
	ν_6	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 $VOCl_3$
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} (Liquid)	cm^{-1} (Gas)	
a_1	ν_1	VO stretch.	1042 C	1035 VS	1042 (1.8) p	
	ν_2	VCl_3 s–stretch.	408 C	408 S	408 (10.0) p	
	ν_3	VCl_3 s–deform.	125 C		125 (3.8) p	
e	ν_4	VCl_3 d–stretch.	502 D	502 VS	502 (2.0) dp	
	ν_5	VCl_3 d–deform.	249 C		249 (1.5) dp	
	ν_6	VCl_3 rock.	164 C		164 (0.8) dp	

References

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

No. 349 Permanganyl fluoride MnO_3F

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$	
a_1	ν_1	MnO_3 s–stretch.	905 B	905.2 M		
	ν_2	MnF stretch.	721 B	720.7 M		
	ν_3	MnO_3 s–deform.	338 B	337.7 W		
e	ν_4	MnO_3 d–stretch.	953 B	952.5 S		
	ν_5	MnO_3 d–deform.	374 B	373.9 W		
	ν_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 ReO_3Cl

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Liquid)	*cm*$^{-1}$ (Liquid)	
a_1	ν_1	ReO_3 s–stretch.	1001 C	1001.5 VS	1001 S, p	
	ν_2	ReO_3 s–deform.	434 C	434 VS	435 M, p	
	ν_3	ReCl stretch.	293 C	293 S		
e	ν_4	ReO_3 d–stretch.	960 C	960 VS	962.5 M, dp	
	ν_5	ReO_3 d–deform.	344 C	343.5 S	344 M, dp	
	ν_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 (960).
[3] Th. A. Müller, B. Krebs, and W. Höltje, Spectrochim. Acta **23A,** 2753 (1967).

No. 351 Rhenium (VII) oxide bromide ReO_3Br

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (CCl_4 soln.)	*cm*$^{-1}$	
a_1	ν_1	ReO_3 s–stretch.	997 C	997 S		
	ν_2	ReO_3 s–deform.	350 C	350 M		
	ν_3	ReBr stretch.	195 C	195 M		
e	ν_4	ReO_3 d–stretch.	963 C	963 VS		
	ν_5	ReO_3 d–deform.	332 C	332 S		
	ν_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 $H^{14}NO_3$

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'	ν_1	OH stretch.	3550 B	3550.0 M		
	ν_2	NO_2 a–stretch.	1708 B	1708.2 VS		
	ν_3	OH bend.	1331 B	1330.7 S		
	ν_4	NO_2 s–stretch.	1325 B	1324.9 VS		
	ν_5	NO_2 scis.	879 B	878.6 S		
	ν_6	NO stretch.	647 B	646.6 W		
	ν_7	NO_2 rock.	579 B	579.0 W		
a''	ν_8	NO_2 wag.	762 B	762.2 S		
	ν_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'	ν_1	OD stretch.	2622 B	2621.5 M		
	ν_2	NO_2 a–stretch.	1687 B	1687.0 VS		
	ν_3	NO_2 s–stretch.	1308 B	1308.4 VS		
	ν_4	OD bend.	1014 B	1013.6 M		
	ν_5	NO_2 scis.	888 B	888.0 S		
	ν_6	NO stretch.	641 B	641.0 S		
	ν_7	NO_2 rock.	541 B	541.0 W		
a''	ν_8	NO_2 wag.	763 B	762.8 S		
	ν_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'	ν_1	OH stretch.	3550 B	3550.0 M		
	ν_2	NO_2 a–stretch.	1672 B	1672.0 VS		
	ν_3	OH bend.	1327 B	1327.0 S		
	ν_4	NO_2 s–stretch.	1321 B	1320.6 S		
	ν_5	NO_2 scis.	871 B	870.8 S		
	ν_6	NO stretch.	647 B	646.6 W		
	ν_7	NO_2 rock.	578 B	578.0 W		
a''	ν_8	NO_2 wag.	744 B	743.6 S		
	ν_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'	ν_1	OD stretch.	2622 B	2621.9 M		
	ν_2	NO_2 a–stretch.	1656 B	1655.5 VS		
	ν_3	NO_2 s–stretch.	1291 B	1290.7 S		
	ν_4	OD bend.	1012 B	1011.5 M		
	ν_5	NO_2 scis.	876 B	876.3 S		
	ν_6	NO stretch.	641 B	640.9 S		
	ν_7	NO_2 rock.	541 B	541.0 VW		
a''	ν_8	NO_2 wag.	743 B	743.4 S		
	ν_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'	ν_1	NO_2 a–stretch.	1759 C	1759.1 VS		
	ν_2	NO_2 s–stretch.	1301 B	1300.9 VS		
	ν_3	OF stretch.	928 B	927.7 S		
	ν_4	NO_2 scis.	804 B	803.7 S		
	ν_5	NO stretch.	633 B	633.0 VW		
	ν_6	NO_2 rock.	455 B	454.5 MS		
	ν_7	OF bend.	303 B	302.6 VW		
a''	ν_8	NO_2 wag.	709 C	708.5 M		
	ν_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 $FO^{15}NO_2$

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'	ν_1	NO a−stretch.	1720 C	1719.8 VS		
	ν_2	NO_2 s−stretch.	1291 B	1290.5 VS		
	ν_3	OF stretch.	928 B	927.5 S		
	ν_4	NO_2 scis.	792 B	791.8 S		
	ν_5	NO stretch.	632 B	631.5 VW		
	ν_6	NO_2 rock.	455 B	454.4 MS		
	ν_7	OF bend.	302 B	301.6 VW		
a''	ν_8	NO_2 wag.	690 C	690.2 M		
	ν_9	OF torsion	151 D	151.2		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 $ClO^{14}NO_2$

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'	ν_1	NO_2 a−stretch.	1735 B	1735.4 VS		
	ν_2	NO_2 s−stretch.	1292 B	1291.9 VS		
	ν_3	OCl stretch.	809 C	809.3 S		
	ν_4	NO_2 scis.	780 C	780.2 MS		
	ν_5	NO stretch.	560 B	560.0 S		
	ν_6	NO_2 rock.	434 B	434.1 M		
	ν_7	OCl bend.	270 C	270 VVW		
a''	ν_8	NO_2 wag.	711 B	710.8 W		
	ν_9	OCl torsion	121 E	121		OC($\nu_5+\nu_7-\nu_9$).

References

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

No. 359 Chloronitrate $ClO^{15}NO_2$

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'	ν_1	NO_2 a–stretch.	1694 B	1694.0 VS		
	ν_2	NO_2 s–stretch.	1280 B	1280.2 VS		
	ν_3	OCl stretch.	805 C	804.7 MS		
	ν_4	NO_2 scis.	773 C	772.9 S		
	ν_5	NO stretch.	557 B	556.8 S		
	ν_6	NO_2 rock.	432 B	432.2 M		
	ν_7	OCl bend.	263 D	263		OC($\nu_5+\nu_7$).
a''	ν_8	NO_2 wag.	694 B	693.7 W		
	ν_9	OCl torsion	122 E	122		OC($\nu_5+\nu_7-\nu_9$).

References

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

No. 360 Thiophosphoryl chlorodifluoride PSF_2Cl

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*$^{-1}$ (Liquid)	
a'	ν_1	PF_2 s–stretch.	946 B	946 VS	939 (3.7) p	
	ν_2	PS stretch.	738 B	738 VS	727 (50) p	
	ν_3	PCl stretch.	541 B	541 S	536 (100) p	
	ν_4	PCl bend.	395 B	395 M	394 (31) p	
	ν_5	PF_2 scis.	361 B	361 M	359 (38) p	
	ν_6	PS ip–bend.	207 C	198	207 (65) p	
a''	ν_7	PF_2 s–stretch.	920 B	920 VS	913 (6.5) dp	
	ν_8	PF_2 rock.	317 B	317 M	314 (14) dp	
	ν_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 $PSFCl_2$

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} (Liquid)	
a'	ν_1	PF stretch.	912 B	912 VS	902 (2) p	
	ν_2	PS stretch.	753 B	753 VS	737 (17) p	
	ν_3	PCl_2 s–stretch.	478 B	478 S	474 (100) p	
	ν_4	PF bend.	331 B	331 M	327 (13) dp	
	ν_5	PS ip–bend.	268 B	268 M	267 (32) p	
	ν_6	PCl_2 scis.	192 D	192 W	193 (65) dp	OV(ν_9).
a''	ν_7	PCl_2 a–stretch.	575 C	575 S	567 (6) dp	
	ν_8	PS op–bend.	319 B	319 M	317 (19) dp	
	ν_9	PCl_2 rock.	192 D	192 W	193 (65) dp	OV(ν_6).

Reference

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

No. 362 Phosphorus difluoride trichloride PCl_3F_2

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} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	PF_2 s–stretch.	633 C		633 M, p	
	ν_2	PCl_3 s–stretch.	387 C		387 S, p	
a_2''	ν_3	PF_2 a–stretch.	867 C	867 VS		
	ν_4	PCl_3 op–deform.	328 C	328 M		
e'	ν_5	PCl_3 d–stretch.	625 C	625 VS	609 VW, dp	
	ν_6	PCl_3 d–deform.	404 C	404 VS	408 M, dp	
	ν_7	PF bend.	122 C		122 S, dp	
e''	ν_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 PCl_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} (Gas)	cm^{-1} (C_6H_6 or CS_2 soln.)	
a_1'	ν_1	PCl_3 s–stretch.	395 D		395 VS, p	
	ν_2	PCl_2 s–stretch.	370 D		370 VW	
a_2''	ν_3	PCl_2 a–stretch.	465 C	465 VS	441 VW	
	ν_4	PCl_3 op–deform.	299 D	299 S (CS_2 soln.)	301	
e'	ν_5	PCl_3 d–stretch.	592 C	592 VS	581 W, p	
	ν_6	PCl_3 d–deform.	273 D	273 S (CS_2 soln.)	281 W, dp	
	ν_7	PCl bend.	100 C	100 W	100 M, dp	
e''	ν_8	PCl bend.	261 D		261 W, dp	

References

[1] R. H. Moureu, P. Sue, and M. Magat, Contribution a l· étude de la structure moleculaire. Vol. commem. Victor Herni, p.125 Maison Desoerg, Liege (1947/48).

[2] IR.R. J. K. Wilmshurst and H. J. Bernstein, J. Chem. Phys. **27,** 661 (1957).

[3] IR.R. G. L. Carlson, Spectrochim. Acta **19,** 1291 (1963).

[4] R. M. J. Taylor and L. A. Woodward, J. Chem. Soc. **1963,** 4670 (1963).

[5] Th. R. R. Holmes, R. M. Deiters, and J. A. Golen, Inorg. Chem. **8,** 2612 (1969).

[6] Th. R. R. Holmes and R. M. Deiters, J. Chem. Phys. **51,** 4043 (1969).

No. 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} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	$SbCl_3$ s-stretch.	357 C		357 (10) p	
	ν_2	$SbCl_2$ s-stretch.	307 C	306 W (liquid)	307 (4) dp	
a_2''	ν_3	$SbCl_2$ a-stretch.	384 C	384 VS		
	ν_4	$SbCl_3$ op-deform.	154 D	154 (CCl_4 soln.)		
e'	ν_5	$SbCl_3$ d-stretch.	398 C	398 VS	397 (2)	
	ν_6	$SbCl_3$ d-deform.	177 C	172 S (CCl_4 soln.)	177 (4) dp	
	ν_7	SbCl bend.	72 D		72 dp	
e''	ν_8	SbCl bend.	165 C		165 (2) dp	

References

[1] IR. J. K. Wilmshurst, 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} (Solid)	cm^{-1} (CH_3NO_2 soln.)	
a_1	ν_1	CH_3 s-stretch.	2920 D	2920 M	2914 (Solid)	
	ν_2	CH_3 s-deform.	1180 D	1180 M	1182 p	
	ν_3	CHg stretch.	531 D	531 M	538 p	
	ν_4	HgI stretch.	184 D	184 M	180 p	
e	ν_5	CH_3 d-stretch.	3008 D	3008 M		
	ν_6	CH_3 d-deform.	1400 D	1400 W		
	ν_7	CH_3 rock.	781 D	781 S		
	ν_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 CH_3GeI_3

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}	
				(Liquid)	(Liquid)	
a_1	ν_1	CH_3 s–stretch.	2911 C	2911 M	2909 W	
	ν_2	CH_3 s–deform.	1225 C	1225 M	1222 W	
	ν_3	CGe stretch.	597 C	597 S	596 M	
	ν_4	GeI_3 s–stretch.	195 C	196 M	195 S	
				(Solid)		
	ν_5	GeI_3 s–deform.	92 C	96 M	92 S	
				(Solid)		
a_2	ν_6	Torsion	123 D	123 VW	123 VW	
				(Solid)		
e	ν_7	CH_3 d–stretch.	2999 C	2999 M	2996 W	
	ν_8	CH_3 d–deform.	1392 C	1392 S	1394	
					(Solid)	
	ν_9	CH_3 rock.	810 C	810 S	809	
					(Solid)	
	ν_{10}	GeI_3 d–stretch.	252 C	252 S	251 M	
	ν_{11}	GeI_3 rock.	147 C		147 M	
	ν_{12}	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 CH_3SnH_3

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}	
				(Gas)		
a_1	ν_1	CH_3 s–stretch.	2933 B	2932.5 W		
	ν_2	SnH_3 s–stretch.	1875 D	1874.5 S		OV(ν_8).
	ν_3	CH_3 s–deform.	1209 B	1209.3 W		
	ν_4	SnH_3 s–deform.	695 B	694.5 S		
	ν_5	SnC stretch.	527 B	526.9 M		
a_2	ν_6	Torsion	109 C			MW[1].
e	ν_7	CH_3 d–stretch.	3005 B	3005.4 W		
	ν_8	SnH_3 d–stretch.	1875 B	1874.5 S		OV(ν_2).
	ν_9	CH_3 d–deform.	1417 B	1417.0 W		
	ν_{10}	CH_3 rock.	774 C	774.1 M		
	ν_{11}	SnH_3 d–deform.	741 C	741.3 M		
	ν_{12}	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_3 CH_3SnD_3

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s–stretch.	2930 D	2930 M		
	ν_2	SnD_3 s–stretch.	1352 D	1352.0 S		OV(ν_9).
	ν_3	CH_3 s–deform.	1205 C	1204.5 S		
	ν_4	SnC stretch.	509 C	509.1 M		
	ν_5	SnD_3 s–deform.	493 C	493.0 S		
a_2	ν_6	Torsion	101 C			MW[1].
e	ν_7	CH_3 d–stretch.	3000 D	3000 W		
	ν_8	CH_3 d–deform.	1400 D	1400 W		
	ν_9	SnD_3 d–stretch.	1352 C	1352.0 S		OV(ν_2).
	ν_{10}	CH_3 rock.	765 D	765 W		
	ν_{11}	SnD_3 d–deform.	503 C	502.5 S		
	ν_{12}	SnD_3 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_3–stannane CD_3SnH_3

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s–stretch.	2144 B	2144.3 M		
	ν_2	SnH_3 s–stretch.	1889 D	1889.0 S		OV(ν_8).
	ν_3	CD_3 s–deform.	920 B	920.2 M		
	ν_4	SnH_3 s–deform.	704 B	703.5 S		
	ν_5	SnC stretch.	478 B	478.0 M		
a_2	ν_6	Torsion	88 C			MW[1].
e	ν_7	CD_3 d–stretch.	2255 C	2254.5 M		
	ν_8	SnH_3 d–stretch.	1889 B	1889.0 S		OV(ν_2).
	ν_9	CD_3 d–deform.	1017 C	1017.1 W		
	ν_{10}	SnH_3 d–deform.	738 B	738.1 M		
	ν_{11}	CD_3 rock.	628 B	628.4 S		
	ν_{12}	SnH_3 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 CF_3CN

Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CN stretch.	2278 B	2278.3	2274 S, p	
	ν_2	CF_3 s–stretch.	1227 B	1227.2	1222 VW	
	ν_3	CC stretch.	802 B	801.7	818 M, p	
	ν_4	CF_3 s–deform.	522 B	521.8	521 M, p	
e	ν_5	CF_3 d–stretch.	1214 B	1214.3	1192 W	
	ν_6	CF_3 d–deform.	618 B	618.3	620 W, dp	
	ν_7	CF_3 rock.	463 B	462.7	463 W, dp	
	ν_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 ClCCCN

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.)	
σ^+	ν_1	CN stretch.	2297 C	2297 VS	2290 VS, p	
	ν_2	C≡C stretch.	2194 B	2194 W	2196 M, p	
	ν_3	C–C stretch.	1093 C	1093 S	1103 W, p	
	ν_4	CCl stretch.	527 B	527 M	530 M, p	
π^+	ν_5	CCN bend.	483 B	483 S	487 S	
	ν_6	CCC bend.	333 C	333 M	338 M	
	ν_7	CCCl bend.	145 D		145 VW	

References

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

No. 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.)	
σ^+	ν_1	CN stretch.	2292 C	2292 VS	2276 VS, p	
	ν_2	C≡C stretch.	2150 C	2150 S	2123 W	
	ν_3	C–C stretch.	1054 B	1054 VW	1052 W	
	ν_4	CBr stretch.	419 B	419 W	418 M, p	
π^+	ν_5	CCN bend.	485 B	485 S	489 S	
	ν_6	CCC bend.	312 B	312 M	317 S	
	ν_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 ICCCN

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.)	
σ^+	ν_1	CN stretch.	2270 C	2270 S	2265 VS, p	
	ν_2	C≡C stretch.	2131 C	2131 M	2125 M, p	
	ν_3	C–C stretch.	1031 C	1031 S	1034 W, p	
	ν_4	CI stretch.	364 B	364 W	356 M	
π^+	ν_5	CCN bend.	496 B	496 M	497 S, dp	
	ν_6	CCC bend.	309 C	309 W	315 M, dp	
	ν_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 CH_2CCHCl

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*$^{-1}$ (Liquid)	
a'	ν_1	CH stretch.	3079 C	3079 S	3062 S, p	OV(ν_{11}).
	ν_2	CH_2 s–stretch.	3009 C	3009 M	2990 S, p	
	ν_3	CCC a–stretch.	1963 C	1963 M	1951 W, dp	
	ν_4	CH_2 scis.	1435 C	1435 S	1419 S, p	
	ν_5	CH bend.	1256 C	1256 VS	1244 W, p	
	ν_6	CCC s–stretch.	1101 C	1101 S	1095 VS, p	
	ν_7	CH_2 wag.	875 C	875 VS	877 W, dp	
	ν_8	CCl stretch.	767 C	767 VS	751 W, dp	
	ν_9	CCC deform.	592 C	592 W		
	ν_{10}	CCCl deform.	494 C	494 M	490 VS, p	
a''	ν_{11}	CH_2 a–stretch.	3079 C	3079 S	3062 S, p	OV(ν_1).
	ν_{12}	CH_2 rock.	999 B	999 W	995 W, dp	
	ν_{13}	CH bend.	822 B	822 S	815 W, dp	
	ν_{14}	CCC deform.	548 B	548 M	546 W, dp	
	ν_{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 CH_2CCHBr

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*$^{-1}$ (Liquid)	
a'	ν_1	CH stretch.	3080 C	3080 M	3060 (46), p	OV(ν_{11}).
	ν_2	CH_2 s–stretch.	3005 C	3005 M	2985 (63), p	
	ν_3	CCC a–stretch.	1961 C	1961 W	1954 (19), p	
	ν_4	CH_2 scis.	1432 B	1432 S	1422	
	ν_5	CH bend.	1217 C	1217 VS	1209 (12)	
	ν_6	CCC s–stretch.	1078 C	1078 W	1086 (29), p	
	ν_7	CH_2 wag.	862 C	862 VS	873 (3), dp	
	ν_8	CBr stretch.	681 C	681 VS	667 (31), p	
	ν_9	CCC deform.	603 C	603 W		
	ν_{10}	CCBr deform.	423 C	423 VW (CS_2 soln.)	426 (33), p	
a''	ν_{11}	CH_2 a–stretch.	3080 C	3080 M	3060 (46), p	OV(ν_1).
	ν_{12}	CH_2 rock.	1000 B	1000 W		
	ν_{13}	CH bend.	812 B	812 S	806 (3), dp	
	ν_{14}	CCC deform.	519 B	519 M		
	ν_{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 CH_2CCHI

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} (Liquid)	
a'	ν_1	CH stretch.	3070 C	3070 M	3057 M	OV(ν_{11}).
	ν_2	CH_2 s–stretch.	3004 C	3004 W	2978 VS	
	ν_3	CCC a–stretch.	1953 C	1953 M	1947 VS	
	ν_4	CH_2 scis.	1425 B	1425 M	1412 VS	
	ν_5	CH bend.	1178 C	1178 VS	1174 S, p	
	ν_6	CCC s–stretch.	1076 C	1076 M	1076 VS, p	
	ν_7	CH_2 wag.	854 C	854 S		
	ν_8	CCC deform.	625 C	625 S	635 W	
	ν_9	CI stretch.	609 C	609 S		
	ν_{10}	CCI drform.	387 C		387 S, p	
a''	ν_{11}	CH_2 a–stretch.	3070 C	3070 M	3057 M	OV(ν_1).
	ν_{12}	CH_2 rock.	995 B	995 W		
	ν_{13}	CH bend.	807 B	807 S		
	ν_{14}	CCC deform.	485 B	485 W		
	ν_{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 CF_3CCH

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch.	3327 B	3327.3 S	3316 (9) p	
	ν_2	C≡C stretch.	2165 C	2165.4 S	2156 (80) p	FR($\nu_4+\nu_6+\nu_{10}$).
	ν_3	CF_3 s–stretch.	1253 B	1253.2 VS	1250 (1b)	
	ν_4	C–C stretch.	812 B	811.9 W	810 (50) p	
	ν_5	CF_3 s–deform.	536 B	536.1 M	537 (11) p	
e	ν_6	CF_3 d–stretch.	1179 B	1179.2 VS	1155 (5b) dp	
	ν_7	CH bend.	686 B	685.5 S	696 (6) dp	
	ν_8	CF_3 d–deform.	612 B	611.9 M	606 (4) dp	
	ν_9	CF_3 rock.	453 B	453.0 M	445 (6) dp	
	ν_{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 CF_3CCD

Symmetry C_{3v} **Symmetry number $\sigma = 3$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch.	2626 B	2626.0 M		
	ν_2	C≡C stretch.	2014 B	2013.9 S		
	ν_3	CF_3 s–stretch.	1250 B	1249.7 VS		
	ν_4	C–C stretch.	808 B	808.4 W		
	ν_5	CF_3 s–deform.	529 B	528.9 M		
e	ν_6	CF_3 d–stretch.	1179 B	1179.0 VS		
	ν_7	CD bend.	539 B	538.5 S		
	ν_8	CF_3 d–deform.	611 B	611.3 M		
	ν_9	CF_3 rock.	456 B	455.5 M		
	ν_{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 $CHCCH_2F$

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} (Liquid)	
a'	ν_1	CH stretch.	3338 C	3338 S	3330 (4), p	
	ν_2	CH_2 s–stretch.	2955 C	2955 M	2960 (22), p	
	ν_3	C≡C stretch.	2150 C	2150 W	2135 (43), p	
	ν_4	CH_2 scis.	1465 C	1465 VW	1458 (3), dp	
	ν_5	CH_2 wag.	1381 C	1381 S	1374 (3), dp	
	ν_6	CF stretch.	1039 C	1039 VS		
	ν_7	C–C stretch.	940 C	940 M	935 (6), p	
	ν_8	CH bend.	675 C	675 S (CS_2 soln.)	692 (1), dp	
	ν_9	CCF deform.	539 C	539 W	544 (3), p	
	ν_{10}	CCC deform.	211 C		211 (10), dp	
a''	ν_{11}	CH_2 a–stretch.	2972 C	2972 M	2986 (7), dp	
	ν_{12}	CH_2 twist.	1242 D	1240 VW	1242 (1), dp	
	ν_{13}	CH_2 rock.	1018 D	1018 W	1012 (3b), p	
	ν_{14}	CH bend.	635 C	635 S	646 (1b), dp	
	ν_{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 $CHCCH_2Cl$
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} (Liquid)	
a'	ν_1	CH stretch.	3335 C	3335 VS	3305 (2), p	
	ν_2	CH_2 s–stretch.	2968 C	2968 M	2957 (29), p	
	ν_3	C≡C stretch.	2147 C	2147 W	2130 (35), p	
	ν_4	CH_2 scis.	1441 C	1441 M	1432 (2), p	
	ν_5	CH_2 wag.	1271 C	1271 VS	1267 (5), p	
	ν_6	C–C stretch.	960 C	960 S	961 (2), dp	
	ν_7	CCl stretch.	725 C	725 VS	713 (12), p	
	ν_8	CH bend.	650 D	650 S	650 (2b)	
				(CS_2 soln.)		
	ν_9	CCCl deform.	451 C	451	452 (5), p	
	ν_{10}	CCC deform.	186 D		186 (10), dp	
a''	ν_{11}	CH_2 a–stretch.	3002 C	3002 M	2995 (4), dp	
	ν_{12}	CH_2 twist.	1179 B	1179 W	1174 (1), dp	
	ν_{13}	CH_2 rock.	908 D		908 (1), dp	
	ν_{14}	CH bend.	637 D	637 M	650 (2b), dp	
	ν_{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 $CHCCH_2Br$

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*$^{-1}$ (Liquid)	
a'	ν_1	CH stretch.	3335 C	3335 S	3305 (2), p	
	ν_2	CH_2 s–stretch.	2976 C	2976 W	2958 (20), p	
	ν_3	C≡C stretch.	2138 D	2138 VW	2125 (36), p	
	ν_4	CH_2 scis.	1431 C	1431 W	1425 (2), dp	
	ν_5	CH_2 wag.	1218 C	1218 S	1214 (9), p	
	ν_6	C–C stretch.	961 C	961 M	962 (3), p	
	ν_7	CH bend.	652 C	652 VS (CS_2 soln.)		
	ν_8	CBr stretch.	621 C	621 S (CS_2 soln.)	618 (22), p	
	ν_9	CCBr deform.	399 C	399 (soln.)	399 (9), p	
	ν_{10}	CCC deform.	168 C		168 (10), p	
a''	ν_{11}	CH_2 a–stretch.	3006 C	3006 (CS_2 soln.)	3008 (4), p	
	ν_{12}	CH_2 twist.	1152 D	1152 VW	1146 (1)	
	ν_{13}	CH_2 rock.	866 D		866 (1), dp	
	ν_{14}	CH bend.	637 C	637 S		
	ν_{15}	CCC deform.	314 C		314 (3), dp	

Reference

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

No. 382 Propargyl iodide $CHCCH_2I$
Symmetry C_S **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency cm^{-1}	Infrared cm^{-1}	Raman cm^{-1}	Comments
				(Gas)	(Liquid)	
a	ν_1	CH stretch.	3335 C	3335 S		
	ν_2	CH_2 s–stretch.	2958 C	2958 (CS_2 soln.)	2957 VS	
	ν_3	C≡C stretch.	2130 C	2130 C (CCl_4 soln.)	2128 VS	
	ν_4	CH_2 scis.	1423 C	1423 W	1414	
	ν_5	CH_2 wag.	1160 C	1160 M	1160 VS	
	ν_6	C–C stretch.	959 C	959 W	964 S	
	ν_7	CH bend.	640 C	640 S	650 VW,b	OV(ν_{14}).
	ν_8	CI stretch.	570 C	570 W	567 VS	
	ν_9	CCI deform.	364 C		364 S	
	ν_{10}	CCC deform.	157 C		157 M	
a″	ν_{11}	CH_2 a–stretch.	3008 D	3008 (CS_2 soln.)	2990 b	
	ν_{12}	CH_2 twist.	1116 D	1116 (CS_2 soln.)		
	ν_{13}	CH_2 rock.	810 E[a]			
	ν_{14}	CH bend.	640 D	640 S	650 VW, b	OV(ν_7).
	ν_{15}	CCC deform.	314 C		314 VW	

[a] Estimated from the corresponding frequencies of other propargyl halides.

Reference

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

No. 383 Chlorodiacetylene ClCCCCH

Symmetry $C_{\infty x}$ **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}	
σ^+	ν_1	CH stretch.	3327 C	3327 VS		
	ν_2	C≡C a–stretch.	2252 C	2252 VS		
	ν_3	C≡C s–stretch.	2071 C	2071 M		
	ν_4	C–C stretch.	1093 C	1093 S		
	ν_5	CCl stretch.	525 C	525 S		
π	ν_6	CH bend.	621 B	621 VS		
	ν_7	CCCC a–bend.	463 B	463 S		
	ν_8	CCCC s–bend.	335 C	335 M		
	ν_9	CCCl bend.	133 E	133		OC($\nu_1+\nu_9$, $\nu_6+\nu_9$, $\nu_7+\nu_9$).

Reference

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

No. 384 Bromodiacetylene BrCCCCH

Symmetry $C_{\infty x}$ **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}	
σ^+	ν_1	CH stretch.	3335 C	3335 VS		
	ν_2	C≡C a–stretch.	2237 C	2237 S		
	ν_3	C≡C s–stretch.	2095 C	2095 W		
	ν_4	C–C stretch.	1046 C	1046 M		
	ν_5	CBr stretch.	425 C	425 M		
π	ν_6	CH bend.	623 C	623 VS		
	ν_7	CCCC a–bend.	470 B	470 S		
	ν_8	CCCC s–bend.	355 B	355 M		
	ν_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 $C_{\infty v}$ **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$	
σ^+	ν_1	CH stretch.	3332 C	3332 VS		
	ν_2	C≡C a–stretch.	2211 C	2211 S		
	ν_3	C≡C s–stretch.	2060 C	2060 VW		
	ν_4	C–C stretch.	1025 D	1025 VW		
				(CS_2 soln.)		
	ν_5	CI stretch.	362 C	362 M		
π	ν_6	CH bend.	623 B	623 VS		
	ν_7	CCCC a–bend.	473 B	473 M		
	ν_8	CCCC s–bend.	357 C	357 W		
	ν_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 $D_{\infty h}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	*cm*$^{-1}$ (Gas)	*cm*$^{-1}$ (CCl_4 soln.)	
σ_g^+	ν_1	CN s–stretch.	2235 C	ia	2235 VS, p	
	ν_2	C≡C s–stretch.	2183 C	ia	2183 M, p	
	ν_3	C–C s–stretch.	1288 C	ia	1287.5 W, p	
	ν_4	C–C stretch.	571	ia	571 W, dp	
σ_u^+	ν_5	CN a–stretch.	2266 B	2266 S	ia	
	ν_6	C≡C a–stretch.	2097 B	2097 M	ia	
	ν_7	C–C a–stretch.	717 B	717 S	ia	
π_g	ν_8	Bend.	501 C	ia	501 M, dp	
	ν_9	Bend.	455 C	ia	455 W, dp	
					(C_6H_{14} soln.)	
	ν_{10}	Bend.	170 D	ia	170 W, b, dp	
π_u	ν_{11}	Bend.	491 B	490.5 VS	ia	
	ν_{12}	Bend.	276 B	276 VS	ia	
	ν_{13}	Bend.	62 B	61.5 VS	ia	

Reference

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