

Tables of Molecular Vibrational Frequencies

Part 5.

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The compilations of fundamental vibrational frequencies of molecules previously published as NSRDS-NBS-6, NRSD-NBS-11, NSRDS-NBS-17, and NSRDS-NBS-39, are extended to 58 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 has recently appeared, which includes revised versions of all the tables in ref. [1] plus tables for 52 additional molecules (a total of 223 molecules).

2. Molecules Selected and Their Ordering

The present volume contains tables of fundamental vibrational frequencies for 58 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. [3, 4, and 5] contain good compilations of data for them.

Rotational isomers are treated as independent molecular species, and a separate table is made for each of the isomers. When the gas and liquid state spectra are significantly different from each other, they are tabulated separately.

The molecules are ordered according to the following rules:

- (a) Number of carbon atoms.
- (b) Total number of atoms.
- (c) Molecular shape: linear, planar, and non-planar.
- (d) Molecular symmetry, in descending order of the number symmetry elements. Isotopically substituted molecules directly follow the normal species regardless of their symmetry.
- (e) Atomic number of central atom (ascending order).
- (f) Atomic number of the other atoms (ascending order).

Molecules are first divided into groups by the items (a) and (b) and the ordering of molecules in each group is given by the items (c), (d), (e), and (f). A complete list in the order presented is given at the beginning of the tables. The molecules are numbered starting with number 224, continuing the designations of NSRDS-NBS-39.

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. [6 and 7].

¹ Figures in brackets indicate the literature references.

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. [7], page 508.

3.3. Symmetry Species

In the tables 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. [7]. 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. [7].

TABLE I. Ordering of symmetry species

(In the present volume 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 _{3v}	A ₁ , A ₂ , E ₁ , E ₂
C _{∞v}	Σ ⁺ , Σ ⁻ , π, Δ, Φ, ...
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 _{∞h}	Σ _g ⁺ , Σ _u ⁺ , Σ _g ⁻ , Σ _u ⁻ , π _g , π _u , Δ _g , Δ _u , Φ _g , Φ _u , ...
C ₃	A, E
C ₆	A, B, E ₁ , E ₂
S ₆	A _g , A _u , E _g , E _u
C _{3h}	A', A'', E', E''
C _{4h}	A _g , A _u , B _g , B _u , E _g , E _u
C _{6h}	A _g , A _u , B _g , B _u , E _{1g} , E _{1u} , E _{2g} , E _{2u}
T _d , O	A ₁ , A ₂ , E, F ₁ , F ₂
O _h	A _{1g} , A _{1u} , A _{2g} , A _{2u} , E _g , E _u , F _{1g} , F _{1u} , F _{2g} , F _{2u}
T	A, E, F

3.4. 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 the C₂X₆ type of molecule we adopt the numbering given in ref. [7], although it is based on D_{3h} symmetry. 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.

3.5. Approximate Type of Mode

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

TABLE II. Definition of local symmetry coordinates

- | Point group | Symmetry species | Approximate type of mode |
|---|------------------|---|
| (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: $(4\Delta\alpha - \Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y})/\sqrt{20}$ |
| | | CH ₂ wagging: $(\Delta\beta_{1X} + \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$ |
| | | CH ₂ twisting: $(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y})/2$ |
| | | CH ₂ rocking: $(\Delta\beta_{1X} - \Delta\beta_{2X} + \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$ |
| (c) Local symmetry coordinates for the CH group (see fig. 1c) | | |
| | | CH stretching: 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 following abbreviations are used for the type of mode:

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

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

3.6. Selected Value of Frequency

The fundamental frequency ν_i is defined as the difference between the term values $G(v_i=1, \text{ and other } v_j=0)$ and $G(v_i=0, \text{ and other } v_j=0)$ 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 top molecule, the frequency listed contains the nonvibrational part $A'\zeta^2$, where A' is the rotational constant of

the vibrational level and ζ is the Coriolis coupling constant. This is in accord with the definition of ν_0 given in ref. [7], 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.

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. [9] 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. [8].

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

3.7. Infrared and Raman Spectra

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

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

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis*
A	cm^{-1} 0 ~ 1	(i) Gas, grating spectrometer, rotational fine structure accurately analyzed. (ii) Gas, grating spectrometer, a sharp <i>Q</i> branch.
B	1 ~ 3	(i) Gas, grating spectrometer, rotational fine structure partly analyzed. (ii) Gas, prism spectrometer, fairly high resolution (e.g., 700 ~ 1000 cm^{-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.

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

3.8. Comments

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

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

3.9. Footnotes and References

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

and Th stand for infrared, Raman, microwave, and theoretical, respectively.

4. Acknowledgements

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5. References

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6. List of Tables of Molecular Vibrational Frequencies

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224	Nitrogen dioxide $^{14}\text{NO}_2$	195	253	Trichlorosilane SiHCl_3	205
225	Nitrogen dioxide $^{15}\text{NO}_2$	195	254	Trichlorosilane- <i>d</i> SiDCl_3	205
226	Sulfur dichloride SCl_2	195	255	Tribromosilane SiHBr_3	205
227	Nitrosyl fluoride $^{16}\text{O}^{14}\text{NF}$	196	256	Phosphoryl fluoride POF_3	206
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233	Nitrosyl chloride $^{18}\text{O}^{14}\text{NCl}$	198	262	Germyl chloride- <i>d</i> ₃ GeD_3Cl	208
234	Nitrosyl chloride $^{18}\text{O}^{15}\text{NCl}$	198	263	Germyl bromide GeH_3Br	208
235	Nitrosyl bromide $^{16}\text{O}^{14}\text{NBr}$	198	264	Germyl bromide- <i>d</i> ₃ GeD_3Br	208
236	Nitrosyl bromide $^{16}\text{O}^{15}\text{NBr}$	199	265	Germyl iodide GeH_3I	209
237	Nitrosyl bromide $^{18}\text{O}^{15}\text{NBr}$	199	266	Germyl iodide- <i>d</i> ₃ GeD_3I	209
238	Boron trifluoride $^{10}\text{BF}_3$	199	267	Trichlorogermane GeHCl_3	209
239	Boron trifluoride $^{11}\text{BF}_3$	200	268	Tribromogermane GeHBr_3	210
240	Sulfur trioxide SO_3	200	269	Sulfuryl fluoride SO_2F_2	210
241	Nitryl fluoride F^{14}NO_2	200	270	Sulfuryl chloride SO_2Cl_2	211
242	Nitryl fluoride F^{15}NO_2	201	271	Selenium dioxide difluoride SeO_2F_2	211
243	Nitryl chloride $\text{Cl}^{14}\text{NO}_2$	201	272	Tellurium hexafluoride TeF_6	212
244	Nitryl chloride $\text{Cl}^{15}\text{NO}_2$	201	273	Digermane GeH_3GeH_3	212
245	Hydrazoic acid HN_3	202	274	Digermane- <i>d</i> ₆ GeD_3GeD_3	213
246	Hydrazoic acid- <i>d</i> ₁ DN_3	202	275	Methylsilane CH_3SiH_3	213
247	Hydrogen peroxide H_2O_2	202	276	Methylsilane- <i>d</i> ₃ CH_3SiD_3	214
248	Thionyl fluoride SOF_2	203	277	Methylgermane CH_3GeH_3	214
249	Thionyl chloride SOCl_2	203	278	Methyl- <i>d</i> ₃ -germane CD_3GeH_3	215
250	Thionyl bromide SOBr_2	204	279	Cyanogen C_2N_2	215
251	Trifluorosilane SiHF_3	204	280	Carbon suboxide C_3O_2	216
252	Trifluorosilane- <i>d</i> SiDF_3	204	281	Carbon subsulfide C_3S_2	216

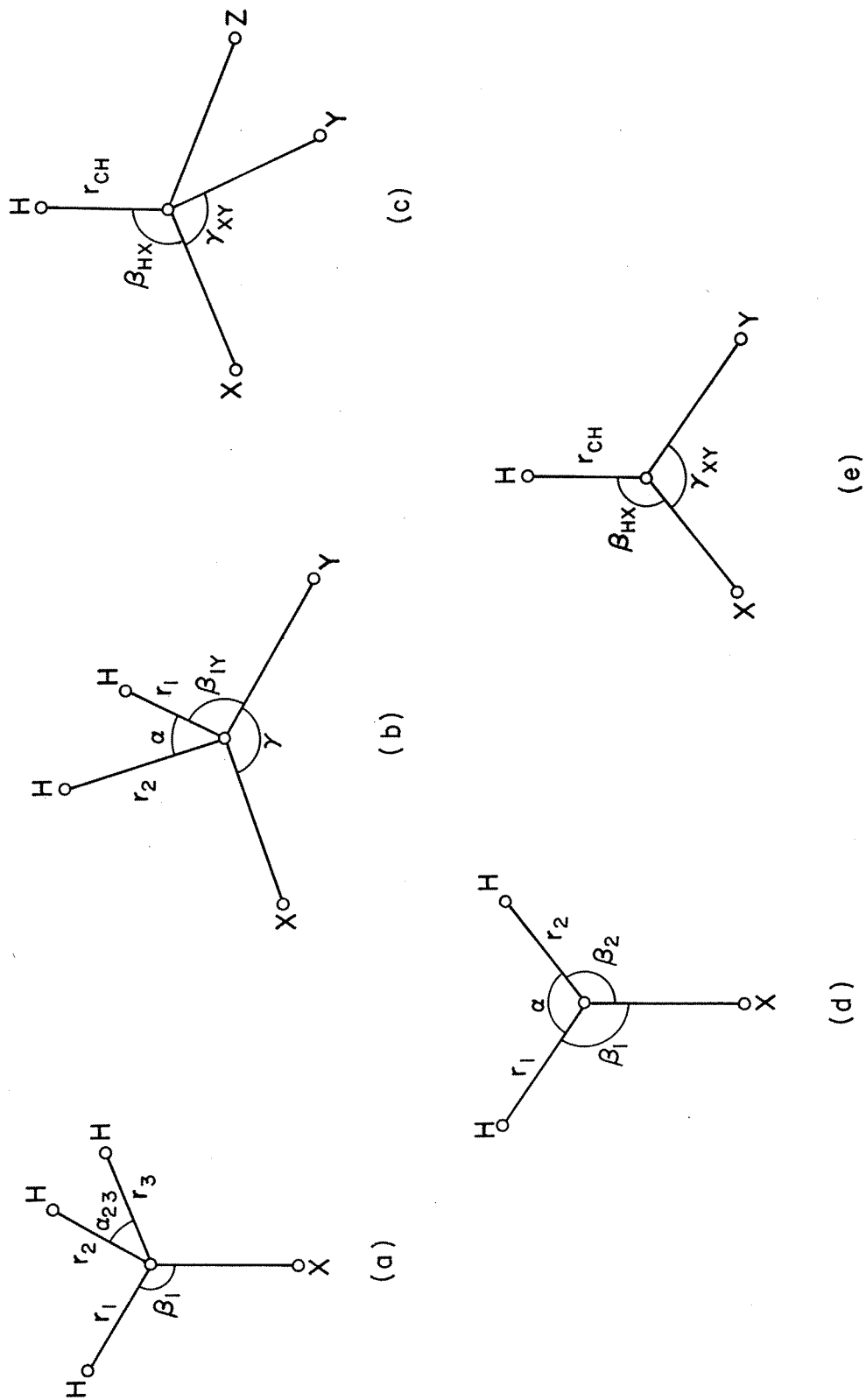


FIGURE 1. Parameters of methyl, methylene, and methin groups.

No. 224

Nitrogen dioxide

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1318 B	1318 W		
	ν_2	Bend.	750 B	749.8 S		
b_1	ν_3	Anti. stretch.....	1618 B	1617.8 VS		

Reference

- [1] IR. E. T. Arakawa and A. H. Nielsen, J. Mol. Spectry. **2**, 413 (1958).
 [2] IR. J. W. Keller and A. H. Nielsen, J. Chem. Phys. **29**, 252 (1958).

No. 225

Nitrogen dioxide

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.	1306 B	1306 W		
	ν_2	Bend.	740 B	740.2 S		
b_1	ν_3	Anti. stretch.....	1580 B	1580.3 VS		

Reference

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

No. 226

Sulfur dichloride

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.	525 D	525 VS	514 (10), p	
	ν_2	Bend.	208 D		208 (5), p	
b_1	ν_3	Anti. stretch.....	535 D		535 (1),	

References

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No. 227

Nitrosyl fluoride

 $^{16}\text{O}^{14}\text{NF}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a'	ν_1	NO stretch.	1844 B	cm^{-1} (Gas)	cm^{-1}		
	ν_2	NF stretch.	766 B				1843.5 VS
	ν_3	Bend.	520 C				765.8 VS
						519.9 VS	

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No. 228

Nitrosyl fluoride

 $^{16}\text{O}^{15}\text{NF}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a'	ν_1	NO stretch.	1812 C	cm^{-1} (Gas)	cm^{-1}		
	ν_2	NF stretch.	749 C				1811.8 VS
	ν_3	Bend.	517 C				748.7 VS
						517.4 VS	

Reference

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

No. 229

Nitrosyl fluoride

 $^{18}\text{O}^{14}\text{NF}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a'	ν_1	NO stretch.	1796 C	cm^{-1} (Gas)	cm^{-1}		
	ν_2	NF stretch.	758 C				1795.6 VS
	ν_3	Bend.	511 C				757.8 VS
						511.3 VS	

Reference

See No. 228 ($^{16}\text{O}^{15}\text{NF}$).

J. Phys. Chem. Ref. Data, Vol. 1, No. 1, 1972

No. 230

Nitrosyl fluoride

 $^{18}\text{O}^{15}\text{NF}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1763 C	cm^{-1} (Gas) 1763.0 VS	cm^{-1}	
	ν_2	NF stretch.....	740 C	740.4 VS		
	ν_3	Bend.....	509 C	509.3 VS		

Reference

See No. 228 ($^{16}\text{O}^{15}\text{NF}$).

No. 231

Nitrosyl chloride

 $^{16}\text{O}^{14}\text{NCl}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1800 C	cm^{-1} (Gas) 1799.7 VS	cm^{-1}	
	ν_2	NCl stretch.....	596 C	595.8 VS		
	ν_3	Bend.....	332 C	331.9 VS		

References

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

No. 232

Nitrosyl chloride

 $^{16}\text{O}^{15}\text{NCl}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1769 C	cm^{-1} (Gas) 1768.9 VS	cm^{-1}	
	ν_2	NCl stretch.....	582 C	581.7 VS		
	ν_3	Bend.....	330 C	329.9 VS		

References

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

No. 233

Nitrosyl chloride

 $^{18}\text{O}^{14}\text{NCl}$ Symmetry C_s Symmetry number $\sigma=1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1751 C	cm^{-1} (Gas) {1752.7 VS} {1749.0 VS} 588.4 VS 324.9 VS	cm^{-1}	FR($3\nu_2$).
	ν_2	NCl stretch.....	588 C			
	ν_3	Bend.....	325 C			

Reference

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

No. 234

Nitrosyl chloride

 $^{18}\text{O}^{15}\text{NCl}$ Symmetry C_s Symmetry number $\sigma=1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1721 C	cm^{-1} (Gas) 1720.6 VS 573.9 VS 323.2 VS	cm^{-1}	
	ν_2	NCl stretch.....	574 C			
	ν_3	Bend.....	323 C			

Reference

See No. 233 ($^{18}\text{O}^{14}\text{NCl}$).

No. 235

Nitrosyl bromide

 $^{16}\text{O}^{14}\text{NBr}$ Symmetry C_s Symmetry number $\sigma=1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1799 C	cm^{-1} (Gas) 1799.0 VS 542.0 VS 266.4 S	cm^{-1}	
	ν_2	NBr stretch.....	542 C			
	ν_3	Bend.....	266 C			

References

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

No. 236

Nitrosyl bromide

 $^{16}\text{O}^{15}\text{NBr}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1768 C	cm^{-1} (Gas) 1768.3 VS 527.8 VS 264 S	cm^{-1}	
	ν_2	NBr stretch.....	528 D			
	ν_3	Bend.....	264 C			

Reference

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

No. 237

Nitrosyl bromide

 $^{18}\text{O}^{15}\text{NBr}$ Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NO stretch.....	1720 C	cm^{-1} (Gas) 1719.5 VS 521.5 VS 257.0 S	cm^{-1}	
	ν_2	NBr stretch.....	522 C			
	ν_3	Bend.....	257 C			

Reference

See No. 236 ($^{16}\text{O}^{15}\text{NBr}$).

No. 238

Boron trifluoride

 $^{10}\text{BF}_3$ Symmetry D_{3h} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'_1 a''_2 e'	ν_1	Sym. stretch.....	888 B	cm^{-1} (Gas) ia 719.3 S 1502.5 S 482.0 M	cm^{-1} 888 VS ia 1481 VW 482 W, b	
	ν_2	Op-deform.....	719 A			
	ν_3	Deg. stretch.....	1503 A			
	ν_4	Deg. deform.....	482 B			

References

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

No. 239

Boron trifluorideSymmetry D_{3h} Symmetry number $\sigma=6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'_1	ν_1	Sym. stretch.....	888 B	ia	888 VS	
a''_2	ν_2	Op-deform.....	691 A	691.2 S	ia	
e'	ν_3	Deg. stretch.....	1449 B	1449 S	1448 VW	
	ν_4	Deg. deform.....	480 B	480.4 M	482 b	

ReferenceSee No. 238 ($^{10}\text{BF}_3$).

No. 240

Sulfur trioxideSymmetry D_{3h} Symmetry number $\sigma=6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'_1	ν_1	Sym. stretch.....	1068 B	ia	1068 VS, p	
a''_2	ν_2	Op-deform.....	530 B	529.65 S	ia	
e'	ν_3	Deg. stretch.....	1391 A	1391.3 VS	1385 W (liquid)	
	ν_4	Deg. deform.....	499 B	498.5 M		

References

- [1] R. H. Gerding and W. J. Nijverd, Rec. trav. chim. **59**, 1206 (1940).
- [2] IR. R. W. Lovejoy, J. H. Colwell, D. F. Eggers, and G. D. Halsey, J. Chem. Phys. **36**, 612 (1962).
- [3] IR. R. Bent and W. R. Lander, Spectrochim. Acta **19**, 931 (1963).
- [4] R. K. Stopperka, Z. anorg. allgem. Chem. **345**, 277 (1966).
- [5] IR. J. B. Milne and A. Ruoff, J. Mol. Spectry. **23**, 408 (1967).
- [6] IR. R. K. Thomas and H. Thompson, Proc. Roy. Soc. London A **314**, 329 (1970).

No. 241

Nitryl fluorideSymmetry C_{2v} Symmetry number $\sigma=2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.....	1310 B	1309.6 VS		
	ν_2	NF stretch.....	822 B	822.4 VS		
	ν_3	NO_2 scis.....	568 C	567.8 S		
b_1	ν_4	NO_2 a-stretch.....	1792 B	1791.5 VS		
	ν_5	NO_2 rock.....	560 C	559.6 S		
b_2	ν_6	Op-deform.....	742 B	742.0 M		

References

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

No. 242

Nitryl fluoride

 $F^{15}NO_2$ Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.....	1298 B	1298.0 VS		
	ν_2	NF stretch.....	809 B	808.5 VS		
	ν_3	NO_2 scis.....	567 C	567.1 S		
b_1	ν_4	NO_2 a-stretch.....	1751 B	1750.5 VS		
	ν_5	NO_2 rock.....	559 C	558.9 S		
b_2	ν_6	Op-deform.....	722 B	722.0 M		

References

See No. 241 ($F^{14}NO_2$).

No. 243

Nitryl chloride

 $Cl^{14}NO_2$ Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.....	1286 C	{ 1318.5 S } { 1267.1 VS }		FR($2\nu_6$).
	ν_2	NCl stretch.....	793 B	792.6 VS		
	ν_3	NO_2 scis.....	370 C	369.6 VS		
b_1	ν_4	NO_2 a-stretch.....	1685 B	1684.6 VS		
	ν_5	NO_2 rock.....	408 C	408.1 VW		
b_2	ν_6	Op-deform.....	652 C	652.3 M		

References

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

No. 244

Nitryl chloride

 $Cl^{15}NO_2$ Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	NO_2 s-stretch.....	1286 D	{ 1318.5 S } { 1267.1 VS }		FR ($2\nu_6$).
	ν_2	NCl stretch.....	793 B	792.6 VS		
	ν_3	NO_2 scis.....	370 C	369.6 VS		
b_1	ν_4	NO_2 a-stretch.....	1685 B	1684.6 VS		
	ν_5	NO_2 rock.....	408 C	408.1 VW		
b_2	ν_6	Op-deform.....	652 C	652.3 M		

References

See No. 243 ($Cl^{14}NO_2$).

No. 245

Hydrazoic acid

Symmetry C_sSymmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	ν_1	NH stretch.....	3336 B	3336 M		
	ν_2	N≡N stretch.....	2140 B	2139.8 VS		
	ν_3	NH bend.....	1264 B	1263.7 M		
	ν_4	N-N stretch.....	1151 B	1150.5 VS		
<i>a''</i>	ν_5	NNN bend.....	534 B	534.2 W		
	ν_6	NNN bend.....	607 B	607.0 VW		

References

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

No. 246

Hydrazoic acid-*d*₁Symmetry C_sSymmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	ν_1	ND stretch.....	2478 B	2478 M		FR ($\nu_3 + \nu_4$).
	ν_2	N≡N stretch.....	2112 C	2112 VS		
	ν_3	ND bend.....	954 B	953.8 S		
	ν_4	N-N stretch.....	1184 B	1183.7 M		
<i>a''</i>	ν_5	NNN bend.....	492 B	492.2 W		
	ν_6	NNN bend.....	588 B	588.4 VW		

See references of No. 245 (HN₃).

No. 247

Hydrogen peroxide

Symmetry C₂Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i>	ν_1	OH stretch.....	3599 B	3599.2	3364 P	
	ν_2	OH bend.....	1402 E		1402 P	
	ν_3	OO stretch.....	877 C	877	880 P	
<i>b</i>	ν_4	Torsion.....	371 B	{ 370.7		
			243 C			
	ν_5	OH stretch.....	3608 B	3607.9		
	ν_6	OH bend.....	1266 D	1266		

References

- [1] IR. P. A. Giguère, J. Chem. Phys. **18**, 88 (1950).
 [2] IR. P. A. Giguère and O. Bain, J. Phys. Chem. **56**, 340 (1952).
 [3] IR. O. Bain and P. A. Giguère, Can. J. Chem. **33**, 527 (1955).
 [4] R. R. C. Taylor and P. C. Cross, J. Chem. Phys. **24**, 41 (1956).
 [5] IR. R. L. Redington, W. B. Olson, and P. C. Cross, J. Chem. Phys. **36**, 1311 (1962).
 [6] IR. R. H. Hunt, R. A. Leacock, C. W. Peters and K. T. Hecht, J. Chem. Phys. **42**, 1931 (1965).

No. 248

Thionyl fluoride

Symmetry C_sSymmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Gas)	
<i>a'</i>	ν_1	SO stretch.....	1333 D	{ 1340.8 S 1330.9 S	1339.3 VS 1329.9 VS	} FR ($\nu_2 + \nu_3$).
	ν_2	SF ₂ s-stretch.....	808 B	808.2 VS	808.3 VS	
	ν_3	OSF deform.....	530 B	530.4 M	529.6 S	
	ν_4	SF ₂ scis.....	378 D	377.8 W	379.5 W	
<i>a''</i>	ν_5	SF ₂ a-stretch.....	747 C	747.0 VS	746.8 W	
	ν_6	OSF deform.....	393 D	392.5 W	398.6 M (Liquid)	

References

- [1] IR. J. K. O'Loane and M. K. Wilson, J. Chem. Phys. **23**, 1314 (1955).
 [2] R. P. Bender and J. M. Wood, Jr., J. Chem. Phys. **23**, 1316 (1955).
 [3] IR. F. Seel and R. Budenz, Chem. Ber. **98**, 251 (1965).
 [4] IR.R. E. L. Pace and H. V. Samuelson, J. Chem. Phys. **44**, 3682 (1966).

No. 249

Thionyl chloride

Symmetry C_sSymmetry number $\sigma = 1$

Sym. class.	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a'</i>	ν_1	SO stretch.....	1251 C	1251 VS	1230 W, p	
	ν_2	SOCl ₂ s-stretch.....	492 C	492 VS	490 M, p	
	ν_3	OSCl deform.....	344 D		344 S, p	
	ν_4	SOCl ₂ scis.....	194 D		194 M, p	
<i>a''</i>	ν_5	SOCl ₂ a-stretch.....	455 C	455 VS	445 W, dp	
	ν_6	OSCl deform.....	284 D		284 M, dp	

References

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

No. 250

Thionyl bromide**Symmetry C_s****Symmetry number $\sigma = 1$**

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹	<i>cm</i> ⁻¹ (Liquid)	
<i>a'</i>	ν_1	SO stretch.....	1121 D		1121 (2)p	
	ν_2	SBr ₂ s-stretch.....	405 D		405 (7)p	
	ν_3	OSBr deform.....	267 D		267 (10)p	
<i>a''</i>	ν_4	SBr ₂ scis.....	120 D		120 (10)p	
	ν_5	SBr ₂ a-stretch.....	379 D		379 (5)dp	
	ν_6	OSBr deform.....	223 D		223 (7)dp	

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

No. 251

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	ν_1	SiH stretch.....	2315 B	2315 M		
	ν_2	SiF ₃ s-stretch.....	859 B	859 S		
	ν_3	SiF ₃ s-deform.....	425 C	425 M		
<i>e</i>	ν_4	SiF ₃ d-stretch.....	999 C	999 VS		
	ν_5	SiH bend.....	845 C	845 S		
	ν_6	SiF ₃ d-deform.....	305 B	305 M		

Reference[1] IR. C. Newman, S. R. Polo, and M. K. Wilson, Spectrochim. Acta **15**, 793 (1959).

No. 252

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	ν_1	SiD stretch.....	1688 B	1688 M		
	ν_2	SiF ₃ s-stretch.....	854 C	854 S		
	ν_3	SiF ₃ s-deform.....	422 B	422 M		
<i>e</i>	ν_4	SiF ₃ d-stretch.....	994 D	994 VS		
	ν_5	SiD bend.....	629 C	629 M		
	ν_6	SiF ₃ d-deform.....	302 B	302 M		

Reference[1] IR. C. Newman, S. R. Polo, and M. K. Wilson, Spectrochim. Acta **15**, 793 (1959).

No. 253

Trichlorosilane

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	SiH stretch.....	2261 B	2260.9 S	2258 p	
	ν_2	SiCl ₃ s-stretch.....	499 B	498.6 S	489 p	
	ν_3	SiCl ₃ s-deform.....	254 B	253.7 M	250 p	
<i>e</i>	ν_4	SiH bend.....	811 B	810.8 VS	799 dp	
	ν_5	SiCl ₃ d-stretch.....	600 B	600.1 VS	587 dp	
	ν_6	SiCl ₃ d-deform.....	176 B	175.5 M	179 dp	

References

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

No. 254

Trichlorosilane-d

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	ν_1	SiD stretch.....	1647 B	1647.1 S		
	ν_2	SiCl ₃ s-stretch.....	496 B	495.9 S		
	ν_3	SiCl ₃ s-deform.....	252 B	252.0 M		
<i>e</i>	ν_4	SiD bend.....	634 B	633.8 VS		
	ν_5	SiCl ₃ d-stretch.....	550 B	550.0 VS		
	ν_6	SiCl ₃ d-deform.....	175 B	174.5 M		

Reference

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

No. 255

Tribromosilane

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	SiH stretch.....	2236 D		2236 p	
	ν_2	SiBr ₃ s-stretch.....	362 D		362 p	
	ν_3	SiBr ₃ s-deform.....	166 D		166 p	
<i>e</i>	ν_4	SiH bend.....	770 D		770 dp	
	ν_5	SiBr ₃ d-stretch.....	470 D		470 dp	
	ν_6	SiBr ₃ d-deform.....	115 D		115 dp	

Reference

- [1] R. M. M. Delwaulle and M. F. François, C.R. **230**, 743 (1950).

No. 256

Phosphoryl fluoride

POF₃Symmetry C_{3v}Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	PO stretch.....	1415 B	1415 M	1395 p	OV(ν_3) in Raman.
	ν_2	PF ₃ s-stretch.....	873 B	873 M	875 p	
	ν_3	PF ₃ s-deform.....	473 B	473 S	476	
<i>e</i>	ν_4	PF ₃ d-stretch.....	990 C	990 VS	982 dp	
	ν_5	PF ₃ d-deform.....	485 C	485 M	476 dp	
	ν_6	PO bend.....	337 D		337 dp	

References

- [1] R. M. L. Delwaille and F. François, C.R. **222**, 550 (1946).
 [2] IR. H. S. Gutowsky and A. D. Liehr, J. Chem. Phys. **20**, 1652 (1952).

No. 257

Phosphoryl chloride

POCl₃Symmetry C_{3v}Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	PO stretch.....	1290 D		1290	
	ν_2	PCl ₃ s-stretch.....	486 D		486	
	ν_3	PCl ₃ s-deform.....	267 D		267	
<i>e</i>	ν_4	PCl ₃ d-stretch.....	581 D		581	
	ν_5	PO bend.....	337 D		337	
	ν_6	PCl ₃ d-deform.....	193 D		193	

Reference

- [1] R. M. L. Delwaille and F. François, J. chim. Physique **45**, 50 (1948).

No. 258

Phosphoryl bromide

POBr₃Symmetry C_{3v}Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	PO stretch.....	1261 D		1261	
	ν_2	PBr ₃ s-stretch.....	340 D		340	
	ν_3	PBr ₃ s-deform.....	173 D		173	
<i>e</i>	ν_4	PBr ₃ d-stretch.....	488 D		488	
	ν_5	PO bend.....	267 D		267	
	ν_6	PBr ₃ d-deform.....	118 D		118	

Reference

See No. 257 (POCl₃).

No. 259

Germyl fluoride

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
a ₁	ν_1	GeH ₃ s-stretch.....	2121 C	2120.6 S		
	ν_2	GeH ₃ s-deform.....	859 C	859.0 VS		
	ν_3	GeF stretch.....	689 B	689.1 S		
e	ν_4	GeH ₃ d-stretch.....	2132 B	2131.7 S		
	ν_5	GeH ₃ d-deform.....	874 B	874.0 S		
	ν_6	GeH ₃ rock.....	643 B	642.6 M		

References

- [1] IR. J. E. Griffiths, T. N. Srivastava, and M. Onyszczuk, Can. J. Chem. **40**, 579 (1962).
 [2] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).
 [3] IR. K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).

No. 260

Germyl fluoride-d₃Symmetry C_{3v}Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
a ₁	ν_1	GeD ₃ s-stretch.....	1525 C	1525		
	ν_2	GeD ₃ s-deform.....	696 B	696		
	ν_3	GeF stretch.....	618 C	618		
e	ν_4	GeD ₃ d-stretch.....	1535 B	1535		
	ν_5	GeD ₃ d-deform.....	635 C	635		
	ν_6	GeD ₃ rock.....	466 C	466		

Reference

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

No. 261

Germyl chloride

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
a ₁	ν_1	GeH ₃ s-stretch.....	2120 C	2119.9		
	ν_2	GeH ₃ s-deform.....	848 B	847.5		
	ν_3	GeCl stretch.....	422 C	421.7		
e	ν_4	GeH ₃ d-stretch.....	2129 B	2128.9		
	ν_5	GeH ₃ d-deform.....	874 B	874.1		
	ν_6	GeH ₃ rock.....	602 B	602.2		

References

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

No. 262

Germyl chloride- d_3 GeD_3Cl Symmetry C_{3v} Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeD_3 s-stretch.....	1518 C	1518		
	ν_2	GeD_3 s-deform.....	609 C	609		
	ν_3	GeCl stretch.....	422 C	422		
e	ν_4	GeD_3 d-stretch.....	1530 C	1530		
	ν_5	GeD_3 d-deform.....	630 C	630		
	ν_6	GeD_3 rock.....	434 C	434		

Reference

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

No. 263

Germyl bromide

 GeH_3Br Symmetry C_{3v} Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeH_3 s-stretch.....	2115 C	2115.2		
	ν_2	GeH_3 s-deform.....	833 C	832.7		
	ν_3	GeBr stretch.....	308 C	307.7		
e	ν_4	GeH_3 d-stretch.....	2127 B	2126.7		
	ν_5	GeH_3 d-deform.....	871 B	870.9		
	ν_6	GeH_3 rock.....	578 B	578.2		

References

- [1] IR. J. E. Griffiths, T. N. Srivastava, and M. Onyszchuk, Can. J. Chem. **40**, 579 (1962).
 [2] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).
 [3] IR. K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).

No. 264

Germyl bromide- d_3 GeD_3Br Symmetry C_{3v} Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeD_3 s-stretch.....	1514 C	1514		
	ν_2	GeD_3 s-deform.....	596 C	596		
	ν_3	GeBr stretch.....	305 C	305		
e	ν_4	GeD_3 d-stretch.....	1530 C	1530		
	ν_5	GeD_3 d-deform.....	621 C	621		
	ν_6	GeD_3 rock.....	420 C	420		

Reference

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

No. 265

Germyl iodide

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	ν_1	GeH ₃ s-stretch.....	2110 C	2110.1		
	ν_2	GeH ₃ s-deform.....	808 C	808.2		
	ν_3	GeI stretch	248 C	248.2		
<i>e</i>	ν_4	GeH ₃ d-stretch.....	2121 B	2120.7		
	ν_5	GeH ₃ d-deform.....	854 B	853.6		
	ν_6	GeH ₃ rock.....	558 B	558.3		

References

- [1] IR. D. E. Freeman, K. H. Rhee, and M. K. Wilson, J. Chem. Phys. **39**, 2908 (1963).
 [2] IR. K. H. Rhee and M. K. Wilson, J. Chem. Phys. **43**, 331 (1965).

No. 266

Germyl iodide-d₃Symmetry C_{3v}Symmetry number $\sigma=3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	ν_1	GeD ₃ s-stretch.....	1508 C	1508		
	ν_2	GeD ₃ s-deform.....	582 C	582		
	ν_3	GeI stretch.....	249 C	249		
<i>e</i>	ν_4	GeD ₃ d-stretch.....	1525 C	1525		
	ν_5	GeD ₃ d-deform.....	603 C	603		
	ν_6	GeD ₃ rock.....	404 C	404		

Reference

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

No. 267

Trichlorogermene

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	GeH stretch.....	2159 D		2159 p	
	ν_2	GeCl ₃ s-stretch....	409 D		409 p	
	ν_3	GeCl ₃ s-deform....	181 D		181 p	
<i>e</i>	ν_4	GeH bend.....	699 D		699 dp	
	ν_5	GeCl ₃ d-stretch....	438 D		438 dp	
	ν_6	GeCl ₃ d-deform....	149 D		149 dp	

Reference

- [1] R. M. M. Delwaille and M. F. François, C.R. **228**, 1007 (1949).

No. 268

Tribromogermane

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	GeH stretch.....	2116 D		2116 p	
	ν_2	GeBr ₃ s-stretch.....	273 D		273 p	
	ν_3	GeBr ₃ s-deform.....	128 D		128 p	
<i>e</i>	ν_4	GeH bend.....	674 D		674 dp	
	ν_5	GeBr ₃ d-stretch.....	325 D		325 dp	
	ν_6	GeBr ₃ d-deform.....	95 E		95 dp	

Reference

- [1] R. M. M. Delwaille and M. F. François, C.R. **230**, 743 (1950).

No. 269

Sulfuryl fluoride

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Gas)	
<i>a</i> ₁	ν_1	SO ₂ s-stretch.....	1269 C	1269 S	1270 M	
	ν_2	SF ₂ s-stretch.....	848 C	848 S	847 S	
	ν_3	SO ₂ scis.....	544 D	544.3 M	543 M	
	ν_4	SF ₂ scis.....	385 D	384.5 VW		
<i>a</i> ₂	ν_5	SF ₂ twist.....	388 C	ia	388 W	
<i>b</i> ₁	ν_6	SO ₂ a-stretch.....	1502 C	1502 S	1502 VW	
	ν_7	SO ₂ rock.....	553 D	552.8 M		
<i>b</i> ₂	ν_8	SF ₂ a-stretch.....	885 C	885 S	883 VW	
	ν_9	SO ₂ wag.....	539 D	539.4 M		

References

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

No. 270

Sulfuryl chloride

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	SO ₂ s-stretch.....	1205 C	1205 S	1182 S, p	
	ν_2	SO ₂ scis.....	577 D	577 VS	560 VS, p	
	ν_3	SO ₂ s-stretch.....	408 D		408 VS, p	
	ν_4	SO ₂ scis.....	218 D		218 VS, p	
<i>a</i> ₂	ν_5	SO ₂ twist.....	282 D	ia	282 S, dp	
<i>b</i> ₁	ν_6	SO ₂ a-stretch.....	1434 C	1434 S	1414 M, dp	
	ν_7	SO ₂ rock.....	388 D		388 S, dp	
<i>b</i> ₂	ν_8	SO ₂ a-stretch.....	586 D	586 VS	580 VW, dp	
	ν_9	SO ₂ wag.....	362 D		362 sh, dp	

References

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

No. 271

Selenium dioxide difluoride

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	SeO ₂ s-stretch.....	973 C	973 S	969 S, p	
	ν_2	SeF ₂ s-stretch.....	700 C	700 S	702 S, p	
	ν_3	SeO ₂ scis.....	360 C	360 S	357 M	
	ν_4	SeF ₂ scis.....	284 C	284 W	280 M	
<i>a</i> ₂	ν_5	SeF ₂ twist.....	272 E			OC(2 ν_5).
<i>b</i> ₁	ν_6	SeO ₂ a-stretch.....	1059 C	1059 S	1059 W	
	ν_7	SeO ₂ rock.....	335 D	335 S	334 M	OV(ν_7).
<i>b</i> ₂	ν_8	SeF ₂ a-stretch.....	756 C	756 W		
	ν_9	SeO ₂ wag.....	335 D	335 S	334 M	OV(ν_7).

References

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

No. 272

Tellurium hexafluoride

Symmetry O_hSymmetry number $\sigma = 24$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.....	697 B	ia	697.1 VS	OC($2\nu_6$) [3].
e_g	ν_2	Deg. stretch.....	670 C	ia	670.3 W	
f_{1u}	ν_3	Deg. stretch.....	751 C	751.0	ia	
	ν_4	Deg. deform.....	327 C	326.5	ia	
f_{2g}	ν_5	Deg. deform.....	314 C	ia	314 W	
f_{2u}	ν_6	Deg. deform.....	197 E	ia	ia	

References

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

No. 273

Digermene

Symmetry D_{3d}Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	GeH ₃ s-stretch.....	2068 C	ia	2068 S, p	$\left. \begin{array}{l} \text{OC}(\nu_9 + 2\nu_4) \\ \text{OC}(\nu_7 + 2\nu_4) \\ \text{OC}(\nu_7 - 2\nu_4) \\ \text{OC}(\nu_6 - 2\nu_4) \end{array} \right\}$
	ν_2	GeH ₃ s-deform.....	832 C	ia	832 VW, p	
	ν_3	GeGe stretch.....	268 C	ia	268.4 S, p	
a_{1u}	ν_4	Torsion.....	146 E	ia	ia	
a_{2u}	ν_5	GeH ₃ s-stretch.....	2077 B	2077.0 VS	ia	
	ν_6	GeH ₃ s-deform.....	756 B	756.0 VS	ia	
e_u	ν_7	GeH ₃ d-stretch.....	2091 B	2090.7 S	ia	
	ν_8	GeH ₃ d-deform.....	879 B	879.0 S	ia	
	ν_9	GeH ₃ rock.....	370 B	370.3 M	ia	
e_g	ν_{10}	GeH ₃ d-stretch.....	2081 E	ia		
	ν_{11}	GeH ₃ d-deform.....	880 C	ia	879.6 M, dp	
	ν_{12}	GeH ₃ rock.....	567 C	ia	566.6 W, dp	

References

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

No. 274

Digermene- d_6 Symmetry D_{3d} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	GeD_3 s-stretch.....	1484 C	ia	1483.7 S, p	CF[3].
	ν_2	GeD_3 s-deform.....	600 C	ia	600 VW, p	
	ν_3	GeGe stretch.....	264 C	ia	264 S, p	
a_{1u}	ν_4	Torsion.....	^a 106 E	ia	ia	
a_{2u}	ν_5	GeD_3 s-stretch.....	1490 B	1489.9 VS	ia	
	ν_6	GeD_3 s-deform.....	546 C	546.2 S	ia	
e_u	ν_7	GeD_3 d-stretch.....	1511 C	1511 S	ia	
	ν_8	GeD_3 d-deform.....	630 B	629.7 M	ia	
	ν_9	GeD_3 rock.....	262 C	262 S	ia	
e_g	ν_{10}	GeD_3 d-stretch.....	1501 D	ia	1501	
	ν_{11}	GeD_3 d-deform.....	626 C	ia	626.1 M, dp	
	ν_{12}	GeD_3 rock.....	412 C	ia	412.0 W, dp	

^a From the product rule.

References

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

No. 275

Methylsilane

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch.....	2898 E	{ 2928.8 M 2867.4 M }	}	FR ($\nu_2 + \nu_5$).
	ν_2	SiH_3 s-stretch.....	2169 C	2169 S		
	ν_3	CH_3 s-deform.....	1260 C	1260 M		
	ν_4	SiH_3 s-deform.....	940 C	940 VS		
	ν_5	CSi stretch.....	700 C	700 S		
a_2	ν_6	Torsion.....	187 D	ia		{ 187.6 (A) 186.9 (E) } MW.
e	ν_7	CH_3 d-stretch.....	2982 A	2981.6 M		
	ν_8	SiH_3 d-stretch.....	2166 A	2165.7 S		
	ν_9	CH_3 d-deform.....	1403 C	1403 M		
	ν_{10}	SiH_3 d-deform.....	980 D	^a 980		
	ν_{11}	CH_3 rock.....	868 B	867.5 S		
	ν_{12}	SiH_3 rock.....	540 C	540 M		

^a The band origin is not determined clearly.

References

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

No. 276

Methylsilane-*d*₃Symmetry C_{3v}

Symmetry number σ = 3

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	<i>ν</i> ₁	CH ₃ s-stretch	2923 A	2923.4 M		{172.1 (A)} {171.9 (E)} ^{MW.}
	<i>ν</i> ₂	SiD ₃ s-stretch	1558 C	1558 M		
	<i>ν</i> ₃	CH ₃ s-deform	1262 C	1262 S		
	<i>ν</i> ₄	CSi stretch	741 C	741 VS		
	<i>ν</i> ₅	SiD ₃ s-deform	652 C	652 S		
<i>a</i> ₂	<i>ν</i> ₆	Torsion	172 D	ia		
<i>e</i>	<i>ν</i> ₇	CH ₃ d-stretch	2982 A	2981.8 M		
	<i>ν</i> ₈	SiD ₃ d-stretch	1577 C	1577 VS		
	<i>ν</i> ₉	CH ₃ d-deform	1401 C	1401 M		
	<i>ν</i> ₁₀	CH ₃ rock	825 C	825 S		
	<i>ν</i> ₁₁	SiD ₃ d-deform	668 C	668 S		
	<i>ν</i> ₁₂	SiD ₃ rock	433 C	433		

References

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

No. 277

Methylgermane

Symmetry C_{3v}

Symmetry number σ = 3

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	<i>ν</i> ₁	CH ₃ s-stretch	2938 B	2937.8 S		{158.1 (A)} {156.1 (E)} ^{MW.}
	<i>ν</i> ₂	GeH ₃ s-stretch	2085 B	2084.8 S		
	<i>ν</i> ₃	CH ₃ s-deform	1254 B	1254.1 M		
	<i>ν</i> ₄	GeH ₃ s-deform	843 B	842.5 VS		
	<i>ν</i> ₅	CGe stretch	602 B	601.6 VS		
<i>a</i> ₂	<i>ν</i> ₆	Torsion	157 D	ia		
<i>e</i>	<i>ν</i> ₇	CH ₃ d-stretch	2997 B	2997.2 S		
	<i>ν</i> ₈	GeH ₃ d-stretch	2084 B	2084.3 S		
	<i>ν</i> ₉	CH ₃ d-deform	1428 C	1427.7 W		
	<i>ν</i> ₁₀	GeH ₃ d-deform	900 C	900.4 S		
	<i>ν</i> ₁₁	CH ₃ rock	848 C	847.5 S		
	<i>ν</i> ₁₂	GeH ₃ rock	506 C	505.9 S		

References

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

No. 278

Methyl-*d*₃-germaneCD₃GeH₃Symmetry C_{3v}

Symmetry number σ=3

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
a ₁	ν ₁	CD ₃ s-stretch.....	2090 C	2090.1 S		
	ν ₂	GeH ₃ s-stretch.....	2073 C	2073 S		
	ν ₃	CD ₃ s-deform.....	978 C	977.5 S		
	ν ₄	GeH ₃ s-deform.....	844 C	844.3 S		
	ν ₅	CGe stretch.....	550 B	549.6 S		
a ₂	ν ₆	Torsion.....	132 D	ia		{131.7 (A)} {131.5 (E)} MW.
e	ν ₇	CD ₃ d-stretch.....	2248 B	2247.5 S		
	ν ₈	GeH ₃ d-stretch.....	2089 B	2089.0 S		
	ν ₉	CD ₃ d-deform.....	1032 B	1032.0 M		
	ν ₁₀	GeH ₃ d-deform.....	904 B	903.9 S		
	ν ₁₁	CD ₃ rock.....	713 C	713 S		
	ν ₁₂	GeH ₃ rock.....	452 B	451.8 S		

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No. 279

Cyanogen

C₂N₂Symmetry D_{∞h}

Symmetry number σ=2

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹ (Liquid)	
σ _g ⁺	ν ₁	CN s-stretch.....	2330 B	^a 2329.9	2328.5 VS, p	
	ν ₂	NN stretch.....	851 D	ia	850.6 M, p	
σ _u ⁺	ν ₃	CN a-stretch.....	2158 A	2157.85 VS	ia	
π _g	ν ₄	CCN bend.....	507 D	ia	507.2 S	
π _u	ν ₅	CCN bend.....	233 B	^a 233.1	240 W	

^a Determined from difference bands [3].

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No. 280

Carbon suboxide

Symmetry $D_{\infty h}$ Symmetry number $\sigma=2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	CO stretch.....	2185 B	ia	2185 W	
	ν_2	CC stretch.....	820 B	ia	820 W, p	
σ_u^+	ν_3	CO stretch.....	2258 B	2258 S	ia	
	ν_4	CC stretch.....	1573 B	1573 S	ia	
π_g	ν_5	CCO bend.....	584 B	ia	584 W	
	ν_6	CCO bend.....	550 B	550 S	ia	
π_u	ν_7	CCC bend.....	63 B	63 VW	ia	

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No. 281

Carbon subsulfide

Symmetry $D_{\infty h}$ Symmetry number $\sigma=2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (CS ₂ soln.)	
σ_g^+	ν_1	CC stretch.....	1663 D	ia	1663 S	
	ν_2	CS stretch.....	485 D	ia	485 S, p	
σ_u^+	ν_3	CC stretch.....	2089 B	2088.5 VS	ia	
	ν_4	CS stretch.....	1019 B	1019.2 S	ia	
π_g	ν_5	CCS bend.....	470 D	ia	470 M	
	ν_6	CCS bend.....	502 C	502 VW	ia	
π_u	ν_7	CCC bend.....	94 C	94 W	ia	

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