Tables of Molecular Vibrational Frequencies. Part 8

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Part 8

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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 49 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). Tables covering 160 more molecules have appeared as Parts 5, 6, and 7 of the series in earlier issues [3, 4, 5] of this journal.

A second Consolidated Volume is now in preparation, and will be published as a supplement to the *Journal of Physical and Chemical Reference Data*. It will bring together under a single cover revised tables for all the molecules treated since ref. [2], plus some updating of that text. The planned consolidation will include indexes to all the published tables.

2. Molecules Selected

The present volume contains tables of fundamental vibrational frequencies for 49 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. [6], [7], and [8] 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 387, continuing the designations of Part 7 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. [9] and [10].

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. [10], 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. [10]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be

defined uniquely. In such cases we generally follow the notation adopted in ref. [10].

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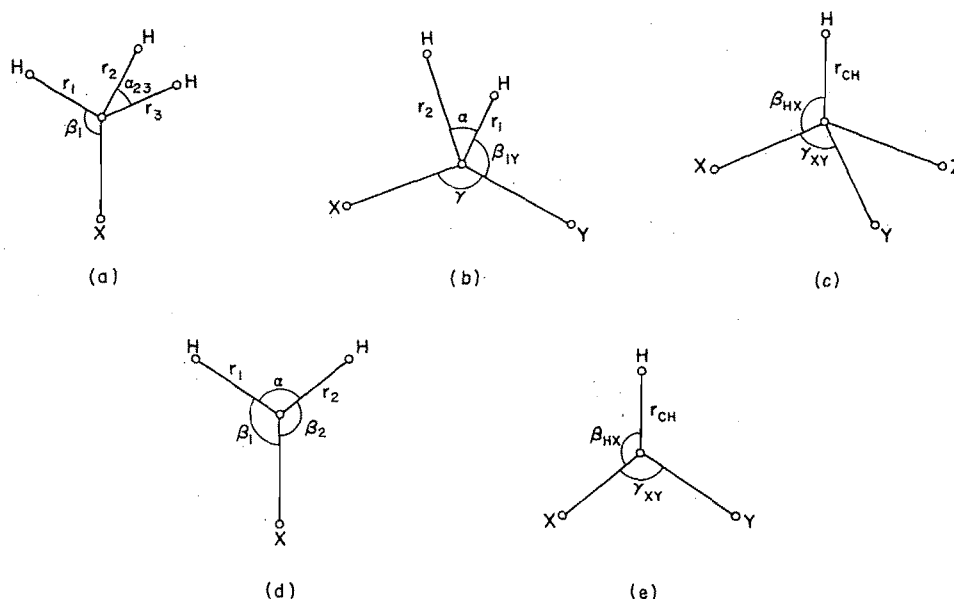
FIGURE 1. Parameters of methyl, methylene, and methin groups.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis*
	cm^{-1}	
A	0 ~ 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^{-1} for NaCl prism).
C	3 ~ 6	(i) Gas, prism spectrometer, low resolution (e.g., 1000 ~ 2000 cm^{-1} for NaCl prism).
		(ii) Solid, liquid or solution, accurate measurement.
D	6 ~ 15	(i) Gas, prism spectrometer, very low resolution (e.g., > 2000 cm^{-1} for NaCl prism).
		(ii) Solid, liquid or solution, inaccurate measurement.
E	15 ~ 30	(i) Value estimated from Fermi resonance doublet.
		(ii) Value estimated from overtone or combination tone.
		(iii) Calculated frequency.

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

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

[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 non-vibrational 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. [10], 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. [12] 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. [11].

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 accord-ance 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.
EL	Derived from analysis of electronic transitions.

3.9. Footnotes and References

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

4. Acknowledgements

5. References

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6. List of Tables of Molecular Vibrational Frequencies

No. 387   Ozone $^{16}O_3$
   Symmetry C_{2v}   **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1103 A	1103.157 VW		
	ν_2	Bend.	701 B	701.42 W		
b_1	ν_3	Antisym. stretch.	1042 A	1042.096 S		

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

No. 388   Ozone $^{18}O_3$
   Symmetry C_{2v}   **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Xe Matrix)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1038 C	1038 W		
	ν_2	Bend.	660 C	660 W		
b_1	ν_3	Antisym. stretch.	974 C	974 S		

Reference
[1] IR.   L. Brewer and J. Ling–Fai Wang, J. Chem. Phys. **56**, 759 (1972).

No. 389   Germanium (II) chloride   GeCl$_2$
Symmetry C$_{2v}$ Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	399 C	399	399 p	
	ν_2	Bend.	159 C		159 p	
b_1	ν_3	Antisym. stretch.	374 D	374	362 dp (Ar Matrix)	

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No. 390   Tin (II) fluoride   SnF$_2$
Symmetry C$_{2v}$ Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1}	
a_1	ν_1	Sym. stretch.	593 D	592.7		
	ν_2	Bend.	197 D	197		
b_1	ν_3	Antisym. stretch.	571 D	570.9		

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

No. 391   **Tin (II) chloride**   **SnCl₂**
      Symmetry C₂ᵥ   **Symmetry number σ = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	352 C	354	352 p	
	ν_2	Bend.	120 C		120 p	
b_1	ν_3	Antisym. stretch.	334 D	334	332 (Ar Matrix)	

References
See No. 389(GeCl₂).

No. 392   **Tin (II) bromide**   **SnBr₂**
      Symmetry C₂ᵥ   **Symmetry number σ = 2**

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	Sym. stretch.	244 D		244 (Ar Matrix)	
	ν_2	Bend.	80 C		80	
b	ν_3	Antisym. stretch.	231 D		231 (Ar Matrix)	

References
See No. 389(GeCl₂).

No. 393 **Lead (II) fluoride** PbF_2

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1}	
a_1	ν_1	Sym. stretch.	531 D	531.2		
	ν_2	Bend.	165 D	165		
b_1	ν_3	Antisym. stretch.	507 D	507.2		

Reference
See No. 390(SnF_2).

No. 394 **Lead (II) chloride** $PbCl_2$

Symmetry C_{2v} **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Ar Matrix)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	314 C	322	314 p	
	ν_2	Bend.	99 C		99 p	
b_1	ν_3	Antisym. stretch.	299 D	299	300 dp (Ar Matrix)	

References
See No. 389($GeCl_2$).

No. 395   **Aluminum trichloride** $AlCl_3$
 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} (Ar Matrix)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.	375 C	380.2	375 p	
	ν_2	Sym. deform.	183 C	182.8		
e	ν_3	Deg. stretch.	595 C	594.7		
	ν_4	Deg. deform.	150 C	149.2	150	

References
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[3] IR.   M. L. Lesiecki and J. S. Shirk, J. Chem. Phys. **56**, 4171 (1972).

No. 396   **Titanium tetrachloride** $TiCl_4$
 Symmetry T_d   **Symmetry number $\sigma = 12$**

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	Sym. stretch.	389 B	ia, 388[a]	389	
e	ν_2	Deg. deform.	114 B	ia, 119[a]	114	
f_2	ν_3	Deg. stretch.	498 C	498.5	498	
	ν_4	Deg. deform.	136 C	136	136	

[a] Estimated from combination bands.

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

No. 397   Titanium tetrabromide   TiBr$_4$
    Symmetry T$_d$ Symmetry number $\sigma = 12$

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	Sym. stretch.	232 B	ia	231.5	
e	ν_2	Deg. deform.	69 B	ia	68.5	
f_2	ν_3	Deg. stretch.	393 C	383 VS	393	
	ν_4	Deg. deform.	88 C		88	

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

No. 398   Titanium tetraiodide   TiI$_4$
    Symmetry T$_d$ Symmetry number $\sigma = 12$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (C$_6$H$_{12}$ soln.)	cm^{-1} (C$_6$H$_{12}$ soln.)	
a_1	ν_1	Sym. stretch.	162 D	ia	162 VS, p	
e	ν_2	Deg. deform.	51 D	ia	51 M, dp	
f_2	ν_3	Deg. stretch.	322 D	322 VS	324 M, dp	
	ν_4	Deg. deform.	67 D	67 M		

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

No. 399　　　**Zirconium tetrachloride**　　　$ZrCl_4$

Symmetry T_d　　　　　　　　　　　　　　　　　　　**Symmetry number** $\sigma = 12$

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	Sym. stretch.	377 B	ia, 388[a]	377 VS, p	
e	ν_2	Deg. deform.	98 B	ia, 102[a]	98	
f_2	ν_3	Deg. stretch.	418 C	421	418 VW	
	ν_4	Deg. deform.	113 C	112[a]	113	

[a] Estimated from combination bands.

References

[1] IR.　　　　J. K. Wilmshurst, J. Mol. Spectry. **5**, 343 (1960).

[2] IR.　　　　A. Büchler, J. B. Berkowitz–Mattuck, and D. H. Dugre, J. Chem. Phys. **34**, 2202 (1961).

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

No. 400　　　**Zirconium tetrabromide**　　　$ZrBr_4$

Symmetry T_d　　　　　　　　　　　　　　　　　　　**Symmetry number** $\sigma = 12$

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	Sym. stretch.	223 B	ia	222.5	
e	ν_2	Deg. deform.	60 B	ia	60	
f_2	ν_3	Deg. stretch.	315 C		315	
	ν_4	Deg. deform.	72 C		72	

Reference

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

No. 401   **Zirconium tetraiodide**   **ZrI₄**

    Symmetry Tₐ   **Symmetry number $\sigma = 12$**

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	Sym. stretch.	158 B	ia	158	
e	ν_2	Deg. deform.	43 B	ia	43	
f_2	ν_3	Deg. stretch.	254 C		254	
	ν_4	Deg. deform.	55 C		55	

Reference
See No. 400(ZrBr₄).

No. 402   **Hafnium tetrachloride**   **HfCl₄**

    Symmetry Tₐ   **Symmetry number $\sigma = 12$**

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	Sym. stretch.	382 B	ia	382	
e	ν_2	Deg. deform.	102 B	ia	101.5	
f_2	ν_3	Deg. stretch.	390 C	393	390	
	ν_4	Deg. deform.	112 C		112	

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

No. 403   **Hafnium tetrabromide**   **HfBr$_4$**

Symmetry T$_d$ **Symmetry number $\sigma = 12$**

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	Sym. stretch.	236 B	ia	235.5	
e	ν_2	Deg. deform.	63 B	ia	63	
f_2	ν_3	Deg. stretch.	273 C		273	
	ν_4	Deg. deform.	71 C		71	

Reference
See No. 400(ZrBr$_4$).

No. 404   **Hafnium tetraiodide**   **HfI$_4$**

Symmetry T$_d$ **Symmetry number $\sigma = 12$**

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	Sym. stretch.	158 B	ia	158	
e	ν_2	Deg. deform.	55 C	ia	55	
f_2	ν_3	Deg. stretch.	224 C		224	
	ν_4	Deg. deform.	63 C		63	

Reference
See No. 400(ZrBr$_4$).

No. 405   Iodine heptafluoride   IF$_7$

Symmetry D^{5h}   **Symmetry number $\sigma = 10$**

Sym. class	No.	Approximate type of mode[a]	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	IF$_{ax}$ s−stretch.	676 C	ia	676 W, p	
	ν_2	IF$_{eq}$ s−stretch.	635 C	ia	635 S, p	
a_2''	ν_3	IF$_{ax}$ a−stretch.	672 C	672 VS	ia	
	ν_4	F$_{eq}$IF$_{ax}$ deform.	257 C	257 W	ia	
e_1'	ν_5	IF$_{eq}$ a−stretch.	746 C	746 S, b	ia	
	ν_6	F$_{eq}$IF$_{eq}$ deform.	425 C	425 VS	ia	
	ν_7	F$_{ax}$IF$_{ax}$ deform.	363 C	363 S	ia	
e_1''	ν_8	F$_{eq}$IF$_{ax}$ deform.	310 C	ia	310 W, dp	
e_2'	ν_9	IF$_{eq}$ a−stretch.	510 C	ia	510 W, dp	
	ν_{10}	F$_{eq}$IF$_{eq}$ deform.	352 C	ia	352 W, dp	
e_2''	ν_{11}	F$_{eq}$IF$_{ax}$ deform.	200 D	ia	ia	CF[2]. OC($\nu_2+\nu_{11}$, $\nu_5+\nu_{11}$).

[a] F$_{ax}$ and F$_{eq}$ represent the axial and equatorial fluorine atoms, respectively.

References

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

No. 406   Thiocarbonyl chloride   CSCl$_2$

Symmetry C$_{2v}$ **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CS stretch.	1137 C	1137 VS	1121 (10)	
	ν_2	CCl$_2$ s–stretch.	505 C	505 M	496 (5)	
	ν_3	CCl$_2$ scis.	220 D	220 VW, b	200 (1)	
b_1	ν_4	CCl$_2$ a–stretch.	816 C	816 VS		
	ν_5	CS deform.	294 C	294	287 (3)	
b_2	ν_6	op–Bend.	473 C	473 W		

References

[1] R.   H. W. Thompson, J. Chem. Phys. **6**, 748 (1938).

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

[3] IR.   M. J. Hopper, J. W. Russell, and J. Overend, Spectrochim. Acta **28A**, 1215 (1972).

No. 407   Thiocarbonyl bromochloride   CSBrCl

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	CS stretch.	1130 C	1130 S	1125 W, p	
	ν_2	CCl stretch.	764 C	764 S	761 W	
	ν_3	CBr stretch.	438 C	438 M	437 S, p	
	ν_4	CBrCl deform.	256 D	256 W (liquid)	257 M, p	
	ν_5	CS deform.	222 D	222 VW (liquid)	222 M, p	
a''	ν_6	op–Bend.	405 E			CF [1].

Reference

[1] IR.R.Th.   J. L. Brena and D. C. Moule, Spectrochim. Acta **28A**, 809 (1972).

No. 408   Chlorotrifluoromethane   CClF$_3$

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} (Gas)	
a_1	ν_1	CF$_3$ s–stretch.	1105 C	1105 VS	1106 W, p	
	ν_2	CCl stretch.	781 C	781 S	781.7 VS, p	
	ν_3	CF$_3$ s–deform.	476 C		475.8 S, p	
e	ν_4	CF$_3$ d–stretch.	1212 C	1212 VS	1217 W, dp	
	ν_5	CF$_3$ d–deform.	563 C	563 M	560 W, dp	
	ν_6	CCl bend.	350 C		350 M, dp	

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

No. 409   Bromotrifluoromethane   CBrF$_3$

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} (Gas)	
a_1	ν_1	CF$_3$ s–stretch.	1089 C	1089 VS	1082 (8) p	
	ν_2	CF$_3$ s–deform.	760 C	760 VS	761 (9) p	
	ν_3	CBr stretch.	349 C	350[a]	349 (7) p	
e	ν_4	CF$_3$ d–stretch.	1210 C	1210 VS	1207 (8) dp	
	ν_5	CF$_3$ d–deform.	547 C	547 M	541 (2) dp	
	ν_6	CBr bend.	306 C	297[a]	306 (2) dp	

[a] Estimated from overtone and combination bands.

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

No. 410   Trifluoroiodomethane CF_3I
    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	CF_3 s−stretch.	1080 C	1080 VS	1056	
	ν_2	CF_3 s−deform.	742 C	742 VS	741	
	ν_3	CI stretch.	286 E	286*	284*	
e	ν_4	CF_3 d−stretch.	1187 C	1187 VS	1168	
	ν_5	CF_3 d−deform.	537 C	537	537	
	ν_6	CI bend.	260 E	260*	260*	

* Estimated from overtone and combination bands.

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

No. 411   Trichlorofluoromethane CCl_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	CF stretch.	1085 C	1085 S	1090 VW, p	
	ν_2	CCl_3 s−stretch.	535 C	535 M	535 VS, p	
	ν_3	CCl_3 s−deform.	350 C	350 VS	349.5 S, p	
e	ν_4	CCl_3 d−deform.	847 C	847 VS	847 M, dp	
	ν_5	CF bend.	394 C	401 VW	394 S, dp	
	ν_6	CCl_3 d−deform.	241 C		241 S, dp	

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

No. 412   Trichloroiodomethane CCl_3I

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	CCl_3 s–stretch.	684 D	684 VS	687 W, b, p	
	ν_2	CI stretch.	390 D	390 M	405 W, p	
	ν_3	CCl_3 s–deform.	224 D	224 W	224 W	
e	ν_4	CCl_3 d–stretch.	755 D	755 VS		
	ν_5	CCl_3 d–deform.	284 D	284 W	288 W, dp	
	ν_6	CI bend.	188 D	188 M		

Reference
[1] IR.R.   R. H. Mann and P. M. Manis, J. Mol. Spectry. **45**, 65 (1973).

No. 413   Tribromofluoromethane CBr_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}	cm^{-1} (Liquid)	
a_1	ν_1	CF stretch.	1069 D		1069 p	
	ν_2	CBr_3 s–stretch.	398 D		398 p	
	ν_3	CBr_3 s–deform.	218 D		218 p	
e	ν_4	CBr_3 d–stretch.	743 D		743 dp	
	ν_5	CF bend.	306 D		306 dp	
	ν_6	CBr_3 d–deform.	150 D		150 dp	

References
[1] R.   M. L. Delwaulle and F. François, Comptes Rendus **214**, 828 (942).
[2] R.   M. L. Delwaulle and F. François, J. Phys. (Paris) **7**, 15 (1946).
[3] Th.   A. G. Meister, S. E. Rosson, and F. F. Cleveland, J. Chem. Phys. **18**, 346 (1950).
[4] Th.   L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 414   **Dichlorodifluoromethane** CCl_2F_2
      Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CF_2 s−stretch.	1101 C	1101 S	1098 M	
	ν_2	CCl_2 s−stretch.	667 C	667 S	667.2 S, p	
	ν_3	CF_2 scis.	458 D		457.5 S	
	ν_4	CCl_2 scis.	262 C		261.5 S, dp	
a_2	ν_5	CF_2 twist.	322 C	ia	322 W, dp	
b_1	ν_6	CF_2 a−stretch.	1159 C	1159 S	1167 W, dp	
	ν_7	CF_2 rock.	446 C	446 W		
b_2	ν_8	CCl_2 a−stretch.	902 E	922 VS	923 W, dp	
				882 VS		$FR(\nu_3+\nu_9)$.
	ν_9	CF_2 wag.	437 C	437 W	433 M	

References
See No. 408(CCl_3F).

No. 415   **Dibromodifluoromethane** CBr_2F_2

     Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CF_2 s–stretch.	1090 C	1090	1077 W, p	
	ν_2	CF_2 scis.	623 C	623	624 W, p	
	ν_3	CBr_2 s–stretch.	340 D		340 S, p	
	ν_4	CBr_2 scis.	168 D		168 M, p	
a_2	ν_5	CF_2 twist.	281 D	ia	281 W, dp	
b_1	ν_6	CF_2 a–stretch.	1153 C	1153 VS	1141 VW, dp	
	ν_7	CF_2 rock.	369 D		369 VW, dp	
b_2	ν_8	CBr_2 a–stretch.	831 C	831 VS	816 W, dp	
	ν_9	CF_2 wag.	325 D		325 VW, dp	

References

[1] R.   G. Glockler and G. R. Leader, J. Chem. Phys. **7**, 553 (1939).

[2] IR.   E. K. Plyler and N. Acquista, J. Res. NBS **48**, 92 (1952).

[3] IR.   C. E. Decker and F. F. Cleveland, J. Chem. Phys. **21**, 189 (1953).

[4] IR.R.   C. E. Decker, A. G. Meister, F. F. Cleveland, and R. B. Bernstein, J. Chem. Phys. **21**, 1781 (1953).

[5] Th.   L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 416   Bromodichlorofluoromethane   CBrCl$_2$F

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	CF stretch.	1080 C	1080 VS	1070 (3) p	
	ν_2	CCl$_2$ s—stretch.	796 C	796 VS	783 (12) p	
	ν_3	CBr stretch.	502 C	502 M (liquid)	504 (100) p	
	ν_4	CCl$_2$ scis.	339 D		339 (14) p	
	ν_5	CBrF scis.	306 D		306 (98) p	
	ν_6	CCl$_2$ wag.	218 D		218 (53) p	
a''	ν_7	CCl$_2$ a—stretch.	838 C	838 VS	831 (5) dp	
	ν_8	CCl$_2$ twist.	392 D		392 (10) dp	
	ν_9	CCl$_2$ rock.	204 D		204 (34) dp	

References

[1] R.   M. L. Delwaulle and F. François, Comptes Rendus **214**, 828 (1942).

[2] IR.R.   R. L. Gilbert, E. A. Piotrowski, J. M. Dowing, and F. F. Cleveland, J. Chem. Phys. **31**, 1633 (1959).

[3] Th.   L. H. Ngai and R. H. Mann, J. Mol. Spectry. **38**, 322 (1971).

No. 417   **Dibromochlorofluoromethane**   **CBr$_2$ClF**

       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	CF stretch.	1075 C	1075 VS	1059 (2) p	
	ν_2	CCl stretch.	806 E	795 VS	793 (4) p	
				814 VS	815 (5) p	FR($\nu_3+\nu_4$).
	ν_3	CBr$_2$ s–stretch.	460 C	460 W (liquid)	464 (58) p	
	ν_4	CClF scis.	341 D		341 (17) p	
	ν_5	CBr$_2$ scis.	268 D		268 (100) p	
	ν_6	CBr$_2$ wag.	162 D		162 (50) p	
a''	ν_7	CBr$_2$ a–stretch.	754 C	754 VS	742 (11) dp	
	ν_8	CBr$_2$ twist.	308 D		308 (6) dp	
	ν_9	CBr$_2$ rock.	196 D		196 (20) dp	

References

See No. 416(CBrCl$_2$F).

No. 418   **Bromoiodoacetylene** C_2BrI

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} (CS_2 soln.)	
σ^+	ν_1	CC stretch.	2166 B	2166 S	2153 VS	
	ν_2	CBr stretch.	782 C	782 M	775 VW	
	ν_3	CI stretch.	222 D		222 M, p	
π	ν_4	CBr bend.	304 D		304 VS, dp	
	ν_5	CI bend.	122 B	122 S		

Reference

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

No. 419   Glyoxal $C_2H_2O_2$

Symmetry C_{2h}   **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	CH stretch.	2843 B	ia		EL[4].
	ν_2	CO stretch.	1745 B	ia		EL[4].
	ν_3	CH bend.	1338 D	ia		OC[1].
	ν_4	CC stretch.	1065 B	ia		EL[4].
	ν_5	CCO deform.	551 B	ia		EL[3].
a_u	ν_6	CH bend.	801 B	801.36 M		
	ν_7	Torsion	127 B	126.5 W		EL[3].
b_g	ν_8	CH bend.	1048 B	ia		[5].
b_u	ν_9	CH stretch.	2835 B	2835.07 VS		
	ν_{10}	CO stretch.	1732 C	1732 VS		
	ν_{11}	CH bend.	1312 B	1312.38 S		
	ν_{12}	CCO deform.	339 B	338.55 S		

References

[1] IR.R.   R. K. Harris, Spectrochim. Acta **20**, 1129 (1964).

[2] IR.   A. R. H. Cole and G. A. Osborne, J. Mol. Spectry. **36**, 276 (1970).

[3] EL.   F. W. Birss, J. M. Brown, A. R. H. Cole, A. Loftus, S. L. N. G. Krishnamachari, G. A. Osborne, J. Puldus, D. A. Ramsay, and L. Watmann, Can. J. Phys. **48**, 1230 (1970).

[4] EL.   W. Holzer and D. A. Ramsay, Can. J. Phys. **48**, 1759 (1970).

[5] IR.   A. R. H. Cole and G. A. Osborne, Spectrochim. Acta **27A**, 2461 (1971).

No. 420 **Glyoxal–d** C_2HDO_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	CH stretch.	2835 B	3835.2 S		
	ν_2	CD stretch.	2130 B	2130.2 S		
	ν_3	CO s–stretch.	1735 D	1735 M		
	ν_4	CO a–stretch.	1717 C	177 VS		
	ν_5	CH bend.	1335 B	1335.0 W		
	ν_6	CC stretch.	1104 E			CF[1].
	ν_7	CD bend.	972 B	971.6 M		
	ν_8	CCO s–deform.	542 D	542[a]		EL[2].
	ν_9	CCO a–deform.	323 B	323.7 S		
a''	ν_{10}	CH bend.	999 D	999 W		
	ν_{11}	CO bend.	688 D			CF.[b]
	ν_{12}	Torsion	124 B	123.9 W		

[a] From the analyses of electronic transitions.

[b] From the product rule.

References

[1] Th. T. Fukuyama, Ph. D. Thesis (University of Tokyo, 1970).

[2] IR. A. R. H. Cole and G. A. Osborne, Spectrochim. Acta **27A**, 2461 (1971).

No. 421   Glyoxal–d₂ $C_2D_2O_2$
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared		Raman		Comments
			cm^{-1}	cm^{-1} (Gas)		cm^{-1} (Gas)		
a_g	ν_1	CD stretch.	2138 D	ia				OC[5].
	=.	CO stretch.	1722 C	ia				OC[5].
	ν_3	CD bend.	1130 D	ia				OC[5].
	ν_4	CC stretch.	915 E	ia				CF[3].
	ν_5	CCO deform.	537 B	ia				EL[2].
a_u	ν_6	CD bend.	630 D					CF[1].[a]
	ν_7	Torsion	118 B	118.2	W			EL[2].
b_g	ν_8	CD bend.	911 D	ia				CF[1].[a]
b_u	ν_9	CD stretch.	2130 C	2130	S			
	ν_{10}	CO stretch.	1710 C	1710	VS			
	ν_{11}	CH bend.	1010 B	1010.12	M			
	ν_{12}	CCO deform.	311 B	311.05	M			

[a] From the product rule

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

No. 422   **Acetyl fluoride**   **CH_3COF**

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_3 d–stretch.	3043 C	3043 W	3043 VW	
	ν_2	CH_3 s–stretch.	2955 C	2955 VW	2952 S	
	ν_3	C=O stretch.	1870 C	1870 VS	1847 S	
	ν_4	CH_3 d–deform.	1440 C	1440 W	1440 W	
	ν_5	CH_3 s–deform.	1378 C	1378 M	1379 W	
	ν_6	CF stretch.	1188 C	1188 VS	1178 VW	
	ν_7	CH_3 rock.	1000 C	1000 M	1003 M	
	ν_8	CC stretch.	826 C	826 S	822 S	
	ν_9	OCF deform.	598 C	598 W	602 M	
	ν_{10}	OCF deform.	420 D	420 VW	428 W	
a''	ν_{11}	CH_3 d–stretch.	3004 C	3004 W	3004 VW	
	ν_{12}	CH_3 d–deform.	1437 D	1437 W	1440 W	
	ν_{13}	CH_3 rock.	054 C	1054 M		
	ν_{14}	C=O op–bend.	567 C	567 W	573 W	
	ν_{15}	CH_3 torsion	123 E			CF[1].

References

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

No. 423   **Acetyl fluoride–d₃** CD_3COF

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	CD_3 d–stretch.	2274 D	2286 M	2272 W	
				2263 M		FR($\nu_3+\nu_{10}$).
	ν_2	CD_3 s–stretch.	2144 C	2144 W	2140 S	
	ν_3	C=O stretch.	1869 C	1869 VS	1849 M	
	ν_4	CF stretch.	1204 C	1204 VS	1196 VW	
	ν_5	CD_3 s–deform.	1149 C	1149 W		
	ν_6	CD_3 d–deform.	1030 C	1030 S	1030 W	
	ν_7	CD_3 rock.	839 C	839 M	845 M	
	ν_8	CC stretch.	778 C	778 S	774 M	
	ν_9	OCF deform.	575 C	575 M	578 M	
	ν_{10}	OCF deform.	395 D	395 VW	378 W	
a''	ν_{11}	CD_3 d–stretch.	2242 C	2242 W	2250 W	
	ν_{12}	CD_3 d–deform.	1057 C	1057 M	1053 W	
	ν_{13}	CD_3 rock.	915 C	915 M		
	ν_{14}	C=O op–bend.	491 C	491 M	495 W	
	ν_{15}	CD_3 torsion	93 E			CF[1].

References

[1] MW.   L. Pierce and L. C. Krisher, J. Chem. Phys. **31,** 875 (1959).

[2] IR.   C. V. Berney, R. L. Redington and K. C. Lin, J. Chem. Phys. **53,** 1713 (1970).

[3] IR.R.   C. V. Berney and A. D. Cormier, Spectrochim. Acta **28A,** 1813 (1972).

No. 424   Dimethylzinc CH_3ZnCH_3

Symmetry $D_{3h}'(G^+_{36})^a$ **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CH_3 s–stretch.	2900 C	ia	2900 S, p	
	ν_2	CH_3 s–deform.	1157 C	ia	1157 S, p	
	ν_3	CZn s–stretch.	503 C	ia	503 VS, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CH_3 s–stretch.	2915 C	2915 S	ia	
	ν_6	CH_3 s–deform.	1183 C	1183 M	ia	
	ν_7	CZn a–stretch.	613 C	613	ia	
e'	ν_8	CH_3 d–stretch.	2966 C	2966 S	2947	
	ν_9	CH_3 d–deform.	1301 C	1301 M	1302 W	
	ν_{10}	CH_3 rock.	704 C	704 S		
	ν_{11}	CZnC deform.	134 D		134 sh	
e''	ν_{12}	CH_3 d–stretch.	2843 C	2843	2830	
	ν_{13}	CH_3 d–deform.	1434 C		1434 W	
	ν_{14}	CH_3 rock.	620 C		620 M	

a Free rotation [3,5].

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

No. 425   **Dimethylzinc-d_6** CD_3ZnCD_3

Symmetry $D_{3h}'(G^+_{36})^a$ Symmetry number $\sigma = 6$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CD_3 s–stretch.	2109 C	ia	2109 S, p	
	ν_2	CD_3 s–deform.	898 C	ia	898 S, p	
	ν_3	CZn s–stretch.	458 C	ia	458 S, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CD_3 s–stretch.	2117 C	2117 M	ia	
	ν_6	CD_3 s–deform.	934 C	934 M	ia	
	ν_7	CZn a–stretch.	554 C	554 S	ia	
e'	ν_8	CD_3 d–stretch.	2219 C	2219 M	2206 M	
	ν_9	CD_3 d–deform.	960 C	960 W		
	ν_{10}	CD_3 rock.	585 D	585 sh		
	ν_{11}	CZnC deform.	96 D		96 sh	
e''	ν_{12}	CD_3 d–stretch.	2073 C	2073 W	2075 sh	
	ν_{13}	CD_3 d–deform.	1006 C	1006 W		
	ν_{14}	CD_3 rock.	495 C		495 W, p	

^{a} Free rotation [1].

Reference

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

No. 426   **Dimethylcadmium CH$_3$CdCH$_3$**

Symmetry D$_{3h}$'(G$^+{}_{36}$)^a   **Symmetry number σ = 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	CH$_3$ s–stretch.	2903 C	ia	2903 S, p	
	ν_2	CH$_3$ s–deform.	1127 C	ia	1127 S, p	
	ν_3	CCd s–stretch.	459 C	ia	459 S, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CH$_3$ s–stretch.	2923 C	2923 S	ia	
	ν_6	CH$_3$ s–deform.	1136 C	1136 M	ia	
	ν_7	CCd a–stretch.	535 C	535 S	ia	
e'	ν_8	CH$_3$ d–stretch.	2980 C	2980 VS		
	ν_9	CH$_3$ d–deform.	1315 C	1315	1324	
	ν_{10}	CH$_3$ rock.	700 C	700 S		
	ν_{11}	CCdC deform.	124 C	124 W	120 W, b	
e''	ν_{12}	CH$_3$ d–stretch.	2859 C	2859	2834 M	
	ν_{13}	CH$_3$ d–deform.	1427 C		1427 W	
	ν_{14}	CH$_3$ rock.	634 C		634 M, dp	

^{a} Free rotation [3,5].

References

[1] R.   F. Fehér, W. Kolb, and L. Leverenz, Z. Naturforsh. **2a**, 454 (1947).

[2] IR.   H. S. Gutowsky, J. Amer. Soc. **71**, 3194 (1949).

[3] IR.R.   J.-L. Bribes, Ph. D. Thesis, (Universite des Sciences et Techniques du Languedoc 1971).

[4] Th.   A. M. W. Bakke, J. Mol. Spectry. **41**, 1 (1972).

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

No. 427   Dimethylcadmium–d_6 CD_3CdCD_3

Symmetry $D_{3h}'(G^+{}_{36})^a$ Symmetry number $\sigma = 6$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CD_3 s–stretch.	2112 C	ia	2112 S, p	
	ν_2	CD_3 s–deform.	873 C	ia	873 S, p	
	ν_3	CCd s–stretch.	419 C	ia	419 S, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CD_3 s–stretch.	2120 C	2120 S	ia	
	ν_6	CD_3 s–deform.	900 C	900 W	ia	
	ν_7	CCd a–stretch.	492 C	492 S	ia	
e'	ν_8	CD_3 d–stretch.	2229 C	2229 S	2214 M, dp	
	ν_9	CD_3 d–deform.	1047 D		1047 W	
	ν_{10}	CD_3 rock.	538 C	538 S		
	ν_{11}	CCdC deform.	109 D		109 sh	
e''	ν_{12}	CD_3 d–stretch.	2080 D	2080	2086 sh	
	ν_{13}	CD_3 d–deform.	1126 C		1126	
	ν_{14}	CD_3 rock.	476 C		476 M, dp	

a Free rotation [1].

Reference

See No. 425(CD_3ZnCD_3).

No. 428   **Dimethylmercury CH_3HgCH_3**

Symmetry $D_{3h}'(G^+_{36})^a$ **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CH_3 s−stretch.	2911 C	ia	2911 VS, p	
	ν_2	CH_3 s−deform.	1182 C	ia	1182 VS, p	
	ν_3	CHg s−stretch.	515 C	ia	515 VS, p	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CH_3 s−stretch.	2925 D	2925 b	ia	
	ν_6	CH_3 s−deform.	1191 C	1191 M	ia	
	ν_7	CHg a−stretch.	540 C	540 VS	ia	
e'	ν_8	CH_3 d−stretch.	2962 C	2962 S		
	ν_9	CH_3 d−deform.	1397 C		1397 W, dp	
	ν_{10}	CH_3 rock.	780 C	780 VS	779 VW, dp	
	ν_{11}	CHgC deform.	161 C		161 M, dp	
e''	ν_{12}	CH_3 d−stretch.	2874 C		2874 S, p	
	ν_{13}	CH_3 d−deform.	1442 C		1442 W, dp	
	ν_{14}	CH_3 rock.	699 C	700 sh	699 M, dp	

a Free rotation [3,6].

References

[1] IR.R.   H. S. Gutowsky, J. Chem. Phys. **17**, 128 (1949).
[2] Th.IR.   D. R. J. Boyd, R. L. Williams and H. W. Thompson, Nature **167**, 766 (1951).
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[5] Th.   A. M. W. Bakke, J. Mol. Spectry. **41**, 1 (1972).
[6] Th.   J. R. Durig and S. C. Brown, J. Mol. Spectry. **45**, 338 (1973).

No. 429   Dimethylmercury-d_6 CD_3HgCD_3

Symmetry $D_{3h}'(G^+_{36})^a$ **Symmetry number $\sigma = 6$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CD_3 s–stretch.	2111 C	ia	2111 M, p	
	ν_2	CD_3 s–deform.	909 C	ia	909 VS, p	
	ν_3	CHg s–stretch.	471 C	ia.	471	
a_1''	ν_4	Torsion		ia	ia	
a_2''	ν_5	CD_3 s–stretch.	2114 C	2114 S	ia	
	ν_6	CD_3 s–deform.	931 C	931 M	ia	
	ν_7	CHg a–stretch.	491 C	491 VS	ia	
e'	ν_8	CD_3 d–stretch.	2224 C	2224	2224 S, dp	
	ν_9	CD_3 d–deform.	1030 C	1030 M	1030 W, dp	
	ν_{10}	CD_3 rock.	598 C	598 VS		
	ν_{11}	CHgC deform.	141 C		141 S, dp	
e''	ν_{12}	CD_3 d–stretch.	2039 C	2039	2044 M, p	
	ν_{13}	CD_3 d–deform.	1050 C		1050 VW, p	
	ν_{14}	CD_3 rock.	525 C		525 M, sh, dp	

a free rotation [2,4].

References

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

No. 430   Azomethane CH_3NNCH_3

Symmetry C_{2h}   **Symmetry number $\sigma = 2$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CH_3 d–stretch.	2977 C	ia	2977 M, dp	
	ν_2	CH_3 s–stretch.	2916 C	ia	2916 S, p	
	ν_3	NN stretch.	1580 C	ia	1580 VW, p	
	ν_4	CH_3 d–deform.	1434 C	ia	1434 M	
	ν_5	CH_3 s–deform.	1380 C	ia	1380 W	
	ν_6	CN stretch.	1176 C	ia	1176 VW	
	ν_7	CH_3 rock.	916 C	ia	916 M	
	ν_8	CCN bend.	589 C	ia	589 VS, p	
a_u	ν_9	CH_3 d–stretch.	2966 D	2966 W, sh (solid)	ia	
	ν_{10}	CH_3 d–deform.	1438 C	1438	ia	
	ν_{11}	CH_3 rock.	1109 C	1109 W	ia	
	ν_{12}	CCN bend.	312 D	312 S (solid)	ia	
	ν_{13}	CH_3 torsion	222 D	222 VW	ia	
b_g	ν_{14}	CH_3 d–stretch.	2982 D	ia	2982 VS (solid)	
	ν_{15}	CH_3 d–deform.	1447 D	ia	1447 S (solid)	
	ν_{16}	CH_3 rock.	1010 D	ia	1010 VW	
	ν_{17}	CH_3 torsion	223 D	ia	223 W (solid)	
b_u	ν_{18}	CH_3 d–stretch.	2982 C	2982 VS	ia	
	ν_{19}	CH_3 s–stretch.	2926 C	2926 VS	ia	
	ν_{20}	CH_3 d–deform.	1445 C	1445 S	ia	
	ν_{21}	CH_3 s–deform.	1393 C	1393 M	ia	
	ν_{22}	CN stretch.	1300 C	1300 VW	ia	
	ν_{23}	CH_3 rock.	1009 C	1009 W	ia	
	ν_{24}	CCN bend.	352 C	352 M	ia	

Reference

[1] IR.R.   J. R. Durig, C. B. Pate, and W. C. Harris, J. Chem. Phys. **56**, 5652 (1972).

No. 431   Azomethane–d_6 CD_3NNCD_3
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CD_3 d–stretch.	2227 C	ia	2227 M	
	ν_2	CD_3 s–stretch.	2117 C	ia	2117 S, p	
	ν_3	NN stretch.	1563 C	ia	1563 VW, dp	
	ν_4	CN stretch.	1125 C	ia	1125 W, p	
	ν_5	CD_3 d–deform.	1042 C	ia	1042 M	
	ν_6	CD_3 s–deform.	1035 D	ia	1035 (solid)	
	ν_7	CD_3 rock.	764 C	ia	764 M, p	
	ν_8	CNN bend.	524 C	ia	524 VS, p	
a_u	ν_9	CD_3 d–stretch.	2178 C	2178 VW	ia	
	ν_{10}	CD_3 d–deform.	1043 D	1043 S (solid)	ia	
	ν_{11}	CD_3 rock.	894 D	894 S, b	ia	OV(ν_{23}).
	ν_{12}	CCN bend.	273 C	273 M	ia	
	ν_{13}	CD_3 torsion	166 D	166 VW (solid)	ia	
b_g	ν_{14}	CD_3 d–stretch.	2250 C	ia	2250 M	
	ν_{15}	CD_3 d–deform.	1057 C	ia	1057 M (solid)	
	ν_{16}	CD_3 rock.	792 D	ia	792 W	
	ν_{17}	CD_3 torsion.	183 D	ia	183 W (solid)	
b_u	ν_{18}	CD_3 d–stretch.	2239 C	2239 VS	ia	
	ν_{19}	CD_3 s–stretch.	2111 C	2111 M	ia	
	ν_{20}	CN stretch.	1116 D	1116 VW (solid)	ia	
	ν_{21}	CD_3 d–deform.	1047 C	1047 M	ia	
	ν_{22}	CD_3 s–deform.	1029 C	1029 sh	ia	
	ν_{23}	CD_3 rock.	894 D	894 S, b	ia	OV(ν_{11}).
	ν_{24}	CNN bend.	304 C	304 M	ia	

Reference
See No.430(CH_3NNCH_3).

No. 432   1-Chloro-3,3,3-trifluoropropyne   CF$_3$CCCl
    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)	(Liquid)			
a_1	ν_1	C≡C stretch.	2270 C	2270 VS	2266 S, p	
	ν_2	CF$_3$ s−stretch.	1276 C	1276 VS	1272 W	
	ν_3	C−C stretch.	937 C	937 S	933 S, p	
	ν_4	CCl stretch.	723 C	723 S	723 S, p	
	ν_5	CF$_3$ s−deform.	377 C	377 W	374 S, p	
e	ν_6	CF$_3$ d−stretch.	1174 C	1174 VS	1153 W, b	
	ν_7	CF$_3$ d−deform.	606 C	606 M	603 W	
	ν_8	CF$_3$ rock.	448 D		448 M, dp	
	ν_9	CCCCl deform.	311 C	311 W	316 VS, dp	
	ν_{10}	CCCCl deform.	97 D		97 VS, dp	

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

No. 433   1-Bromo-3,3,3-trifluoropropyne   CF$_3$CCBr
    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)	(Liquid)	
a_1	ν_1	C≡C stretch.	2243 C	2243 S	2236 M, p	
	ν_2	CF$_3$ s−stretch.	1275 C	1275 VS	1267 W	
	ν_3	C−C stretch.	883 C	883 S	879 S, p	
	ν_4	CBr stretch.	687 C	687 S	684 M, p	
	ν_5	CF$_3$ s−deform.	285 D	285 M	292 VS	
e	ν_6	CF$_3$ d−stretch.	1176 C	1176 VS	1155 W, b	
	ν_7	CF$_3$ d−deform.	607 C	607 M	606 W	
	ν_8	CF$_3$ rock.	455 D	455 VW	452 S	
	ν_9	CCCBr deform.	278 D	278 VW, sh		
	ν_{10}	CCCBr deform.	90 D		90 VS, dp	

Reference
See No. 432(CF$_3$CCCl).

No. 434 1-Iodo-3,3,3-trifluoropropyne CF_3CCI

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	C≡C stretch.	2218 C	2218 S	2207 S, p	
	ν_2	CF_3 s-stretch.	1264 C	1264 VS	1253 W	
	ν_3	C-C stretch.	857 C	857 M	857 S, p	
	ν_4	CI stretch.	661 C	661 S	658 M	
	ν_5	CF_3 s-deform.	250 D	250 W, sh	254 VS, p	
e	ν_6	CF_3 d-stretch.	1174 C	1174 VS	1150 W, b	
	ν_7	CF_3 d-deform.	608 C	608 W	605 W	
	ν_8	CF_3 rock.	450 C	450 W	449 M, dp	
	ν_9	CCCI deform.	263 C	263 M	267 VS, dp	
	ν_{10}	CCCI deform.	85 D		85 VS, dp	

Reference
See No. 432(CF_3CCCl).

No. 435   **Diethynyl ketone   (HC≡C)₂CO**
   Symmetry C₂ᵥ   Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
			cm^{-1}	cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch.	3325 C	3325 S	3275 W, b	OV(ν_{13}).
	ν_2	C≡C stretch.	2097 C	2098 VS, sh (liquid)	2097 VS, p	
	ν_3	CO stretch.	1669 C	1669 S	1636 S, p	
	ν_4	C–C stretch.	739 C	739 VW	749 M, p	
	ν_5	CH bend.	648 C	648 S		
	ν_6	C–C–C deform.	571 C		571 W	
	ν_7	C≡C–C deform.	122 C	122 VW		
a_2	ν_8	CH bend.	712 C	ia	712 VW, dp	
	ν_9	C≡C–C deform.	268 C	ia	268 M	
b_1	ν_{10}	CH bend.	729 C	729 S	733 VW (solid)	
	ν_{11}	CO op–bend.	688 C	688 S	689 VW	
	ν_{12}	C≡C–C deform.	190 C	190 VW	200 W	
b_2	ν_{13}	CH stretch.	3325 C	3325 S	3275 VW, b	OV(ν_1).
	ν_{14}	C≡C stretch.	2115 C	2115 S	2107 M	
	ν_{15}	C–C stretch.	1144 C	1144 VS		
	ν_{16}	CH bend.	682 C	682 M		
	ν_{17}	CO ip–bend.	548 C	548 M		
	ν_{18}	C≡C–C deform.	229 C	229 VW	239 M	

Reference
[1] IR.R.   F. A. Miller, B. M. Harney, and J. Tyrrell, Spectrochim. Acta **27A**, 1003 (1971).