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ALEXANDER B. TROWBRIDGE, *Secretary*,
NATIONAL BUREAU OF STANDARDS · A. V. ASTIN, *Director*

Tables of Molecular Vibrational Frequencies Part 2.

Takehiko Shimanouchi

University of Tokyo

Tokyo, Japan

NSRDS-NBS 11

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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. The 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 classifications 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 eleventh publication in a new NBS series known as the National Standard Reference Data Series.

A. V. Astin, *Director.*

Contents

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Tables of Molecular Vibrational Frequencies

Part 2.

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 I published as NSRDS–NBS–6, 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 I. The fundamental frequencies are obtained mainly from the infrared and Raman spectra. When these are not avialable, 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. These 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: Data, force constants, infrared spectra, modes of vibration, molecular vibrational frequencies, molecular spectra, Raman spectra.

1. 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. These data may also be useful to those who utilize infrared or Raman spectra as a technique in analytical chemistry.

This is the second 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 report, which has been published as NSRDS-NBS 6, contains data for 59 molecules. This second report contains another 54 molecules with the serial numbers 60 113. These molecules have been selected from compounds for which experimental data are available and normal coordinate treatments have been made in detail. General comments on the procedures by which the tables are prepared and on the explanations of notation and abbreviations are given in Part 1 (NSRDS-NBS 6). Only the important notation 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 me in the planning, the preparation, and the publication of the tables.

The author also acknowledges the assistance of his colleagues at the University of Tokyo: I. Nakagawa, A. Hirakawa, I. Suzuki, M. Tasumi, T. Fujiyama, I. Harada, M. Ishii, T. Ueda, H. Yoshioka, and K. Ishii.

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 38

Molecule: Diborane $^{10}B_2H_6$

Symmetry D_{2n} **Symmetry number $\sigma = 4$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared [6]	Raman [8]	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	BH_2 sym. stretch	2537 C	ia	2537 VS	
	ν_2	BH ring stretch	2110 C	ia	2110 S	
	ν_3	BH_2 scissors	1186 C	ia	1186 M	
	ν_4	Ring deform	816 C	ia	816 S [b] 820 (2) (liquid)	
a_u	ν_5	BH_2 twist	829 D	[a] 829 VW	ia	
b_{1g}	ν_6	BH ring stretch	1768 C	ia	1768 W	
	ν_7	BH_2 wag	1044 E	ia	.....	OC($\nu_5+\nu_7$) [6].
b_{1u}	ν_8	BH_2 anti. stretch	2625 C	2625 VS	ia	
	ν_9	BH_2 rock	955 E	.....	ia	CF [9].
	ν_{10}	Ring puckering	368 C	368 S	ia	
b_{2g}	ν_{11}	BH_2 anti. stretch	2640 E	ia	2640 W, b	
	ν_{12}	BH_2 rock	930 E	ia	.....	OC($\nu_{10}+\nu_{12}$) [6].
b_{2u}	ν_{13}	BH ring stretch	[b] 1920 E	1882 M (1992 W)	ia	
b_{2u}	ν_{14}	BH_2 wag	977 C	977 S	ia	
b_{3g}	ν_{15}	BH_2 twist	1012 E	ia	.....	CF.[c]
b_{3u}	ν_{16}	BH_2 sym. stretch	2528 C	2528 VS	ia	
	ν_{17}	BH ring stretch. and deform.	1606 C	1606 VVS	ia	
	ν_{18}	BH_2 scissors	1181 C	1181 VS	ia	

[a] Forbidden by the selection rule, observed very weakly, and also confirmed by a combination band.
[b] Corrected for a presumed shift due to Fermi resonance.
[c] Expected frequency from ν_{15} of $^{11}B_2H_6$.

References

[1] R. T. F. Anderson and A. B. Burg, J. Chem. Phys. **6,** 586 (1938).
[2] IR.R. F. Stitt, J. Chem. Phys. **9,** 780 (1941).
[3] Th. R. P. Bell and H. C. Longuet-Higgins, Proc. Roy. Soc. (London) **A183,** 357 (1945).
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[5] IR.R. A. N. Webb, J. T. Neu, and K. S. Pitzer, J. Chem. Phys. **17,** 1007 (1949).
[6] IR.R. R. C. Lord and E. Nielsen, J. Chem. Phys. **19,** 1 (1951).
[7] IR. W. J. Lehman, J. F. Ditter, and J. Shapiro, J. Chem. Phys. **29,** 1248 (1958).
[8] R. R. C. Taylor and A. R. Emergy, Spectrochim. Acta **10,** 419 (1958).
[9] Th. T. Ogawa and T. Miyazawa, Spectrochim. Acta **20,** 557 (1964).

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Symmetry D_{2h} **Symmetry number $\sigma = 4$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared [2]	Raman [2]	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	BD_2 sym. stretch	[a] 1860 E	ia	1880 VS, p 1833 S, p	FR($2\nu_3$).
	ν_2	BD ring stretch	1511 C	ia	1511 VS, p	
	ν_3	BD_2 scissors	929 C	ia	929 p	
	ν_4	Ring deform	726 C	ia	726 VS, p	
a_u	ν_5	BD_2 twist	592 D	[b] 592 VVW	ia	OC($\nu_5+\nu_7$).[b] OC($\nu_5+\nu_{15}$).
b_{1g}	ν_6	BD ring stretch	1273 C	ia	1273 (2) dp	
	ν_7	BD_2 wag	870 E	ia	.....	OC($\nu_5+\nu_7$).
b_{1u}	ν_8	BD_2 anti. stretch	1999 C	1999 VS	ia	
	ν_9	BD_2 rock	705 E	.....	ia	OC($\nu_9+\nu_{10}$).
	ν_{10}	Ring puckering	262 C	262M	ia	
b_{2g}	ν_{11}	BD_2 anti. stretch	[a] 1980 E	ia	1975 (9) dp (2000 (5)) dp	FR($\nu_6+\nu_{15}$).
	ν_{12}	BD_2 rock	740 E	ia	.....	OC($\nu_{10}+\nu_{12}$).
b_{2u}	ν_{13}	BD ring stretch	[a] 1465 E	1491 M 1459 MS	ia	FR($\nu_5+\nu_7$).
b_{2u}	ν_{14}	BD_2 wag	728 C	728 S	ia	
b_{3g}	ν_{15}	BD_2 twist	730 C	ia	730 (4) dp	
b_{3u}	ν_{16}	BD_2 sym. stretch	1845 C	1857 VS (1799 S)	ia	FR($\nu_3+\nu_{18}$).
	ν_{17}	BD ring stretch. and deform.	1205 C	1205 VVS	ia	
	ν_{18}	BD_2 scissors	881 C	881 VS	ia	

[a] Corrected for a presumed shift due to Fermi resonance.
[b] Forbidden, by the selection rule, observed very weakly, and also confirmed by a combination band.

References

[1] IR. A. N. Webb, J. T. Neu, and K. S. Pitzer, J. Chem. Phys. **17**, 1007 (1949).
[2] IR. R. R. C. Lord and E. Nielsen, J. Chem. Phys. **19**, 1 (1951).
[3] R. R. C. Taylor and A. R. Emergy, Spectrochim. Acta **10**, 419 (1958).
[4] Th. T. Ogawa and T. Miyazawa, Spectrochim. Acta **20**, 557 (1964).

Symmetry D_{2h} **Symmetry number $\sigma = 4$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared [6]	Raman [6],	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	BH_2 sym. stretch.....	2524 C	ia	2524 (10) p	
	ν_2	BH ring stretch.....	2104C	ia	2104 (10) p	
	ν_3	BH_2 scissors.....	1180 C	ia	1180 (7)	
	ν_4	Ring deform.....	794 C	ia	794 (10) p	
a_u	ν_5	BH_2 twist.....	829 D	[a] 829 VW	ia	OC($\nu_5+\nu_7$).[a] OC($\nu_5+\nu_9$).
b_{1g}	ν_6	BH ring stretch.....	[b] 1768 E	ia	1788 (1) dp 1747 (1) dp	FR($\nu_5+\nu_9$).
	ν_7	BH_2 wag.....	1035 E	ia	.....	OC($\nu_5+\nu_7$).
b_{1u}	ν_8	BH_2 anti. stretch.....	2612 C	2612 VS	ia	
	ν_9	BH_2 rock.....	950 E	.....	ia	OC($\nu_5+\nu_9$). OC($\nu_9+\nu_{10}$).
	ν_{10}	Ring puckering.....	368 C	368 S	ia	
b_{2g}	ν_{11}	BH_2 anti. stretch.....	2591 C	ia	2591 (9) dp	
	ν_{12}	BH_2 rock.....	920 E	ia	.....	OC($\nu_{10}+\nu_{12}$).
b_{2u}	ν_{13}	BH ring stretch.....	[b] 1915 E	1887 M (1999 W)	ia	
	ν_{14}	BH_2 wag.....	973 C	973 S	ia	
b_{3g}	ν_{15}	BH_2 twist.....	1012 C	ia	1012 (5) dp	
b_{3u}	ν_{16}	BH_2 sym. stretch.....	2525 C	2525 VS	ia	
	ν_{17}	BH ring stretch. and deform.	1602 C	1602 VVS	ia	
	ν_{18}	BH_2 scissors.....	1177 C	1177 VS	ia	

[a] Forbidden by the selection rule, observed very weakly, and also confirmed by a combination band.
[b] Corrected for a presumed shift due to Fermi resonance.

References

[1] R. T. F. Anderson and A. B. Burg, J. Chem. Phys. **6**, 586 (1938).
[2] IR. R. F. Stitt, J. Chem. Phys. **9**, 780 (1941).
[3] Th. R. P. Bell and H. C. Longuet-Higgins, Proc. Roy. Soc. (London) **A183**, 357 (1945).
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[5] IR. R. A. N. Webb, J. T. Neu, and K. S. Pitzer, J. Chem. Phys. **17**, 1007 (1949).
[6] IR. R. R. C. Lord and E. Nielsen, J. Chem. Phys. **19**, 1 (1951).
[7] IR. W. J. Lehman, J. F. Ditter, and J. Shapiro, J. Chem. Phys. **29**, 1248 (1958).
[8] R. R. C. Taylor and A. R. Emergy, Spectrochim. Acta **10**, 419 (1958).
[9] Th. T. Ogawa and T. Miyazawa, Spectrochim. Acta **20**, 557 (1964).

Molecule: Silicon tetrabromide $SiBr_4$ No. 63

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	$SiBr_4$ sym. stretch.....	249 C	ia	249 (4) p	
e	ν_2	$SiBr_4$ deg. deform.....	90 C	ia	90 (3)	
f_2	ν_3	$SiBr_4$ deg. stretch.....	487 C	.....	487 (1)	
	ν_4	$SiBr_4$ deg. deform.....	137 C	.....	137 (3)	

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[2] G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
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Molecule: Silicon tetrachloride $SiCl_4$ No. 64

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	$SiCl_4$ sym. stretch	424 C	ia	424 (5) p	
e	ν_2	$SiCl_4$ deg. deform.....	150 C	ia	150 (4)	
f_2	ν_3	$SiCl_4$ deg. stretch.....	621 C	621 VS	610 (2b)	
	ν_4	$SiCl_4$ deg. deform.....	221 C	.....	221 (4)	

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[1] G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] R. M. L. Delwaulle, J. Phys. Chem. **56,** 355 (1952).
[3] R. IR. A. L. Smith, J. Chem. Phys. **21,** 1997 (1953).
[4] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London) **A240,** 499 (1957).
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Molecule: Silicon tetrafluoride SiF_4 No. 65

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	SiF_4 sym. stretch	801 C	ia	800 S	
e	ν_2	SiF_4 deg. deform	264 C	ia	268 W	
f_2	ν_3	SiF_4 deg. stretch	1032 B	[a] 1031.8 S	1010 W	
	ν_4	SiF_4 deg. deform	389 B	[a] 389.35 S	390 W	

[a] $^{28}Si^{23}F_4$.

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[2] IR. J. Heicklen and V. Knight, Spectrochim. Acta **20,** 295 (1964).
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Molecule: Silane SiH_4 No. 66

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}	
a_1	ν_1	SiH_4 sym. stretch	2187 B	ia	2187.0 S	
e	ν_2	SiH_4 deg. deform	975 C	[a] 974.6	978 W	
f_2	ν_3	SiH_4 deg. stretch	2191 A	2190.6		
	ν_4	SiH_4 deg. deform	914 B	914.2		

[a] Coriolis interaction between ν_2 and ν_4.

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Molecule: Silane-d_2 SiH_2D_2 No. 67

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	SiH_2 sym. stretch	2189 C	2189 S		
	ν_2	SiD_2 sym. stretch	1587 C	1587 S		
	ν_3	SiH_2 scissors	944 B	944 W		
	ν_4	SiD_2 scissors	683 B	682.5 M		
a_2	ν_5	SiH_2 twist	844 E	ia	.....	CF [1].
b_1	ν_6	SiH_2 anti. stretch	2183 C	2183 S		
	ν_7	SiH_2 rock	743 B	743 S		
b_2	ν_8	SiD_2 anti. stretch	1601 C	1601 S		
	ν_9	SiH_2 wag	862 B	862 M		

Reference

[1] IR.Th. J. H. Meal and M. K. Wilson, J. Chem. Phys. **24**, 385 (1956).

Molecule: Silane-d_3 $SiHD_3$ No. 68

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	SiH stretch	2182 C	2182 M		
	ν_2	SiD_3 sym. stretch	1573 C	1573 S		
	ν_3	SiD_3 sym. deform	683 C	683 S	.....	SF(ν_6).
e	ν_4	SiD_3 deg. stretch	1598 C	1598 S		
	ν_5	SiH bend	851 B	851 S		
	ν_6	SiD_3 deg. deform	683 C	683 S	.....	SF(ν_3).

References

[1] IR. J. H. Meal and W. K. Wilson, J. Chem. Phys. **24**, 385 (1956).
[2] IR. I. W. Levin and W. T. King, J. Chem. Phys. **37**, 1375 (1962).

Molecule: Silane-d_4 SiD_4 No. 69

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}	
a_1	ν_1	SiD_4 sym. stretch.....	1558 E	.....	.....	CF [4].
e	ν_2	SiD_4 deg. deform.....	700 E	.....	.....	CF [4].
f_2	ν_3	SiD_4 deg. stretch.....	1597 B	1597 S		
	ν_4	SiD_4 deg. deform.....	681 C	681 S		

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Molecule: Silicon tetriodide SiI_4 No. 70

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}	
a_1	ν_1	SiI_4 sym. stretch.....	168 C	ia	168 S, p	
e	ν_2	SiI_4 deg. deform.....	63 C	ia	63 M, dp	
f_2	ν_3	SiI_4 deg. stretch.....	405 C	.....	405 W, dp	
	ν_4	SiI_4 deg. deform.....	94 C	.....	94 S, dp	

Reference

[1] R. M. L. Delwaulle, J. Phys. Chem. **56,** 355 (1952).

Molecule: Germane GeH_4 No. 71

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}	
a_1	ν_1	GeH_4 sym. stretch.....	2106 B	ia	2106 S, p	
e	ν_2	GeH_4 deg. deform.....	931 D	[a] 930.9	920 W	
f_2	ν_3	GeH_4 deg. stretch.....	2114 B	2113.6	2106 W (liquid)	
	ν_4	GeH_4 deg. deform.....	819 B	819.3	816 W (liquid)	

[a] Coriolis interaction between ν_2 and ν_4.

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[3] G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[4] IR.R. L. P. Lindeman and M. K. Wilson, Z. Physik. Chem. (Frankfurt) **9,** 29 (1956).
[5] IR. A. A. Chalmers and D. C. McKean, Spectrochim. Acta **21,** 1941 (1965).

Molecule: Germane-d_1 GeH_3D No. 72

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	GeH_3 sym. stretch	2106 C	.....	2106	
	ν_2	GeD stretch.....	1520 B	1520.4 M		
	ν_3	GeH_3 sym. deform.....	820 C	820 S		
e	ν_4	GeH_3 deg. stretch.....	2112 B	2112 S		
	ν_5	GeH_3 deg. deform.....	901 C	901 W		
	ν_6	GeH_3 rock.....	706 C	706 S		

References

[1] IR. L. P. Lindeman and M. K. Wilson, J. Chem. Phys. **22,** 1723 (1954).
[2] IR.R. L. P. Lindeman and M. K. Wilson, Z. Physik. Chem. (Frankfurt) **9,** 29 (1956).

Molecule: Germane-d_2 GeH_2D_2 No. 73

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	GeH_2 sym. stretch.....	2112 C	2112		
	ν_2	GeD_2 sym. stretch.....	1512 C	1512		
	ν_3	GeH_2 scissors.....	881 B	881		
	ν_4	GeD_2 scissors.....	620 C	620		
a_2	ν_5	GeH_2 twist.....	807 E	807		
b_1	ν_6	GeH_2 anti. stretch.....	2112 C	2112		
	ν_7	GeH_2 rock.....	657 C	657		
b_2	ν_8	GeD_2 anti. stretch.....	1522 C	1522		
	ν_9	GeH_2 wag.....	770 C	770		

Reference

[1] IR. L. P. Lindeman and M. K. Wilson, Z. Physik. Chem. (Frankfurt) **9**, 29 (1956).

Molecule: Germane-d_3 $GeHD_3$ No. 74

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	GeH stretch.....	2112 B	2112.4		
	ν_2	GeD_3 sym. stretch.....	1504 B	.....	1504	
	ν_3	GeD_3 sym. deform.....	593 C	595		
e	ν_4	GeD_3 deg. stretch.....	1522 C	1522		
	ν_5	GeH bend.....	792 B	792.3		
	ν_6	GeD_3 deg. deform.....	625 C	625		

References

[1] IR. L. P. Lindeman and M. K. Wilson, J. Chem. Phys. **22**, 1723 (1954).
[2] IR.R. L. P. Lindeman and M. K. Wilson, Z. Physik. Chem. (Frankfurt) **9**, 29 (1956).

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Molecule: Germane-d_4 GeD_4 No. 75

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}	
a_1	ν_1	GeD_4 sym. stretch.....	1504 C	ia	1504	
e	ν_2	GeD_4 deg. deform.....	665 D	[a] 665 W		
f_2	ν_3	GeD_4 deg. stretch.....	1522 B	1522.2 S		
	ν_4	GeD_4 deg. deform.....	596 C	596 S		

[a] Coriolis interaction between ν_2 and ν_4.

Reference

[1] IR.R. L. P. Lindeman and M. K. Wilson, Z. Physik. Chem. (Frankfurt) **9**, 29 (1956).

Molecule: Nitrogen trifluoride NF_3 No. 76

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	NF_3 sym. stretch.....	1032 C	1032 S	1050	
	ν_2	NF_3 sym. deform.....	647 C	647 W	667	
e	ν_3	NF_3 deg. stretch.....	905 C	905 S	905	
	ν_4	NF_3 deg. deform.....	493 C	493 W	515	

References

[1] IR. C. R. Bailey, S. C. Carson, and J. W. Thompson, J. Chem. Phys. **5**, 274 (1937).
[2] IR. M. K. Wilson and S. R. Polo, J. Chem. Phys. **20**, 1716 (1952).
[3] IR.R. E. L. Pace and L. Pierce, J. Chem. Phys. **23**, 1248 (1955).
[4] IR. P. N. Schatz and I. W. Levin, J. Chem. Phys. **29**, 475 (1958).
[5] Th. P. N. Schatz, J. Chem. Phys. **29**, 481 (1958).

Molecule: Phosphorus trichloride PCl_3 No. 77

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	PCl_3 sym. stretch.....	504 C	504	510 (10) p	
	ν_2	PCl_3 sym. deform.....	252 C	252	257 (6) p	
e	ν_3	PCl_3 deg. stretch.....	482 C	482	480 (3) dp	
	ν_4	PCl_3 deg. deform.....	198 C	198	190 (10) dp	

References

[1] R. K. W. F. Kohlrausch, Der Smekal-Raman Effekt, Ergänzungsband, 1931–1937, J. Springer, Berlin, 1938.
[2] IR. P. W. Davais and R. A. Oetzen, J. Mol. Spectry. **2**, 253 (1958).
[3] IR. V. Lorenzelli, Compt. Rend. **252**, 3219 (1961).
[4] Th. A. M. Mirri, F. Scappini, and P. G. Favero, Spectrochim. Acta **21**, 965 (1965).

Molecule: Phosphorus trifluoride PF_3 No. 78

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	PF_3 sym. stretch.....	892 C	892 S	890 (10)	
	ν_2	PF_3 sym. deform.....	487 C	487 M	486 (3)	
e	ν_3	PF_3 deg. stretch.....	860 D	860 S	840 (10)	
	ν_4	PF_3 deg. deform.....	344 C	344 M		

References

[1] R. D. M. Yost and T. F. Anderson, J. Chem. Phys. **2**, 624 (1934).
[2] IR. H. S. Gutowsky and A. D. Liehr, J. Chem. Phys. **20**, 1652 (1952).
[3] IR. M. K. Wilson and S. R. Polo, J. Chem. Phys. **20**, 1716 (1952).
[4] Th. A. M. Mirri, F. Scappini, and P. G. Favero, Spectrochim. Acta **21**, 965 (1965).

Molecule: Tribromochloromethane CBr_3Cl No. 79

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (C_6H_6 CCl_4 soln.)	
a_1	ν_1	CCl stretch	745 C	747 S (CS_2 soln.)	748 (1)	
	ν_2	CBr_3 sym. stretch	327 C	329 W (C_7H_{14} soln.)	326 (10) p	
	ν_3	CBr_3 sym. deform	211 C	.....	210 (10) p	SF(ν_5).
e	ν_4	CBr_3 deg. stretch	677 C	675 S (CS_2 soln.)	677 (4) dp	
	ν_5	CCl bend. (ν_6)	211 E	.....	.....	SF(ν_3).
	ν_6	CBr_3 deg. deform. (ν_5)	140 C	.....	141 (7) dp	

References

[1] R.IR. A. G. Meister, S. E. Rosser, and F. F. Cleveland, J. Chem. Phys. **18,** 346 (1950).
[2] IR. E. K. Plyler, W. H. Smith, and N. Acquista, J. Res. NBS **44,** 503 (1950), RP2097.
[3] R. M. L. Delwaulle, M. B. Buisset, and M. Delhaye, J. Am. Chem. Soc. **74,** 5768 (1952).
[4] R. R. H. Krupp, S. M. Ferogle, and A. Weber, J. Chem. Phys. **24,** 355 (1956).

Molecule: Dibromodichloromethane CBr_2Cl_2 No. 80

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CCl_2 sym. stretch	733 C	733 VS	734 (1) p	
	ν_2	CBr_2 sym. stretch	380 C	377 W	380 (10) p	
	ν_3	CCl_2 scissors (ν_4)	242 C	.....	242 (6) p	
	ν_4	CBr_2 scissors (ν_3)	154 C	.....	154 (4) p	
a_2	ν_5	CCl_2 twist	175 C	.....	175 (2) dp	
b_1	ν_6	CBr_2 anti. stretch	683 C	683 VS	684 (3) dp	
	ν_7	CCl_2 wag	230 C	.....	229 (2) dp	
b_2	ν_8	CCl_2 anti. stretch	768 C	768 VS	771 (0) dp	
	ν_9	CCl_2 rock	262 C	.....	262 (1) dp	

References

[1] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47,** 202 (1951), RP 2245.
[2] R. IR. A. Davis, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **20,** 454 (1952).

Molecule: Bromotrichlromethane $CBrCl_3$ No. 81

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	CCl_3 sym. stretch	716 C	719 VS	716.3 (2) p	
	ν_2	CBr stretch	422 C	420 W	422.3 (10) p	
	ν_3	CCl_3 sym. deform	247 C	.....	247.3 (5) p	
e	ν_4	CCl_3 deg. stretch	775 C	773 VS	775.3 (1) dp	
	ν_5	CBr bend. (ν_6)	295 C	294 W	295.0 (3) dp	
	ν_6	CCl_3 deg. deform. (ν_5)	193 C	.....	193.3 (4) dp	

References

[1] R. J. P. Zietlow, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **18,** 1076 (1950).
[2] IR. J. R. Madigan and F. F. Cleveland, J. Chem. Phys. **19,** 119 (1951).
[3] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47,** 202 (1951), RP 2245.

Molecule: Dibromomethane CH_2Br_2 No. 82

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 sym. stretch	2989 C	2989 W	2988 M, p	
	ν_2	CH_2 scissors	1389 C	1389 M	1387 M, p	
	ν_3	CBr_2 sym. stretch	579 C	579 M	577 S, p	
	ν_4	CBr_2 scissors	174 C	.....	174 S, p	
a_2	ν_5	CH_2 twist	1096 C	[a] 1096 W	1089 W, dp	
b_1	ν_6	CH_2 anti. stretch	3065 C	3065 S	3061 W, dp	
	ν_7	CH_2 rock	813 C	813 M		
b_2	ν_8	CH_2 wag	1192 C	1192 S	1183 W, dp	
	ν_9	CBr_2 anti. stretch	638 C	638 S	639 W, dp	

[a] Apparently the C_{2v} selection rule does not hold in the liquid state.

References

[1] R. J. Wagner, Z. Physik. Chem. **B45,** 69 (1939).
[2] R. M. L. Delwaulle and F. Francois, J. Phys. Radium **7,** 15 (1946).
[3] IR. E. K. Plyler, W. A. Smith, and N. Acquista, J. Res. NBS **44,** 503 (1950) RP2097.
[4] IR. I. Suzuki, unpublished work.

Molecule: Dibromomethane-d_1 $CHDBr_2$ No. 83

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch	3030 C	3030 M		
	ν_2	CD stretch	2247 C	2247 W		
	ν_3	CH bend	1245 C	1245 W		
	ν_4	CD bend	702 C	702 M		
	ν_5	CBr_2 sym. stretch	563 C	563 M		
	ν_6	CBr_2 scissors	[a] 174 D	.....		
a''	ν_7	CH bend	1151 C	1151 S		
	ν_8	CD bend	836 C	836 M		
	ν_9	CBr_2 anti. stretch	622 C	622 W		

[a] Assumed to have the same value as the corresponding frequencies of CH_2Br_2 and CD_2Br_2.

References

[1] IR. I. Suzuki, unpublished work.

Molecule: Dibromomethane-d_2 CD_2Br_2 No. 84

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

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_2 sym. stretch	2192 C	2192 M	2195	
	ν_2	CD_2 scissors	1028 C	1028 W	1023	
	ν_3	CBr_2 sym. stretch	553 C	553 W	548	
	ν_4	CBr_2 scissors	174 C	.....	174	
a_2	ν_5	CD_2 twist	779 C	[a] 779 W		
b_1	ν_6	CD_2 anti. stretch	2313 C	2313 S	2235	
	ν_7	CD_2 rock	637 C	637 M		
b_2	ν_8	CD_2 wag	901 C	901 S		
	ν_9	CBr_2 anti. stretch	779 C	779 S		

[a] Apparently the C_{2v} selection rule does not hold in the liquid state.

References

[1] R. B. Trumpy, Z. Physik. **100,** 250 (1936).
[2] IR. I. Suzuki, unpublished work.

Molecule: Chlorobromomethane CH_2ClBr No. 85

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} (Liquid)	
a'	ν_1	CH_2 sym. stretch	3003 A	3003 S	2986 M, p	
	ν_2	CH_2 scissors	1482 D	[a] 1482 M	1410 M, p	
	ν_3	CH_2 wag	1231 B	1231 S	1229 W, p	
	ν_4	CCl stretch	744 B	744 VS	731 M, p	
	ν_5	CBr stretch	614 B	614 S	606 S, p	
	ν_6	CCl_2 scissors	229 C	.....	229 S, p	
a''	ν_7	CH_2 anti. stretch	3066 B	3066 W	3055 M, dp	
	ν_8	CH_2 twist	1128 C	1127 W (liquid)	1130 W	
	ν_9	CH_2 rock	852 B	852 W	848 W	

[a] The corresponding frequency in the liquid state is found at 1407 cm^{-1}. This band may be assigned to the overtone of the CCl stretching vibration.

References

[1] IR. E. K. Plyler, W. A. Smith, and W. Acquista, J. Res. NBS **44**, 503 (1950) RP2097.
[2] IR.R. A. Weber, A. G. Meister, and F. F. Cleveland, J. Chem. Phys. **21**, 930 (1953).
[3] IR.R. A. N. Tanaka, K. V. Narasimham, A. G. Meister, J. M. Dowling, F. F. Cleveland, S. Sundaram, E. A. Piotrowski, R. B. Bernstein, and S. I. Miller, J. Mol. Spectry. **15**, 319 (1965).
[4] IR. I. Suzuki, unpublished work.

Molecule: Chlorobromomethane-d_1 CHDClBr No. 86

Symmetry C_1 **Symmetry number $\sigma = 1$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a	ν_1	CH stretch	3031 C	[a] 3031 S	3024 S, p	
	ν_2	CD stretch	2252 C	[a] 2252 M	2245 S, p	
	ν_3	CH bend	1262 C	[a] 1262 S	1264 W, p	
	ν_4	CH bend	1188 B	1188 M	1179 W, p	
	ν_5	CD bend	868 B	868 M	867 W	
	ν_6	CD bend	746 B	746 W	743 VW	
	ν_7	CCl stretch	711 B	711 S	707 M, p	
	ν_8	CBr stretch	607 C	607 W	586 S, p	
	ν_9	CBrCl scissors	228 C	.....	228 S, p	

[a] The value in the liquid state.

References

[1] IR.R. A. N. Tanaka, K. V. Narasimham, A. G. Meister, F. F. Cleveland, S. Sundaram, F. A. Piotrowski, R. B. Bernstein, and S. I. Miller, J. Mol. Spectry. **15**, 319 (1965).

Molecule: Chlorobromomethane-d_2 CD_2ClBr No. 87

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} (Liquid)	
a'	ν_1	CD_2 sym. stretch	2208 B	2208 S	2196 M, p	
	ν_2	CD_2 scissors	1050 B	1050 W	1042 M, p	
	ν_3	CD_2 wag	936 B	936 S	922 W, p	
	ν_4	CCl stretch	717 B	717 S	702 M, p	
	ν_5	CBr stretch	582 B	582 S	574 S, p	
	ν_6	CBrCl scissors	226 C	.....	226 S, p	
a''	ν_7	CD_2 anti. stretch	2305 C	[a] 2305 S	2305 W, dp	
	ν_8	CD_2 twist	811 B	811 W	809 W, dp	
	ν_9	CD_2 rock	667 C	[a] 668 W	667 W, dp	

[a] The value in the liquid state.

References

[1] IR.R. A. N. Tanaka, K. V. Narasimham, A. G. Meister, J. M. Dowling, F. F. Cleveland, S. Sundaram, E. A. Piotrowski, R. B. Bernstein, and S. I. Miller, J. Mol. Spectry. **15**, 319 (1965).

Molecule: Formaldehyde H_2CO No. 88

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	2766 E	2766.4 S	2781.6 S	
	ν_2	CO stretch	1746 A	1746.1 VS	1742.3 W	
	ν_3	CH_2 scissors	1501 A	1500.6 S	1499.7 M	
b_1	ν_4	CH_2 anti. stretch	[a] 2843 E	2843.4 VS	2866 W	
	ν_5	CH_2 rock	1247 B	1247.4 S		
b_2	ν_6	CH_2 wag	1164 B	1163.5 S		

[a] The frequency has uncertainty due to the Fermi resonance between ν_4 and $\nu_2 + \nu_5$.

References

[1] R. D. W. Davidson, B. P. Stoicheff, and H. J. Bernstein, J. Chem. Phys. **22**, 289 (1954).
[2] IR. H. H. Blau, Jr. and H. H. Nielsen, J. Mol. Spectry. **1**, 124 (1957).
[3] IR. K. B. Harvey and J. F. Ogilvie, Can. J. Chem. **40**, 85 (1962).

Molecule: Formaldehyde-d_1 HDCO No. 89

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 stretch	[a] 2844 E	2844.1 S	2846.2 S	
	ν_2	CD stretch	[b] 2121 B	2120.7 S	2120.3 S	
	ν_3	CO stretch	1723 A	1723.4 VS	1723.2 VS	
	ν_4	CHD scissors	1400 A	1400.0 S	1397.4 M	
	ν_5	CHD rock	1041 E	1041 S		
a''	ν_6	CHD wag	1074 E	1074 S		

[a] The frequency has uncertainty due to the Fermi resonance between ν_1 and $\nu_3+\nu_5$.
[b] The frequency has uncertainty due to the Fermi resonances among ν_2, $2\nu_6$, and $2\nu_5$.

References

[1] IR.R. D. W. Davidson, B. P. Stoicheff, and H. J. Bernstein, J. Chem. Phys. **22**, 289 (1954).

Molecule: Formaldehyde-d_2 D_2CO No. 90

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	CD_2 sym. stretch	[a] 2056 E	2056.4 S		
	ν_2	CO stretch	1700 C	1700 VS		
	ν_3	CD_2 scissors	1106 C	1106.0 S		
b_1	ν_4	CD_2 anti. stretch	2160 E	2160.3 VS		
	ν_5	CD_2 rock	990 E	990.2 S		
b_2	ν_6	CD_2 wag	938 E	938 S		

[a] The frequency has uncertainty due to the Fermi resonance between ν_1 and $2\nu_3$.

References

[1] IR. E. S. Ebers and H. H. Nielsen, J. Chem. Phys. **6**, 311 (1938).

Molecule: Methylbromide CH_3Br No. 91

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.....	2935 E	2972 M 2861 M	2972 VS 2862 W	FR($2\nu_5$).
	ν_2	CH_3 sym. deform.....	1305 A	1305 S	1309 W	
	ν_3	CBr stretch.....	611 A	611 S	609 S	
e	ν_4	CH_3 deg. stretch.....	3057 A	3056.7 S	3068 VS	
	ν_5	CH_3 deg. deform.....	1443 A	1442.8 M	1456 M	
	ν_6	CH_3 rock.....	954 A	954.3 M	956 VW	

References

[1] R. H. L. Welsh, M. F. Crawford, T. R. Thomas, and G. R. Love, Can. J. Phys. **30,** 577 (1952).
[2] IR. H. B. Weissman, R. B. Bernstein, S. E. Rosser, A. G. Meister, and F. F. Cleveland, J. Chem. Phys. **23,** 544 (1955).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38,** 443 (1965).
[4] IR. Y. Morino, J. Nakamura, and S. Yamamoto, Bull. Chem. Soc. Japan **38,** 459 (1965).
[5] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22,** 647 (1966).

Molecule: Methylbromide-d_3 CD_3Br No. 92

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.....	2157 E	2157 VS	.....	FR($2\nu_5$).
	ν_2	CD_3 sym. deform.....	993 A	993.4 VS		
	ν_3	CBr stretch.....	578 A	577.9 S		
e	ν_4	CD_3 deg. stretch.....	2296 A	2296.3 M		
	ν_5	CD_3 deg. deform.....	1056 A	1055.6 S		
	ν_6	CD_3 rock.....	713 A	713.1 M		

References

[1] IR. H. B. Weissman, R. B. Bernstein, S. E. Roser, A. G. Meister, and F. F. Cleveland, J. Chem. Phys. **23,** 544 (1955).
[2] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38,** 443 (1965).
[3] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22,** 639 (1966).

Molecule: Methylchloride CH_3Cl No. 93

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.....	2937 E	2966.7 M 2878.7 M	2955 VS, p 2861 M	FR($2\nu_5$).
	ν_2	CH_3 sym. deform.....	1355 A	1354.9 S	1370 VW, p	
	ν_3	CCl stretch.....	732 A	732.1 S	709 VS, p	
e	ν_4	CH_3 deg. stretch.....	3042 A	3042.4 S	3036 M, dp	
	ν_5	CH_3 deg. deform.....	1452 A	1452.1 M	1446 W, dp	
	ν_6	CH_3 rock.....	1017 A	1017.3 M	1016 W, dp	

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[1] R. J. Wagner, Z. Physik. Chem. **B40**, 439 (1938).
[2] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) **A222**, 443 (1954).
[3] IR. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1964).
[4] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[5] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22**, 669 (1966).

Molecule: Methylchloride-d_3 CD_3Cl No. 94

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.....	2141 E	2161 S 2103 M	.....	FR($2\nu_5$).
	ν_2	CD_3 sym. deform.....	1029 A	1029 S		
	ν_3	CCl stretch.....	695 A	695 S		
e	ν_4	CD_3 deg. stretch.....	2283 A	2283.4 S		
	ν_5	CD_3 deg. deform.....	1060 A	1059.9 M		
	ν_6	CD_3 rock.....	768 A	767.7 M		

References

[1] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) **A222**, 443 (1954).
[2] IR. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1964).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[4] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22**, 659 (1966).

Molecule: Methylfluoride CH_3F No. 95

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_3 sym. stretch.....	2930 E	2964 VS 2863 S	.....	FR($2\nu_5$).
	ν_2	CH_3 sym. deform.....	1464 A	1464 S		
	ν_3	CF stretch.....	1049 A	1048.6 S		
e	ν_4	CH_3 deg. stretch.....	3006 A	3005.8 S		
	ν_5	CH_3 deg. deform.....	1467 A	1466.5 M		
	ν_6	CH_3 rock.....	1182 A	1182.4 M		

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[4] IR. W. L. Smith and I. M. Mills, J. Mol. Spectry. **11,** 11 (1963).
[5] IR. E. W. Jones, E. J. L. Popplewell, and H. W. Thompson, Proc. Roy. Soc. (London) **A290,** 490 (1966).

Molecule: Methylfluoride-d_3 CD_3F No. 96

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.....	2110 E	2090 2150	.....	FR($2\nu_5$).
	ν_2	CD_3 sym. deform.....	1136 A	1136		
	ν_3	CF stretch.....	991 A	991		
e	ν_4	CD_3 deg. stretch.....	2258 A	2258		
	ν_5	CD_3 deg. deform.....	1072 A	1072		
	ν_6	CD_3 rock.....	903 A	903		

References

[1] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) **A222,** 443 (1954).
[2] IR. W. F. Edgell and L. Parts, J. Am. Chem. Soc. **78,** 2358 (1956).
[3] IR. E. W. Jones, E. J. L. Popplewell, and H. W. Thompson, Proc. Roy. Soc. (London) **A290,** 490 (1966).

Molecule: Methyliodide CH_3I No. 97

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_3 sym. stretch.....	2933 E	2969.8 M 2861.0 M	.....	FR($2\nu_5$).
	ν_2	CH_3 sym. deform.....	1252 A	1251.5 S		
	ν_3	Cl stretch.....	533 A	532.8 S		
e	ν_4	CH_3 deg. stretch.....	3060 A	3060.3 S		
	ν_5	CH_3 deg. deform.....	1437 A	1437.4 M		
	ν_6	CH_3 rock.....	882 A	882.4 M		

References

[1] Th. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1957).
[2] IR. E. W. Jones and H. W. Thompson, Proc. Roy. Soc. (London) **A288**, 50 (1965).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[4] IR. Y. Morino, J. Nakamura, and S. Yamamoto, to be published.

Molecule: Methyliodide-d_3 CD_3I No. 98

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.....	2130 E	2155.1 2081.0	.....	FR($2\nu_5$).
	ν_2	CD_3 sym. deform.....	951 A	950.7		
	ν_3	CI stretch.....	501 A	501.4		
e	ν_4	CD_3 deg. stretch.....	2298 E	2298		
	ν_5	CD_3 deg. deform.....	1049 A	1049.3		
	ν_6	CD_3 rock.....	656 A	655.9		

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[1] Th. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1957).
[2] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Proc. Roy. Soc. (London) **A288**, 39 (1965).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[4] IR. Y. Morino, J. Nakamura, and S. Yamamoto, to be published.

Molecule: Methylamine CH_3NH_2 No. 99

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

Sym. class	No.	Approximate type of mode	Selected value of frequency		Infrared [2]	Raman [1]	Comments
					cm^{-1}	cm^{-1}	
a'	ν_1	NH_2 sym. stretch	3361	B	3361 W	3360 VS	
	ν_2	CH_3 deg. stretch	2961	B	2961 VS	2960 VS	
	ν_3	CH_3 sym. stretch	2820	B	2820 VS	2820 S	
	ν_4	NH_2 scissors	1623	B	1623 S		
	ν_5	CH_3 deg. deform	1473	B	1473 S	1460 M	
	ν_6	CH_3 sym. deform	1430	B	1430 M		
	ν_7	CH_3 rock	1130	A	1130 M		
	ν_8	CN stretch	1044.2	A	1044 S	1044 S	
	ν_9	NH_2 wag	780.1	A [3]	780 VS	781 W	
a''	ν_{10}	NH_2 anti. stretch	3427	C	3427 W	3470 W	
	ν_{11}	CH_3 deg. stretch	2985	C	2985 VS		
	ν_{12}	CH_3 deg. deform	1485	D	[a] 1485		
	ν_{13}	NH_2 twist	1419	D	.....	.....	CF.[b]
	ν_{14}	CH_3 rock	1195	D	[a] 1195		
	ν_{15}	CN torsion	268	A	200 ~ 330		

[a] Estimated from ^RQ branch frequency.

[b] Calculated from the force constants which correlate the frequencies of CH_3NH_2, CH_3ND_2, CD_3NH_2, and CD_3ND_2 including the ND_2 twisting frequency of CD_3NH_2.

References

[1] R. J. S. Kirby-Smith and L. G. Booner, J. Chem. Phys. **7**, 880 (1939).
[2] IR. A. P. Gray and R. C. Lord, J. Chem. Phys. **26**, 690 (1957).
[3] IR. M. Tsuboi, A. Y. Hirakawa, T. Ino, T. Sasaki, and K. Tamagake, J. Chem. Phys.
[4] IR. M. Tsuboi, A. Y. Hirakawa, and K. Tamagake, to be published.

Molecule: **Methylamine-d_2** **CH_3ND_2 (gas)** No. 100

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared [2]	Raman [1]	Comments
				cm^{-1}	cm^{-1}	
a'	ν_1	ND_2 sym. stretch	2479 B	2479 W	2450 S	
	ν_2	CH_3 deg. stretch	2961 B	2961 VS	2969 M	
	ν_3	CH_3 sym. stretch	2817 B	2817 S	2824 M	
	ν_4	ND_2 scissors (ν_7, ν_9)	1234 B	1234 S	1214 M	
	ν_5	CH_3 deg. deform	1468 B	1468 S	1473 M	
	ν_6	CH_2 sym. deform	1430 B	1430 M		
	ν_7	CH_3 rock. (ν_4)	1117 A	1117 S		
	ν_8	CN stretch. (ν_4)	997 A	997 S	995 S	
	ν_9	ND_2 wag	625.4 [3]	624 VS		
a''	ν_{10}	ND_2 anti. stretch	2556 B	2556 M	2527 M	
	ν_{11}	CH_3 deg. stretch	2985 C	2985 VS		
	ν_{12}	CH_3 deg. deform	1485 D	[a] 1485		
	ν_{13}	ND_2 twist. (ν_{14})	1058 D	.....	.....	CF.[b]
	ν_{14}	CH_3 rock. (ν_{13})	1187 C	1187 M		
	ν_{15}	CN torsion	228	180 ~ 280 S		

[a] Estimated from ^RQ branch frequency.

[b] Calculated from the force constants which correlate the frequencies of CH_3NH_2, CH_3ND_2, CD_3NH_2, and CD_3ND_2 including the ND_2 twisting frequency of CD_3NH_2.

References

[1] R. J. T. Edsall and H. Schinberg. J. Chem. Phys. **8**, 520 (1940).
[2] IR. A. P. Gray and R. C. Lord. J. Chem. Phys. **26**, 690 (1957).
[3] IR. M. Tsuboi. A. Y. Hirakawa. T. Sasaki. and K. Tamagake. to be published.
[4] IR. M. Tsuboi. A. Y. Hirakawa. and K. Tamagake. to be published.

Molecule: **Methylamine-d_3** **CD_3NH_2 (gas)** No. 101

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

Sym. class	No.	Approximate type of mode	Selected value of frequency		Infrared [1]	Raman	Comments
					cm^{-1}	cm^{-1}	
a'	ν_1	NH_2 sym. stretch	3361	B	3361 W		
	ν_2	CD_3 deg. stretch	2203	B	2203 VS		
	ν_3	CD_3 sym. stretch	2077	A	2077 VS		
	ν_4	NH_2 scissors (ν_9)	1624	B	1624 S		
	ν_5	CD_3 deg. deform	1065	D			CF.[a]
	ν_6	CD_3 sym. deform	1142	A	1142 S		
	ν_7	CD_3 rock. (ν_9)	913	A	913 S		
	ν_8	CN stretch. (ν_6)	973	B	973 M		
	ν_9	NH_2 wag. (ν_7)	740.4	A [2]	740 VS		
a''	ν_{10}	NH_2 anti. stretch	3427	C	3427 W		
	ν_{11}	CD_3 deg. stretch	2236	C	2236 VS		
	ν_{12}	CD_3 deg. deform	1077	C	1077 W		
	ν_{13}	NH_2 twist	1416	C	1416 W		
	ν_{14}	CD_3 rock	926	D			CF.[a]
	ν_{15}	CN torsion	247	D			CF.[a]

[a] Calculated from the force constants which correlate the frequencies of CH_3NH_2, CH_3ND_2, CD_3NH_2, and CD_3ND_2.

References

[1] IR. A. P. Gray and R. C. Lord, J. Chem. Phys. **26,** 690 (1957).
[2] IR. M. Tsuboi, A. Y. Hirakawa, and K. Tamagake, to be published.

Molecule: Methylamine-d_5 CD_3ND_2(Gas) No. 102

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared [1]	Raman	Comments
				cm^{-1}	cm^{-1}	
a'	ν_1	ND_2 sym. stretch	2477 B	2477 W		
	ν_2	CD_3 deg. stretch	2202 B	2202 VS		
	ν_3	CD_3 sym. stretch	2073 B	2073 VS		
	ν_4	ND_2 scissors (ν_7, ν_9)	1227 B	1227 S		
	ν_5	CD_3 deg. deform	1065 D			CF.[a]
	ν_6	CD_3 sym. deform	1123 B	1123 M		
	ν_7	CD_3 rock. (ν_8, ν_9)	880 B	880 M		
	ν_8	CN stretch (ν_6, ν_7)	942 A	942 S		
	ν_9	ND_2 wag	601 A	601 VS		
a''	ν_{10}	ND_2 anti. stretch	2556 C	2556 W		
	ν_{11}	CD_3 deg. stretch	2238 C	2238 VS		
	ν_{12}	CD_3 deg. deform	1077 C	1077 W		
	ν_{13}	ND_2 twist (ν_{14})	1072 D			CF.[a]
	ν_{14}	CD_3 rock	910 B	910 M		
	ν_{15}	CN torsion	201 D			CF.[a]

[a] Calculated from the force constants which correlate the frequencies of CH_3NH_2. CH_3ND_2. CD_3NH_2. and CD_3ND_2.

References

[1] IR. A. P. Gray and R. C. Lord. J. Chem. Phys. **26**, 690 (1957).

Molecule: Methylcyanide CH_3CN No. 103

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	2965 A	2965.3 M	2942 VS	
	ν_2	CN stretch	2267 A	2267.3 M	2249 S	
	ν_3	CH_3 sym. deform	1400 C	1400.0 S	1376 M	
	ν_4	CC stretch	920 A	919.9 S	918 S	
e	ν_5	CH_3 deg. stretch	3009 A	3009.0 S	2999 S	
	ν_6	CH_3 deg. deform	1454 A	1454.0 S	1440 M. b	
	ν_7	CH_3 rock	1041 A	1041.0 M	1124 VW	
	ν_8	CCN bend	361 A	361.0 S	380 S	

References

[1] R. A. Dadieu. Monatsh. **57**, 437 (1931).
[2] R. A. W. Reitz and R. Skrabel. Monatsh. **70**, 398 (1937).
[3] IR.R. P. Venkatesvarlu. J. Chem. Phys. **19**, 293 (1951).
[4] IR.R. H. W. Thompson and R. L. Williams. Trans Faraday Soc. **48**, 502 (1952).
[5] IR. F. W. Parker. A. H. Nielsen. and W. H. Fletcher. J. Mol. Spectry. **1**, 107 (1957).
[6] IR. I. Nakagawa and T. Shimanouchi. Spectrochim. Acta **18**, 513 (1962).

Molecule: Methylcyanide-d_3 CD_3CN No. 104

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.....	2107 A	2106.9		
	ν_2	CN stretch.....	2278 A	2277.5		
	ν_3	CD_3 sym. deform.....	1112 A	1112.2		
	ν_4	CC stretch.....	831 A	831.4		
e	ν_5	CD_3 deg. stretch.....	2258 A	2258.4		
	ν_6	CD_3 deg. deform.....	1046 A	1045.7		
	ν_7	CD_3 rock.....	847 A	846.6		
	ν_8	CCN bend.....	333 A	333.2		

References

[1] IR. Y. Morino and J. Nakamura, to be published.

Molecule: Ethylene oxide C_2H_4O No. 105

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} (Liquid)	
a_1	ν_1	CH_2 sym. stretch.....	3006 C	3006 S	3005 S, p	SF(ν_9).
	ν_2	CH_2 scissors.....	1498 B	1498 W	1490 W, p	
	ν_3	Ring stretch. (ring breath).....	1271 B	1271 S	1266 S, p	
	ν_4	CH_2 wag.....	1130 D	1118 W (CS_2 soln.)	1120 M, p	
	ν_5	Ring stretch+deform.....	877 B	877 VS	867 M, dp	
a_2	ν_6	CH_2 anti. stretch.....	3065 D	ia	3063 W, dp	SF(ν_{13}).
	ν_7	CH_2 twist.....	1300 E	ia		
	ν_8	CH_2 rock.....	860 E	ia		
b_1	ν_9	CH_2 sym. stretch.....	3006 C	3006 S	3005 S, p	SF(ν_1).
	ν_{10}	CH_2 scissors.....	1472 B	1472 W		
	ν_{11}	CH_2 wag.....	1151 D	1151 M	1150 W, dp	
	ν_{12}	Ring stretch+deform.....	890 E	.....	.....	CF [4].
b_2	ν_{13}	CH_2 anti. stretch.....	3065 B	3065 S	3063 W, dp	SF(ν_6).
	ν_{14}	CH_2 twist.....	1142 D	1142 M	1150 W, dp	
b_2	ν_{15}	CH_2 rock.....	822 B	822 M	807 M, dp	

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[3] R.IR. H. W. Thompson and W. T. Cave, Trans. Faraday Soc. **47**, 946 (1951).
[4] IR. R. C. Lord and B. Nolin, J. Chem. Phys. **24**, 656 (1956).
[5] R.IR. W. J. Potts, Spectrochim. Acta **21**, 511 (1965).

Molecule: **Ethylene oxide-d_4** C_2D_4O No. 106

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} (Liquid)	
a_1	ν_1	CD_2 sym. stretch.....	2204 C	.....	2204 S	
	ν_2	CD_2 scissors.....	1311 C	1311 M	1301 VS	
	ν_3	Ring stretch. (ring breath).....	1013 C	1014 W	1013 S	
	ν_4	CD_2 wag.....	970 C	970 VS	952 M	
	ν_5	Ring stretch. + deform.....	755 C	755 VS	755 M	
a_2	ν_6	CD_2 anti. stretch.....	2250 C	ia	2250 W	
	ν_7	CD_2 twist.....	1083 D	ia	1083 VW	
	ν_8	CD_2 rock.....	581 C	ia	581 W	
b_1	ν_9	CD_2 sym. stretch.....	2174 C	2174 VS	2157 M	
	ν_{10}	CD_2 scissors.....	1145 D	1145 VW		
	ν_{11}	CD_2 wag.....	952 D	.....	952 M	
	ν_{12}	Ring stretch. + deform.....	809 C	809 S	786 M	
b_2	ν_{13}	CD_2 anti. stretch.....	2317 C	2317 VS	2319 S	
	ν_{14}	CD_2 twist.....	896 C	896 S	896 W	
	ν_{15}	CD_2 rock.....	577 C	577 W		

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[1] IR. C. W. Arnold and F. A. Matsen, Bull. Am. Phys. Soc. **29**, 8 (1954).
[2] R.IR. R. C. Lord and B. Nolin, J. Chem. Phys. **24**, 656 (1956).

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} (Liquid)	
a'	ν_1	NH stretch	3338 B	3338 W	3302 M, p	
	ν_2	CH_2 anti. stretch	3079 D	3079 S	3059 M, dp	SF(ν_{11}).
	ν_3	CH_2 sym. stretch	3015 D	3015 S	2999 VS, p	SF(ν_{12}).
	ν_4	CH_2 scissors	1482 B	1482 W	1471 W, p	
	ν_5	Ring stretch. (ring breath)	1211 B	1211 S	1212 VS, p	
	ν_6	CH_2 twist	1095 D	1095 S	1088 W, p	
	ν_7	CH_2 wag	1090 D	1090 S	1088 W, p	
	ν_8	NH bend	998 C	998 M	1028 W	
	ν_9	Ring stretch. + deform.	856 B	856 VS	855 M, dp	
	ν_{10}	CH_2 rock	773 B	773 S	787 W, dp	
a''	ν_{11}	CH_2 anti. stretch	3079 D	3079 S	3059 M, dp	SF(ν_2).
	ν_{12}	CH_2 sym. stretch	3015 D	3015 S	2999 VS, p	SF(ν_3).
	ν_{13}	CH_2 scissors	1463 B	1463 W	1452 W, dp	
	ν_{14}	CH_2 twist	1268 C	1268 M	1276 VW	
a''	ν_{15}	NH bend	1237 C	1237 M	1297 W, p	
	ν_{16}	CH_2 wag	1131 B	1131 M	1130 VW	
	ν_{17}	Ring stretch. + deform.	904 B	904 S		
	ν_{18}	CH_2 rock	817 D	.....	817 M, dp	

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[1] R.IR. H. W. Thompson and W. T. Cave, Trans. Faraday Soc. **47**, 951 (1951).
[2] IR. H. T. Hoffman, Jr., G. E. Evans, and G. Glockler, J. Am. Chem. Soc. **73**, 3028 (1951).
[3] R.IR. W. J. Potts, Spectrochim. Acta **21**, 511 (1965).

Molecule: Cyclopropane C_3H_6 No. 108

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1'	ν_1	CH_2 sym. stretch	3038 C	ia	3038 S, p	
	ν_2	CH_2 scissors	1475 D	ia	1504 W, p 1453 W, p	FR($2\nu_{14}$).
	ν_3	Ring stretch. (ring breath)	1188 C	ia	1188 S, p	
a_1''	ν_4	CH_2 twist	1133 D	ia	ia	
a_2'	ν_5	CH_2 wag	1078 D	ia	ia	
a_2''	ν_6	CH_2 anti. stretch	3101 C	3101 S	ia	
	ν_7	CH_2 rock	852 C	852 S	ia	
e'	ν_8	CH_2 sym. stretch	3025 C	3025 VS	3019 VS, p	
	ν_9	CH_2 scissors	1442 C	1442 M	1443 M, dp	
	ν_{10}	CH_2 wag	1028 C	1028 S	1023 VW (liquid).	
	ν_{11}	Ring stretch. + deform.	866 C	866 VS	866 S, dp	
e''	ν_{12}	CH_2 anti. stretch	3082 C	ia	3090 S, dp	
	ν_{13}	CH_2 twist	1178 C	ia	1178 M	
	ν_{14}	CH_2 rock	739 C	ia	739 W, dp	

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[1] R.IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York 1945), and the references cited there.
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[4] R. P. M. Mathai, G. G. Shepherd, and H. L. Welsh, Can. J. Phys. **34**, 1448 (1956).
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Molecule: **Cyclopropane-d_6** **C_3D_6** No. 109

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

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1'	ν_1	CD_2 sym. stretch.....	2236 C	ia	2236 VS, p	
	ν_2	CD_2 scissors.....	1274 C	ia	1274 S, p	
	ν_3	Ring stretch. (ring breath).....	956 C	ia	956 S, p	
a_1''	ν_4	CD_2 twist.....	801 E	ia	ia	CF.
a_2'	ν_5	CD_2 wag.....	873 E	ia	ia	CF.
a_2''	ν_6	CD_2 anti. stretch.....	2336 C	2336 VS	ia	
	ν_7	CD_2 rock.....	614 C	614 W	ia	
e'	ν_8	CD_2 sym. stretch.....	2211 C	2211 VS	2204 W, dp	
	ν_9	CD_2 scissors.....	1074 C	1074 S	1068 W, dp	
	ν_{10}	CD_2 wag.....	887 C	887 M	884 M, dp	
	ν_{11}	Ring stretch. + deform.....	720 C	720 VS	721 M, dp	
e''	ν_{12}	CD_2 anti. stretch.....	2329 C	ia	2329 S, p	
	ν_{13}	CD_2 twist.....	928 E	ia	.....	CF.
	ν_{14}	CD_2 rock.....	528 C	ia	528 W, dp	

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Molecule: Cyclobutane C_4H_8 No. 110

Symmetry $D_{2d}(D_{4h})$ **Symmetry number $\sigma = 4(8)$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
$a_1(a_{1g})$	ν_1	CH_2 sym. stretch.....	[a] 2895 D	ia	2916 p 2866 p	FR($2\nu_2$, $2\nu_{13}$).
	ν_2	CH_2 scissors.....	1443 C	ia	1443 p	SF(ν_{13}).
	ν_3	CC stretch. (ring breathing).....	1001 C	ia	1001 p	SF(ν_{14}).
$a_1(b_{1u})$	ν_4	CH_2 anti. stretch.....	2975 E	ia	.....	CF [3].
	ν_5	CH_2 rock.....	741 C	ia	741 dp	
	ν_6	Ring puckering.....	200 E	ia	.....	CF [3].
$a_2(a_{2g})$	ν_7	CH_2 wag.....	1260 E	ia	ia	CF [3].
$a_2(b_{2u})$	ν_8	CH_2 twist.....	1257 E	ia	ia	CF [3].
$b_1(b_{1g})$	ν_9	CH_2 wag.....	1219 C	ia	1219 dp	
	ν_{10}	CC stretch. (ring deform.).....	926 C	ia	926 dp	
$b_1(a_{1u})$	ν_{11}	CH_2 twist.....	1222 E	ia	.....	CF [3].
$b_2(b_{2g})$	ν_{12}	CH_2 sym. stretch.....	2893 E	.....	.....	CF [3].
	ν_{13}	CH_2 scissors.....	1443 C	.....	1443 dp	SF(ν_2).
	ν_{14}	CCC deform. (ring deform.).....	1001 D	.....	(1001 p)	SF(ν_3).
$b_2(a_{2u})$	ν_{15}	CH_2 anti. stretch.....	2987 C	2987 S		
	ν_{16}	CH_2 rock.....	627 C	627 S		
$e(e_g)$	ν_{17}	CH_2 anti. stretch.....	2952 C	.....	2952 dp?	
	ν_{18}	CH_2 twist.....	1223 C	1223 W		
	ν_{19}	CH_2 rock.....	749 C	749 W		
$e(e_u)$	ν_{20}	CH_2 sym. stretch.....	2887 D	2997 2878		
	ν_{21}	CH_2 scissors.....	1447 C	1447 S		
	ν_{22}	CH_2 wag.....	1257 C	1257 S		
	ν_{23}	CC stretch. and CCC deform. (ring deform.).....	898 C	898 S		

[a] Corrected for a presumed shift due to Fermi resonance.

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Molecule: **Cyclobutane-d_8** C_4D_8 No. 111

Symmetry $D_{2d}(D_{4h})$ **Symmetry number $\sigma = 4(8)$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared [1]	Raman [1]	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
$a_1(a_{1g})$	ν_1	CD_2 sym. stretch	2124 E	ia	.....	CF [2].
	ν_2	CD_2 scissors	1160 C	ia	1160 p	
	ν_3	CC stretch. (ring breathing)	882 C	ia	882 p	
$a_1(b_{1u})$	ν_4	CD_2 anti. stretch	2224 E	ia	.....	CF [2].
	ν_5	CD_2 rock	632 E	ia	.....	CF [2].
	ν_6	Ring puckering	151 E	ia	.....	CF [2].
$a_2(a_{2g})$	ν_7	CD_2 wag	1010 E	ia	ia	CF [2].
$a_2(b_{2u})$	ν_8	CD_2 twist	889 E	ia	ia	CF [2].
$b_1(b_{1g})$	ν_9	CD_2 wag	1078 C	ia	1078 dp	
	ν_{10}	CC stretch. (ring deform.)	746 C	ia	746 dp	
$b_1(a_{1u})$	ν_{11}	CD_2 twist	864 E	ia	.....	CF [2].
$b_2(b_{2g})$	ν_{12}	CD_2 sym. stretch	2115 E	.....	.....	CF [2].
	ν_{13}	CD_2 scissors	1040 D	.....	1040 dp	
	ν_{14}	CCC deform. (ring deform.)	938 D	.....	938 dp	SF(ν_{18}).
$b_2(a_{2u})$	ν_{15}	CD_2 anti. stretch	2242 C	2242 S		
	ν_{16}	CD_2 rock	483 C	483 S		
$e(e_g)$	ν_{17}	CD_2 anti. stretch	2230 C	.....	2230 dp?	
	ν_{18}	CD_2 twist	938 D	.....	938 dp	SF(ν_{14}).
	ν_{19}	CD_2 rock	556 C	556 W		
$e(e_g)$	ν_{20}	CD_2 sym. stretch	2103 E	.....	.....	CF [2].
	ν_{21}	CD_2 scissors	1078 C	1078 S		
	ν_{22}	CD_2 wag	1048 C	1048 S		
	ν_{23}	CC stretch. and CCC deform. (ring. deform.)	734 C	734 S		

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[1] IR.R. R. C. Lord and D. G. Rea (to be published). Preliminary account presented at 3d Meeting, European Molecular Spectroscopy Group, Oxford, England, 1955.

[2] Th. R. C. Lord and I. Nakagawa, J. Chem. Phys. **39**, 2951 (1963).

Molecule: Polyethylene $(CH_2)_n$ No. 112

Symmetry D_{2h} **Symmetry number $\sigma = 4$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Solid)	
a_g	ν_1	CH_2 sym. stretch.....	2848 C	ia	2848 S	
	ν_2	CH_2 scissors.....	1440 C	ia	1440 M	
	ν_3	CC stretch. + CCC deform.....	1131 C	ia	1131 M	
b_{1g}	ν_4	CH_2 wag.....	1415 C	ia	1415 W	
	ν_5	CC stretch.....	1061 C	ia	1061 M	
b_{2g}	ν_6	CH_2 twist.....	1295 C	ia	1295 M	
b_{3g}	ν_7	CH_2 anti. stretch.....	2883 C	ia	2883 S	
	ν_8	CH_2 rock.....	1168 C	ia	1168 W	
a_u	ν_9	CH_2 twist.....	1050 D	ia	ia	[a].
b_{1u}	ν_{10}	CH_2 anti. stretch.....	2919 C	2919 S	ia	
	ν_{11}	CH_2 rock.....	725 C	731 S 720 S	ia	[b].
b_{2u}	ν_{12}	CH_2 sym. stretch.....	2851 C	2851 S	ia	
	ν_{13}	CH_2 scissors.....	1468 C	1473 S 1463 S	ia	[b].
b_{3u}	ν_{14}	CH_2 wag.....	1176 C	1176 VW	ia	

[a] 1063 cm^{-1} is given to this frequency in reference 6.

[b] Doublet due to the crystal field effect [1, 8].

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Molecule: Perdeuterated Polyethylene $(CD_2)_n$ No. 113

Symmetry D_{2h} **Symmetry number $\sigma = 4$**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Solid)	
a_g	ν_1	CD_2 sym. stretch.....	2102 C	ia	2102 S	
	ν_2	CD_2 scissors.....	1146 C	ia	1146 M	
	ν_3	CC stretch. + CCC deform.....	966 E	ia	966 VW	
b_{1g}	ν_4	CD_2 wag.....	1249 C	ia	1249 W	
	ν_5	CC stretch.....	820 E	ia	.....	CF [5].
b_{2g}	ν_6	CD_2 twist.....	916 C	ia	916 M	
b_{3g}	ν_7	CD_2 anti. stretch.....	2197 C	ia	2197 M	
	ν_8	CD_2 rock.....	991 C	ia	991 M	
a_u	ν_9	CD_2 twist.....	743 E	ia	ia	CF [5].
b_{1u}	ν_{10}	CD_2 anti. stretch.....	2192 C	2192 S	ia	
	ν_{11}	CD_2 rock.....	526 C	528 M 522 M	ia	[a].
b_{2u}	ν_{12}	CD_2 sym. stretch.....	2088 C	2088 S	ia	
	ν_{13}	CD_2 scissors.....	1090 C	1092 S 1087 S	ia	[a].
b_{3u}	ν_{14}	CD_2 wag.....	889 E	.....	ia	CF [5].

[a] Doublet due to the crystal field effect [5].

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