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Tables of Molecular Vibrational Frequencies

Part 3.

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UNITED STATES DEPARTMENT OF COMMERCE
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Tables of Molecular Vibrational Frequencies Part 3.

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Foreword

The National Standard Reference Data System is a government-wide effort to give to the technical community of the United States optimum access to the quantitative data of physical science, critically evaluated and compiled for convenience. This program was established in 1963 by the President's Office of Science and Technology, acting upon the recommendation of the Federal Council for Science and Technology. The National Bureau of Standards has been assigned responsibility for administering the effort. The general objective of the System is to coordinate and integrate existing data evaluation and compilation activities into a systematic, comprehensive program, supplementing and expanding technical coverage when necessary, establishing and maintaining standards for the output of the participating groups, and providing mechanisms for the dissemination of the output as required.

The NSRDS is conducted as a decentralized operation of nation-wide scope with central coordination by NBS. It comprises a complex of data centers and other activities, carried on in government agencies, academic institutions, and nongovernmental laboratories. The independent operational status of existing critical data projects is maintained and encouraged. Data centers that are components of the NSRDS produce compilations of critically evaluated data, critical reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data.

For operational purposes, NSRDS compilation activities are organized into seven categories as listed below. The data publications of the NSRDS, which may consist of monographs, loose-leaf sheets, computer tapes, or any other useful product, will be classified as belonging to one or another of these categories. An additional "General" category of NSRDS publications will include reports on detailed classification schemes, lists of compilations considered to be Standard Reference Data, status reports, and similar material. Thus, NSRDS publications will appear in the following eight categories:

Category	*Title*
1	General
2	Nuclear Properties
3	Atomic and Molecular Properties
4	Solid State Properties
5	Thermodynamic and Transport Properties
6	Chemical Kinetics
7	Colloid and Surface Properties
8	Mechanical Properties of Materials

The present compilation is in category 3 of the above list. It constitutes the seventeenth publication in a new NBS series known as the National Standard Reference Data Series.

A. V. Astin, *Director.*

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Tables of Molecular Vibrational Frequencies

Part 3.

T. Shimanouchi

A compilation of vibrational frequency data for selected molecules is being conducted at the University of Tokyo in cooperation with the National Standard Reference Data Program of the National Bureau of Standards as a part of an international effort to compile and evaluate physical and chemical data. This report, as a continuation of Part 1 published as NSRDS–NBS–6, and Part 2 published as NSRDS–NBS–11, contains fundamental vibrational frequencies of 54 molecules together with vibrational assignments, sources of data, brief comments, and citations of references. The procedures used for the preparation of tables are the same as given in Part 1. The fundamental frequencies are obtained mainly from the infrared and Raman spectra. When these are not available, other experimental data such as microwave results are taken into account. The selection of vibrational fundamentals from observed data is based upon careful studies of the spectral data and comprehensive mathematical analyses. The tables were designed to provide a concise summary needed for the computation of ideal gas thermodynamic properties. They may also provide a convenient source of information to those who require vibrational energy levels and related properties in molecular spectroscopy, analytical chemistry, and other fields of physics and chemistry.

Key Words: Molecular, vibrational, frequencies, data, tables, spectral.

I. Introduction

A compilation of vibrational frequency data for selected molecules is being conducted as a part of a broad program on the compilation and critical evaluation of physical and chemical data of many substances. Vibrational frequency data of molecules are not only useful in research on molecular structure, but are also essential to accurate computation of ideal gas thermodynamic properties. These tables will be a convenient source of information in any field of physics or chemistry in which the vibrational energy levels and related properties are needed. The data may also be useful to those who utilize infrared or Raman spectra as a technique in analytical chemistry.

This is the third of a series of annual reports being prepared in cooperation with the National Standard Reference Data Program of the National Bureau of Standards. The first and the second report which have been published as NSRDS–NBS–6 and NSRDS–NBS–11, contain data for 113 molecules. This third report contains 58 additional molecules with the serial numbers 114–171. These molecules have been selected from the molecules for which the experimental data are available and for which the normal coordinate treatments were made in detail. General comments on the procedures by which the tables are made and on the explanations of notations and abbreviations used are given in Part 1 (NSRDS–NBS–6). Only the important notations and abbreviations are reproduced in the following tables.

The author expresses his sincere thanks to many members of the National Bureau of Standards, especially C. W. Beckett, D. R. Lide, Jr., E. L. Brady, and S. A. Rossmassler who helped in the planning, the preparation, and the publication of the tables.

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TABLE 1. *Abbreviations for approximate type of mode*

stretch.	stretching	twist.	twisting
deform.	deformation	wag.	wagging
rock.	rocking	bend.	bending
sym.	symmetric	deg.	degenerate
anti.	antisymmetric		

TABLE 2. *Uncertainty for the selective values of frequencies*

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

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

TABLE 3. *Abbreviations used with "infrared" and "Raman"*

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

The intensity of a Raman line may also be indicated by (1) ~ (10), which gives a rough estimation of relative intensity.

TABLE 4. *Abbreviations used in "Comments"*

FR	Fermi Resonance with an overtone or a combination tone indicated in the parentheses which follow
OC	Frequency estimated from an overtone or a combination tone indicated in the parentheses
CF	Calculated frequency
SF	Calculation shows that the frequency approximately equals that of the vibration indicated in the parentheses
TA	Tentative assignment
OV	Overlapped by the band indicated in the parentheses
ρ	Depolarization degree

II. Tables of Vibrational Frequencies

Pages 5 to 39

Molecule: Hydrogen oxide H_2O **No. 114**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	OH_2 sym. stretch.....	3657 A	3656.7	3654	
	ν_2	OH_2 deform.....	1595 A	1594.6		
b_1	ν_3	OH_2 anti. stretch.....	3756 A	3755.8		

References

[1] R. E. F. Barker and W. W. Slater, J. Chem. Phys. **3**, 660 (1935).
[2] IR. N. Gailar and E. K. Plyler, J. Chem. Phys. **24**, 1139 (1956).

Molecule: Hydrogen oxide-d_1 HDO **No. 115**
Symmetry C_s Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'	ν_1	OH stretch.....	3707 A	3707.5		
	ν_2	OD stretch.....	2727 A	2726.7	2718	
	ν_3	OHD deform.....	1402 A	1402.2		

References

[1] R. E. F. Barker and W. W. Slater, J. Chem. Phys. **3**, 660 (1935).
[2] IR. N. Gailar and E. K. Plyler, J. Chem. Phys. **24**, 1139 (1956).

Molecule: Hydrogen oxide-d_2 D_2O **No. 116**
Symmetry C_{2v} Symmetry number $\sigma=2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	OD_2 sym. stretch.....	2671 A	2671.5	2666	
	ν_2	OD_2 deform.....	1178 A	1178.3		
b_1	ν_3	OD_2 anti. stretch.....	2788 A	2788.0		

References

[1] R. E. F. Barker and W. W. Slater, J. Chem. Phys. **3**, 660 (1935).
[2] IR. N. Gailar and E. K. Plyler, J. Chem. Phys. **24**, 1139 (1956).

Molecule: Nitrous oxide $^{14}N_2O$ **No. 117**
Symmetry $C_{\infty v}$ Symmetry number $\sigma=1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ^+	ν_1	NN stretch.....	2224 A	2223.7 VS	2224 W	
	ν_2	NO stretch.....	1285 A	1284.9 VS	1287 VS	
π	ν_3	NNO bend.....	589 A	588.7 S	589 W	

References

[1] R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik," Berlin, Göttingen, Heidelberg (1951).
[2] IR. J. Pliva, J. Mol. Spectry. **12**, 360 (1964).
[3] IR. R. P. Grosso and T. K. McCubbin, Jr., J. Mol. Spectry. **13**, 240 (1964).

Molecule: Nitrous oxide $^{14}N^{15}NO$ **No. 118**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	NN stretch.....	2202 A	2201.6		
	ν_2	NO stretch.....	1270 A	1269.9		
π	ν_3	NNO bend.....	585 A	585.3		

Reference

[1] IR. R. P. Grosso and T. K. McCubbin, Jr., J. Mol. Spectry. **13**, 240 (1964).

Molecule: Nitrous oxide $^{15}N_2O$ **No. 119**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	NN stretch.....	2155 A	2154.7		
	ν_2	NO stretch.....	1265 A	1265.3		
π	ν_3	NNO bend.....	572 A	571.9		

Reference

[1] IR. R. P. Grosso and T. K. McCubbin, Jr., J. Mol. Spectry. **13**, 240 (1964).

Molecule: Oxygen difluoride F_2O **No. 120**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	F_2O sym. stretch.....	928 B	928 S		
	ν_2	F_2O deform.....	461 B	461 S		
b_1	ν_3	F_2O anti. stretch.....	831 B	831 VS		

References

[1] R.IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR.Th. H. J. Bernstein and J. Powling, J. Chem. Phys. **18**, 685 (1950).
[3] IR.Th. E. A. Jones, J. S. Kirby-Smith, P. J. H. Woltz, and A. H. Nielsen, J. Chem. Phys. **19**, 337 (1951).

Molecule: Oxygen dichloride Cl_2O **No. 121**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Cl_2O sym. stretch.....	631 C	630.7 VS (solid)		
	ν_2	Cl_2O deform.....	296 C	296.4 W (solid)		
b_1	ν_3	Cl_2O anti. stretch.....	686 C	685.9 S		

References

[1] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and the references cited there.
[2] IR.Th. K. Hedberg, J. Chem. Phys. **19**, 509 (1951).
[3] IR.Th. M. M. Rochkind and G. C. Pimentel, J. Chem. Phys. **42**, 1361 (1965).

Molecule: Silyl fluoride SiH_3F **No. 122**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiH_3 sym. stretch.....	2206 D	2206		
	ν_2	SiH_3 sym. deform.....	990 C	990 S		
	ν_3	SiF stretch.....	872 B	872 M		
e	ν_4	SiH_3 deg. stretch.....	2196 C	2196 M		
	ν_5	SiH_3 deg. deform.....	956 C	[a]956 M		
	ν_6	SiH_3 rock.....	728 B	728.1 M		

[a] The band center was re-estimated by Duncan on the basis of the data by Newman, et al.

References

[1] IR. F. A. Andersen and B. Bak, Acta Chem. Scand. **8**, 738 (1954).
[2] IR. C. Newman, J. K. O'Loane, S. R. Polo, and M. K. Wilson, J. Chem. Phys. **25**, 855 (1956).
[3] Th. J. L. Duncan, Spectrochim. Acta **20**, 1807 (1964).

Molecule: Silyl chloride SiH_3Cl **No. 123**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiH_3 sym. stretch.....	2201 D	2201		
	ν_2	SiH_3 sym. deform.....	949 D	949		
	ν_3	SiCl stretch.....	551 C	551 S		
e	ν_4	SiH_3 deg. stretch.....	2195 B	2195 S		
	ν_5	SiH_3 deg. deform.....	954 B	954.4 S		
	ν_6	SiH_3 rock.....	664 B	664.0 M		

References

[1] IR. A. Monfils, J. Chem. Phys. **19**, 138(1951).
[2] IR. A. Monfils, Compt. Rend. **236**, 795 (1953).
[3] IR. C. Newman, J. K. O'Loane, S. R. Polo, and M. K. Wilson, J. Chem. Phys. **25**, 855 (1956).
[4] Th. J. L. Duncan, Spectrochim. Acta **20**, 1807 (1964).

Molecule: Silyl bromide SiH_3Br **No. 124**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiH_3 sym. stretch.....	2200 D	2200		
	ν_2	SiH_3 sym. deform.....	930 C	930 S		
	ν_3	SiBr stretch.....	430 C	430 M		
e	ν_4	SiH_3 deg. stretch.....	2196 C	2196 S		
	ν_5	SiH_3 deg. deform.....	950 B	950.4 S		
	ν_6	SiH_3 rock.....	633 B	632.6 S		

References

[1] IR. D. W. Mayo, H. E. Opitz, and J. S. Peake, J. Chem. Phys. **23**, 1344 (1955).
[2] IR. C. Newman, J. K. O'Loane, S. R. Polo, and M. K. Wilson, J. Chem. Phys. **25**, 855 (1956).
[3] Th. J. L. Duncan, Spectrochim. Acta **20**, 1807(1964).

Molecule: Hydrogen sulfide H_2S **No. 125**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SH_2 sym. stretch.....	2354 A	2353.9		
	ν_2	SH_2 deform.....	1183 A	1182.7		
b_1	ν_3	SH_2 anti. stretch.....	2615 A	2614.6		

References

[1] IR. H. C. Allen, Jr., L. R. Blaine, E. K. Plyler, and P. C. Cross, J. Chem. Phys. **24**, 35 (1956).
[2] IR. H. C. Allen, Jr., L. R. Blaine, E. K. Plyler, and P. C. Cross, J. Chem. Phys. **25**, 1132 (1956).

Molecule: Hydrogen sulfide-d_2 D_2S **No. 126**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Solid)	
a_1	ν_1	SD_2 sym. stretch.....	1892 C	1892	1832	
	ν_2	SD_2 deform.....	855 C	855		
b_1	ν_3	SD_2 anti. stretch.....	1900 C	1900	1853	

Reference

[1] R.IR. J. B. Lohman, F. P. Reding, and F. Horing, J. Chem. Phys. **19**, 252 (1951).

Molecule: Sulfur hexafluoride SF_6 **No. 127**
Symmetry O_h Symmetry number $\sigma = 24$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	SF stretch.....	772 C	ia	772.4 (10)	
e_g	ν_2	SF stretch.....	642 C	ia	642 (2) (liquid)	
f_{1u}	ν_3	SF stretch.....	932 C	932	ia	
	ν_4	FSF deform.....	613 C	613	ia	
f_{2g}	ν_5	FSF deform.....	522 C	ia	522 (2) (liquid)	
f_{2u}	ν_6	FSF deform.....	344 E	ia	ia	OC ($\nu_2 + \nu_6$, $\nu_5 + \nu_6$).[2]

References

[1] R. D. M. Yost, C. C. Steffens, and S. T. Gross, J. Chem. Phys. **2**, 311 (1934).
[2] IR. J. Gaunt, Trans. Faraday Soc. **49**, 1122 (1953).

Molecule: Germanium tetrachloride $GeCl_4$ **No. 128**
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)	
a_1	ν_1	$GeCl_4$ sym. stretch.....	396 C	.....	396 (10)	
e	ν_2	$GeCl_4$ deg. deform.....	134 C	.....	134 (6)	
f_2	ν_3	$GeCl_4$ deg. stretch.....	453 C	.....	453 (1)	
	ν_4	$GeCl_4$ deg. deform.....	172 C	.....	172 (6)	

References

[1] R. R. R. Haun and W. D. Harkins, J. Am. Chem. Soc. **54**, 3917 (1932).
[2] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London) **A240**, 499 (1957).

Molecule: Germanium tetrabromide $GeBr_4$ **No. 129**
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)	
a_1	ν_1	$GeBr_4$ sym. stretch.....	235 C	.....	235	
e	ν_2	$GeBr_4$ deg. deform.....	79 C	.....	79	
f_2	ν_3	$GeBr_4$ deg. stretch.....	327 C	.....	327	
	ν_4	$GeBr_4$ deg. deform.....	112 C	.....	112	

Reference

[1] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London) **A240**, 499 (1957).

Molecule: Hydrogen selenide H_2Se **No. 130**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SeH_2 sym. stretch	2345 B	2344.5 S		
	ν_2	SeH_2 deform	1034 A	1034.2 S		
b_1	ν_3	SeH_2 anti. stretch	2358 B	2357.8 S		

References

[1] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York 1945) and the references cited there.
[2] IR.Th. E. D. Palik, J. Mol. Spectry. **3**, 259 (1959).

Molecule: Hydrogen selenide-d_1 HDSe **No. 131**
Symmetry C_s Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	SeH stretch	2352 C	2352		
	ν_2	SeD stretch	1691 C	1691		
	ν_3	SeHD deform	912 C	912		

References

[1] R.IR.Th. D. M. Cameron, W. C. Sears, and H. H. Nielsen, J. Chem. Phys. **7**, 994 (1939).
[2] R.IR. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik," Berlin, Göttingen, Heidelberg (1951).

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Molecule: Selenium hexafluoride SeF_6 **No. 132**
Symmetry O_h Symmetry number $\sigma = 24$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	SeF stretch.....	708 C	ia	708.0 (10)	
e_g	ν_2	SeF stretch.....	662 C	ia	662 (2) (liquid)	
f_{1u}	ν_3	SeF stretch.....	780 C	780	ia	
	ν_4	FSeF deform.....	437 C	437	ia	
f_{2g}	ν_5	FSeF deform.....	405 C	ia	405 (2) (liquid)	
f_{2u}	ν_6	FSeF deform.....	260 E	ia	ia	OC ($\nu_5 + \nu_6$, $\nu_2 + \nu_6$)[2].

References

[1] R. D. M. Yost, C. C. Steffens, and S. T. Gross, J. Chem. Phys. **2**, 311 (1934).
[2] IR. J. Gaunt, Trans. Faraday Soc. **49**, 1122 (1953).

Molecule: Tin (IV) chloride $SnCl_4$ **No. 133**
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)	
a_1	ν_1	$SnCl_4$ sym. stretch.....	366 C	.....	366 (10)	
e	ν_2	$SnCl_4$ deg. deform.....	104 C	.....	104 (5)	
f_2	ν_3	$SnCl_4$ deg. stretch.....	403 C	.....	403 (6)	
	ν_4	$SnCl_4$ deg. deform.....	134 C	.....	134 (6)	

References

[1] R. R. R. Haun and W. D. Harkins, J. Am. Chem. Soc. **54**, 3917 (1932).
[2] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London) **A240**, 499 (1957).

Molecule: Tin (IV) bromide $SnBr_4$ **No. 134**
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)	
a_1	ν_1	$SnBr_4$ sym. stretch.....	220 C	.....	220 (4)	
e	ν_2	$SnBr_4$ deg. deform.....	64 C	.....	64 (2)	
f_2	ν_3	$SnBr_4$ deg. stretch.....	279 C	.....	279 (3)	
	ν_4	$SnBr_4$ deg. deform.....	88 C	.....	88 (4)	

References

[1] R. B. Trumpy, Z. Physik **68**, 675 (1931).
[2] R. R. R. Haun and W. D. Harkins, J. Am. Chem. Soc. **54**, 3917 (1932).
[3] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London) **A240**, 499 (1957).

Molecule: Hydrogen cyanide HCN **No. 135**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ^+	ν_1	CH stretch.....	3311 A	3311.4 S	3313 W	
	ν_2	C ≡ N stretch.....	2097 A	2096.8	2089 S	
π	ν_3	HCN bend.....	712 A	711.9 VS	712 W	

References

[1] R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik", Berlin, Göttingen, Heidelberg (1951).
[2] IR. H. C. Allen, Jr., E. D. Tidwell, and E. K. Plyler, J. Chem. Phys. **25**, 302 (1956).
[3] IR. A. G. Maki and L. R. Blaine, J. Mol. Spectry. **12**, 45 (1964).

Molecule: Hydrogen cyanide-d_1 DCN **No. 136**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ^+	ν_1	CD stretch	2630 A	2630.3	2630	
	ν_2	C ≡ N stretch	1925 A	1925.3	1906	
π	ν_3	DCN bend	569 A	569.1	569	

References

[1] R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik", Berlin, Göttingen, Heidelberg (1951).
[2] IR. H. C. Allen, Jr., E. D. Tidwell, and E. K. Plyler, J. Chem. Phys. **25**, 302 (1956).

Molecule: Formic acid HCOOH (gas) **No. 137**
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}	
a'	ν_1	OH stretch	3570 D	3570 M		
	ν_2	CH stretch	2943 A	2942.8 M		
	ν_3	C = O stretch	1770 C	1770 VS		
	ν_4	CH bend	1387 C	1387 VW		
	ν_5	OH bend (ν_6)	1229 C	1229 W		
	ν_6	CO stretch (ν_5)	1105 A	1105.3 S		
	ν_7	OCO bend	625 C	625 M		
a''	ν_8	CH bend	1033 B	1033 W		
	ν_9	CO torsion	638 C	638 S		

References

[1] IR. V. Z. Williams, J. Chem. Phys. **15**, 232, 243 (1947).
[2] IR. L. M. Sverdlov, Dokl. Akad. Nauk SSSR **91**, 503 (1953).
[3] IR. W. J. Orville Thomas, Research **9**, S15 (1956).
[4] IR. J. K. Wilmshurst, J. Chem. Phys. **25**, 478 (1956).
[5] IR.Th. R. C. Millikan and K. S. Pitzer, J. Chem. Phys. **27**, 1305 (1957).
[6] IR.Th. T. Miyazawa and K. S. Pitzer, J. Chem. Phys. **30**, 1076 (1959).

Molecule: Formic acid-d_2 DCOOD (gas) **No. 138**
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}	
a'	ν_1	OD stretch	2632 A	2632 W		
	ν_2	CD stretch	2232 A	2231.8 M		
	ν_3	C=O stretch	1742 C	1742 VS		
	ν_4	CD bend	945 B	945 M		
	ν_5	OD bend	1040 A	1040 W		
	ν_6	CO stretch	1171 B	1171.3 S		
	ν_7	OCO bend	558 C	558 W		
a''	ν_8	CD bend	873 C	873 W		
	ν_9	CO torsion	491 C	491 W		

References

[1] IR. V. Z. Williams, J. Chem. Phys. **15**, 232, 243 (1947).
[2] IR. L. M. Sverdlov, Dokl. Akad. Nauk SSSR **91**, 503 (1953).
[3] IR. W. J. Orville Thomas, Research **9**, S15 (1956).
[4] IR. J. K. Wilmshurst, J. Chem. Phys. **25**, 478 (1956).
[5] IR.Th. R. C. Millikan and K. S. Pitzer, J. Chem. Phys. **27**, 1305 (1957).
[6] IR.Th. T. Miyazawa and K. S. Pitzer, J. Chem. Phys. **30**, 1076 (1959).

Molecule: Fluoroform CHF_3 **No. 139**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3036 C	3036 S	3062 S, p	
	ν_2	CF_3 sym. stretch	1117 C	.....	1117 VS, p	
	ν_3	CF_3 sym. deform	700 C	700 M	697 S, p	
e	ν_4	CH bend	1372 C	1372 M	1376 S, dp	
	ν_5	CF_3 deg. stretch	1152 C	1152 VS	1160 W, dp	
	ν_6	CF_3 deg. deform	507 C	507 M	508 VS, dp	

References

[1] IR. H. J. Bernstein and G. Herzberg, J. Chem. Phys. **16**, 30 (1948).
[2] R. D. H. Rank, E. R. Shull, and E. L. Pace, J. Chem. Phys. **18**, 885 (1950).
[3] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47**, 202 (1951).

Molecule: Chloroform $CHCl_3$ **No. 140**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH stretch	3034 B	3034.1 M	3030 W	
	ν_2	CCl_3 sym. stretch	680 B	680 S	672 S	
	ν_3	CCl_3 sym. deform	363 C	366 (liquid)	363 M	
e	ν_4	CH bend	1220 B	1219.7 VS	1217 W	
	ν_5	CCl_3 deg. stretch	774 B	774.0 VS	760 W	
	ν_6	CCl_3 deg. deform	261 B	260 (liquid)	261 W	

References

[1] R. J. R. Nielsen and N. E. Ward, J. Chem. Phys. **10**, 81 (1941).
[2] IR;R. J. R. Madigan and F. F. Cleveland, J. Chem. Phys. **19**, 119 (1951).
[3] IR. T. G. Gibian and D. S. Mckinney, J. Am. Chem. Soc. **73**, 1431 (1951).
[4] IR. A. E. Stanevich and N. G. Yaroslavskii, Opt. Spectry. **9**, 31 (1961).
[5] IR. I. Suzuki, unpublished work.

Molecule: Chloroform-d_1 $CDCl_3$ **No. 141**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD stretch	2266 B	2266 W	2255 (2) p	
	ν_2	CCl_3 sym. stretch	659 B	658.5 S	649 (7) p	
	ν_3	CCl_3 sym. deform	369 C	366 W (liquid)	369 (9) p	
e	ν_4	CD bend	914 B	913.9 VS	908 (1) dp	
	ν_5	CCl_3 deg. stretch	749 B	748.5 VS	649 (7) dp	
	ν_6	CCl_3 deg. deform	262 C	262 W (liquid)	262 (10) dp	

References

[1] R. J. P. Zietlow, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **18**, 1076 (1950).
[2] R.IR, V. R. Madigan, F. F. Cleveland, W. M. Boyer, and R. B. Bernstein, J. Chem. Phys. **18**, 1081 (1950).
[3] IR. R. B. Bernstein, A. G. Gordus, and F. F. Cleveland, J. Chem. Phys. **20**, 1979 (1952).
[4] IR. I. Suzuki, unpublished work.

Molecule: Bromoform $CHBr_3$ **No. 142**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3042 B	3042 M	3017 (1) p	
	ν_2	CBr_3 sym. stretch	541 B	541 M	540 (4) p	
	ν_3	CBr_3 sym. deform	222 C	.....	222 (10) p	
e	ν_4	CH bend	1149 B	1149 VS	1143 (2) dp	
	ν_5	CBr_3 deg. stretch	669 B	669 VS	655 (2) dp	
	ν_6	CBr_3 deg. deform	155 C	.....	155 (5) dp	

References

[1] IR.R A. G. Meister, S. E. Rosser, and F. F. Cleveland, J. Chem. Phys. **18**, 346 (1950).
[2] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47**, 202 (1951).
[3] IR. M. T. Forel, J. P. Leicknam, and M. L. Josien, J. Chim. Phys. **57**, 1103 (1960).
[4] IR. L. P. Lindsay and P. N. Schatz, Spectrochim. Acta **20**, 1421 (1964).

Molecule: Bromoform-d_1 $CDBr_3$ **No. 143**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CD stretch	2251 C	2251 M	2247 (4)	
	ν_2	CBr_3 sym. stretch	520 C	521 M	519.3 (7)	
	ν_3	CBr_3 sym. deform	222 C	.....	221.6 (10)	
e	ν_4	CD bend	850 D	858 VS 844 VS	856.5 (3) 840 (3)	FR ($\nu_3 + \nu_5$).
	ν_5	CBr_3 deg. stretch	632 C	632 VS	628.5 (5)	
	ν_6	CBr_3 deg. deform	153 C	.....	153.4 (8)	

References

[1] R. A. G. Meister, S. E. Rosser, and F. F. Cleveland, J. Chem. Phys. **18**, 346 (1950).
[2] IR. M. T. Forel, J. P. Leicknam, and M. L. Josien, J. Chim. Phys. **57**, 1103 (1960).
[3] IR. I. Suzuki, unpublished work.

Molecule: Acetylene C_2H_2 **No. 144**
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	CH stretch.....	3374 C	ia	3373.7 S	
	ν_2	CC stretch.....	1974 C	ia	1973.8 VS	
σ_u^+	ν_3	CH stretch.....	3289 B	3294.9 3281.9	.....	FR ($\nu_2 + \nu_4 + \nu_5$).
π_g	ν_4	CCH deform.....	612 C	ia	[1] 611.8 VW	
π_u	ν_5	CCH deform.....	730 A	730.3		

References

[1] R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945) and references cited there.
[2] IR. H. C. Allen, Jr., E. D. Tidwell, and E. K. Plyler, J. Res. NBS **57**, 213 (1956).
[3] IR. T. A. Wiggins, E. K. Plyler, and E. D. Tidwell, J. Opt. Soc. Am. **51**, 1219 (1961).
[4] IR. E. K. Plyler, E. D. Tidwell, and T. A. Wiggins, J. Opt. Soc. Am. **53**, 589 (1963).
[5] IR. W. J. Lafferty and R. J. Thibault, J. Mol. Spectry. **14**, 79 (1964).
[6] IR. J. F. Scott and K. N. Rao, J. Mol. Spectry. **16**, 15–23 (1965).
[7] IR. J. F. Scott and K. N. Rao, J. Mol. Spectry. **18**, 152 (1965).
[8] IR. J. F. Scott and K. N. Rao, J. Mol. Spectry. **18**, 451 (1965).
[9] IR. J. F. Scott and K. N. Rao, J. Mol. Spectry. **20**, 438 (1966).

Molecule: Acetylene-d_1 C_2HD **No. 145**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CH stretch.....	3336 A	3335.6		
	ν_2	CC stretch.....	1854 A	1853.8		
	ν_3	CD stretch.....	2584 A	2583.6		
π	ν_4	CH bend.....	519 C	.....	518.8 S	
	ν_5	CD bend.....	683 C	.....	683 S	

References

[1] R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR. J. Overend and H. W. Thompson, Proc. Roy. Soc. (London) **A234**, 306 (1955).
[3] IR. H. C. Allen, Jr., E. D. Tidwell, and E. K. Plyler, J. Am. Chem. Soc. **78**, 3034 (1956).
[4] IR. W. J. Lafferty, E. K. Plyler, and E. D. Tidwell, J. Chem. Phys. **37**, 1981 (1962).

Molecule: Acetylene-d_2 C_2D_2 **No. 146**
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	CD stretch.....	2701 C	ia	2700.5 S	
	ν_2	CC stretch.....	1762 C	ia	1762.4 S	
σ_u^+	ν_3	CD stretch.....	2439 A	2439.3		
π_g	ν_4	CCD deform.....	505 C	ia	.....	OC $(\nu_4+\nu_5)$.[1]
π_u	ν_5	CCD deform.....	537 A	536.9		

References

[1] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR. J. Overend and H. A. Thompson, Proc. Roy. Soc. (London) **A232**, 291 (1955).
[3] IR. H. C. Allen, Jr., L. R. Blaine, and E. K. Plyler, J. Res. NBS **56**, 279 (1956).
[4] IR. E. D. Tidwell and E. K. Plyler, J. Opt. Soc. Am. **52**, 656 (1962).

Molecule: Fluoroacetylene HCCF **No. 147**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CH stretch.....	3355 B	3355 VS		
	ν_2	C ≡ C stretch.....	2255 B	2255 VS		
	ν_3	CF stretch.....	1055 B	1055 VS		
π	ν_4	CCH deg. deform.....	578 B	578 VS		
	ν_5	CCF deg. deform.....	367 B	367 M		

References

[1] IR. W. J. Middleton and W. H. Sharkey, J. Am. Chem. Soc. **81**, 803 (1959).
[2] IR. W. S. Richardson and J. H. Goldstein, J. Chem. Phys. **18**, 1314 (1960).
[3] IR. G. R. Hund and M. K. Wilson, J. Chem. Phys. **34**, 1301 (1961).

Molecule: Chloroacetylene HCCCl **No. 148**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CH stretch.....	3340 B	3340 VS		
	ν_2	C ≡ C stretch.....	2110 B	2110 VS		
	ν_3	CCl stretch.....	756 B	756 VS		
π	ν_4	CCH deg. deform.....	604 B	604 S		
	ν_5	CCCl deg. deform.....	326 B	326 W		

References

[1] IR. W. J. Middleton and W. H. Sharkey, J. Am. Chem. Soc. **81,** 803 (1959).
[2] IR. W. S. Richardson and J. H. Goldstein, J. Chem. Phys. **18,** 1314 (1960).
[3] IR. G. R. Hund and M. K. Wilson, J. Chem. Phys. **34,** 1301 (1961).

Molecule: Bromoacetylene HCCBr **No. 149**
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
σ^+	ν_1	CH stretch.....	3325 B	3325 VS		
	ν_2	C ≡ C stretch.....	2085 B	2085 VS		
	ν_3	CBr stretch.....	618 C	618 VS	.....	SF (ν_4).
π	ν_4	CCH deg. deform.....	618 C	618 VS	.....	SF (ν_3).
	ν_5	CCBr deg. deform.....	295 B	295 W		

References

[1] IR. W. J. Middleton and W. H. Sharkey, J. Am. Chem. Soc. **81,** 803 (1959).
[2] IR. W. S. Richardson and J. H. Goldstein, J. Chem. Phys. **18,** 1314 (1960).
[3] IR. G. R. Hund and M. K. Wilson, J. Chem. Phys. **34,** 1301 (1961).

Molecule: Methyl isocyanide CH_3NC **No. 150**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 sym. stretch.....	2966 B	2965.8 M	2951 S	
	ν_2	N = C stretch.....	2166 B	2166.0 M	2161 S	
	ν_3	CH_3 sym. deform.....	1429 D	1429	1414 M	
	ν_4	CC stretch.....	945 B	944.6 M	928 M	
e	ν_5	CH_3 deg. stretch.....	3014 B	3014.3 S	3002 W	
	ν_6	CH_3 deg. deform.....	1467 B	1466.9 S	1456 W	
	ν_7	CH_3 rock.....	1129 B	1129.3 S		
	ν_8	CNC bend.....	263 C	263 W	290 S	

References

[1] R.IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR. H. W. Thompson and R. L. Williams, Trans. Faraday Soc. **48,** 502 (1952).
[3] IR. R. L. Williams, J. Chem. Phys. **25,** 656 (1956).
[4] Th. W. H. Fletcher and C. S. Shoup, Proceedings of the International Symposium on Molecular Structure and Spectroscopy, C204 (Tokyo, 1962).
[5] Th. J. L. Duncan, Spectrochim. Acta **20,** 1197 (1964).

Molecule: Methyl isocyanide-d_3 CD_3NC **No. 151**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 sym. stretch.....	2251 B	2250.6 W		
	ν_2	N = C stretch.....	2165 B	2165.0 W		
	ν_3	CD_3 sym. deform.....	1117 B	1117.4 W		
	ν_4	CC stretch.....	877 B	876.7 M		
e	ν_5	CD_3 deg. stretch.....	2263 B	2262.9 S		
	ν_6	CD_3 deg. deform.....	1058 B	1058.2 S		
	ν_7	CD_3 rock.....	900 B	900.1 S		
	ν_8	CNC bend.....	249 C	248.9	.....	OC ($\nu_2 + \nu_8$).

References

[1] IR. J. G. Mottern and W. H. Fletcher, Spectrochim. Acta **18,** 995 (1962).
[2] IR.Th. W. H. Fletcher and C. S. Shoup, Proceedings of the International Symposium on Molecular Structure and Spectroscopy, C204 (Tokyo, 1962).
[3] Th. J. L. Duncan, Spectrochim. Acta **20,** 1197 (1964).

Molecule: Acetic acid CH_3COOH (gas) **No. 152**
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}	
a'	ν_1	OH stretch	3583 B	3583 M		
	ν_2	CH_3 deg. stretch	3051 B	3051 VW		
	ν_3	CH_3 sym. stretch	2944 B	2944 VW		
	ν_4	C=O stretch	1788 B	1788 VS		
	ν_5	CH_3 deg. deform	1430 C	1430 sh	.....	SF (ν_{14}).
	ν_6	CH_3 sym. deform. (ν_7, ν_8)	1382 B	1382 M		
	ν_7	OH bend. (ν_8, ν_6)	1264 B	1264 M		
	ν_8	CO stretch. (ν_7, ν_6)	1182 B	1182 S		
	ν_9	CH_3 rock	989 B	989 M		
	ν_{10}	CC stretch	847 B	847 W		
	ν_{11}	OCO deform	657 B	657 S		
	ν_{12}	COO deform	581 B	581 M		
a''	ν_{13}	CH_3 deg. stretch	2996 B	2996 VW		
	ν_{14}	CH_3 deg. deform	1430 C	1430 sh	.....	SF (ν_5).
	ν_{15}	CH_3 rock	1048 B	1048 W		
	ν_{16}	COO deform	642 B	642 S		
	ν_{17}	CO torsion	534 B	534 M		
	ν_{18}	CC torsion	93 D	.....	.....	CF.[3]

References

[1] IR. W. Weltner, J. Am. Chem. Soc. **77**, 3941 (1955).
[2] IR. J. K. Wilmshurst, J. Chem. Phys. **25**, 1171 (1956).
[3] IR. M. Haurie and A. Novak, J. Chim. Phys. **62**, 137 (1965).
[4] IR. M. Ohara and T. Shimanouchi, unpublished work.

Molecule: **Acetic acid-d_1** **CH_3COOD (gas)** **No. 153**
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}	
a'	ν_1	CH_3 deg. stretch	3039 B	3039 VW		
	ν_2	CH_3 sym. stretch	2952 B	2952 VW		
	ν_3	OD stretch	2642 B	2642 M		
	ν_4	C=O stretch	1775 B	1775 VS		
	ν_5	CH_3 deg. deform	1440 C	1440 sh	.....	SF (ν_{14}).
	ν_6	CH_3 sym. deform. (ν_8)	1383 B	1383 S		
	ν_7	CO stretch. (ν_6)	1270 B	1270 S		
	ν_8	CH_3 rock	990 D	990 sh		
	ν_9	OD bend	955 B	955 S		
	ν_{10}	CC stretch	840 B	840 W		
	ν_{11}	OCO deform	609 B	609 M		
	ν_{12}	COO deform	543 B	543 M		
a''	ν_{13}	CH_3 deg. stretch	2997 D	2997 VW		
	ν_{14}	CH_3 deg. deform	1440 C	1440 sh	.....	SF (ν_{15}).
	ν_{15}	CH_3 rock	1052 B	1052 W		
	ν_{16}	COO deform	603 B	603 M		
	ν_{17}	CO torsion	415 B	415 M		
	ν_{18}	CC torsion	93 D	.....	.....	CF.[3]

References

[1] IR. W. Weltner, J. Am. Chem. Soc. **77**, 3941 (1955).
[2] IR. J. K. Wilmshurst, J. Chem. Phys. **25**, 1171 (1956).
[3] IR. M. Haurie and A. Novak, J. Chim. Phys. **62**, 137 (1965).
[4] IR. M. Ohara and T. Shimanouchi, unpublished work.

Molecule: ***cis*-1,2-Difluoroethylene** **CHFCHF** **No. 154**
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH stretch	3135 D	3135 W		SF (ν_8).
	ν_2	C=C stretch	1715 C	1715 S		
	ν_3	CH bend	1266 C	1266 S		
	ν_4	CF stretch	1014 C	1014 S		
	ν_5	CF bend	255 D	255 W		
a_2	ν_6	CH bend	866 E	ia	.....	CF.[a]
	ν_7	CC torsion	482 E	ia	.....	CF.[b]
b_1	ν_8	CH stretch	3135 D	3135 W	.....	SF (ν_1).
	ν_9	CH bend	1376 C	1376 S		
	ν_{10}	CF stretch	1127 C	1127 VS		
	ν_{11}	CF bend	768 B	768 S		
b_2	ν_{12}	CH bend	756 B	756 S		

[a] Calculated from a product rule.

[b] Calculated by assuming $\frac{\nu_7(cis)}{\nu_7(trans)} = \frac{\nu_{12}(cis\text{-}d_1)}{\nu_{12}(trans\text{-}d_1)} = \frac{\nu_7(cis\text{-}d_2)}{\nu_7(trans\text{-}d_2)}$.

References

[1] IR. R. N. Haszeldine and B. R. Steele, J. Chem. Soc. (London) **1957**, 2800 (1957).
[2] IR. H. G. Viehe, Chem. Ber. **93**, 1697 (1960).
[3] IR. N. C. Craig and E. A. Entemann, J. Chem. Phys. **36**, 243 (1962).

Molecule: ***cis*-1,2-Difluoroethylene-d_1** **CHFCDF** **No. 155**
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
		s		cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH stretch	3125 D	3125 W		
	ν_2	CD stretch	2364 D	2364 W		
	ν_3	C=C stretch	1692 C	1692 S		
	ν_4	CH bend	1330 C	1330 S		
	ν_5	CF stretch	1167 C	1167 VS		
	ν_6	CF stretch	1033 C	1033 VS		
	ν_7	CD bend	889 B	889 M		
	ν_8	CF bend	757 B	757 S		
	ν_9	CF bend	255 D	255 W		
a''	ν_{10}	CH bend	801 B	801 M		
	ν_{11}	CD bend	633 B	633 M		
	ν_{12}	CC torsion	469 B	469 W		

Reference

[1] IR. N. C. Craig and E. A. Entemann, J. Chem. Phys. **36**, 243 (1962).

Molecule: ***cis*-1,2-Difluoroethylene-d_2** **CDFCDF** **No. 156**
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch	2320 D	2320 W	.....	SF (ν_8).
	ν_2	C=C stretch	1675 C	1675 S		
	ν_3	CF stretch	1054 C	1054 S		
	ν_4	CD bend	847 B	847 M		
	ν_5	CF bend	255 D	255 W		
a_2	ν_6	CD bend	656 E	ia	.....	CF.[a]
	ν_7	CC torsion	459 E	ia	.....	CF.[b]
b_1	ν_8	CD stretch	2320 D	2320 W	.....	SF (ν_1).
	ν_9	CF stretch	1225 C	1225 VS		
	ν_{10}	CD bend	937 B	937 M		
	ν_{11}	CF bend	748 B	748 S		
b_2	ν_{12}	CD bend	597 B	597 M		

[a] Calculated from a product rule.

[b] Calculated by assuming $\frac{\nu_7(cis)}{\nu_7(trans)} = \frac{\nu_{12}(cis\text{-}d_1)}{\nu_{12}(trans\text{-}d_1)} = \frac{\nu_7(cis\text{-}d_2)}{\nu_7(trans\text{-}d_2)}$.

Reference

[1] IR. N. C. Craig and E. A. Entemann, J. Chem. Phys. **36**, 243 (1962).

Molecule: 1,1-Dichloroethylene CH_2CCl_2 **No. 157**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 sym. stretch.....	3035 D	3035 W (CCl_4 soln.)	3035 VS, p	
	ν_2	CC stretch.....	1627 C	1627 VS	1616 VS, p	
	ν_3	CH_2 scissors.....	1400 C	1400 M	1391 M, p	
	ν_4	CCl_2 sym. stretch.....	603 C	603 VS	601 VS, p	
	ν_5	CCl_2 scissors.....	299 C	299 W	299 S, p	
a_2	ν_6	CC torsion.....	686 D	ia	686 M, dp	
b_1	ν_7	CH_2 anti. stretch.....	3130 D	3130 W (CCl_4 soln.)	3130 S, dp	
	ν_8	CH_2 rock.....	1095 C	1095 VS	1088 VW	
	ν_9	CCl_2 anti. stretch.....	800 B	800 VS	788 M, dp	
	ν_{10}	CCl_2 rock.....	372 C	372 M	375 S, dp	
b_2	ν_{11}	CH_2 wag.....	875 B	875 S	874 W	
	ν_{12}	CCl_2 wag.....	460 B	460 S	458 M, dp	

References

[1] IR. H. W. Thompson and P. Torkington, Proc. Roy. Soc. (London) **A184**, 21 (1945).
[2] R. P. Joyner and G. Glocker, J. Chem. Phys. **20**, 302 (1952).
[3] IR.Th. T. Shimanouchi and S. Shimizu, unpublished work.

Molecule: 1,1-Dichloroethylene-d_1 $CHDCCl_2$ **No. 158**
Symmetry C_s Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH stretch.....	3082 D	3082 W (CCl_4 soln.)		
	ν_2	CD stretch.....	2288 D	2288 W (CCl_4 soln.)		
	ν_3	CC stretch.....	1585 C	1585 S		
	ν_4	CHD scissors.....	1280 C	1280 M		
	ν_5	CHD rock.....	999 C	999 VS		
	ν_6	CCl_2 anti. stretch.....	741 C	741 S		
	ν_7	CCl_2 sym. stretch.....	590 C	590 VS		
	ν_8	CCl_2 rock.....	348 C	348 W		
	ν_9	CCl_2 scissors.....	306 E	.....	.....	CF.[1]
a''	ν_{10}	CHD wag.....	819 B	819 S		
	ν_{11}	CC torsion.....	555 C	555 W		
	ν_{12}	CCl_2 wag.....	444 B	444 M		

Reference

[1] IR.Th. T. Shimanouchi and S. Shimizu, unpublished work.

Molecule: 1,1-Dichloroethylene-d_2 CD_2CCl_2 **No. 159**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_2 sym. stretch	2262 D	2262 W (CCl_4 soln.)		
	ν_2	CC stretch	1565 C	1565 VS		
	ν_3	CD_2 scissors	1039 E			CF.[1]
	ν_4	CCl_2 sym. stretch	580 C	580 VS		
	ν_5	CCl_2 scissors	305 E			CF.[1]
a_2	ν_6	CC torsion	488 E	ia		CF.[1]
b_1	ν_7	CD_2 anti. stretch	2380 D	2380 W (CCl_4 soln.)		
	ν_8	CD_2 rock	988 C	998 VS		
	ν_9	CCl_2 anti. stretch	697 C	697 S		SF(ν_{11}).
	ν_{10}	CCl_2 rock	327 C	327 M		
b_2	ν_{11}	CD_2 wag	697 C	697 S		SF(ν_9).
	ν_{12}	CCl_2 wag	439 B	439 S		

Reference

[1] IR.Th. T. Shimanouchi and S. Shimizu, unpublished work.

Molecule: Methylacetylene CH_3CCH **No. 160**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3334 C	3334	3305 M	
	ν_2	CH_3 sym. stretch	2918 E	2941 M, 2881	2941 VS, p	FR ($\nu_2 + 2\nu_7$).[2]
	ν_3	C ≡ C stretch	2142 A	2142.2 M	2142 VS, p	
	ν_4	CH_3 sym. deform	1382 D		1382 S, dp	
	ν_5	C = C stretch	931 C	930.7 W	930 S, p (gas)	
e	ν_6	CH_3 deg. stretch	3008 A	3008.3 M	2971 M	
	ν_7	CH_3 deg. deform	1452 B	1452 M	1448 M	
	ν_8	CH_3 rock	1053 A	1052.5 W	1035 VW	
	ν_9	CCH deform	633 C	633 S	643 S, dp	
	ν_{10}	CCC deform	328 C	328 W	336 VS, dp	

References

[1] R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR. D. R. J. Boyd and H. W. Thompson, Trans. Faraday Soc. **48**, 493 (1952).
[3] Th. J. L. Duncan, Spectrochim. Acta **20**, 1197 (1964).

Molecule: Methylacetylene-1-d_1 CH_3CCD **No. 161**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch	2617 B	2616.8 S		
	ν_2	CH_3 sym. stretch	2920 E	2941.0 M 2881.0 M	.....	FR($\nu_2 + 2\nu_7$).[1]
	ν_3	C ≡ C stretch	[2] 2008			
	ν_4	CH_3 sym. deform	1378 E	1378 W	.....	OV(ν_7).
	ν_5	C − C stretch	886 E	.....	.....	CF.[1]
e	ν_6	CH_3 deg. stretch	3009 B	3008.9 M		
	ν_7	CH_3 deg. deform	1454 B	1453.5 M		
	ν_8	CH_3 rock	1051 B	1051.0 W		
	ν_9	CCD deform	498 B	497.5 S		
	ν_{10}	CCC deform	314 B	314 M		

References

[1] IR. R. J. Grisemthwaite and H. W. Thompson, Trans. Faraday Soc. **50**, 212 (1954).
[2] Th. J. L. Duncan, Spectrochim. Acta **20**, 1197 (1964).

Molecule: Methylacetylene-3,3,3-d_3 CD_3CCH **No. 162**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH stretch	3336 A	3335.8 S		
	ν_2	CD_3 sym. stretch	2110 E	2121.0 M 2077.0 M	.....	FR($\nu_2 + 2\nu_7$).[2]
	ν_3	C ≡ C stretch	2142 A	2142.0 M		
	ν_4	CD_3 sym. deform	1115 B	1115 M		
	ν_5	C − C stretch	830 B	830 W	.....	OV.[1]
e	ν_6	CD_3 deg. stretch	2235 A	2234.9 M		
	ν_7	CD_3 deg. deform	1048 A	1048.2 M		
	ν_8	CD_3 rock	835 A	835.4 W	.....	OV.[1]
	ν_9	CCH deform	633 B	633 S		
	ν_{10}	CCC deform	305 B	304.5 M		

References

[1] IR. M. T. Christensen and H. W. Thompson, Trans. Faraday Soc. **52**, 1439 (1956).
[2] Th. J. L. Duncan, Spectrochim. Acta **20**, 1197 (1964).

Molecule: Methylacetylene-d_4 CD_3CCD **No. 163**
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch.....	2616 A	2616.3 VS		
	ν_2	CD_3 sym. stretch.....	2110 E	2121 M 2077 M	.....	FR ($\nu_2 + 2\nu_7$).[2]
	ν_3	C ≡ C stretch.....	2008 A	2008.4 W		
	ν_4	CD_3 sym. deform.....	1110 A	1110.1 M		
	ν_5	C − C stretch.....	810 E	.....	.....	CF.[1]
e	ν_6	CD_3 deg. stretch.....	2235 A	2234.8 M		
	ν_7	CD_3 deg. deform.....	1048 A	1048.2 M		
	ν_8	CD_3 rock.....	834 A	834.4 W		
	ν_9	CCD deform.....	492 B	492 VS		
	ν_{10}	CCC deform.....	294 B	294 M		

References

[1] IR. H. T. Christensen and H. W. Thompson, Trans. Faraday Soc. **52**, 1439 (1956).
[2] Th. J. L. Duncan, Spectrochim. Acta **20**, 1197 (1964).

Molecule: Propane-2,2-d_2 $CH_3CD_2CH_3$ **No. 164**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 deg. stretch	2974 C	2974 S	.....	SF (ν_{15}).
	ν_2	CH_3 sym. stretch	2883 C	2883 S	.....	SF (ν_{16}).
	ν_3	CD_2 sym. stretch	2141 C	2141 S		
	ν_4	CH_3 deg. deform	1459 C	1459 S		
	ν_5	CH_3 sym. deform	1392 B	1392 M		
	ν_6	CH_3 rock	1166 E	1166 W		
	ν_7	CD_2 scissors	1064 B	1064 M		
	ν_8	CC stretch	843 C	843 W		
	ν_9	CCC deform	362 E	.....	.....	CF.[5]
a_2	ν_{10}	CH_3 deg. stretch	2956 E	ia	.....	OC ($\nu_{18}+\nu_{10}$).[4]
	ν_{11}	CH_3 deg. deform	1453 E	ia	.....	CF.[5]
	ν_{12}	CH_3 rock	1083 E	ia	.....	OC ($\nu_{16}+\nu_{12}$).[4]
	ν_{13}	CD_2 twist	777 E	ia	.....	CF.[5]
	ν_{14}	CH_3 torsion	208 E	ia	.....	OC ($\nu_{18}-\nu_{14}$).[4]
b_1	ν_{15}	CH_3 deg. stretch	2974 C	2974 S	.....	SF (ν_1).
	ν_{16}	CH_3 sym. stretch	2883 C	2883 S	.....	SF (ν_2).
	ν_{17}	CH_3 deg. deform	1461 C	1461 S		
	ν_{18}	CH_3 sym. deform	1374 B	1374 S		
	ν_{19}	CC stretch. + CD_2 wag.	1203 B	1203 S		
	ν_{20}	CH_3 rock. + CC stretch.	964 C	964 W		
	ν_{21}	CD_2 wag. + CH_3 rock	829 C	829 W		
b_2	ν_{22}	CH_3 deg. stretch	2963 C	2963 S		
	ν_{23}	CD_2 anti. stretch	2182 C	2182 S		
	ν_{24}	CH_3 deg. deform	1476 C	1476 S		
	ν_{25}	CH_3 rock	1146 C	1146 W		
	ν_{26}	CD_2 rock	622 B	622 S		
	ν_{27}	CH_3 torsion	222 E	.....	.....	CF.[5]

References

[1] IR. H. L. McMurry and V. Thronton, J. Chem. Phys. **18**, 1515 (1950).
[2] IR. H. L. McMurry and V. Thornton, J. Chem. Phys. **19**, 1014 (1951).
[3] Th. H. Takahashi, Nippon Kagaku Zasshi **82**, 1304 (1961).
[4] IR. J. N. Gayles, Jr. and W. T. King, Spectrochim. Acta **21**, 543 (1965).
[5] Th. T. Shimanouchi and T. Ueda, unpublished work.

Molecule: Propane-1,1,1-d_3 $CH_3CH_2CD_3$ **No. 165**
Symmetry C_s Symmetry number $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_3 deg. stretch	2966 C	2966 S		SF (ν_{17}).
	ν_2	CH_3 sym. stretch	2900 E			CF.[2]
	ν_3	CH_2 sym. stretch	2882 C	2882 M		
	ν_4	CD_3 deg. stretch	2225 C	2225 S		
	ν_5	CD_3 sym. stretch	2075 C	2075 S		
	ν_6	CH_2 scissors	1461 D	1461 S		SF (ν_{20}).
	ν_7	CH_3 deg. deform	1460 D	1460 S		
	ν_8	CH_3 sym. deform	1383 C	1383 S		
	ν_9	CH_2 wag	1332 C	1332 S		
	ν_{10}	CC stretch. + CD_3 sym. deform.	1132 C	1132 M		
	ν_{11}	CH_3 rock + CC stretch.	1101 C	1101 S		
	ν_{12}	CD_3 deg. deform	1062 C	1062 S		
	ν_{13}	CD_3 sym. deform. + CC stretch.	999 D	999 W		
	ν_{14}	CC stretch. + CD_3 rock	846 C	846 M		
	ν_{15}	CD_3 rock. + CC stretch	750 B	750 M		
	ν_{16}	CCC deform	339 E			CF.[2]
a''	ν_{17}	CH_3 deg. stretch	2966 C	2966 S		SF (ν_1).
	ν_{18}	CD_2 anti. stretch	2935 C	2935 S		
	ν_{19}	CD_3 deg. stretch	2214 S	2214 S		
	ν_{20}	CH_3 deg. deform	1461 D	1461 S		SF (ν_6).
	ν_{21}	CH_2 twist	1285 D	1285 W		
	ν_{22}	CH_3 rock	1129 C	1129 M		
	ν_{23}	CD_3 deg. deform	1063 C	1063 S		
	ν_{24}	CH_2 rock	831 B	831 M		
	ν_{25}	CD_3 rock	660 D	660 W		
	ν_{26}	CH_3 torsion	216 E			CF.[2]
	ν_{27}	CD_3 torsion	161 E			CF.[2]

References

[1] IR. J. N. Gayles, Jr. and W. T. King, Spectrochim, Acta **21**, 543 (1965).
[2] Th. T. Shimanouchi and T. Ueda, unpublished work.

Molecule: Propane-1,1,1,3,3,3-d_6 $CD_3CH_2CD_3$ **No. 166**
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}	
a_1	ν_1	CH_2 sym. stretch	2883 B	2883 S		
	ν_2	CD_3 deg. stretch	2225 C	2225 S		SF (ν_{23}).
	ν_3	CD_3 sym. stretch	2091 C	2091 S		SF (ν_{16}).
	ν_4	CH_2 scissors	1467 B	1467 S		
	ν_5	CD_3 sym. deform	1098 E			CF.[4]
	ν_6	CD_3 deg. deform	1066 C	1066 VS		SF (ν_{19}).
	ν_7	CD_3 rock	962 E	962 VW		
	ν_8	CC stretch	744 D	744 W		
	ν_9	CCC deform	315 E			CF.[4]
a_2	ν_{10}	CD_3 deg. stretch	2222 E	ia		CF.[4]
	ν_{11}	CH_2 twist	1257 E	ia		CF.[4]
	ν_{12}	CD_3 deg. deform	1052 E	ia		CF.[4]
	ν_{13}	CD_3 rock	700 E	ia		CF.[4]
	ν_{14}	CD_3 torsion	142 E	ia		OC ($\nu_{14}+\nu_{21}$, $\nu_{21}-2\nu_{14}$).[3]
b_1	ν_{15}	CD_3 deg. stretch	2227 C	2227 S		
	ν_{16}	CD_3 sym. stretch	2091 C	2091 S		SF (ν_3).
	ν_{17}	CH_2 wag	1331 B	1331 M		
	ν_{18}	CC stretch	1131 A	1131 S		
	ν_{19}	CD_3 deg. deform	1066 C	1066 VS		SF (ν_6).
	ν_{20}	CD_3 sym. deform	920 E	920		
	ν_{21}	CD_3 rock	725 B	725 S		
b_2	ν_{22}	CH_2 anti. stretch	2929 B	2929 VS		
	ν_{23}	CD_3 deg. stretch	2225 C	2225 S		SF (ν_2).
	ν_{24}	CD_3 deg. deform	1087 C	1087 S		
	ν_{25}	CH_2 rock	1032 E			CF.[4]
	ν_{26}	CD_3 rock	640 C	640 S		
	ν_{27}	CD_3 torsion	173 E			OC ($\nu_{21}+\nu_{27}-\nu_{14}$).[3]

References

[1] IR. H. L. McMurry and V. Thornton, J. Chem. Phys. **19**, 1014 (1951).
[2] Th. H. Takahashi, Nippon Kagaku Zasshi **82**, 1304 (1961).
[3] IR. J. N. Gayles, Jr. and W. T. King, Spectrochim. Acta **21**, 543 (1965).
[4] Th. T. Shimanouchi and T. Ueda, unpublished work.

Molecule: Propane-d_8 $CD_3CD_2CD_3$ **No. 167**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 deg. stretch	2225 C	2225 VS		
	ν_2	CD_3 sym. stretch	2122 C	2122 S		
	ν_3	CD_2 sym. stretch	2081 C	2081 S		SF (ν_{16}).
	ν_4	CD_3 sym. deform	1086 D	1086 S		SF (ν_{18}).
	ν_5	CD_2 scissors	1064 D	1064 VS		SF (ν_6, ν_{24}).
	ν_6	CD_3 deg. deform	1064 D	1064 VS		SF (ν_5, ν_{24}).
	ν_7	CD_3 rock	959 C	959 W		
	ν_8	CC stretch	712 C	712 M		
	ν_9	CCC deform	313 E			CF.[4]
a_2	ν_{10}	CD_3 deg. stretch	2221 E	ia		CF.[4]
	ν_{11}	CD_3 deg. deform	1064 E	ia		CF.[4]
	ν_{12}	CD_2 twist	945 E	ia		CF.[4]
	ν_{13}	CD_3 rock	659 E	ia		CF.[4]
	ν_{14}	CD_3 torsion	143 E	ia		OC ($\nu_{14}+\nu_{22}$, $\nu_{14}+\nu_{24}$).[3]
b_1	ν_{15}	CD_3 deg. stretch	2224 C	2224 VS		SF (ν_{22}).
	ν_{16}	CD_3 sym. stretch	2081 C	2081 S		SF (ν_3).
	ν_{17}	CC stretch	1203 B	1203 S		
	ν_{18}	CD_3 deg. deform	1086 D	1086 S		SF (ν_4).
	ν_{19}	CD_3 sym. deform	1068 D	1068 VS		
	ν_{20}	CD_2 wag	862 D	862 VW		
	ν_{21}	CD_3 rock	688 C	688 M		
b_2	ν_{22}	CD_3 deg. stretch	2224 C	2224 VS		SF (ν_{15}).
	ν_{23}	CD_2 anti. stretch	2181 E			CF.[4]
	ν_{24}	CD_3 deg. deform	1064 D	1064 VS		SF (ν_5, ν_6).
	ν_{25}	CD_3 rock	949 D	949 W		
	ν_{26}	CD_2 rock	544 D	544 W		
	ν_{27}	CD_3 torsion	172 E			OC ($\nu_{25}+\nu_{27}-\nu_{21}$).[3]

References

[1] IR. H. L. McMurry and V. Thronton, J. Chem. Phys. **19**, 1014 (1951).
[2] Th. H. Takahashi, Nippon Kagaku Zasshi **82**, 1304 (1961).
[3] IR. J. N. Gayles, Jr. and W. T. King, Spectrochim. Acta **21**, 543 (1965).
[4] Th. T. Shimanouchi and T. Ueda, unpublished work.

Molecule: Acetone CH_3COCH_3 **No. 168**
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 deg. stretch	3018 B	3017.6 S	3005.5 S	SF (ν_{13}).
	ν_2	CH_3 sym. stretch	2944 B	2944 S	2922 VS, p	SF (ν_{14}).
	ν_3	CO stretch	1731 B	1731 VS	1710.5 S, p	
	ν_4	CH_3 deg. deform	1435 C	1435 S	1430 S	
	ν_5	CH_3 sym. deform	1364 C	1363.5 VS	1356 W	SF (ν_{16}).
	ν_6	CH_3 rock	1066 C	.....	1066 M, p	
	ν_7	CC stretch	787 C	785 W	786.5 VS, p	
	ν_8	CCC deform	385 B	385 W	393 W	
a_2	ν_9	CH_3 deg. stretch	2963 E	ia	.....	CF.[4]
	ν_{10}	CH_3 deg. deform	1426 E	ia	.....	CF.[4]
	ν_{11}	CH_3 rock	877 E	ia	.....	CF.[4]
	ν_{12}	CH_3 torsion	105 E	ia	.....	CF.[4]
b_1	ν_{13}	CH_3 deg. stretch	3018 B	3017.6 S	3005.5 S	SF (ν_1).
	ν_{14}	CH_3 sym. stretch	2944 B	2944 S	2922 VS	SF (ν_2).
	ν_{15}	CH_3 deg. deform	1410 C	1410 S		
	ν_{16}	CH_3 sym. deform	1364 C	1363.5 VS	.....	SF (ν_5).
	ν_{17}	CC stretch	1216 B	1215.5 VS	1221 M	
	ν_{18}	CH_3 rock	891 C	891 M	902.5 W	
	ν_{19}	CO bend	527 B	527 S	530 M	
b_2	ν_{20}	CH_3 deg. stretch	2970 A	2970.1 S	2967 S	
	ν_{21}	CH_3 deg. deform	1454 C	1454 S		
	ν_{22}	CH_3 rock	1091 B	1090.5 M		
	ν_{23}	CO bend	484 B	484 W	493 W	
	ν_{24}	CH_3 torsion	109 D	109		

References

[1] IR. W. G. Fateley and F. A. Miller, Spectrochim. Acta **18**, 977 (1962).
[2] IR.R.Th. P. Cossee and J. H. Schachtschneider, J. Chem. Phys. **44**, 97 (1966).
[3] IR.R.Th. G. Dellepiane and J. Overend, Spectrochim. Acta **22**, 593 (1966).
[4] IR.R.Th. M. Mikami and T. Shimanouchi, unpublished work.

Molecule: Acetone-α,α,α-d_3 CH_3COCD_3 **No. 169**
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 deg. stretch	3018 A	3017.5 S	3004.5 S	
	ν_2	CH_3 sym. stretch	2922 C		2922 VS, p	
	ν_3	CD_3 deg. stretch	2265 B	2265 M	2256 S	
	ν_4	CD_3 sym. stretch	2115 E	2150 VVW 2095 VW	2141.5 VS, p 2095.5 S, p	FR ($2\nu_9$).
	ν_5	CO stretch	1734 B	1734 VS	1706 S	
	ν_6	CH_3 deg. deform	1430 B	1430 S	1427.5 M	
	ν_7	CH_3 sym. deform	1365 B	1365 VS	1361.5 VW	
	ν_8	CC stretch	1225 B	1224.5 VS	1227.5 W	
	ν_9	CD_3 sym. deform	1058 C		1057.5 W	
	ν_{10}	CH_3 rock. (ν_{11})	1021 C	1021 S	1029.5 W	
	ν_{11}	CD_3 deg. deform. (ν_{10})	1003 C		1003 M, p	
	ν_{12}	CD_3 rock	781 C	781 W	780.5 VW	
	ν_{13}	CC stretch	740 C	735 W	740 VS, p	
	ν_{14}	CO bend	500 B	500 S	504 M	
	ν_{15}	CCC deform	350 B	350 W	356.5 W	
a''	ν_{16}	CH_3 deg. stretch	2968 B	2968 S	2965 S	
	ν_{17}	CD_3 deg. stretch	2222 B	2222 M	2217.5 S	
	ν_{18}	CH_3 deg. deform	1447 C	1447 S		
	ν_{19}	CH_3 rock. (ν_{21})	1035 C	1035 S		
	ν_{20}	CD_3 deg. deform	1002 C	1002 S		
	ν_{21}	CD_3 rock. (ν_{19})	764 D	764 M (solid)		
	ν_{22}	CO bend	435 B	435 W	444 W	
	ν_{23}	CH_3 torsion	106 E			CF.[2]
	ν_{24}	CD_3 torsion	78 E			CF.[2]

References

[1] IR.R.Th. G. Dellepiane and J. Overend, Spectrochim. Acta **22**, 593 (1966).
[2] IR.R.Th. M. Mikami and T. Shimanouchi, unpublished work.

Molecule: **Acetone-d_6** **CD_3COCD_3** **No. 170**
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_3 deg. stretch	2264 B	2263.5 S	.....	SF (ν_{13}).
	ν_2	CD_3 sym. stretch	2123 B	2123 W	2108.5 VS, p	SF (ν_{14}).
	ν_3	CO stretch	1732 B	1732 VS	1700.5 S	
	ν_4	CD_3 sym. deform	1080 C	1080 M	1088 M, p	
	ν_5	CD_3 deg. deform	1035 D	1035 M		
	ν_6	CD_3 rock	887 B	887 W	889 M, p	
	ν_7	CC stretch	689 C	689 W	695.5 VS, p	
	ν_8	CCC deform	320 B	320 W	331 VW	
a_2	ν_9	CD_3 deg. stretch	2219 E	ia	.....	CF.[3]
	ν_{10}	CD_3 deg. deform	1021 E	ia	.....	CF.[3]
	ν_{11}	CD_3 rock	669 E	ia	.....	CF.[3]
	ν_{12}	CD_3 torsion	75 E	ia	.....	CF.[3]
b_1	ν_{13}	CD_3 deg. stretch	2264 B	2263.5 S	2256.5 S	SF (ν_1).
	ν_{14}	CD_3 sym. stretch	2123 B	2123 W	.....	SF (ν_2).
	ν_{15}	CC stretch	1246 B	1246 VS	1248.5 VW	
	ν_{16}	CD_3 sym. deform	1036 D	.....	1036 M	
	ν_{17}	CD_3 deg. deform	1004 C	1004 M	1006 sh	
	ν_{18}	CD_3 rock	726 D	726 W (solid)		
	ν_{19}	CO bend	475 B	475 S	478 W	
b_2	ν_{20}	CD_3 deg. stretch	2227 A	2226.5 S	2222 S	
	ν_{21}	CD_3 deg. deform	1050 C	1050 S		
	ν_{22}	CD_3 rock	960 C	960 M		
	ν_{23}	CO bend	404 B	404 W	410 VW	
	ν_{24}	CD_3 torsion	79 E	.....	.....	CF.[3]

References

[1] IR.R.Th. P. Cossee and J. H. Schachtschneider, J. Chem. Phys. **44**, 97 (1966).
[2] IR.R.Th. G. Dellepiane and J. Overend, Spectrochim. Acta **22**, 593 (1966).
[3] IR.R.Th. M. Mikami and T. Shimanouchi, unpublished work.

Molecule: 1,3-Butadiene $CH_2CHCHCH_2$ **No. 171**
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Solid)	
a_g	ν_1	CH_2 anti. stretch	3087 D	ia	3087 M	
	ν_2	CH stretch	3003 D	ia	3003 M	
	ν_3	CH_2 sym. stretch	2992 D	ia	2992 S	
	ν_4	C=C stretch	1630 D	ia	1630 VS	
	ν_5	CH_2 scissors	1438 D	ia	1438 S	
	ν_6	CH bend	1280 D	ia	1280 S	
	ν_7	C−C stretch	1196 D	ia	1196 S	
	ν_8	CH_2 rock	894 D	ia	894 W	
	ν_9	CCC deform	512 D	ia	512 S	
a_u	ν_{10}	CH bend	1013 B	1013.4 VS	ia	
	ν_{11}	CH_2 wag	908 B	907.8 VS	ia	
	ν_{12}	CH_2 twist	522 B	522.2 M	ia	
	ν_{13}	C−C torsion	162 B	162.3 VW	ia	
b_g	ν_{14}	CH bend	976 D	ia	976 W	
	ν_{15}	CH_2 wag	912 D	ia	912 S	
	ν_{16}	CH_2 twist	770 D	ia	770 VW	
b_u	ν_{17}	CH_2 anti. stretch	3101 B	3100.6 S	ia	
	ν_{18}	CH stretch	3055 B	3054.9 S	ia	
	ν_{19}	CH_2 sym. stretch	2984 B	2984.3 S	ia	
	ν_{20}	C=C stretch	1596 B	1596.0 S	ia	
	ν_{21}	CH_2 scissors	1381 B	1380.7 W	ia	
	ν_{22}	CH bend	1294 B	1294.3 W	ia	
	ν_{23}	CH_2 rock	990 B	989.7 M	ia	
	ν_{24}	CCC deform	301 B	300.6 VW	ia	

References

[1] R. C. M. Richards and J. R. Nielsen, J. Opt. Soc. Am. **40**, 438 (1950).
[2] Th. L. M. Sverdlov and N. V. Tarasova, Opt. Spectry. **9**, 159 (1960).
[3] IR. R. K. Harris, Spectrochim. Acta **20**, 1129 (1964).
[4] IR.R.Th. K. Abe and T. Shimanouchi, to be published.

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