UNITED STATES DEPARTMENT OF COMMERCE

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Tables of Molecular Vibrational Frequencies Consolidated Volume I

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NSRDS–NBS 39

Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 39, 164 pages (June 1972)
NSRDAP

Supersedes and extends the data contained in Tables of Molecular Vibrational Frequencies, NSRDS–NBS–6, Part 1; NSRDS–NBS–11, Part 2; and NSRDS–NBS–17, Part 3.

Issued June 1972

For sale by the Superintendent of Documents, U.S. Government Printing Office
Washington, D.C. 20402 (Order by SD Catalog No. C13.48:39). Price $3
Stock Number 0303–0845

Tables of Molecular Vibrational Frequencies

Consolidated Volume I

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The compilations of fundamental vibrational frequencies of molecules previously published as NSRDS–NBS–6, NSRDS–NBS–11, and NSRDS–NBS–17 have been revised and extended to 52 additional molecules. This consolidated volume includes data on a total of 223 molecules. Selected values of the fundamental vibrational frequencies are given for each molecule, together with observed infrared and Raman spectral data and citations to the original literature. The selection of vibrational fundamentals has been based on careful studies of the spectral data and comprehensive normal-coordinate analyses. An estimate of the accuracy of the selected values is included. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

Key words: Fundamental frequencies; infrared spectra; polyatomic molecules; Raman spectra; vibrational frequencies.

1. Introduction

Establishing the assignment of molecular vibrational frequencies has fundamental importance in elucidating various problems in physics and chemistry. The information concerning the force field and motion of atoms in a molecule can be most directly derived from its vibrational frequencies. If all the vibrational frequencies of a molecule are known, as well as the molecular structure, thermodynamic quantities can be easily computed on the ideal gas model. Thus, the need for a tabulation of evaluated reference data on molecular vibrational frequencies has often been felt by many investigators. In 1964 a project for producing such tables was initiated at the University of Tokyo in cooperation with the National Standard Reference Data System of the National Bureau of Standards. The evaluated data resulting from this project have been published as Tables of Molecular Vibrational Frequencies, Part 1 (NSRDS–NBS–6), Part 2 (NSRDS–NBS–11) and Part 3 (NSRDS–NBS–17). The present volume consists of the contents of these three publications, after extensive revision in the light of new experimental data, plus tables for 52 additional molecules.

2. Molecules Selected and Their Ordering

The present volume contains tables of fundamental vibrational frequencies for 223 molecules. The molecules were selected from basic organic and inorganic molecules for which the vibrational assignments have been established with little ambiguity. The effort of extending the tables to many other important molecules is continuing in this laboratory. Diatomic molecules and electronically excited species are not included in this volume, since refs. [1] and [2][1] contain good compilations of data for them. Rotational isomers are treated as independent molecular species, and a separate table is made for each of the isomers. When the gas and liquid state spectra are significantly different from each other, they are tabulated separately.

The molecules are ordered according to the following rules:

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

Molecules are first divided into groups by the items (a) and (b) and the ordering of molecules in each group is given by the items (c), (d), (e), and (f). A complete list in the order presented is given at the beginning of the tables. Indices by compound name and empirical formula follow the tables.

[1] Figures in brackets indicate the literature references on page 3.

3. Description of Tables

3.1. Symmetry

The symmetry (point group) of each molecule is given by the Schoenflies notation. Detailed discussions of symmetry properties will be found in refs. [3] and [4].

3.2. Symmetry Number

The symmetry number, σ, is used in the calculation of thermodynamic quantities. It is the number of indistinguishable positions into which the molecule can be transformed by simple rigid rotations. A general discussion and pertinent formulas may be found in ref. [4], page 508.

3.3. Symmetry Species

In the table the normal modes are divided into the symmetry species of the point group to which the molecule belongs. The ordering of species in each point group is given in table I, which is a summary of tables 12–30 of ref. [4]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be defined uniquely. In such cases we generally follow the notation adopted in ref. [4].

3.4. Numbering of Frequencies

The numbering is indicated by ν_i given in the second column of each table. The normal modes are first grouped into symmetry species, and then those in each species are ordered from higher to lower values of the frequency. However, we always denote the bending vibration of a linear triatomic molecule as ν_2, following the widely accepted tradition. For the C_2X_6 type of molecule we adopt the numbering given in ref. [4], although it is based on D_{3h} symmetry. For some deuterated compounds the frequencies are arranged so that the same ν_i numbering is given to the corresponding vibrational modes of deuterated and normal compounds.

3.5. Approximate Type of Mode

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

The following abbreviations are used for the type of mode:

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

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

3.6. Selected Value of Frequency

The fundamental frequency ν_i is defined as the difference between the term values $G(v_i = 1$, all other $v_j = 0)$ and $G(v_i = 0$, and other $v_j = 0)$ expressed in cm^{-1}. Fundamental frequencies rather than harmonic frequencies (ω_i) are listed in the table. Although harmonic frequencies are of greater physical significance, they are accurately known only for a small number of polyatomic molecules. The selected values are rounded to the nearest 1 cm^{-1}.

The letter code, A, B, C, D, or E following the selected value of frequency indicates the evaluator's judgment of the accuracy of the value. The basis for estimating accuracy of an observed frequency is given in table III, together with the range of uncertainty in cm^{-1} for each grade.

Frequencies derived from infrared and Raman measurements in the gaseous state are chosen unless otherwise mentioned. When a detailed analysis of the rotational fine structure of an infrared band is available, the band center ν_0 is chosen as the fundamental frequency and given the uncertainty code A (see below). For a well-analyzed perpendicular band of a symmetric top molecule, the frequency listed contains the nonvibrational part $A'\zeta^2$, where A' is the rotational constant of the vibrational level and ζ is the Coriolis coupling constant. This is in accord with the definition of ν_0 given in ref. [4], page 404 and equation (IV, 60).

When the spectra in the gaseous state are not

available, the frequencies observed in the liquid or solid state are listed. When no spectral data have been obtained, the results of normal vibration calculations or of some other methods of estimating frequencies are listed with the grade D or E.

Torsional frequency may be calculated using the barrier height and reduced moment derived from microwave spectroscopy. The value obtained in this way is given as MW (frequency in cm^{-1}) in the "Comments" column or as a footnote for comparison with the value observed or calculated by the normal coordinate treatment. Microwave data are taken from ref. [6] unless otherwise noted.

For many molecules the assignments given in the literature have been checked by normal vibration calculations carried out in this laboratory as part of the project. Revisions in some assignments have been made as a result of these calculations. The details of the normal coordinate treatment and evaluation of force constants may be found in ref. [5].

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

3.7. Infrared and Raman Spectra

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

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

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

3.8. Comments

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

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

3.9. Footnotes and References

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

I acknowledge the assistance of the members of my laboratory at the University of Tokyo in carrying out this project. I also express my sincere thanks to many members of the National Bureau of Standards, particularly to C. W. Beckett, D. R. Lide, Jr., E. L. Brady, and S.A. Rossmassler who offered helpful suggestions in the planning of the tables.

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4. Tables of Vibrational Frequencies

C_0-triatomic molecules

		Page
1	Nitrous oxide, $^{14}N_2O$	9
2	Nitrous oxide, $^{14}N^{15}NO$	9
3	Nitrous oxide, $^{15}N_2O$	10
4	Water, H_2O	10
5	Water-d_1, HDO	10

		Page
6	Water-d_2, D_2O	11
7	Oxygen difluoride, F_2O	11
8	Oxygen dichloride, $^{35}Cl_2{}^{16}O$	12
9	Hydrogen sulfide, H_2S	12
10	Deuterium sulfide, D_2S	13
11	Sulfur dioxide, $^{32}S^{16}O_2$	13
12	Hydrogen selenide, H_2Se	14
13	Hydrogen deuterium selenide, HDSe	14

C_0-four-atomic molecules

14	Ammonia, NH_3	15
15	Ammonia-d_3, ND_3	15
16	Nitrogen trifluoride, NF_3	16
17	Phosphine, PH_3	16
18	Phosphine-d_3, PD_3	17
19	Phosphorus trifluoride, PF_3	17
20	Phosphorus trichloride, PCl_3	18
21	Arsine, AsH_3	18
22	Arsine-d_3, AsD_3	19
23	Stibine, SbH_3	19
24	Stibine-d_3, SbD_3	20

C_0-five-atomic molecules

25	Silane, SiH_4	20
26	Silane-d_2, SiH_2D_2	21
27	Silane-d_3, $SiHD_3$	21
28	Silane-d_4, SiD_4	22
29	Silicon tetrafluoride, SiF_4	22
30	Silicon tetrachloride, $SiCl_4$	23
31	Silicon tetrabromide, $SiBr_4$	23
32	Silicon tetraiodide, SiI_4	24
33	Germane, GeH_4	24
34	Germane-d_1, GeH_3D	25
35	Germane-d_2, GeH_2D_2	25
36	Germane-d_3, $GeHD_3$	26
37	Germane-d_4, GeD_4	26
38	Germanium tetrachloride, $GeCl_4$	27
39	Germanium tetrabromide, $GeBr_4$	27
40	Tin tetrachloride, $SnCl_4$	28
41	Tin tetrabromide, $SnBr_4$	28
42	Silyl fluoride, SiH_3F	29
43	Silyl chloride, SiH_3Cl	29
44	Silyl bromide, SiH_3Br	30
45	Bromotrichlorosilane, $SiBrCl_3$	30
46	Trichloroiodosilane, $SiCl_3I$	31
47	Tribromochlorosilane, $SiBr_3Cl$	31
48	Chlorotriiodosilane, $SiClI_3$	32
49	Dibromodichlorosilane, $SiBr_2Cl_2$	32

C_0-seven-atomic molecules

50	Sulfur hexafluoride, SF_6	33
51	Selenium hexafluoride, SeF_6	33
52	Molybdenum hexafluoride, MoF_6	34
53	Tungsten hexafluoride, WF_6	34
54	Uranium hexafluoride, UF_6	35

C_0-eight-atomic molecules

		Page
55	Diborane, $^{10}B_2H_6$	36
56	Diborane, $^{11}B_2H_6$	37
57	Diborane-d_6, $^{10}B_2D_6$	38

C_1-triatomic molecules

58	Carbon dioxide, $^{12}C^{16}O_2$	39
59	Carbon dioxide, $^{13}C^{16}O_2$	39
60	Carbon disulfide, $^{12}C^{32}S_2$	40
61	Carbonyl sulfide, $^{12}C^{16}O^{32}S$	40
62	Hydrogen cyanide, HCN	41
63	Deuterium cyanide, DCN	41
64	Cyanogen chloride, $^{35}ClCN$	42
65	Cyanogen chloride, $^{37}ClCN$	42
66	Cyanogen bromide, $^{79}BrCN$	43
67	Cyanogen bromide, $^{81}BrCN$	43

C_1-four-atomic molecules

68	Formaldehyde, H_2CO	44
69	Formaldehyde-d_1, HDCO	44
70	Formaldehyde-d_2, D_2CO	45

C_1-five-atomic molecules

71	Methane, CH_4	45
72	Methane-d_1, CH_3D	46
73	Methane-d_2, CH_2D_2	46
74	Methane-d_3, CHD_3	47
75	Methane-d_4, CD_4	47
76	Carbon tetrafluoride, CF_4	48
77	Carbon tetrachloride, CCl_4	48
78	Carbon tetrabromide, CBr_4	49
79	Carbon tetraiodide, CI_4	49
80	Methyl fluoride, CH_3F	50
81	Methyl fluoride-d_3, CD_3F	50
82	Methyl chloride, CH_3Cl	51
83	Methyl chloride-d_3, CD_3Cl	51
84	Methyl bromide, CH_3Br	52
85	Methyl bromide-d_3, CD_3Br	52
86	Methyl iodide, CH_3I	53
87	Methyl iodide-d_3, CD_3I	53
88	Trifluoromethane, CHF_3	54
89	Trichloromethane, $CHCl_3$	54
90	Trichloromethane-d_1, $CDCl_3$	55
91	Tribromomethane, $CHBr_3$	55
92	Tribromomethane-d_1, $CDBr_3$	56
93	Bromotrichloromethane, $CBrCl_3$	56
94	Tribromochloromethane, CBr_3Cl	57
95	Dichloromethane, CH_2Cl_2	57
96	Dichloromethane-d_1, $CHDCl_2$	58
97	Dichloromethane-d_2, CD_2Cl_2	58
98	Dibromomethane, CH_2Br_2	59
99	Dibromomethane-d_1, $CHDBr_2$	59
100	Dibromomethane-d_2, CD_2Br_2	60
101	Dibromodichloromethane, CBr_2Cl_2	60
102	Bromochloromethane, CH_2BrCl	61
103	Bromochloromethane-d_1, CHDBrCl	61
104	Bromochloromethane-d_2, CD_2BrCl	62

Page

105 Formic acid, HCOOH 62
106 Formic acid-d_2, DCOOD 63

C_1-six-atomic molecules

107 Methanol, CH_3OH (Gas) 63
108 Methanol, CH_3OH (Liquid) 64
109 Methanol-d_1, CH_3OD (Gas) 64
110 Methanol-d_1, CH_3OD (liquid) 65
111 Methanol-d_3, CD_3OH (gas) 65
112 Methanol-d_3, CD_3OH (liquid) 66
113 Methanol-d_4, CD_3OD (gas) 66

C_1-seven-atomic molecules

114 Methylamine, CH_3NH_2 67
115 Methylamine-d_2, CH_3ND_2 68
116 Methylamine-d_3, CD_3NH_2 69
117 Methylamine-d_5, CD_3ND_2 70

C_2-four-atomic molecules

118 Acetylene, CHCH 71
119 Acetylene-d_1, CHCD 71
120 Acetylene-d_2, CDCD 72
121 Fluoroacetylene, CHCF 72
122 Chloroacetylene, CHCCl 73
123 Bromoacetylene, CHCBr 73

C_2-six-atomic molecules

124 Ethylene, CH_2CH_2 74
125 Ethylene-d_4, C_2D_4 75
126 Tetrafluoroethylene, CF_2CF_2 75
127 Tetrachloroethylene, CCl_2CCl_2 76
128 Tetrabromoethylene, CBr_2CBr_2 76
129 cis-1,2-Difluoroethylene, CHFCHF 77
130 cis-1,2-Difluoroethylene-d_1, CHFCDF 77
131 cis-1,2-Difluoroethylene-d_2, CDFCDF 78
132 trans-1,2-Dichloroethylene, CHClCHCl 78
133 trans-1,2-Dichloroethylene-d_1, CHClCDCl 79
134 trans-1,2-Dichloroethylene-d_2, CDClCDCl 79
135 cis-1,2-Dichloroethylene, CHClCHCl 80
136 cis-1,2-Dichloroethylene-d_1, CHClCDCl 80
137 cis-1,2-Dichloroethylene-d_2, CDClCDCl 81
138 trans-1,2-Dichloro-1,2-difluoroethylene, CFClCFCl 81
139 1,1-Dichloroethylene, CH_2CCl_2 82
140 1,1-Dichloroethylene-d_1, $CHDCCl_2$ 82
141 1,1-Dichloroethylene-d_2, CD_2CCl_2 83
142 1,1-Dichloro-2,2-difluoroethylene, CF_2CCl_2 83
143 Methyl cyanide, CH_3CN 84
144 Methyl cyanide-d_3, CD_3CN 84
145 Methylisocyanide, CH_3NC 85
146 Methylisocyanide-d_3, CD_3NC 85

C_2-seven-atomic molecules

147 1,2,5-Oxadiazole, $C_2H_2N_2O$ 86
148 Silylacetylene, SiH_3CCH 86

Page

149 Ethylene oxide, C_2H_4O 87
150 Ethylene oxide-d_4, C_2D_4O 88
151 Acetaldehyde, CH_3CHO 89
152 Acetaldehyde-d_1, CH_3CDO 90
153 Acetaldehyde-d_4, CD_3CDO 91

C_2-eight-atomic molecules

154 Ethane, CH_3CH_3 92
155 Ethane-1,1,1-d_3, CH_3CD_3 93
156 Ethane-d_6, CD_3CD_3 94
157 Hexafluoroethane, CF_3CF_3 95
158 Hexachloroethane, CCl_3CCl_3 95
159 Hexabromoethane, CBr_3CBr_3 96
160 1,2-Dichloroethane, CH_2ClCH_2Cl (trans form) 97
161 1,2-Dichloroethane, CH_2ClCH_2Cl (gauche form) 98
162 1,2-Dibromoethane, CH_2BrCH_2Br (trans form) 99
163 1,2-Dibromoethane, CH_2BrCH_2Br (gauche form) 100
164 1-Bromo-2-chloroethane, CH_2ClCH_2Br (trans form) 101
165 1-Bromo-2-chloroethane, CH_2ClCH_2Br (gauche form) 102
166 Fluoroethane, CH_3CH_2F 103
167 Chloroethane, CH_3CH_2Cl 104
168 Bromoethane, CH_3CH_2Br 105
169 Ethylene imine, C_2H_5N 106
170 Methyl formate, $HCOOCH_3$ 107
171 Methyl formate-d_1, $DCOOCH_3$ 108
172 Methyl formate-d_3, $HCOOCD_3$ 109
173 Methyl formate-d_4, $DCOOCD_3$ 110
174 Acetic acid, CH_3COOH 111
175 Acetic acid-d_1, CH_3COOD 112

C_2-nine-atomic molecules

176 Dimethylether, CH_3OCH_3 113
177 Dimethylether-d_3, CH_3OCD_3 114

C_3-seven-atomic molecules

178 Allene CH_2CCH_2 115
179 Methylacetylene, CH_3CCH 116
180 Methylacetylene-d_1, CH_3CCD 116
181 Methyl-d_3-acetylene, CD_3CCH 117
182 Methylacetylene-d_4, CD_3CCD 117
183 Malononitrile, $NCCH_2CN$ 118
184 Malononitrile-d_2, $NCCD_2CN$ 118

C_3-eight-atomic molecules

185 Propenal, CH_2CHCHO 119

C_3-nine-atomic molecules

186 Cyclopropane, C_3H_6 120
187 Cyclopropane-d_6, C_3D_6 121
188 Ethylcyanide, CH_3CH_2CN 122

Page

C_3-ten-atomic molecules

189 Acetone, CH_3COCH_3 123
190 Acetone-α,α,α-d_3, CH_3COCD_3 124
191 Acetone-d_6, CD_3COCD_3 125

C_3-11-atomic molecules

192 Propane, $CH_3CH_2CH_3$ 126
193 Propane-2,2-d_2, $CH_3CD_2CH_3$ 127
194 Propane-1,1,1-d_3, $CH_3CH_2CD_3$ 128
195 Propane-1,1,1,3,3,3-d_6, $CD_3CH_2CD_3$ 129
196 Propane-d_8, $CD_3CD_2CD_3$ 130
197 Methyl acetate, CH_3COOCH_3 131
198 Methyl acetate-d_3, CD_3COOCH_3 132
199 Methyl-d_3-acetate, CH_3COOCD_3 133
200 Methyl acetate-d_6, CD_3COOCD_3 134

C_4-six-atomic molecules

201 Butadiyne, HCCCCH 135

C_4-nine-atomic molecules

202 Furan, C_4H_4O 136
203 Thiophene, C_4H_4S 137
204 Thiophene-d_4, C_4D_4S 138

C_4-ten-atomic molecules

205 1,3-Butadiene, $CH_2CHCHCH_2$ 139
206 1,3-Butadiene-1-d_1 (trans), $CH_2CHCHCHD$ ... 140
207 1,3-Butadiene-1,1,2-d_3, $CH_2CHCDCD_2$ 141
208 1,3-Butadiene-1,1,4,4-d_4, $CD_2CHCHCD_2$ 142
209 1,3-Butadiene-d_6, $CD_2CDCDCD_2$ 143
210 2-Butyne, CH_3CCCH_3 144

C_4-12-atomic molecules

211 Cyclobutane, C_4H_8 145
212 Cyclobutane-d_8, C_4D_8 146
213 2-Methylpropene, $(CH_3)_2CCH_2$ 147
214 2-Methyl-d_3-propene-3,3,3-d_3, $(CD_3)_2CCH_2$ ... 148

C_4-13-atomic molecules

215 2-Butanone $CH_3COCH_2CH_3$ (trans form) 149

C_4-14-atomic molecules

216 n-Butane, $CH_3CH_2CH_2CH_3$ (trans form) 150
217 n-Butane, $CH_3CH_2CH_2CH_3$ (gauche form) 151

C_6-12-atomic molecules

218 Benzene, C_6H_6 152
219 Benzene-d_6, C_6D_6 153

C_6-18-atomic molecules

220 Cyclohexane, C_6H_{12} 154
221 Cyclohexane-d_{12}, C_6D_{12} 155

Polymer

222 Poly (methylene), $(CH_2)_n$ 156
223 Poly (methylene-d_2), $(CD_2)_n$ 157

TABLE I. *Ordering of symmetry species*

(In the present volume small letters are used to designate the species of fundamental frequencies)

Point group	Symmetry species
C_2	A, B
C_s	A′, A″
C_i	A_g, A_u
C_{2v}	A_1, A_2, B_1, B_2
C_{2h}	A_g, A_u, B_g, B_u
D_2	A, B_1, B_2, B_3
D_{2h}	A_g, A_u, B_{1g}, B_{1u}, B_{2g}, B_{2u}, B_{3g}, B_{3u}
C_{3v}	A_1, A_2, E
D_3	A_1, A_2, E
C_{5v}	A_1, A_2, E_1, E_2
$C_{\infty v}$	Σ^+, Σ^-, π, Δ, Φ, ...
C_{4v}, D_4, D_{2d}	A_1, A_2, B_1, B_2, E
C_{6v}, D_6	A_1, A_2, B_1, B_2, E_1, E_2
D_{3d}	A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u
D_{4d}	A_1, A_2, B_1, B_2, E_1, E_2, E_3
D_{3h}	A_1', A_1'', A_2', A_2'', E′, E″
D_{5h}	A_1', A_1'', A_2', A_2'', E_1', E_1'', E_2', E_2''
D_{4h}	A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_g, E_u
D_{6h}	A_{1g}, A_{1u}, A_{2g}, A_{2u}, B_{1g}, B_{1u}, B_{2g}, B_{2u}, E_{1g}, E_{1u}, E_{2g}, E_{2u}
$D_{\infty h}$	Σ_g^+, Σ_u^+, Σ_g^-, Σ_u^-, π_g, π_u, Δ_g, Δ_u, Φ_g, Φ_u, ...
C_3	A, E
C_6	A, B, E_1, E_2
S_6	A_g, A_u, E_g, E_u
C_{3h}	A′, A″, E′, E″
C_{4h}	A_g, A_u, B_g, B_u, E_g, E_u
C_{6h}	A_g, A_u, B_g, B_u, E_{1g}, E_{1u}, E_{2g}, E_{2u}
T_d, O	A_1, A_2, E, F_1, F_2
O_h	A_{1g}, A_{1u}, A_{2g}, A_{2u}, E_g, E_u, F_{1g}, F_{1u}, F_{2g}, F_{2u}
T	A, E, F

TABLE II. *Definition of local symmetry coordinates*

(a) Local symmetry coordinates for the CH_3 group (see fig. 1a)
- CH_3 symmetrical stretching: $(\Delta r_1 + \Delta r_2 + \Delta r_3)/\sqrt{3}$
- CH_3 degenerate stretching: $(2\Delta r_1 - \Delta r_2 - \Delta r_3)/\sqrt{6}$
  $(\Delta r_2 - \Delta r_3)/\sqrt{2}$
- CH_3 symmetrical deformation:
  $(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12} - \Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3)/\sqrt{6}$
- CH_3 degenerate deformation: $(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{6}$
  $(\Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{2}$
- CH_3 rocking: $(2\Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3)/\sqrt{6}$
  $(\Delta\beta_2 - \Delta\beta_3)/\sqrt{2}$.

(b) Local symmetry coordinates for the CH_2 group (see fig. 1b)
- CH_2 symmetrical stretching: $(\Delta r_1 + \Delta r_2)/\sqrt{2}$
- antisymmetrical stretching: $(\Delta r_1 - \Delta r_2)/\sqrt{2}$
- CH_2 scissors: $(4\Delta\alpha - \Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y})/\sqrt{20}$
- CH_2 wagging: $(\Delta\beta_{1X} + \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$
- CH_2 twisting: $(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y})/2$
- CH_2 rocking: $(\Delta\beta_{1X} - \Delta\beta_{2X} + \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$.

(c) Local symmetry coordinates for the CH group (see fig. 1c)
- CH stretching: Δr_{CH}
- CH bending: $(2\Delta\beta_{HX} - \Delta\beta_{HY} - \Delta\beta_{HZ})/\sqrt{6}$
  $(\Delta\beta_{HY} - \Delta\beta_{HZ})/\sqrt{2}$

(d) Local symmetry coordinates for the planar CH_2 group (see fig. 1d)
- CH_2 symmetrical stretching: $(\Delta r_1 + \Delta r_2)/\sqrt{2}$
- CH_2 antisymmetrical stretching: $(\Delta r_1 - \Delta r_2)/\sqrt{2}$
- CH_2 scissors: $(2\Delta\alpha - \Delta\beta_1 - \Delta\beta_2)/\sqrt{6}$
- CH_2 rocking: $(\Delta\beta_1 - \Delta\beta_2)/\sqrt{2}$
- CH_2 wagging: $\Delta\theta \cdot \sin\alpha$.

(e) Local symmetry coordinates for the planar CH group (see fig. 1e)
- CH stretching: Δr_{CH}
- in-plane CH bending: $(\Delta\beta_{HX} - \Delta\beta_{HY})/\sqrt{2}$
- out-of-plane CH bending: $\Delta\theta_H \cdot \sin\gamma_{XY}$.

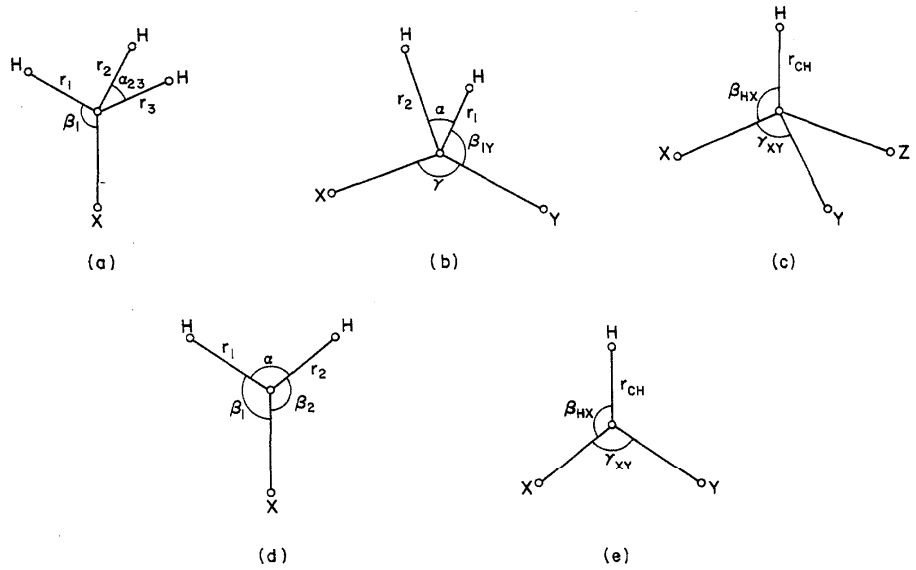

FIGURE 1. *Parameters of methyl, methylene, and methin groups.*

TABLE III. *Uncertainty code for the selected values of frequencies*

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

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

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

Sym. species	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 VW	2224 W	
π	ν_2	Bend	589 A	588.7 S	589 W	
σ^+	ν_3	NO stretch	1285 A	1284.9 VS	1287 VS	

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

Molecule: Nitrous oxide $^{14}N^{15}NO$ No. 2
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	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		
π	ν_2	Bend	585 A	585.3		
σ^+	ν_3	NO stretch	1270 A	1269.9		

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[1] IR. J. Pliva, J. Mol. Spectrosc. **12**, 360 (1964).
[2] IR. R. P. Grosso and T. K. McCubbin, Jr., J. Mol. Spectrosc. **13**, 240 (1964).

Molecule: Nitrous oxide $^{15}N_2O$ No. 3
Symmetry $C_{\infty v}$ **Symmetry number** $\sigma = 1$

Sym. species	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		
π	ν_2	Bend	572 A	571.9		
σ^+	ν_3	NO stretch	1265 A	1265.3		

References

See No. 2.

Molecule: Water H_2O No. 4
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch	3657 A	3656.65	3654	
	ν_2	Bend	1595 A	1594.59		
b_1	ν_3	Antisym. stretch	3756 A	3755.79		

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

Molecule: Water-d_1 HDO No. 5
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'	ν_1	OD stretch	2727 A	2726.73	2718	
	ν_2	Bend	1402 A	1402.20		
	ν_3	OH stretch	3707 A	3707.47		

References

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Molecule: Water-d_2 D_2O No. 6
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch	2671 A	2671.46	2666	
	ν_2	Bend	1178 A	1178.33		
b_1	ν_3	Antisym. stretch	2788 A	2788.05		

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[2] IR. W. S. Benedict, N. Gailar, and E. K. Plyler, J. Chem. Phys. 24, 1139 (1956).

Molecule: Oxygen difluoride F_2O No. 7
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

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

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Molecule: Oxygen dichloride $^{35}Cl_2{}^{16}O$ No. 8
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.....	639 D	638.6 VS (Ar matrix)		
	ν_2	Bend.....	296 C	296.4 W (solid)		
b_1	ν_3	Antisym. stretch.....	686 C	685.9 S		

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Molecule: Hydrogen sulfide H_2S No. 9
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.....	2615 A	2614.6		
	ν_2	Bend.....	1183 A	1182.7		
b_1	ν_3	Antisym. stretch.....	2626 B	2626		

References

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Molecule: Deuterium sulfide D_2S No. 10
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch	1896 A	1896.38	1891.6	
	ν_2	Bend	855 A	855.45		
b_1	ν_3	Antisym. stretch	1999 E	1999		

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Molecule Sulfur dioxide $^{32}S^{16}O_2$ No. 11
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch	1151 B	1151.4 S	1150.5 S, p	
	ν_2	Bend	518 B	517.7 S	524.5 W, p (liquid)	
b_1	ν_3	Antisym. stretch	1362 B	1361.8 S	1336.0 W, dp (liquid)	

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[3] IR. S. R. Polo and M. K. Wilson, J. Chem. Phys. **22**, 900 (1954).

Molecule: Hydrogen selenide H_2Se No. 12
Symmetry C_{2v} Symmetry number $\sigma = 2$

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

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[2] IR.Th. E. D. Palik, J. Mol. Spectrosc. 3, 259 (1959).

Molecule: Hydrogen deuterium selenide HDSe No. 13
Symmetry C_s Symmetry number $\sigma = 1$

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

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[2] IR.R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik," 6. Auflage, I. Band, Atom-und Molekularphysik, 2. Teil, Molekeln, I. (Springer-Verlag, Berlin, Göttingen, Heidelberg, 1951).

Molecule: Ammonia NH_3 No. 14
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared[a]	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	Sym. stretch.....	3337 A	3336.2*s* 3337.2*a*		
	ν_2	Sym. deform.....	950 C	932.5*s* 968.3*a*		
e	ν_3	Deg. stretch.....	3444 A	3443.6*s* 3443.9*a*		
	ν_4	Deg. deform.....	1627 A	1626.1*s* 1627.4*a*		

[a] "*s*" and "*a*" refer to symmetric and antisymmetric levels [2].

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[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
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Molecule Ammonia-d_3 ND_3 No. 15
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared[a]	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.....	2420 C	2420.1*s* 2420.6*a*	.....	FR ($2\nu_4$).
	ν_2	Sym. deform.....	748 B	745.7*s* 749.4*a*		
e	ν_3	Deg. stretch.....	2564 A	2564.0		
	ν_4	Deg. deform.....	1191 B	1191		

[a] "*s*" and "*a*" refer to symmetric and antisymmetric levels [2].

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
[2] IR. W. S. Benedict and E. K. Plyler, Can. J. Phys. **35**, 1235 (1957).
[3] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20**, 523 (1964).

Molecule: Nitrogen trifluoride NF_3 No. 16
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch	1032 B	1032 S	1050	
	ν_2	Sym. deform	647 B	647 W	667	
e	ν_3	Deg. stretch	907 C	907 S	905	
	ν_4	Deg. deform	492 B	492 W	515	

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Molecule: Phosphine PH_3 No. 17
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch	2323 A	2322.9	2306	
	ν_2	Sym. deform	992 B	992.1	979	
e	ν_3	Deg. stretch	2328 B	2327.7		
	ν_4	Deg. deform	1118 A	1118.3	1115	

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Molecule: Phosphine-d_3 PD_3 No. 18
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch	1694 B	1694		
	ν_2	Sym. deform	730 B	730		
e	ν_3	Deg. stretch	1687 D	.....	.....	CF [2].
	ν_4	Deg. deform	806 B	806		

References

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[2] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20**, 523 (1964).

Molecule: Phosphorus trifluoride PF_3 No. 19
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch	892 B	892 S	890 (10)	
	ν_2	Sym. deform	487 B	487 M	486 (3)	
e	ν_3	Deg. stretch	860 C	860 S	840 (10)	
	ν_4	Deg. deform	344 B	344 M		

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Molecule: Phosphorus trichloride PCl_3 No. 20
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	504 C	504	510 (10) p	
	ν_2	Sym. deform.....	252 C	252	257 (6) p	
e	ν_3	Deg. stretch.....	482 C	482	480 (3) dp	
	ν_4	Deg. deform.....	198 C	198	190 (10) dp	

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Molecule Arsine AsH_3 No. 21
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.....	2116 A	2116.1		
	ν_2	Sym. deform.....	906 B	906.0		
e	ν_3	Deg. stretch.....	2123 B	2123.0		
	ν_4	Deg. deform.....	1003 B	1003		

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Molecule: Arsine-d_3 AsD_3 No. 22
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch	1523 B	1523.1		
	ν_2	Sym. deform	660 C	660.0		
e	ν_3	Deg. stretch	1529 C	1529.3		
	ν_4	Deg. deform	714 C	714		

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[1] IR. E. Lee and C. K. Wu, Trans. Faraday Soc. **35**, 1366 (1939).
[2] IR. V. M. McConaghie and H. H. Nielsen, Phys. Rev. **75**, 633 (1949).
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Molecule: Stibine SbH_3 No. 23
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch	1891 B	1890.9		
	ν_2	Sym. deform	782 C	781.5		
e	ν_3	Deg. stretch	1894 C	1894.2		
	ν_4	Deg. deform	831 C	830.9		

References

[1] IR. H. H. Nielsen, J. Chem. Phys. **20**, 759 (1952).
[2] IR. W. H. Haynie and H. H. Nielsen, J. Chem. Phys. **21**, 1839 (1953).
[3] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20**, 523 (1964).

Molecule: Stibine-d_3 SbD_3 No. 24
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.....	1359 B	1358.8		
	ν_2	Sym. deform.....	561 C	561.1		
e	ν_3	Deg. stretch.....	1362 C	1362.0		
	ν_4	Deg. deform.....	593 C	592.5		

References

[1] IR. W. H. Haynie and H. H. Nielsen, J. Chem. Phys. **21**, 1839 (1953).
[2] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20**, 523 (1964).

Molecule: Silane SiH_4 No. 25
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.....	2187 B	ia	2187.0 S	
e	ν_2	Deg. deform.....	975 C	ia, [a]974.6	978 W	
f_2	ν_3	Deg. stretch.....	2191 A	2190.6		
	ν_4	Deg. deform.....	914 B	914.2		

[a] Observed in the infrared through Coriolis interaction with ν_4.

References

[1] R. F. B. Stitt and D. M. Yost, J. Chem. Phys. **4**, 82 (1936).
[2] IR. C. H. Tindal, J. W. Straley, and H. H. Nielsen, Phys. Rev. **62**, 151 (1942).
[3] IR.R G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
[4] IR. D. F. Ball and D. C. McKean, Spectrochim. Acta **18**, 1019; 1029 (1962).
[5] IR. I. W. Levin and W. T. King, J. Chem. Phys. **37**, 1375 (1962).

Molecule: Silane-d_2 SiH_2D_2 No. 26
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiH_2 s-stretch	2189 C	2189 S		
	ν_2	SiD_2 s-stretch	1587 C	1587 S		
	ν_3	SiH_2 scis	944 B	944 W		
	ν_4	SiD_2 scis	683 B	682.5 M		
a_2	ν_5	SiH_2 twist	844 E	ia	.....	CF [1].
b_1	ν_6	SiH_2 a-stretch	2183 C	2183 S		
	ν_7	SiH_2 rock	743 B	743 S		
b_2	ν_8	SiD_2 a-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. 27
Symmetry C_{3v} Symmetry number $\sigma = 3$

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

References

[1] IR. J. H. Meal and M. 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. 28
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	Sym. stretch.....	1558 E	.....	.....	CF [4].
e	ν_2	Deg. deform.....	700 E	.....	.....	CF [4].
f_2	ν_3	Deg. stretch.....	1597 B	1597 S		
	ν_4	Deg. deform.....	681 C	681 S		

References

[1] IR. J. H. Meal and M. K. Wilson, J. Chem. Phys. 24, 385 (1956).
[2] IR. D. F. Ball and D. C. McKean, Spectrochim. Acta 18, 1019; 1029 (1962).
[3] IR. I. W. Levin and W. T. King, J. Chem. Phys. 37, 1375 (1962).
[4] Th. T. Shimanouchi, I. Nakagawa, J. Hiraishi, and M. Ishii, J. Mol. Spectrosc. 19, 78 (1966).

Molecule Silicon tetrafluoride SiF_4 No. 29
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	800 C	ia	800 S	
e	ν_2	Deg. deform.....	268 C	ia	268 W	
f_2	ν_3	Deg. stretch.....	1032 B	1031.8 S	1010 W	
	ν_4	Deg. deform.....	389 B	389.35 S	390 W	

References

[1] IR.R. E. A. Jones, J. S. Kirby-Smith, P. J. H. Woltz, and A. H. Nielsen, J. Chem. Phys. 19, 242 (1951).
[2] IR. J. Heicklen and V. Knight, Spectrochim. Acta 20, 295 (1964).
[3] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta 20, 1089 (1964).
[4] IR.Th. I. W. Levin and S. Abramowitz, J. Chem. Phys. 44, 2562 (1966).
[5] IR.Th. I. W. Levin and S. Abramowitz, J. Res. Nat. Bur. Stand. (U.S.), 72A (Phys. and Chem.), No. 3, 247–249 (1968).

Molecule: Silicon tetrachloride $SiCl_4$ No. 30
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	424 C	ia	424 (5) p	
e	ν_2	Deg. deform.....	150 C	ia	150 (4)	
f_2	ν_3	Deg. stretch.....	621 C	621 VS	610 (2b)	
	ν_4	Deg. deform.....	221 C	.....	221 (4)	

References

[1] IR.R. 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] IR.R. 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), Ser. A,240,499 (1957).
[5] Th. M. Radhakrishnman, Z. Phys. Chem. (Frankfurt am Main) 41, 197 (1964).

Molecule: Silicon tetrabromide $SiBr_4$ No. 31
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	249 C	ia	249 (4) p	
e	ν_2	Deg. deform.....	90 C	ia	90 (3)	
f_2	ν_3	Deg. stretch.....	487 C	.....	487 (1)	
	ν_4	Deg. deform.....	137 C	.....	137 (3)	

References

[1] R. B.Trumpy, Z. Phys. 68, 675 (1931).
[2] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[3] R. M. L. Delwaulle, J. Phys. Chem. 56, 355 (1952).
[4] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London), Ser. A,240, 499 (1957).
[5] Th. M. Radhakrishnan, Z. Phys. Chem. (Frankfurt am Main) 35, 247 (1962).

Molecule: Silicon tetraiodide SiI_4 No. 32
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	168 C	ia	168 S, p	
e	ν_2	Deg. deform.....	63 C	ia	63 M, dp	
f_2	ν_3	Deg. stretch.....	405 C	.....	405 W, dp	
	ν_4	Deg. deform.....	94 C	.....	94 S, dp	

Reference

[1] R. M. L. Delwaulle, J. Phys. Chem. 56, 355 (1952).
[2] R. M. L. Delwaulle and F. François, J. Phys. Radium 15, 206 (1954).

Molecule: Germane GeH_4 No. 33
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.....	2106 B	ia	2106 S, p	
e	ν_2	Deg. deform.....	931 D	ia,[a]930.9	920 W	
f_2	ν_3	Deg. stretch.....	2114 B	2113.6	2106 W (liquid)	
	ν_4	Deg. deform.....	819 B	819.3	816 W (liquid)	

[a] Observed in the infrared through Coriolis interaction with ν_4.

References

[1] IR. J. W. Straley, C. H. Tindal, and H. H. Nielsen, Phys. Rev. 62, 161 (1942).
[2] R. K. Schäfer and J. M. Gonzalez Barredo, Z. Phys. Chem. (Leipzig) 193, 334 (1944.)
[3] IR.R. 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. Phys. Chem. (Frankfurt am Main) 9, 29 (1956).
[5] IR. A. A. Chalmers and D. C. McKean, Spectrochim. Acta 21, 1941 (1965).

Molecule: Germane-d_1 GeH_3D No. 34
Symmetry C_{3v} **Symmetry number** $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	GeH_3 s-stretch	2106 C	.....	2106	
	ν_2	GeD stretch	1520 B	1520.4 M		
	ν_3	GeH_3 s-deform	820 C	820 S		
e	ν_4	GeH_3 d-stretch	2112 B	2112 S		
	ν_5	GeH_3 d-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. Phys. Chem. (Frankfurt am Main) **9**, 29 (1956).

Molecule: Germane-d_2 GeH_2D_2 No. 35
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	GeH_2 s-stretch	2112 C	2112		
	ν_2	GeD_2 s-stretch	1512 C	1512		
	ν_3	GeH_2 scis	881 B	881		
	ν_4	GeD_2 scis	620 C	620		
a_2	ν_5	GeH_2 twist	807 E	807		
b_1	ν_6	GeH_2 a-stretch	2112 C	2112		
	ν_7	GeH_2 rock	657 C	657		
b_2	ν_8	GeD_2 a-stretch	1522 C	1522		
	ν_9	GeH_2 wag	770 C	770		

Reference

[1] IR. L. P. Lindeman and M. K. Wilson, Z. Phys. Chem. (Frankfurtam Main) 9, 29 (1956).

Molecule: Germane-d_3 $GeHD_3$ No. 36
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	GeH stretch	2112 B	2112.4		
	ν_2	GeD_3 s-stretch	1504 B	.....	1504	
	ν_3	GeD_3 s-deform	595 C	595		
e	ν_4	GeD_2 d-stretch	1522 C	1522		
	ν_5	GeH bend	792 B	792.3		
	ν_6	GeD_3 d-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. Phys. Chem. (Frankfurt am Main) 9, 29 (1956).

Molecule: Germane-d_4 GeD_4 No. 37
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch	1504 C	ia	1504	
e	ν_2	Deg. deform	665 D	ia,[a]665 W		
f_2	ν_3	Deg. stretch	1522 B	1522.2 S		
	ν_4	Deg. deform	596 C	596 S		

[a] Observed in the infrared through Coriolis interaction with ν_4.

Reference

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

Molecule: Germanium tetrachloride $GeCl_4$ No. 38
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	396 C	.....	396 (10)	
e	ν_2	Deg. deform.....	134 C	.....	134 (6)	
f_2	ν_3	Deg. stretch.....	453 C	.....	453 (1)	
	ν_4	Deg. deform.....	172 C	.....	172 (6)	

References

[1] R. R. R. Haun and W. D. Harkins, J. Amer. Chem. Soc. 54, 3917 (1932).
[2] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London), Ser. A, 240, 499 (1957).

Molecule: Germanium tetrabromide $GeBr_4$ No. 39
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	235 C	.....	235	
e	ν_2	Deg. deform.....	79 C	.....	79	
f_2	ν_3	Deg. stretch.....	327 C	.....	327	
	ν_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), Ser. A, 240, 499 (1957).

Molecule: Tin tetrachloride $SnCl_4$ No. 40
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	366 C	ia	366 (10)	
e	ν_2	Deg. deform.....	104 C	ia	104 (5)	
f_2	ν_3	Deg. stretch.....	403 C	.....	403 (6)	
	ν_4	Deg. deform.....	134 C	.....	134 (6)	

References

[1] R. R. Haun and W. D. Harkins, J. Amer. Chem. Soc. 54, 3917 (1932).
[2] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London), Ser. A, 240, 499 (1957).

Molecule: Tin tetrabromide $SnBr_4$ No. 41
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	220 C	ia	220 (4)	
e	ν_2	Deg. deform.....	64 C	ia	64 (2)	
f_2	ν_3	Deg. stretch.....	279 C	.....	279 (3)	
	ν_4	Deg. deform.....	88 C	.....	88 (4)	

References

[1] R. B. Trumpy, Z. Phys. 68, 675 (1931).
[2] R. R. R. Haun and W. D. Harkins, J. Amer. Chem. Soc. 54, 3917 (1932).
[3] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London), Ser. A, 240, 499 (1957).

Molecule: Silyl fluoride SiH_3F No. 42
Symmetry C_{3v} Symmetry number $\sigma = 3$

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

[a] The band center was reestimated by Duncan on the basis of the data of Newman et al. [3].

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. 43
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiH_3 s-stretch	2201 D	2201	.....	OV (ν_4).
	ν_2	SiH_3 s-deform	949 D	949	.....	OV (ν_5).
	ν_3	SiCl stretch	551 C	551 S		
e	ν_4	SiH_3 d-stretch	2195 B	2195 S		
	ν_5	SiH_3 d-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, C. R. **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. 44
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	SiH_3 s-stretch	2200 D	2200	.....	OV (ν_4).
	ν_2	SiH_3 s-deform	930 C	930 S		
	ν_3	SiBr stretch	430 C	430 M		
e	ν_4	SiH_3 d-stretch	2196 C	2196 S		
	ν_5	SiH_3 d-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: Bromotrichlorosilane $SiBrCl_3$ No. 45
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	$SiCl_3$ s-stretch	545 C	.....	545 W, p	
	ν_2	SiBr stretch	368 C	.....	368 S, p	
	ν_3	$SiCl_3$ s-deform	191 C	.....	191 M, p	
e	ν_4	$SiCl_3$ d-stretch	610 C	.....	610 M, dp	
	ν_5	$SiCl_3$ rock	205 C	.....	205 M, dp	
	ν_6	$SiCl_3$ d-deform	135 C	.....	135 M, dp	

References

[1] R. M. L. Delwaulle, M. B. Buisset, and M. Delhaye, J. Amer. Chem. Soc. **74**, 5768 (1952).
[2] R. M. L. Delwaulle, J. Phys. Chem. **56**, 355 (1952).
[3] Th. Y. Kakiuchi, Bull. Chem. Soc. Japan **26**, 260 (1953).

Molecule: Trichloroiodosilane $SiCl_3I$ No. 46
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	$SiCl_3$ s-stretch	519 C		519 W, p	
	ν_2	SiI stretch	333 C		333 S, p	
	ν_3	$SiCl_3$ s-deform	169 C		169 M, p	
e	ν_4	$SiCl_3$ d-stretch	600 C		600 W, dp	
	ν_5	$SiCl_3$ rock	197 C		197 W, dp	
	ν_6	$SiCl_3$ d-deform	123 C		123 M, dp	

References

See No. 45.

Molecule: Tribromochlorosilane $SiBr_3Cl$ No. 47
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	SiCl stretch	579 C		579 W, p	
	ν_2	$SiBr_3$ s-stretch	288 C		288 S, p	
	ν_3	$SiBr_3$ s-deform	159 C		159 M, p	
e	ν_4	$SiBr_3$ d-stretch	498 C		498 M, dp	
	ν_5	$SiBr_3$ d-deform	173 C		173 W, dp	
	ν_6	SiCl bend	101 C		101 M, dp	

References

See No. 45.

Molecule: Chlorotriiodosilane $SiClI_3$ No. 48
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	SiCl stretch	557 C		557 W, p	
	ν_2	SiI_3 s-stretch	220 C		220 S, p	
	ν_3	SiI_3 s-deform	114 C		114 S, p	
e	ν_4	SiI_3 d-stretch	411 C		411 W, dp	
	ν_5	SiI_3 d-deform	134 C		134 W, dp	
	ν_6	SiCl bend	73 C		73 S, dp	

References

See No. 45.

Molecule: Dibromodichlorosilane $SiBr_2Cl_2$ No. 49
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	$SiCl_2$ s-stretch	563 C		563 M, p	
	ν_2	$SiBr_2$ s-stretch	326 C		326 S, p	
	ν_3	$SiCl_2$ scis	182 C		182 S, p	
	ν_4	$SiBr_2$ scis	111 C		111 M, p	
a_2	ν_5	$SiCl_2$ twist	122 C		122 M, p	
b_1	ν_6	$SiCl_2$ a-stretch	605 C		605 W, dp	
	ν_7	$SiCl_2$ rock	191 E		191 VW	
b_2	ν_8	$SiBr_2$ a-stretch	508 C		508 W, dp	
	ν_9	$SiBr_2$ rock	174 C		174 W, dp	

References

See No. 45.

Molecule: Sulfur hexafluoride SF_6 No. 50
Symmetry O_h Symmetry number $\sigma = 24$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.....	774 B	ia	773.5 VS	
e_g	ν_2	Deg. stretch.....	642 B	ia	641.7 W	
f_{1u}	ν_3	Deg. stretch.....	948 C	947.5	ia	
	ν_4	Deg. deform.....	616 C	615.5	ia	
f_{2g}	ν_5	Deg. deform.....	525 C	ia	525 W	
f_{2u}	ν_6	Deg. deform.....	347 E	ia	ia	OC ($2\nu_6$) [3].

References

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

Molecule: Selenium hexafluoride SeF_6 No. 51
Symmetry O_h Symmetry number $\sigma = 24$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.....	707 B	ia	706.9 VS	
e_g	ν_2	Deg. stretch.....	659 B	ia	658.7 W	
f_{1u}	ν_3	Deg. stretch.....	780 C	780	ia	
	ν_4	Deg. deform.....	437 C	437	ia	
f_{2g}	ν_5	Deg. deform.....	405 C	ia	405 W	
f_{2u}	ν_6	Deg. deform.....	264 E	ia	ia	OC ($2\nu_6$) [3].

References

[1] IR.R. B. Weinstock and G. L. Goodman, Advan. Chem. Phys. 9, 169 (1966), and references cited there.
[2] IR. S. Abramowitz and I. W. Levin, Inorg. Chem. 6, 538 (1967).
[3] R. H. H. Claassen, G. L. Goodman, J. H. Holloway, and H. Selig, J. Chem. Phys. 53, 341 (1970).

Molecule: Molybdenum hexafluoride MoF_6 No. 52
Symmetry O_h Symmetry number $\sigma = 24$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.....	742 B	ia	741.5 VS, p	
e_g	ν_2	Deg. stretch.....	652 B	ia	651.6 W, dp	
f_{1u}	ν_3	Deg. stretch.....	741 C	741 VS	ia	
	ν_4	Deg. deform.....	264 C	264 S	ia	
f_{2g}	ν_5	Deg. deform.....	318 C	ia	318 W, dp	
f_{2u}	ν_6	Deg. deform.....	116 E	ia	ia	OC ($2\nu_6$) [3].

References

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[3] R. H. H. Claassen, G. L. Goodman, J. H. Holloway, and H. Selig, J. Chem. Phys. 53, 341 (1970).

Molecule: Tungsten hexafluoride WF_6 No. 53
Symmetry O_h Symmetry number $\sigma = 24$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.....	771 B	ia	771.0 VS, p	
e_g	ν_2	Deg. stretch.....	677 B	ia	677.2 W, dp	
f_{1u}	ν_3	Deg. stretch.....	712 C	712 VS	ia	
	ν_4	Deg. deform.....	258 C	258 S	ia	
f_{2g}	ν_5	Deg. deform.....	320 C	ia	320 W, dp	
f_{2u}	ν_6	Deg. deform.....	127 E	ia	ia	OC ($2\nu_6$) [3].

References

[1] IR.R. B. Weinstock and G. L. Goodman, Advan. Chem. Phys. 9, 169 (1966), and references cited there.
[2] IR. S. Abramowitz and I. W. Levin, Inorg. Chem. 6, 538 (1967).
[3] R. H. H. Claassen and H. Selig, Israel J. Chem. 7, 499 (1969).

Molecule: Uranium hexafluoride UF_6 No. 54
Symmetry O_h Symmetry number $\sigma = 24$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.....	667 B	ia	667.1 VS	
e_g	ν_2	Deg. stretch.....	533 B	ia	532.5 W	
f_{1u}	ν_3	Deg. stretch.....	626 C	626	ia	
	ν_4	Deg. deform.....	186 C	186.2	ia	
f_{2g}	ν_5	Deg. deform.....	202 C	ia	202 W	
f_{2u}	ν_6	Deg. deform.....	142 E	ia	ia	OC ($2\nu_6$) [3].

References

[1] IR.R. B. Weinstock and G. L. Goodman, Advan. Chem. Phys. 9, 169 (1966), and references cited there.
[2] IR. B. Frice and H. H. Claassen, J. Chem. Phys. 46, 4603 (1967).
[3] R. H. H. Claassen, G. L. Goodman, J. H. Halloway, and H. Selig, J. Chem. Phys. 53, 341 (1970).

Molecule: Diborane $^{10}B_2H_6$ No. 55
Symmetry D_{2h} Symmetry number $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	BH_2 s-stretch	2537 C	ia	2537 VS	
	ν_2	Ring stretch	2110 C	ia	2110 S	
	ν_3	BH_2 scis	1186 C	ia	1186 M	
	ν_4	Ring deform	816 C	ia	816 S	
a_u	ν_5	BH_2 twist	833 C	ia, [a]833.1 VW	ia	
b_{1g}	ν_6	Ring stretch	1768 C	ia	1768 W	
	ν_7	BH_2 wag	850 E	ia	.....	OC ($\nu_7 + \nu_{10}$).
b_{1u}	ν_8	BH_2 a-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 a-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}	Ring stretch	1920 E	1882 M, (1992 W)	ia	FR ($\nu_9 + \nu_{15}$).
	ν_{14}	BH_2 wag	977 C	977 S	ia	
b_{3g}	ν_{15}	BH_2 twist	1012 E	ia	.....	CF.[b]
b_{3u}	ν_{16}	BH_2 s-stretch	2528 C	2528 VS	ia	
	ν_{17}	Ring deform	1606 C	1606 VS	ia	
	ν_{18}	BH_2 scis	1181 C	1181 VS	ia	

[a] Observed very weakly and also confirmed by combination bands.
[b] Estimated 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).
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[4] IR. W. C. Price, J. Chem. Phys. 16, 894 (1948).
[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. Nelsen, J. Chem. Phys. 19, 1 (1951).
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[11] IR. W. L. Smith and I. M. Mills, J. Chem. Phys. 41, 1479 (1964).

Molecule: **Diborane** $^{11}B_2H_6$ No. 56
Symmetry D_{2h} **Symmetry number** $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	BH_2 s-stretch	2524 C	ia	2524 (10) p	
	ν_2	Ring stretch	2104 C	ia	2104 (10) p	
	ν_3	BH_2 scis	1180 C	ia	1180 (7)	
	ν_4	Ring deform	794 C	ia	794 (10) p	
a_u	ν_5	BH_2 twist	833 C	ia, [a]833.1 VW	ia	
b_{1g}	ν_6	Ring stretch	1768 E	ia	1788 (1) dp 1747 (1) dp	FR ($\nu_5 + \nu_9$).
	ν_7	BH_2 wag	850 E	ia	.....	OC ($\nu_7 + \nu_{10}$).
b_{1u}	ν_8	BH_2 a-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 a-stretch	2591 C	ia	2591 (9) dp	
	ν_{12}	BH_2 rock	915 E	ia	.....	OC ($\nu_{10} + \nu_{12}$).
b_{2u}	ν_{13}	Ring stretch	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 s-stretch	2525 C	2525 VS	ia	
	ν_{17}	Ring deform	1602 C	1602 VS	ia	
	ν_{18}	BH_2 scis	1177 C	1177 VS	ia	

[a] Observed very weakly and also confirmed by combination bands.

References

See No. 55.

Molecule **Diborane-d_6** $^{10}B_2D_6$ No. 57

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	BD_2 s-stretch	1860 E	ia	1880 VS, p 1833 S, p	FR ($2\nu_3$).
	ν_2	Ring stretch	1511 C	ia	1511 VS, p	
	ν_3	BD_2 scis	929 C	ia	929 p	
	ν_4	Ring deform	726 C	ia	726 VS, p	
a_u	ν_5	BD_2 twist	592 D	[a]592 VW	ia	
b_{1g}	ν_6	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 a-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	262 M	ia	
b_{2g}	ν_{11}	BD_2 a-stretch	1980 E	ia	1975 (9) dp (2000 (5))dp	
	ν_{12}	BD_2 rock	740 E	ia	.....	OC ($\nu_{10} + \nu_{12}$).
b_{2u}	ν_{13}	Ring stretch	1465 E	1491 M 1459 MS	ia	FR ($\nu_5 + \nu_7$).
	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 s-stretch	1845 C	1857 VS (1799 S)	ia	FR ($\nu_3 + \nu_{18}$).
	ν_{17}	Ring deform	1205 C	1205 VS	ia	
	ν_{18}	BD_2 scis	881 C	881 VS	ia	

[a] Observed very weakly and also confirmed by combination bands.

References

[1] IR. A. N. Webb, J. T. Neu, and K. S. Pitzer, J. Chem. Phys. **17**, 1007 (1949).
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[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).

Molecule: Carbon dioxide $^{12}C^{16}O_2$ No. 58
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	Sym. stretch.....	1333 C	ia	1388.15 1285.40	FR ($2\nu_2$).
π_u	ν_2	Bend.....	667 A	667.38 S	ia	
σ_u^+	ν_3	Antisym. stretch.....	2349 A	2349.16 VS	ia	

References

[1] IR. E. K. Plyler, L. R. Blaine, and E. D. Tidwell, J. Res. NBS **55**, 183 (1955).
[2] IR. C. P. Courtoy, Can. J. Phys. **35**, 608 (1957).
[3] R. B. P. Stoicheff, Can. J. Phys. **36**, 218 (1958).
[4] IR. C. P. Courtoy, Ann. Sci. Soc. Bruxelles (1) **73**, 5 (1959).
[5] Th. G. A. Amat and M. Pimbert, J. Mol. Spectrosc. **16**, 278 (1965).
[6] IR. H. R. Gordon and T. K. McCubbin, Jr., J. Mol. Spectrosc. **18**, 73 (1965); **19**, 137 (1966).
[7] IR. A. Chedin and Z. Cihla, Cah. Phys. **21**, 129 (1967).

Molecule: Carbon dioxide $^{13}C^{16}O_2$ No. 59
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	Sym. stretch.....	1334 C	ia	1369.90 1266.03	FR ($2\nu_2$).
π_u	ν_2	Bend.....	649 A	648.91 S	ia	
σ_u^+	ν_3	Antisym. stretch.....	2283 A	2283.48 VS	ia	

References

[1] R. B. P. Stoicheff, Can. J. Phys. **35**, 608 (1957).
[2] IR. C. P. Courtoy, Ann. Sci. Soc. Bruxelles (1), **73**, 5 (1959).
[3] Th. G. Amat and M. Pimbert, J. Mol. Spectrosc. **16**, 278 (1965).
[4] Th. I. Suzuki, J. Mol. Spectrosc. **25**, 479 (1968).

Molecule: Carbon disulfide $^{12}C^{32}S_2$ No. 60
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	Sym. stretch.....	658 A	ia	657.98	
π_u	ν_2	Bend.....	397 B	396.8	ia	
σ_u^+	ν_3	Antisym. stretch.....	1535 B	1535.35	ia	

References

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[2] R. B. P. Stoicheff, Can. J. Phys. 36, 218 (1958).
[3] IR. D. Ager, E. K. Plyler, and E. D. Tidwell, J. Res. Nat. Bur. Stand. (U.S.), 66A (Phys. and Chem.) No. 3, 259–264 (1962).

Molecule: Carbonyl sulfide $^{12}C^{16}O^{32}S$ No. 61
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ^+	ν_1	CO stretch.....	2062 A	2062.22	2050 W	
π	ν_2	Bend.....	520 A	520.41	521 W dp	
σ^+	ν_3	CS stretch.....	859 B	858.95	858 M p	

References

[1] R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik," 6. Auflage, I. Band, Atom-und Molekularphysik, 2. Teil, Molekeln I. (Springer-Verlag, Berlin, Göttingen, Heidelberg, 1951).
[2] IR. A. G. Maki, E. K. Plyler, and E. D. Tidwell, J. Res. Nat. Bur. Stand. (U.S.), 66A, (Phys. and Chem.) No. 2, 163–167 (1962).

Molecule: Hydrogen cyanide HCN No. 62
Symmetry $C_{\infty v}$ Symmetry number $\delta = 1$

Sym. species	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	3311.47 S	3313 W	
π	ν_2	Bend	712 A	711.98 VS	712 W	
σ^+	ν_3	CN stretch	2097 A	2096.85 W	2089 S	

References

[1] R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik," 6. Auflage, I. Band, Atom-und Molekularphysik, 2. Teil, Molekeln I. (Springer-Verlag, Berlin, Göttingen, Heidelberg, 1951).
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[3] IR. A. G. Maki and L. R. Blaine, J. Mol. Spectrosc. 12, 45 (1964).

Molecule: Deuterium cyanide DCN No. 63
Symmetry $C_{\infty v}$ Symmetry number $\delta = 1$

Sym. species	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	2630.30 S	2630	
π	ν_2	Bend	569 A	569.04 VS	569	
σ^+	ν_3	CN stretch	1925 A	1925.26 W	1906	

References

[1] R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik," 6. Auflage, I. Band, Atom-und Molekularphysik, 2. Teil, Molekeln I. (Springer-Verlag, Berlin, Göttingen, Heidelberg, 1951).
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[3] IR. A. G. Maki, E. K. Plyler, and R. Thibault, J. Opt. Soc. Amer. 54, 869 (1964).

Molecule: Cyanogen chloride $^{35}ClCN$ No. 64
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ^+	ν_1	CN stretch	2216 A	2215.6 VS	2206 (10)	
π	ν_2	Bend	378 A	380 S	394 (3)	RP [2].
σ^+	ν_3	CCl stretch	744 C	782.6 S 714.0 S	730 (5)	FR ($2\nu_2$) [2].

References

[1] IR.R. W. O. Freitag and E. R. Nixon, J. Chem. Phys. 24, 109 (1956), and references cited there.
[2] IR. W. J. Lafferty, D. R. Lide, and R. A. Toth, J. Chem. Phys. 43, 2063 (1965).

Molecule: Cyanogen chloride $^{37}ClCN$ No. 65
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ^+	ν_1	CN stretch	2215 A	2215.3 VS	2206 (10)	
π	ν_2	Bend	378 A	380 S	394 (3)	RP [2].
σ^+	ν_3	CCl stretch	736 C	.....	730 (5)	FR ($2\nu_2$) [2].

References

See No. 64.

Molecule: Cyanogen bromide $^{79}BrCN$ No. 66
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ^+	ν_1	CN stretch	2198 A	2198.3	2191	
π	ν_2	Bend	342 A	341.5	357	RP [2].
σ^+	ν_3	CBr stretch	575 C	575	568	

References

[1] IR.R. W. O. Freitag and E. R. Nixon, J. Chem. Phys. **24**, 109 (1956), and references cited there.
[2] IR. A. G. Maki and C. T. Gott, J. Chem. Phys. **36**, 2282 (1962).
[3] IR. A. G. Maki, J. Chem. Phys. **38**, 1261 (1963).

Molecule: Cyanogen bromide $^{81}BrCN$ No. 67
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
σ^+	ν_1	CN stretch	2198 A	2198.3	2191	
π	ν_2	Bend	342 A	341.5	357	RP [2].
σ^+	ν_3	CBr stretch	575 C	575	568	

References

See No. 66.

Molecule: Formaldehyde H_2CO No. 68
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_2 s-stretch	2783 A	2782.5 S	2781.6 S	
	ν_2	CO stretch	1746 A	1746.1 VS	1742.3 W	
	ν_3	CH_2 scis	1500 A	1500.1 S	1499.7 M	
b_1	ν_4	CH_2 a-stretch	2843 A	2843.1 VS	2866 W	
	ν_5	CH_2 rock	1249 A	1249.1 S		
b_2	ν_6	CH_2 wag	1167 A	1167.3 S		

References

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Molecule: Formaldehyde-d_1 HDCO No. 69
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'	ν_1	CH stretch	2844 D	2844.1 S	2846.2 S	FR ($\nu_3 + \nu_5$).
	ν_2	CD stretch	2121 D	2120.7 S	2120.3 S	FR ($2\nu_6$, $2\nu_5$).
	ν_3	CO stretch	1723 A	1723.4 VS	1723.2 VS	
	ν_4	CHD scis	1400 B	1400.0 S	1397.4 M	
	ν_5	CHD rock	1041 D	1041 S		
a''	ν_6	CHD wag	1074 C	1074 S		

Reference

[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. 70
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_2 s-stretch	2056 D	2056.4 S	.....	FR ($2\nu_3$).
	ν_2	CO stretch	1700 B	1700 VS		
	ν_3	CD_2 scis	1106 C	1106.0 S		
b_1	ν_4	CD_2 a-stretch	2160 C	2160.3 VS		
	ν_5	CD_2 rock	990 C	990.2 S		
b_2	ν_6	CD_2 wag	938 E	938 S		

Reference

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

Molecule: Methane CH_4 No. 71
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch	2917 A	ia	2917.0	
e	ν_2	Deg. deform	1534 A	ia, [a]1533	1533.6	
f_2	ν_3	Deg. stretch	3019 A	3018.9	3019.5	
	ν_4	Deg. deform	1306 C	1306.2		

[a] Observed in the infrared through Coriolis interaction with ν_4 [5].

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[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
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Molecule: Methane-d_1 CH_3D No. 72
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_3 s-stretch.....	2945 E	2973 M 2914 M	.....	FR ($2\nu_5$).
	ν_2	CD stretch.....	2200 A	2200.0 M		
	ν_3	CH_3 s-deform.....	1300 C	1300 M	1306	
e	ν_4	CH_3 d-stretch.....	3017 B	3016.9 S		
	ν_5	CH_3 d-deform	1471 C	1471 W		
	ν_6	CH_3 rock.....	1155 C	1155 M	1156	

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Molecule: Methane-d_2 CH_2D_2 No. 73
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_2 s-stretch.....	2974 C	2976 M	2974	
	ν_2	CD_2 s-stretch.....	2202 C	2202 W		
	ν_3	CH_2 scis.....	1436 C	1436 W		
	ν_4	CD_2 scis.....	1033 C	1033 S	1034	
a_2	ν_5	CH_2 twist.....	1333 C	ia, [a]1329 W	1333	
b_1	ν_6	CH_2 a-stretch.....	3013 C	3013 S		
	ν_7	CH_2 rock.....	1090 C	1090 S	1090	
b_2	ν_8	CD_2 a-stretch.....	2234 C	2234 M		
	ν_9	CH_2 wag.....	1234 C	1234 M		

[a] Observed in the infrared through Coriolis interaction with ν_9.

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
[2] IR. J. K. Wilmshurst and H. J. Bernstein, Can. J. Chem. 35, 226 (1957).

Molecule: Methane-d_3 CHD_3 No. 74
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH stretch	2993 C	2993 M		
	ν_2	CD_3 s-stretch	2142 C	2142 M	2141	
	ν_3	CD_3 s-deform	1003 C	1003 M		
e	ν_4	CD_3 d-stretch	2263 C	2263 M	2269	
	ν_5	CD_3 rock	1291 C	1291 M	1299	
	ν_6	CD_3 d-deform	1036 C	1036 S	1046	

References

See No. 73.

Molecule: Methane-d_4 CD_4 No. 75
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch	2109 B	ia	2108.9	
e	ν_2	Deg. deform	1092 B	ia, [a]1092	1091.9	
f_2	ν_3	Deg. stretch	2259 A	2259.3	2259.3	
	ν_4	Deg. deform	996 B	996.0		

[a] Observed in the infrared through Coriolis interaction with ν_4 [5].

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[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
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Molecule: Carbon tetrafluoride CF_4 No. 76
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	Sym. stretch.....	909 B	ia	908.5 S	
e	ν_2	Deg. deform.....	435 B	ia	435.0 S	
f_2	ν_3	Deg. stretch.....	1281 D	1282.6 VS 1260.9 VW	1283.0 W 1263 VW	FR ($2\nu_4$).
	ν_4	Deg. deform.....	632 B	631.73 VS	631.2 S	

References

[1] R. D. M. Yost, E. N. Lassettre, and S. T. Gross, J. Chem. Phys. 4, 325 (1936).
[2] IR. C. R. Baeley, J. B. Hale, and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 167, 555 (1938).
[3] IR.Th. E. K. Plyler and W. S. Benedict, J. Res. NBS 47, 202 (1951), RP 2245.
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[5] IR.Th. W. F. Edgell and R. E. Moynihan, J. Chem. Phys. 27, 155 (1957).
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Molecule: Carbon tetrachloride CCl_4 No. 77
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	Sym. stretch.....	459 C	ia	458.7 (10) p	
e	ν_2	Deg. deform.....	217 C	ia	217.0 (7) dp	
f_2	ν_3	Deg. stretch.....	776 E	789 VS 768 VS	790.4 (4) dp 761.7 (4) dp	FR ($\nu_1 + \nu_4$).
	ν_4	Deg. deform.....	314 C	309.9 W (liquid)	313.5 (9) dp	

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] R. J. P. Zietlow, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. 18, 1076 (1950).
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Molecule: Carbon tetrabromide CBr_4 No. 78
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Benzene soln.)	
a_1	ν_1	Sym. stretch.....	267 C	ia	267 (7) p	
e	ν_2	Deg. deform.....	122 C	ia	122 (10) dp	
f_2	ν_3	Deg. stretch.....	672 C	672 VS	671 (1) dp	
	ν_4	Deg. deform.....	182 C	.....	182 (4) dp	

References

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Molecule: Carbon tetraiodide CI_4 No. 79
Symmetry T_d Symmetry number $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Solid)	
a_1	ν_1	Sym. stretch.....	178 D	ia	178 (10)	
e	ν_2	Deg. deform.....	90 D	ia	90 (4)	
f_2	ν_3	Deg. stretch.....	555 D	555 VS		
	ν_4	Deg. deform.....	125 E	[a] 123 W, 127 W	123 (5)	

[a] Crystal field splitting.

Reference

[1] IR.R. H. Stammreich, Y. Tovares, and D. Bassi, Spectrochim. Acta 17, 661 (1961).

Molecule: Methylfluoride CH_3F No. 80
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch	2930 E	2964 VS 2863 S	.....	FR ($2\nu_5$).
	ν_2	CH_3 s-deform	1464 A	1464 S		
	ν_3	CF stretch	1049 A	1048.6 S		
e	ν_4	CH_3 d-stretch	3006 A	3005.8 S		
	ν_5	CH_3 d-deform	1467 A	1466.5 M		
	ν_6	CH_3 rock	1182 A	1182.4 M		

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[1] IR. K. P. Yates and H. H. Nielsen, Phys. Rev. **71**, 349 (1947).
[2] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London), **Ser. A, 222,** 443 (1954).
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Molecule: Methylfluoride-d_3 CD_3F No. 81
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch	2110 E	2090 2150	.....	FR ($2\nu_5$).
	ν_2	CD_3 s-deform	1136 A	1136		
	ν_3	CF stretch	991 A	991		
e	ν_4	CD_3 d-stretch	2258 A	2258		
	ν_5	CD_3 d-deform	1072 A	1072		
	ν_6	CD_3 rock	903 A	903		

References

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[2] IR. W. F. Edgell and L. Parts, J. Amer. Chem. Soc. **78**, 2358 (1956).
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Molecule: Methylchloride CH_3Cl No. 82
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 s-stretch	2937 E	2967.78 M 2879.28 M	2955 VS, p 2861 M	FR ($2\nu_5$).
	ν_2	CH_3 s-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 d-stretch	3039 B	3039.31 S 3042.75 S	3036 M, dp	FR ($3\nu_6$) [6, 8].
	ν_5	CH_3 d-deform	1452 A	1452.1 M	1446 W, dp	
	ν_6	CH_3 rock	1017 A	1017.3 M	1016 W, dp	

References

[1] R. J. Wagner, Z. Phys. Chem. **B40,** 439 (1938).
[2] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London), **Ser. A, 222,** 443 (1954).
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Molecule: Methylchloride-d_3 CD_3Cl No. 83
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch	2160 A	2160.28 S		
	ν_2	CD_3 s-deform	1029 A	1028.7 S		
	ν_3	CCl stretch	701 A	701.4 S		
e	ν_4	CD_3 d-stretch	2283 A	2283.3 S		
	ν_5	CD_3 d-deform	1060 A	1059.9 M		
	ν_6	CD_3 rock	768 A	767.6 M		

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Molecule: Methylbromide CH_3Br No. 84
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 s-stretch	2935 E	2972 M 2862.1 M	2972 VS 2862 W	FR ($2\nu_5$).
	ν_2	CH_3 s-deform	1306 A	1305.9 S	1309 W	
	ν_3	CBr stretch	611 A	611.1 S	609 S	
e	ν_4	CH_3 d-stretch	3056 A	3056.35 S	3068 VS	
	ν_5	CH_3 d-deform	1443 A	1442.7 M	1456 M	
	ν_6	CH_3 rock	955 A	954.7 M	956 VW	

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[6] IR. T. L. Barnett and T. H. Edwards, J. Mol. Spectrosc. **20,** 352 (1966).

Molecule: Methylbromide-d_3 CD_3Br No. 85
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch	2160 A	2159.8 VS		
	ν_2	CD_3 s-deform	992 A	992.0 VS		
	ν_3	CBr stretch	577 A	576.7 S		
e	ν_4	CD_3 d-stretch	2297 A	2297.3 M		
	ν_5	CD_3 d-deform	1056 A	1055.6 S		
	ν_6	CD_3 rock	713 A	713.0 M		

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[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).
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Molecule: Methyliodide CH_3I No. 86
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch	2933 E	2969.8 M 2861.0 M	.....	FR ($2\nu_5$).
	ν_2	CH_3 s-deform	1252 A	1251.5 S		
	ν_3	CI stretch	533 A	532.8 S		
e	ν_4	CH_3 d-stretch	3060 A	3060.06 S		
	ν_5	CH_3 d-deform	1436 C	1435.5 M	.....	FR ($\nu_3 + \nu_6$).
	ν_6	CH_3 rock	882 A	882.4 M		

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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 and H. W. Thompson, Proc. Roy. Soc. (London), **Ser. A, 288**, 50 (1965).
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[5] IR. T. L. Barnett and T. H. Edwards, J. Mol. Spectrosc. **23**, 302 (1967).

Molecule: Methyliodide-d_3 CD_3I No. 87
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch	2130 E	2155.1 2081.0	.....	FR ($2\nu_5$).
	ν_2	CD_3 s-deform	951 A	950.7		
	ν_3	CI stretch	501 A	501.4		
e	ν_4	CD_3 d-stretch	2298 A	2298		
	ν_5	CD_3 d-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), **Ser. A, 288**, 39 (1965).
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[4] IR. R. W. Peterson and T. H. Edwards, J. Mol. Spectrosc. **38**, 1 (1971).

Molecule: Trifluoromethane CHF_3 No. 88
Symmetry C_{3v} Symmetry number $\sigma = 3$

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

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[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).
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Molecule: Trichloromethane $CHCl_3$ No. 89
Symmetry C_{3v} Symmetry number $\sigma = 3$

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

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[5] IR. I. Suzuki, unpublished.

Molecule: Trichloromethane-d_1 $CDCl_3$ No. 90
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD stretch	2266 C	2266 W	2255 (2) p	
	ν_2	CCl_3 s-stretch	659 B	658.5 S	649 (7) p	
	ν_3	CCl_3 s-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 d-stretch	749 B	748.5 VS	735 (2) dp	
	ν_6	CCl_3 d-deform	262 C	262 W (liquid)	262 (10) dp	

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[3] IR. R. B. Bernstein, A. G. Gordus, and F. F. Cleveland, J. Chem. Phys. **20**, 1979 (1952).
[4] IR. I. Suzuki, unpublished.

Molecule: Tribromomethane $CHBr_3$ No. 91
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3042 B	3042 M	3017 (6) p	
	ν_2	CBr_3 s-stretch	541 B	541 M	540 (4) p	
	ν_3	CBr_3 s-deform	222 C	.....	222 (10) p	
e	ν_4	CH bend	1149 B	1149 VS	1143 (2) dp	
	ν_5	CBr_3 d-stretch	669 B	669 VS	655 (2) dp	
	ν_6	CBr d-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: Tribromomethane-d_1 $CDBr_3$ No. 92
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	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 s-stretch	521 C	521 M	519.3 (7)	
	ν_3	CBr_3 s-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 d-stretch	632 C	632 VS	628.5 (5)	
	ν_6	CBr_3 d-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.

Molecule: Bromotrichloromethane $CBrCl_3$ No. 93
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CCl_3 s-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 s-deform	247 C	.....	247.3 (5) p	
e	ν_4	CCl_3 d-stretch	775 C	773 VS	775.3 (1) dp	
	ν_5	CBr bend	295 C	294 W	295.0 (3) dp	
	ν_6	CCl_3 d-deform	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: Tribromochloromethane CBr_3Cl No. 94
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (CS_2, C_7H_{14} soln.)	cm^{-1} (C_6H_6, CCl_4 soln.)	
a_1	ν_1	CCl stretch	747 C	747 S (CS_2 soln.)	748 (1)	
	ν_2	CBr_3 s-stretch	329 C	329 W (C_7H_{14} soln.)	326 (10) p	
	ν_3	CBr_3 s-deform	210 C	.....	210 (10) p	
e	ν_4	CBr_3 d-stretch	675 C	675 S (CS_2 soln.)	677 (4) dp	
	ν_5	CCl bend	211 E	.....	.....	CF [1].
	ν_6	CBr_3 d-deform	141 C	.....	141 (7) 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, 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. Amer. Chem. Soc. 74, 5768 (1952).
[4] R. R. H. Krupp, S. M. Ferogle, and A. Weber, J. Chem. Phys. 24, 355 (1956).

Molecule: Dichloromethane CH_2Cl_2 No. 95
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_2 s-stretch	2999 B	2999 M	2996 S, p	
	ν_2	CH_2 scis	1467 C	1467 W	1430.1 W, p	
	ν_3	CCl_2 s-stretch	717 B	717 M	713 S, p	
	ν_4	CCl_2 scis	282 B	284 (liquid)	281.5 M, p	
a_2	ν_5	CH_2 twist	1153 B	[a]ia	1153 VW	
b_1	ν_6	CH_2 a-stretch	3040 B	3045 (liquid)	3040 S, dp	
	ν_7	CH_2 rock	898 B	897.7 M	893 VW	
b_2	ν_8	CH_2 wag	1268 B	1268 S	1265 (liquid)	
	ν_9	CCl_2 a-stretch	758 B	758 VS		

[a] In the spectrum of liquid CH_2Cl_2, a weak band is found at 1156 cm^{-1}, which may be assigned to ν_5.

References

[1] R. H. L. Welsh, M. F. Crawford, T. R. Thomas, and C. R. Love, Can. J. Phys. 30, 577 (1952).
[2] IR. T. Shimanouchi and I. Suzuki, J. Mol. Spectrosc. 8, 222 (1962).
[3] IR.R. F. E. Palma, E. A. Piotrowski, S. Sundaram, and F. F. Cleveland, J. Mol. Spectrosc. 13, 119 (1964).

Molecule: Dichloromethane-d_1 $CHDCl_2$ No. 96
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch	3024 B	3024	3019 M, p	
	ν_2	CD stretch	2249 B	2249	2246 M, p	
	ν_3	CH bend	1282 B	1282	1276 VW	
	ν_4	CD bend	778 C	778 (liquid)	779 W, p	
	ν_5	CCl_2 s-stretch	692 B	692	682 S, p	
	ν_6	CCl_2 scis	283 B	.....	283 M, p	
a''	ν_7	CH bend	1223 A	1222.9	1221 VW	
	ν_8	CD bend	890 A	889.8	886 VW	
	ν_9	CCl_2 a-stretch	738 B	738	725 W, dp	

References

[1] IR. T. Shimanouchi and I. Suzuki, J. Mol. Spectrosc, 8, 222 (1962).
[2] IR.R. F. E. Palma, E. A. Piotrowski, S. Sundaram, and F. F. Cleveland, J. Mol. Spectrosc. 13, 119 (1964).

Molecule: Dichloromethane-d_2 CD_2Cl_2 No. 97
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_2 s-stretch	2205 B	2205 W	2198 M, p	
	ν_2	CD_2 scis	1052 D	.....	1052 VW, p	
	ν_3	CCl_2 s-stretch	687 B	687 M	677 VS, p	
	ν_4	CCl_2 scis	282 C	.....	282 S, p	
a_2	ν_5	CD_2 twist	826 C	ia	826 VW	
b_1	ν_6	CD_2 a-stretch	2304 C	2304 (liquid)	2304 VW	
	ν_7	CD_2 rock	[a]712 D	.....	.....	OV (ν_9).
b_2	ν_8	CD_2 wag	957 B	957 VS		
	ν_9	CCl_2 a-stretch	727 B	727 VS	716 W	

[a] Calculated from product rule [1].

References

[1] IR. T. Shimanouchi and I. Suzuki, J. Mol. Spectrosc. 8, 222 (1962).
[2] IR.R. F. E. Palma, E. A. Piotrowski, S. Sundaram, and F. F. Cleveland, J. Mol. Spectrosc. 13, 119 (1964).

Molecule: Dibromomethane CH_2Br_2 No. 98
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_2 s-stretch	3009 C	3009 W	3008 (1)	
	ν_2	CH_2 scis	1382 C	1382 VW	1402 (0)	
	ν_3	CBr_2 s-stretch	588 C	588 M	584 (10)	
	ν_4	CBr_2 scis	169 C	.....	169 (10)	
a_2	ν_5	CH_2 twist	1095 D	ia	[a]1095	
b_1	ν_6	CH_2 a-stretch	3073 B	3073 VW	[a]3064	
	ν_7	CH_2 rock	812 B	812 M	[a]813	
b_2	ν_8	CH_2 wag	1195 B	1195 VS	[a]1194	
	ν_9	CBr a-stretch	653 B	653 VS	640 (0)	

[a] Liquid.

References

[1] R. J. Wagner, Z. Phys. 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.R. R. S. Dennen, E. A. Piotrowski, and F. F. Cleveland, J. Chem. Phys. 49, 4385 (1968).

Molecule: Dibromomethane-d_1 $CHDBr_2$ No. 99
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch	3040 C	3040 W	3028 VW, p	
	ν_2	CD stretch	2249 D	2249 W (liquid)	2245 W, p	
	ν_3	CH bend	1220 C	701 W	1239 W, p	
	ν_4	CD bend	701 C	1220 W	702 M, p	
	ν_5	CBr_2 s-stretch	565 C	565 VW	561 S, p	
	ν_6	CBr_2 scis	172 D	.....	172 VS, p	
a''	ν_7	CH bend	1154 B	1154 VS		
	ν_8	CD bend	838 B	838 VS	835 VW, dp	
	ν_9	CBr_2 a-stretch	632 B	632 VS	623 W, dp	

References

[1] IR.R. R. S. Dennen, E. A. Piotrowski, and F. F. Cleveland, J. Chem. Phys. 49, 4385 (1968).

Molecule: Dibromomethane-d_2 CD_2Br_2 No. 100
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_2 s-stretch	2214 C	2214 W	2195 M, p	
	ν_2	CD_2 scis	1026 D	1026 (liquid)	1028 W, p	
	ν_3	CBr_2 s-stretch	559 C	559 M	551 S, p	
	ν_4	CBr_2 scis	172 D	.....	172 VS, p	
a_2	ν_5	CD_2 twist	782 D	ia	782 W, p	
b_1	ν_6	CD_2 a-stretch	2324 C	2324 W	2313 VW, dp	
	ν_7	CD_2 rock	625 B	625 VS	636 VW	
b_2	ν_8	CD_2 wag	907 B	907 VS	902 W, dp	
	ν_9	CBr_2 a-stretch	608 C	608 (liquid)	612 M, dp	

References

[1] R. B. Trumpy, Z. Phys. **100**, 250 (1936).
[2] IR.R. R. S. Dennen, E. A. Piotrowski, and F. F. Cleveland, J. Chem. Phys. **49**, 4385 (1968).

Molecule: Dibromodichloromethane CBr_2Cl_2 No. 101
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CCl_2 s-stretch	733 C	733 VS	734 (1) p	
	ν_2	CBr_2 s-stretch	380 C	377 W	380 (10) p	
	ν_3	CCl_2 scis	242 C	.....	242 (6) p	
	ν_4	CBr_2 scis	154 C	.....	154 (4) p	
a_2	ν_5	CCl_2 twist	175 C	ia	175 (2) dp	
b_1	ν_6	CBr_2 a-stretch	683 C	683 VS	684 (3) dp	
	ν_7	CCl_2 wag	229 C	.....	229 (2) dp	
b_2	ν_8	CCl_2 a-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] IR.R. A. Davis, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **20**, 454 (1952).

Molecule: Bromochloromethane CH_2BrCl No. 102
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_2 s-stretch	3003 A	3003 S	2986 M, p	
	ν_2	CH_2 scis	1482 E	[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	CBrCl scis	229 C	.....	229 S, p	
a''	ν_7	CH_2 a-stretch	3066 B	3066 W	3055 M, dp	
	ν_8	CH_2 twist	1128 C	1128 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 N. 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. Spectrosc. 15, 319 (1965).
[4] IR. I. Suzuki, unpublished.

Molecule: Bromochloromethane-d_1 CHDBrCl No. 103
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a	ν_1	CH stretch	3031 C	3031 S (liquid)	3024 S, p	
	ν_2	CD stretch	2252 C	2252 M (liquid)	2246 S, p	
	ν_3	CH bend	1262 C	1262 S (liquid)	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 scis	228 C	.....	228 S, p	

Reference

[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. Spectrosc. 15, 319 (1965).

Molecule: Bromochloromethane-d_2 CD_2BrCl No. 104
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CD_2 s-stretch	2208 B	2208 S	2196 M, p	
	ν_2	CD_2 scis	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 scis	226 C	.....	226 S, p	
a''	ν_7	CD_2 a-stretch	2305 C	2302 S (liquid)	2305 W, dp	
	ν_8	CD_2 twist	811 B	811 W	809 W, dp	
	ν_9	CD_2 rock	667 C	668 W (liquid)	667 W, dp	

Reference

See No. 103.

Molecule: Formic acid HCOOH No. 105
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OH stretch	3570 D	3570 M		
	ν_2	CH stretch	2943 C	2942.8 M		
	ν_3	C=O stretch	1770 C	1770 VS		
	ν_4	CH bend	1387 C	1387 VW		
	ν_5	OH bend	1229 C	1229 W		
	ν_6	C−O stretch	1105 C	1105.3 S		
	ν_7	OCO deform	625 C	625 M		
a''	ν_8	CH bend	1033 C	1033 W		
	ν_9	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).
[7] Th. K. Nakamoto and S. Kishida, J. Chem. Phys. **41**, 1554 (1964).

Molecule: Formic acid-d_2 DCOOD — No. 106
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OD stretch	2632 C	2632 W		
	ν_2	CD stretch	2232 C	2231.8 M		
	ν_3	C=O stretch	1742 C	1742 VS		
	ν_4	CD bend	945 C	945 M		
	ν_5	OD bend	1040 C	1040 W		
	ν_6	C−O stretch	1171 C	1171.3 S		
	ν_7	OCO deform	558 C	558 W		
a''	ν_8	CD bend	873 C	873 W		
	ν_9	Torsion	491 C	491 W		

References

See No. 105.

Molecule: Methanol CH_3OH (gas) — No. 107
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'	ν_1	OH stretch	3681 A	3681 M		
	ν_2	CH_3 d-stretch	3000 C	3000 M		
	ν_3	CH_3 s-stretch	2844 A	2844 S		
	ν_4	CH_3 d-deform	1477 B	1477 M	.....	OV (ν_{10})
	ν_5	CH_3 s-deform	1455 A	1455 M		
	ν_6	OH bend	1345 B	1345 S		
	ν_7	CH_3 rock	1060 D	1060 W	.....	OV (ν_8)
	ν_8	CO stretch	1033 A	1033 VS	1032 (2)	
a''	ν_9	CH_3 d-stretch	2960 C	2960 S	2955 (4)	
	ν_{10}	CH_3 d-deform	1477 B	1477 M	.....	OV (ν_4)
	ν_{11}	CH_3 rock	1165 C	.....	1165 (1) (liquid)	
	ν_{12}	Torsion	295 (A) 200 (E)	80∼300	.....	MW:[a] 295 (A) 200 (E)

[a] The value of ν_{12} is undefined because of the large coupling between internal and overall rotations. The MW values quoted are the calculated separations between the lowest rotational levels (J = K = 0) of the ground and first excited torsional states [2, 5].

References

[1] R. J. R. Nielsen and N. E. Ward, J. Chem. Phys. **10**, 81 (1942).
[2] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[3] IR. C. Tanaka, K. Kuratani, and S. Mizushima, Spectrochim. Acta **9**, 265 (1957).
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[7] IR. M. Falk and E. Whalley, J. Chem. Phys. **34**, 1554 (1961) and references cited there.
[8] Th. G. Zerbi, J. Overend, and B. Crawford, J. Chem. Phys. **38**, 122 (1963).
[9] IR.Th. C. Tanaka and T. Shimanouchi, unpublished.

Molecule: Methanol CH_3OH (liquid) No. 108
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a'	ν_1	OH stretch	3328 D	3328 vb	3270 3480	
	ν_2	CH_3 d-stretch	2980 C	2980 M	2993 (3)	
	ν_3	CH_3 s-stretch	2834 C	2834 S	2834 (10)	
	ν_4	CH_3 d-deform	1480 C	1480 M	1464 (5b)	OV (ν_{10}).
	ν_5	CH_3 s-deform	1450 C	1450 M		
	ν_6	OH bend	1418 C	1418 M, b		
	ν_7	CH_3 rock	1115 C	1115 M	1107 (2)	
	ν_8	CO stretch	1030 C	1030 VS	1033 (6)	
a''	ν_9	CH_3 d-stretch	2946 C	2946 S	2940 (9)	
	ν_{10}	CH_3 d-deform	1480 C	1480 M	1464 (5b)	OV (ν_4).
	ν_{11}	CH_3 rock	1165 C	.....	1165 (1)	
	ν_{12}	Torsion	655 D	655 vb		

References

[1] R. S. Mizushima, Y. Morino, and G. Okamoto, Bull. Chem. Soc. Japan 11, 698 (1936).
[2] R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecule, (Van Nostrand, New York, 1945).
[3] IR.R. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961), and references cited there.
[4] IR.Th. C. Tanaka and T. Shimanouchi, unpublished.

Molecule: Methanol-d_1 CH_3OD(gas) No. 109
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OD stretch	2718 A	2718 M		
	ν_2	CH_3 d-stretch	3000 C	3000 M	.....	SF (ν_2 of CH_3OH).
	ν_3	CH_3 s-stretch	2843 A	2843 S		
	ν_4	CH_3 d-deform	1473 B	1473 M	.....	OV (ν_{10}).
	ν_5	CH_3 s-deform	1456 A	1456 M		
	ν_6	OD bend	864 A	864 S		
	ν_7	CH_3 rock	1230 B	1230 W		
	ν_8	CO stretch	1040 A	1040 VS		
a''	ν_9	CH_3 d-stretch	2960 C	2960 S	.....	SF (ν_9 of CH_3OH).
	ν_{10}	CH_3 d-deform	1473 B	1473 M	.....	OV (ν_4).
	ν_{11}	CH_3 rock	1160 C	1160 VW		
	ν_{12}	Torsion	213 E	.....	.....	CF [5, 6].

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Molecule: Methanol-d_1 CH_3OD (liquid) No. 110
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a'	ν_1	OD stretch	2467 D	2467 vb	2420–2560	
	ν_2	CH_3 d-stretch	2978 M	2978 M	2992 (3)	
	ν_3	CH_3 s-stretch	2838 C	2838 S	2834 (10)	
	ν_4	CH_3 d-deform	1469 C	1469 M	1463 (5b)	OV (ν_{10}).
	ν_5	CH_3 s-deform	1449 C	1449 M		
	ν_6	OD bend	940 C	940 M, b	955 (1)	
	ν_7	CH_3 rock	1231 C	1231 W	1226 (0)	
	ν_8	CO stretch	1038 C	1038 VS	1029 (6)	
a''	ν_9	CH_3 d-stretch	2951 C	2951 S	2943 (9)	
	ν_{10}	CH_3 d-deform	1469 C	1469 M	1463 (5b)	OV (ν_4).
	ν_{11}	CH_3 rock	1163 C	.....	1163 (1)	
	ν_{12}	Torsion	475 D	475 vb		

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Molecule: Methanol-d_3 CD_3OH (gas) No. 111
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OH stretch	3690 D	3690 S		
	ν_2	CD_3 d-stretch	2260 E	2260 M, sh		
	ν_3	CD_3 s-stretch	2077 C	2077 S		
	ν_4	CD_3 d-deform	1047 D	1047 W		
	ν_5	CD_3 s-deform	1134 C	1134 VS		
	ν_6	OH bend	1297 C	1297 VS		
	ν_7	CD_3 rock	858 C	858 M		
	ν_8	CO stretch	988 C	988 VS		
a''	ν_9	CD_3 d-stretch	2235 D	2235 S		
	ν_{10}	CD_3 d-deform	1075 C	1075 W		
	ν_{11}	CD_3 rock	877 D	877 M		
	ν_{12}	Torsion	256 E			CF [1, 3].

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Molecule: Methanol-d_3 CD_3OH (liquid) No. 112
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a'	ν_1	OH stretch	3310 D	3310 S, vb	3350 W, vb	
	ν_2	CD_3 d-stretch	2235 D	[a]2235 M	2230 M, dp	
	ν_3	CD_3 s-stretch	2078 C	2078 S	2074 VS, p	
	ν_4	CD_3 d-deform	1069 C	1069 W	1072 M, dp	OV (ν_{10}).
	ν_5	CD_3 s-deform	1122 C	1122 VS	1127 M, p	
	ν_6	OH bend	1391 C	1391 S, b	1360 VW, vb	
	ν_7	CD_3 rock	882 C	882 M	894 M, dp	OV (ν_{11}).
	ν_8	CO stretch	982 C	982 VS	986 VS, p	
a''	ν_9	CD_3 d-stretch	2213 D	[a]2213 M	2213 VW	
	ν_{10}	CD_3 d-deform	1069 C	1069 W	1072 M, dp	OV (ν_4).
	ν_{11}	CD_3 rock	882 D	882 M	894 M, dp	OV (ν_7).
	ν_{12}	Torsion	665 D	665 S, vb		

[a] The value obtained in the vitreous solid (−180 °C).

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[2] Th. C. Tanaka and T. Shimanouchi, unpublished.

Molecule: Methanol-d_4 CD_3OD (gas) No. 113
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OD stretch	2724 D	2724 S		
	ν_2	CD_3 d-stretch	2260 E	2260	.....	SF (ν_2 of CD_3OH).
	ν_3	CD_3 s-stretch	2080 C	2080 S		
	ν_4	CD_3 d-deform	1024 D	1024 W		
	ν_5	CD_3 s-deform	1135 C	1135 VS		
	ν_6	OD bend	1060 D	1060 W		
	ν_7	CD_3 rock	776 C	776 S		
	ν_8	CO stretch	983 C	983 VS		
a''	ν_9	CD_3 d-stretch	2228 D	2228 S		
	ν_{10}	CD_3 d-deform	1080 C	1080 W		
	ν_{11}	CD_3 rock	892 C	892 W		
	ν_{12}	Torsion	196 E	.....	.....	CF [1, 3].

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Molecule: Methylamine CH_3NH_2 No. 114
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'	ν_1	NH_2 s-stretch	3361 B	3361 W	3360 VS	
	ν_2	CH_3 d-stretch	2961 B	2961 VS	2960 VS	
	ν_3	CH_3 s-stretch	2820 B	2820 VS	2820 S	
	ν_4	NH_2 scis	1623 B	1623 S		
	ν_5	CH_3 d-deform	1473 B	1473 S	1460 M	
	ν_6	CH_3 s-deform	1430 B	1430 M		
	ν_7	CH_3 rock	1130 A	1130 M		
	ν_8	CN stretch	1044 A	1044 S	1044 S	
	ν_9	NH_2 wag	780 A	780 VS	781 W	
a''	ν_{10}	NH_2 a-stretch	3427 C	3427 W	3470 W	
	ν_{11}	CH_3 d-stretch	2985 C	2985 VS		
	ν_{12}	CH_3 d-deform	1485 D	[a]1485		
	ν_{13}	NH_2 twist	1419 D	.....	.....	CF [5].
	ν_{14}	CH_3 rock	1195 D	[a]1195		
	ν_{15}	Torsion	268 B	268	.....	MW: 272 (A). 265 (E).

[a] Estimated from ^RQ branch frequency.

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Molecule: Methylamine-d_2 CH_3ND_2
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a'	ν_1	ND_2 s-stretch	2479 B	2479 W	2450 S	
	ν_2	CH_3 d-stretch	2961 B	2961 VS	2969 M	
	ν_3	CH_3 s-stretch	2817 B	2817 S	2824 M	
	ν_4	ND_2 scis	1234 B	1234 S	1214 M	
	ν_5	CH_3 d-deform	1468 B	1468 S	1473 M	
	ν_6	CH_3 s-deform	1430 B	1430 M		
	ν_7	CH_3 rock	1117 A	1117 S		
	ν_8	CN stretch	997 A	997 S	995 S	
	ν_9	ND_2 wag	625 A	625 VS		
a''	ν_{10}	ND_2 a-stretch	2556 B	2556 M	2527 M	
	ν_{11}	CH_3 d-stretch	2985 C	2985 VS		
	ν_{12}	CH_3 d-deform	1485 D	[a]1485		
	ν_{13}	ND_2 twist	1058 E	.....	.....	CF [5].
	ν_{14}	CH_3 rock	1187 C	1187 M		
	ν_{15}	Torsion	228 C	228 S		

[a] Estimated from ^RQ branch frequency.

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Molecule: Methylamine-d_3 CD_3NH_2 No. 116
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	NH_2 s-stretch	3361 B	3361 W		
	ν_2	CD_3 d-stretch	2203 B	2203 VS		
	ν_3	CD_3 s-stretch	2077 A	2077 VS		
	ν_4	NH_2 scis	1624 B	1624 S		
	ν_5	CD_3 d-deform	1065 D	.....	.....	CF [3].
	ν_6	CD_3 s-deform	1142 A	1142 S		
	ν_7	CD_3 rock	913 A	913 S		
	ν_8	CN stretch	973 B	973 M		
	ν_9	NH_2 wag	740 A	740 VS		
a''	ν_{10}	NH_2 a-stretch	3427 C	3427 W		
	ν_{11}	CD_3 d-stretch	2236 C	2236 VS		
	ν_{12}	CD_3 d-deform	1077 C	1077 W		
	ν_{13}	NH_2 twist	1416 C	1416 W		
	ν_{14}	CD_3 rock	926 D	.....	.....	CF [3].
	ν_{15}	Torsion	247 D	.....	.....	CF [3].

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Molecule: Methylamine-d_5 CD_3ND_2 No. 117
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	ND_2 s-stretch	2477 B	2477 W		
	ν_2	CD_3 d-stretch	2202 B	2202 VS		
	ν_3	CD_3 s-stretch	2073 B	2073 VS		
	ν_4	ND_2 scis	1227 B	1227 S		
	ν_5	CD_3 d-deform	1065 D	.....	.....	CF [2.]
	ν_6	CD_3 s-deform	1123 B	1123 M		
	ν_7	CD_3 rock	880 B	880 M		
	ν_8	CN stretch	942 A	942 S		
	ν_9	ND_2 wag	601 A	601 VS		
a''	ν_{10}	ND_2 a-stretch	2556 C	2556 W		
	ν_{11}	CD_3 d-stretch	2238 C	2238 VS		
	ν_{12}	CD_3 d-deform	1077 C	1077 W		
	ν_{13}	ND_2 twist	1072 D	.....	.....	CF [2].
	ν_{14}	CD_3 rock	910 B	910 M		
	ν_{15}	Torsion	201 C	.....	.....	CF [2]. MW: 200 (A). 203 (E).

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Molecule: Acetylene CHCH No. 118
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	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 S 3281.9 VS	ia	FR ($\nu_2 + \nu_4 + \nu_5$).
π_g	ν_4	CH bend	612 C	ia	611.8 VW	
π_u	ν_5	CH bend	730 A	730.3 VS	ia	

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Molecule: Acetylene-d_1 CHCD No. 119
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ^+	ν_1	CH stretch	3336 A	3335.6 S	3335 S	
	ν_2	CC stretch	1854 A	1853.8 M	1851 S	
	ν_3	CD stretch	2584 A	2583.6 S		
π	ν_4	CH bend	518 A	518.38 S	.....	RP [4].
	ν_5	CD bend	678 A	677.8 S	.....	RP [4].

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Molecule: Acetylene-d_2 CDCD No. 120
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	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	2439.24 S	ia	
π_g	ν_4	CD bend	505 C	ia	.....	OC ($\nu_4 + \nu_5$) [1].
π_u	ν_5	CD bend	537 A	536.9 VS	ia	

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Molecule: Fluoroacetylene CHCF No. 121
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	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	CC stretch	2255 B	2255 VS		
	ν_3	CF stretch	1055 B	1055 VS		
π	ν_4	CH bend	578 B	578 VS		
	ν_5	CCF bend	367 B	367 M		

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Molecule: Chloroacetylene CHCCl No. 122
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	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	CC stretch	2110 B	2110 VS		
	ν_3	CCl stretch	756 B	756 VS		
π	ν_4	CH bend	604 B	604 S		
	ν_5	CCCl bend	326 B	326 W		

References

See No. 121.

Molecule: Bromoacetylene CHCBr No. 123
Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

Sym. species	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	CC stretch	2085 B	2085 VS		
	ν_3	CBr stretch	618 C	618 VS	.....	SF (ν_4).
π	ν_4	CH bend	618 C	618 VS	.....	SF (ν_3).
	ν_5	CCBr bend	295 B	295 W		

References

See No. 121.

Molecule: Ethylene CH_2CH_2 No. 124
Symmetry D_{2h} **Symmetry number** $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	CH_2 s-stretch	3026 B	ia	3026.4 (10)p	
	ν_2	CC stretch	1623 D	ia	1622.6 (8)p	FR ($2\nu_{10}$).
	ν_3	CH_2 scis	1342 B	ia	1342.2 (10)p	
a_u	ν_4	CH_2 twist	1023 E	ia	ia	OC ($\nu_4 + \nu_6$) [7].
b_{1g}	ν_5	CH_2 a-stretch	3103 B	ia	3102.5 (1)dp	
	ν_6	CH_2 rock	1236 C	ia	1236 (1)dp (liquid)	
b_{1u}	ν_7	CH_2 wag	949 A	949.3 M	ia	
b_{2g}	ν_8	CH_2 wag	943 C	ia	943 (1)dp (liquid)	
b_{2u}	ν_9	CH_2 a-stretch	3106 B	3105.5 S	ia	
	ν_{10}	CH_2 rock	826 A	826.0 W	ia	
b_{3u}	ν_{11}	CH_2 s-stretch	2989 A	2988.66 S	ia	
	ν_{12}	CH_2 scis	1444 B	1443.5 S	ia	

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Molecule: Ethylene-d_4 C_2D_4 No. 125
Symmetry D_{2h} Symmetry number $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CD_2 s-stretch	2251 C	ia	2251 VS	
	ν_2	CC stretch	1515 C	ia	1515 VS	
	ν_3	CD_2 scis	981 C	ia	981 M	
a_u	ν_4	CD_2 twist	728 E	ia	ia	CF [4].
b_{1g}	ν_5	CD_2 a-stretch	2304 C	ia	2304 W	
	ν_6	CD_2 rock	1009 E	ia	.....	OC ($\nu_6 + \nu_{10}$).
b_{1u}	ν_7	CD_2 wag	720 B	720.0 VS	ia	
b_{2g}	ν_8	CD_2 wag	780 C	ia	780 W	
b_{2u}	ν_9	CD a-stretch	2345 C	2345 S	ia	
	ν_{10}	CD_2 rock	586 E	.....	ia	CF.[a]
b_{3u}	ν_{11}	CD_2 a-stretch	2200 C	2200.2 S	ia	
	ν_{12}	CD_2 scis	1078 C	1077.9 S	ia	

[a] From product rule.

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Molecule: Tetrafluoroethylene CF_2CF_2 No. 126
Symmetry D_{2h} Symmetry number $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	CC stretch	1872 C	ia	1872 M, p	
	ν_2	CF_2 s-stretch	778 C	ia	777.9 S, p	
	ν_3	CF_2 scis	394 C	ia	394 W, p	
a_u	ν_4	CF_2 twist	190 E	ia	ia	CF [3].
b_{1g}	ν_5	CF_2 a-stretch	1340 D	ia	1340 VW	
	ν_6	CF_2 rock	551 D	ia	551 M (liquid)	
b_{1u}	ν_7	CF_2 wag	406 C	406 S	ia	
b_{2g}	ν_8	CF_2 wag	508 D	ia	508 S (liquid)	
b_{2u}	ν_9	CF_2 a-stretch	1337 C	1337 S	ia	
	ν_{10}	CF_2 rock	218 C	218 S	ia	
b_{3u}	ν_{11}	CF_2 s-stretch	1186 C	1186 S	ia	
	ν_{12}	CF_2 sciss	558 C	558 S	ia	

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[2] R. A. Monfils and J. Duchesne, J. Chem. Phys. 18, 1415 (1950).
[3] IR. D. E. Mann, N. Acquista, and E. K. Plyler, J. Res. NBS 52, 67 (1954), RP2474.

Molecule: Tetrachloroethylene CCl_2CCl_2 No. 127
Symmetry D_{2h} Symmetry number $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_g	ν_1	CC stretch	1571 D	ia	1571 (7)p	
	ν_2	CCl_2 s-stretch	447 D	ia	447 (10)p	
	ν_3	CCl_2 scis	237 D	ia	237 (7)p	
a_u	ν_4	CCl_2 twist	110 E	ia	ia	OC ($2\nu_4$) [2].
b_{1g}	ν_5	CCl_2 a-stretch	1000 D	ia	1000 (0)	
	ν_6	CCl_2 rock	347 D	ia	347 (4)dp	
b_{1u}	ν_7	CCl_2 wag	288 D	288 M	ia	
b_{2g}	ν_8	CCl_2 wag	512 D	ia	512 (4)dp	
b_{2u}	ν_9	CCl_2 a-stretch	908 C	908 S (CS_2 soln.)	ia	
	ν_{10}	CCl_2 rock	176 C	176 S	ia	
b_{3u}	ν_{11}	CCl_2 s-stretch	777 C	777 S (CS_2 soln.)	ia	
	ν_{12}	CCl_2 scis	310 C	310 W	ia	

References

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[2] IR. D. E. Mann, N. Acquista, and E. K. Plyler, J. Res. NBS **52**, 67 (1954), RP2474.
[3] IR. D. E. Mann, J. H. Meal and E. K. Plyler, J. Chem. Phys. **24**, 1018 (1956).

Molecule: Tetrabromoethylene CBr_2CBr_2 No. 128
Symmetry D_{2h} Symmetry number $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_g	ν_1	CC stretch	1535 E	ia	1547 (2)p 1515 (1)p	FR ($2\nu_9$) [1].
	ν_2	CBr_2 s-stretch	265 D	ia	265 (10)p	
	ν_3	CBr_2 scis	144 D	ia	144 (1)p	
a_u	ν_4	CBr_2 twist	66 E	ia	ia	CF [2].
b_{1g}	ν_5	CBr_2 a-stretch	880 D	ia	880 (1)dp	
	ν_6	CBr_2 rock	208 D	ia	208 (2)dp	
b_{1u}	ν_7	CBr_2 wag	245 C	245 S	ia	
b_{2g}	ν_8	CBr_2 wag	464 D	ia	464 (1)dp	
b_{2u}	ν_9	CBr_2 a-stretch	766 C	766 S	ia	
	ν_{10}	CBr_2 rock	119 C	119 M	ia	
b_{3u}	ν_{11}	CBr_2 s-stretch	635 C	635 S	ia	
	ν_{12}	CBr_2 scis	188 C	188 M	ia	

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[1] R. F. E. Malherbe, G. Allen, and H. J. Bernstein, Can. J. Chem. **31**, 1223 (1953).
[2] IR. D. E. Mann, J. H. Meal, and E. K. Plyler, J. Chem. Phys. **24**, 1018 (1956).

Molecule: cis-1,2-Difluoroethylene CHFCHF No. 129
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH stretch	3135 D	3135 W	.....	SF (ν_8).
	ν_2	CC stretch	1715 C	1715 S		
	ν_3	CH bend	1266 C	1266 S		
	ν_4	CF stretch	1014 C	1014 S		
	ν_5	CCF deform	255 D	255 W		
a_2	ν_6	CH bend	866 E	ia	.....	CF.[a]
	ν_7	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}	CCF deform	768 B	768 S		
b_2	ν_{12}	CH bend	756 B	756 S		

[a] From product rule.

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

References

[1] IR. R. N. Haszeldine and B. R. Steele, J. Chem. Soc. 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. 130
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH stretch	3125 D	3125 W		
	ν_2	CD stretch	2364 D	2364 W		
	ν_3	CC 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	CCF deform	757 B	757 S		
	ν_9	CCF deform	255 D	255 W		
a''	ν_{10}	CH bend	801 B	801 M		
	ν_{11}	CD bend	633 B	633 M		
	ν_{12}	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. 131
Symmetry C_{2v} Symmetry number $\sigma = 2$

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

[a] From product rule.

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

Reference

See No. 130.

Molecule: trans-1,2-Dichloroethylene CHClCHCl No. 132
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CH stretch	3073 C	ia	3073 S, p	
	ν_2	CC stretch	1578 C	ia	1578 S, p	
	ν_3	CH bend	1274 C	ia	1274 S, p	
	ν_4	CCl stretch	846 C	ia	846 S, p	
	ν_5	CCCl deform	350 C	ia	350 S, p	
a_u	ν_6	CH bend	900 B	899.8 VS	ia	
	ν_7	Torsion	227 C	227 M	ia	
b_g	ν_8	CH bend	763 B	ia	763 M, dp	
b_u	ν_9	CH stretch	3090 C	3090 S	ia	
	ν_{10}	CH bend	1200 B	1200 S	ia	
	ν_{11}	CCl stretch	828 B	828 VS	ia	
	ν_{12}	CCCl deform	250 D	250 W	ia	

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR.R. H. J. Bernstein and D. A. Ramsey, J. Chem. Phys. 17, 556 (1949).
[3] IR.R. H. J. Bernstein and A. D. E. Pullin, Can. J. Chem. 30, 963 (1952).
[4] IR.R. K. S. Pitzer and J. L. Hollenberg, J. Amer. Chem. Soc. 76, 1493 (1954).
[5] Th. J. M. Dowling, J. Chem. Phys. 25, 284 (1956).
[6] — — Aoki and T. Shimanouchi, unpublished.

Molecule: trans-1,2-Dichloroethylene-d_1 CHClCDCl No. 133
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch	3087 C	3087 S	3074 M	
	ν_2	CD stretch	2310 C	2310 S	2304 M	
	ν_3	CC stretch	1574 D	1574 W (liquid)	1574 S	
	ν_4	CH bend	1241 C	1241 S	1238 S	
	ν_5	CD bend	963 C	963 VS	957 S	
	ν_6	CCl stretch	823 C	825 VS (liquid)	823 W	
	ν_7	CCl stretch	775 B	775 VS	775 M	
	ν_8	CCCl deform	348 C	.....	348 VS	
	ν_9	CCCl deform	245 E	.....	.....	CF [6].
a''	ν_{10}	CH bend	830 C	830 VS	834 W	
	ν_{11}	CD bend	660 B	660 S	659 W	
	ν_{12}	Torsion	224 E	.....	.....	CF [5, 6].

References

See No. 132.

Molecule: trans-1,2-Dichloroethylene-d_2 CDClCDCl No. 134
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CD stretch	2325 C	ia	2325 S	
	ν_2	CC stretch	1570 C	ia	1570 S	
	ν_3	CD bend	992 C	ia	992 S	
	ν_4	CCl stretch	765 C	ia	765 M	
	ν_5	CCCl deform	346 C	ia	346 S	
a_u	ν_6	CD bend	660 B	660 S	ia	
	ν_7	Torsion	221 E	.....	ia	CF [5, 6].
b_g	ν_8	CD bend	657 C	ia	657 M	
b_u	ν_9	CD stretch	2290 C	2290 S	ia	
	ν_{10}	CD bend	916 C	916 VS	ia	
	ν_{11}	CCl stretch	791 C	791 VS	ia	
	ν_{12}	CCCl deform	240 E	.....	ia	CF [6].

References

See No. 132.

Molecule: cis-1,2-Dichloroethylene CHClCHCl
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

No. 135

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3077 C	.....	3077	
	ν_2	CC stretch	1587 C	1590 S (liquid)	1587 S, p	
	ν_3	CH bend	1179 C	1183 W (liquid)	1179 S, p	
	ν_4	CCl stretch	711 C	714 S (liquid)	711 S, p	
	ν_5	CCCl deform	173 C	.....	173 S, p	
a_2	ν_6	CH bend	876 C	ia	876 W, dp	
	ν_7	Torsion	406 C	ia	406 S, dp	
b_1	ν_8	CH stretch	3072 C	3072		
	ν_9	CH bend	1303 C	1303		
	ν_{10}	CCl stretch	857 B	857		
	ν_{11}	CCCl deform	571 B	571	563 M, dp	
b_2	ν_{12}	CH bend	697 B	697		

References

See No. 132.

Molecule: cis-1,2-Dichloroethylene-d_1 CHClCDCl
Symmetry C_s **Symmetry number** $\sigma = 1$

No. 136

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH stretch	3076 C	3076 S (liquid)	3078 VS	
	ν_2	CD stretch	2306 C	2306 S	2299 VS	
	ν_3	CC stretch	1562 C	1562 S	1553 S	
	ν_4	CH bend	1253 C	1253 VS	1245 M	
	ν_5	CD bend	957 C	957 VS	950 M	
	ν_6	CCl stretch	788 B	788 VS	781 W	
	ν_7	CCl stretch	711 C	711 VS	703 VS	
	ν_8	CCl bend	558 C	558 S	561 S	
	ν_9	CCl bend	175 D	.....	175 VS	
a''	ν_{10}	CH bend	822 C	822 VS	817 W	
	ν_{11}	CD bend	589 C	589 VS	590 W	
	ν_{12}	Torsion	387 C	.....	387 S	

References

See No. 132.

Molecule: cis-1,2-Dichloroethylene-d_2 **CDClCDCl** No. 137
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD stretch	2325 C	.....	2325 S	
	ν_2	CC stretch	1575 C	1575 S	1570 S	
	ν_3	CD bend	850 C	.....	850 M	
	ν_4	CCl stretch	700 C	700 S	689 S	
	ν_5	CCCl deform	171 C	.....	171 S	
a_2	ν_6	CD bend	686 E	ia	.....	CF [6].
	ν_7	Torsion	368 C	ia	368 M	
b_1	ν_8	CD stretch	2280 B	2280	2280 S	
	ν_9	CD bend	1051 B	1051	1040 VS	
	ν_{10}	CCl stretch	766 B	766	761 VS	
	ν_{11}	CCCl deform	558 C	.....	558 S	
b_2	ν_{12}	CD bend	540 C	.....	540 S	

References

See No. 132.

Molecule: trans-1,2-Dichloro-1,2-difluoroethylene **CClFCClF** No. 138
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CC stretch	1707 C	ia	1707 VS, p	
	ν_2	CF stretch	1186 C	ia	1186 W, p	
	ν_3	CCl stretch	632 C	ia	632 M, p	
	ν_4	CF bend	425 C	ia	425 M, p	
	ν_5	CCl bend	288 C	ia	288 M, p	
a_u	ν_6	CFCl wag	333 C	333 M	ia	
	ν_7	Torsion	140 D	.....	ia	CF [2].
b_g	ν_8	CFCl wag	529 C	ia	529 M, dp	
b_u	ν_9	CF stretch	1190 E	1214 VS 1167 VS	ia	FR ($\nu_5 + \nu_{10}$).
	ν_{10}	CCl stretch	892 B	892 VS	ia	
	ν_{11}	CF bend	426 C	426 M	ia	
	ν_{12}	CCl bend	175 C	175 M	ia	

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Molecule: 1,1-Dichloroethylene CH_2CCl_2 No. 139
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 s-stretch	3035 D	[a]3035 W	3035 VS, p	
	ν_2	CC stretch	1627 C	1627 VS	1616 VS, p	
	ν_3	CH_2 scis	1400 C	1400 M	1391 M, p	
	ν_4	CCl_2 s-stretch	603 C	603 VS	601 VS, p	
	ν_5	CCl_2 scis	299 C	299 W	299 S, p	
a_2	ν_6	Torsion	686 D	ia	686 M, dp	
b_1	ν_7	CH_2 a-stretch	3130 D	[a]3130 W	3130 S, dp	
	ν_8	CH_2 rock	1095 C	1095 VS	1088 VW	
	ν_9	CCl_2 a-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	

[a] CCl_4 solution.

References

[1] IR. H. W. Thompson and P. Torkington, Proc. Roy. Soc. (London), **Ser. A, 184,** 21 (1945).
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Molecule: 1,1-Dichloroethylene-d_1 $CHDCCl_2$ No. 140
Symmetry C_s Symmetry number $\sigma = 1$

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

[a] CCl_4 solution.

Reference

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

Molecule: 1,1-Dichloroethylene-d_2 CD_2CCl_2 No. 141
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_2 s-stretch	2262 D	[a]2262 W		
	ν_2	CC stretch	1565 C	1565 VS		
	ν_3	CD_2 scis	1039 E			CF [1].
	ν_4	CCl_2 s-stretch	580 C	580 VS		
	ν_5	CCl_2 scis	305 E			CF [1].
a_2	ν_6	Torsion	488 E	ia		CF [1].
b_1	ν_7	CD_2 a-stretch	2380 D	[a]2380 W		
	ν_8	CD_2 rock	998 C	998 VS		
	ν_9	CCl_2 a-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		

[a] CCl_4 solution.

Reference

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

Molecule: 1,1-Dichloro 2,2-difluoroethylene CF_2CCl_2 No. 142
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CC stretch	1749 B	1749 VS	1738.8 S	
	ν_2	CF stretch	1032 B	1032 VS	1027.6 M	
	ν_3	CCl stretch	622 C	622 M	623.0 S	
	ν_4	CF_2 scis	434 C	434	433.8 VS	
	ν_5	CCl_2 scis	258 C	258 S	258 VS	
a_2	ν_6	Torsion	167 D		167 VW	
b_1	ν_7	CF stretch	1327 B	1327 VS	1313 VW	
	ν_8	CCl stretch	989 B	989 VS	986 VW	
	ν_9	CF_2 rock	459 C	459 VW	454 W	
	ν_{10}	CCl_2 rock	192 C	192	187.8 W	
b_2	ν_{11}	CF_2 wag	564 C	564 S	560.8 VS	
	ν_{12}	CCl_2 wag	323 C	323 W		

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Molecule: Methylcyanide CH_3CN No. 143

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 s-stretch	2954 A	2954.1 M	2942 VS	
	ν_2	CN stretch	2267 A	2266.5 M	2249 S	
	ν_3	CH_3 s-deform	1385 C	.....	1376 M	OC ($\nu_3 + \nu_4$).
	ν_4	CC stretch	920 A	920.2 S	918 S	
e	ν_5	CH_3 d-stretch	3009 A	3009.2 S	2999 S	
	ν_6	CH_3 d-deform	1448 D	1447.9 S	1440 M, b	FR ($\nu_7 + \nu_8$).
	ν_7	CH_3 rock	1041 A	1040.8 M		
	ν_8	CCN bend	362 B	362 S	380 S	

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Molecule: Methylcyanide-d_3 CD_3CN No. 144

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_3 s-stretch	2126 A	2125.6	2112 S	
	ν_2	CN stretch	2278 A	2277.6	2258 S	
	ν_3	CD_3 s-deform	1110 B	1110	1103 W	
	ν_4	CC stretch	831 A	831.3	834 W	
e	ν_5	CD_3 d-stretch	2257 A	2256.6	2258 S	
	ν_6	CD_3 d-deform	1046 A	1046.4	1041 W	
	ν_7	CD_3 rock	847 A	846.6		
	ν_8	CCN bend	331 B	331.2	346 M	

References

[1] IR.R. J. C. Evans and H. J. Bernstein, Can. J. Chem. **33**, 1746 (1955).
[2] IR. W. H. Fletcher and C. S. Shoup, Proceedings of International Symposium on Molecular Structure and Spectroscopy C 204 (Tokyo, 1962).
[3] Th. J. L. Duncan, Spectrochim. Acta **20**, 1197 (1964).

Molecule: Methyl isocyanide CH_3NC No. 145
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 s-stretch	2966 B	2965.8 M	2951 S	
	ν_2	NC stretch	2166 B	2166.0 M	2161 S	
	ν_3	CH_3 s-deform	1429 D	1429	1414 M	
	ν_4	CN stretch	945 B	944.6 M	928 M	
e	ν_5	CH_3 d-stretch	3014 B	3014.3 S	3002 W	
	ν_6	CH_3 d-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	

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[1] IR.R. 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).
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[5] Th. J. L. Duncan, Spectrochim. Acta 20, 1197 (1964).

Molecule: Methyl isocyanide-d_3 CD_3NC No. 146
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch	2251 B	2250.6 W		
	ν_2	NC stretch	2165 B	2165.0 W		
	ν_3	CD_3 s-deform	1117 B	1117.4 W		
	ν_4	CN stretch	877 B	876.7 M		
e	ν_5	CD_3 d-stretch	2263 B	2262.9 S		
	ν_6	CD_3 d-deform	1058 B	1058.2 S		
	ν_7	CD_3 rock	900 B	900.1 S		
	ν_8	CNC bend	249 C	.....	.....	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).
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Molecule: 1,2,5-Oxadiazole $C_2H_2N_2O$ No. 147
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3140 C	3140 VW	3144 VS, p	
	ν_2	ip-Ring II	1418 B	1418 S	1422 VS, p	
	ν_3	ip-Ring III	1316 B	1316 M	1315 VS, p	
	ν_4	CH ip-bend	1038 D	1039 sh	1038 W, p	
	ν_5	ip-Ring IV	1006 B	1006 S	998 M, p	
	ν_6	ip-Ring VII	872 C	872 S	864 M, p	
a_2	ν_7	CH op-bend	824 D	ia, 824 sh (liquid)	824 VW, dp	
	ν_8	op-Ring I	635 E	ia	.....	OC ($2\nu_8$, $\nu_4 + \nu_8$, $\nu_8 + \nu_{12}$).
b_1	ν_9	CH stretch	3133 D	3133 sh (liquid)		
	ν_{10}	ip-Ring I	1546 D	1546 VW (liquid)		
	ν_{11}	CH ip-bend	1177 B	1177 M	1172 VW, dp	
	ν_{12}	ip-Ring V	952 B	952 S	951 W, dp	
	ν_{13}	ip-Ring VI	889 B	889 S		
b_2	ν_{14}	CH op-bend	839 B	839 VS		
	ν_{15}	op-Ring II	631 B	631 W	626 VW, dp	

Reference

[1] IR.R. G. Sbrana, M. Ginanneschi, and M. P. Marzocchi, Spectrochim. Acta **23A**, 1757 (1967).

Molecule: Silylacetylene SiH_3CCH No. 148
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH stretch	3311 B	3311.4 M		
	ν_2	SiH_3 s-stretch	2192 B	2192.4 VS		
	ν_3	CC stretch	2055 B	2054.9 S		
	ν_4	SiH_3 s-deform	935 B	935.3 VS		
	ν_5	SiC stretch	659 D	[a]659 S		
e	ν_6	SiH_3 d-stretch	2193 A	2192.9 VS		
	ν_7	SiH_3 d-deform	946 D	[a]946.4 VS		
	ν_8	SiH_3 rock	685 D	[a]685.4 VS		
	ν_9	CH bend	668 D	[a]668 VS		
	ν_{10}	SiCC deform	220 E	220		

[a] These frequencies are taken from ref. 1. The band centers of ν_5, ν_7, ν_8, and ν_9 given in ref. 2 are different from the values listed in this table by 10–20 cm^{-1}, due to the different assignment of the vibration-rotation lines.

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[1] IR. E. A. V. Ebsworth, S. G. Frankiss, and W. J. Jones, J. Mol. Spectrosc. 13, 9 (1964).
[2] IR. R. B. Reeves, R. E. Wilde, and D. W. Robinson, J. Chem. Phys. 40, 125 (1964).

Molecule: Ethylene oxide C_2H_4O No. 149
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 s-stretch	3006 C	3006 S	3005 S, p	
	ν_2	CH_2 scis	1498 B	1498 W	1490 W, p	
	ν_3	Ring stretch	1271 B	1271 S	1266 S, p	
	ν_4	CH_2 wag	1120 D	1118 W (CS_2 soln.)	1120 M, p	
	ν_5	Ring deform	877 B	877 VS	867 M, dp	
a_2	ν_6	CH_2 a-stretch	3063 D	ia	3063 W, dp	OV (ν_{13}).
	ν_7	CH_2 twist	1300 E	ia		
	ν_8	CH_2 rock	860 E	ia		
b_1	ν_9	CH_2 s-stretch	3006 C	3006 S	3005 S, p	OV (ν_1).
	ν_{10}	CH_2 scis	1472 B	1472 W		
	ν_{11}	CH_2 wag	1151 D	1151 M	1150 W, dp	
	ν_{12}	Ring deform	892 D	892 VS		
b_2	ν_{13}	CH_2 a-stretch	3065 B	3065 S	3063 W, dp	
	ν_{14}	CH_2 twist	1142 D	1142 M	1150 W, dp	
	ν_{15}	CH_2 rock	822 B	822 M	807 M, dp	

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[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
[2] IR.Th. Hs. H. Günthard, B. Messikommer, and M. Kohler, Helv. Chim. Acta 33, 1809 (1950).
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[4] IR. R. C. Lord and B. Nolin, J. Chem. Phys. 24, 656 (1956).
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Molecule: Ethylene oxide-d_4 C_2D_4O No. 150
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_2 s-stretch	2204 C	.....	2204 S	
	ν_2	CD_2 scis	1311 C	1311 M	1301 VS	
	ν_3	Ring stretch	1013 C	1014 W	1013 S	
	ν_4	CD_2 wag	970 C	970 VS	952 M	
	ν_5	Ring deform	755 C	755 VS	755 M	
a_2	ν_6	CD_2 a-stretch	2250 D	ia	2250 W	
	ν_7	CD_2 twist	1083 D	ia	1083 VW	
	ν_8	CD_2 rock	581 D	ia	581 W	
b_1	ν_9	CD_2 s-stretch	2174 C	2174 VS	2157 M	
	ν_{10}	CD_2 scis	1145 D	1145 VW		
	ν_{11}	CD_2 wag	952 D	.....	952 M	
	ν_{12}	Ring deform	809 C	809 S	786 M	
b_2	ν_{13}	CD_2 a-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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[2] IR.R. R. C. Lord and B. Nolin, J. Chem. Phys. **24**, 656 (1956).

Molecule: Acetaldehyde CH_3CHO No. 151
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch	3005 C	3005 M	3001 W	
	ν_2	CH_3 s-stretch	2917 D	.....	2917 S, p	
	ν_3	CH stretch	2822 C	2822 M	2843 W, p	
	ν_4	CO stretch	1743 C	1743 VS	1714 S, p	
	ν_5	CH_3 d-deform	1441 C	1441 S	1426 S	
	ν_6	CH bend	1400 C	1400 S	1391 S	
	ν_7	CH_3 s-deform	1352 C	1352 S	1342 M	
	ν_8	CC stretch	1113 C	1113 S	1109 M, p	
	ν_9	CH_3 rock	919 C	919 M	911 M	
	ν_{10}	CCO deform	509 C	509 S	512 S, p	
a''	ν_{11}	CH_3 d-stretch	2967 C	2967 M	2964 W	
	ν_{12}	CH_3 d-deform	1420 C	1420 S	1426 S, dp	
	ν_{13}	CH_3 rock	867 C	867 M	885 M	
	ν_{14}	CH bend	763 C	763 W	767 M, dp	
	ν_{15}	Torsion	150 C	150 W	.....	MW: 150 (A), 148 (E) [2].

References

[1] IR.R. J. C. Evans and H. J. Bernstein, Can. J. Chem. 34, 1084 (1956).
[2] MW. D. R. Herschbach, J. Chem. Phys. 31, 91 (1959).
[3] IR. W. G. Fateley and F. A. Miller, Spectrochim. Acta 19, 389 (1963).
[4] IR.R.Th. P. Cossee and J. H. Schachtschneider, J. Chem. Phys. 44, 97 (1966).

Molecule: Acetaldehyde-d_1 CH_3CDO No. 152
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch	3028 C	3028 M	2998 W	
	ν_2	CH_3 s-stretch	2917 D	.....	2917 S, p	
	ν_3	CD stretch	2071 C	2071 W	2097 W, p	
	ν_4	CO stretch	1743 C	1743 VS	1702 S, p	
	ν_5	CH_3 d-deform	1442 C	1442 S	1426 S	
	ν_6	CD bend	1109 C	1109 S	1111 S, p	
	ν_7	CD_3 s-deform	1353 C	1353 S	1343 M	
	ν_8	CC stretch	1043 C	1043 W	1080 W	
	ν_9	CH_3 rock	849 C	849 M	858 M	
	ν_{10}	CCO deform	500 C	500 S	505 M, p	
a''	ν_{11}	CH_3 d-stretch	2970 C	2970 M	2965 W	
	ν_{12}	CH_3 d-deform	1420 C	1420 S	1426 S	
	ν_{13}	CH_3 rock	802 C	802 W	820 W, sh	
	ν_{14}	CD bend	668 C	668 W	674 W, dp	
	ν_{15}	Torsion	145 D	145		

References

[1] IR.R. J. C. Evans and H. J. Bernstein, Can. J. Chem. 34, 1084 (1956).
[2] IR.R.Th. P. Cossee and J. H. Schachtschneider, J. Chem. Phys. 44, 97 (1966).

Molecule: Acetaldehyde-d_4 CD_3CDO No. 153
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value o frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CD_3 d-stretch	2265 C	2265 W		
	ν_2	CD_3 s-stretch	2130 C	2130 W	2128	
	ν_3	CD stretch	2060 C	2060 M	2072	
	ν_4	CO stretch	1737 C	1737 VS	1706	
	ν_5	CD_3 d-deform	1045 C	1045 M	1090	
	ν_6	CD bend	938 C	938 M		
	ν_7	CD_3 s-deform	1028 C	1028 M	1024	SF (ν_{12}).
	ν_8	CC stretch	1151 C	1151 S	1153	
	ν_9	CD_3 rock	747 C	747 W	762	
	ν_{10}	CCO deform	436 C	436 S	422.4	
a''	ν_{11}	CD_3 d-stretch	2225 C	2225 W		
	ν_{12}	CD_3 d-deform	1028 C	1028 M	1024	SF (ν_7).
	ν_{13}	CD_3 rock	573 C	573 W		
	ν_{14}	CD bend	670 D	.....	.....	CF [5].
	ν_{15}	Torsion	116 C	116 W	.....	MW [3].

References

[1] R. R. W. Wood, J. Chem. Phys. 4, 536 (1936).
[2] IR.R. J. Carrell Morris, J. Chem. Phys. 11, 230 (1943).
[3] MW. D. R. Herschbach, J. Chem. Phys. 31, 91 (1959).
[4] IR. W. G. Fateley and F. A. Miller, Spectrochim. Acta 19, 389 (1963).
[5] IR.R.Th. P. Cossee and J. H. Schactschneider, J. Chem. Phys. 44, 97 (1966).

Molecule: Ethane CH_3CH_3 No. 154
Symmetry D_{3d} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	CH_3 s-stretch	2954 B	ia	2953.7	
	ν_2	CH_3 s-deform	1388 B	ia	1388.4	
	ν_3	CC stretch	995 A	ia	994.8	
a_{1u}	ν_4	Torsion	289 B	289	ia	
a_{2u}	ν_5	CH_3 s-stretch	2896 B	2895.8	ia	
	ν_6	CH_3 s-deform	1379 A	1379.2	ia	
e_g	ν_7	CH_3 d-stretch	2969 A	ia	2968.7	
	ν_8	CH_3 d-deform	1468 A	ia	1468.1	
	ν_9	CH_3 rock	1190 E	ia	.....	OC [2, 3].
e_u	ν_{10}	CH_3 d-stretch	2985 A	2985.4	ia	
	ν_{11}	CH_3 d-deform	1469 C	1469	ia	FR ($\nu_4 + \nu_{12}$).
	ν_{12}	CH_3 rock	822 A	821.6	ia	

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[3] IR. G. E. Hansen and D. M. Dennison, J. Chem. Phys. **20**, 313 (1952).
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[5] IR.R. R. Van Riet, Bull. Roy. Acad. Belg. **1955**, 188.
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[8] IR. A. R. H. Cole, W. J. Lafferty, and R. J. Thibault, J. Mol. Spectrosc. **29**, 365 (1969).
[9] IR. I. Nakagawa and T. Shimanouchi, J. Mol. Spectrosc. **39**, 255 (1971).

Molecule: Ethane-d_3 CH_3CD_3
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_3 s-stretch.....	2912 E	2955.1 S	2955.5	FR ($2\nu_9$).
				2897.4 S	2898.2	
	ν_2	CD_3 s-stretch.....	2098 E	2139.6 S 2089.7 S	.....	FR ($2\nu_{11}$).
	ν_3	CH_3 s-deform.....	1387 B	1386.6 W		
	ν_4	CD_3 s-deform.....	1122 B	1122.0 W		
	ν_5	CC stretch.....	904 A	903.8 VW	904.7	
a_2	ν_6	Torsion.....	253 B	253 VW		
e	ν_7	CH_3 d-stretch.....	2977 D	2976.5 S	2976.6	
	ν_8	CD_3 d-stretch.....	2240 E	2240 S		
	ν_9	CH_3 d-deform.....	1471 A	1471.1 M		
	ν_{10}	CH_3 rock.....	1115 B	1115.0 W		
	ν_{11}	CD_3 d-deform.....	1066 B	1065.7 M	1062.6	
	ν_{12}	CD_3 rock.....	678 A	678.4 M		

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[2] R. D. E. Shaw and H. L. Welsh, Can. J. Phys. 45, 3823 (1967).
[3] IR. S. Weiss and G. E. Leroi, J. Chem. Phys. 48, 962 (1968).
[4] IR.Th. I. Nakagawa and T. Shimanouchi, J. Mol. Spectrosc. 39, 255 (1971).

Molecule: Ethane-d_6 CD_3CD_3 No. 156
Symmetry D_{3d} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	CD_3 s-stretch	2083 B	ia	2083.0	
	ν_2	CD_3 s-deform	1155 A	ia	1154.5	
	ν_3	CC stretch	843 A	ia	843.0	
a_{1u}	ν_4	Torsion	208 B	208	ia	
a_{2u}	ν_5	CD_3 s-stretch	2087 B	2087.4	ia	
	ν_6	CD_3 s-deform	1077 B	1077.1	ia	
e_g	ν_7	CD_3 d-stretch	2226 A	ia	2225.6	
	ν_8	CD_3 d-deform	1041 B	ia	1041	
	ν_9	CD_3 rock	970 C	ia	970 (liquid)	
e_u	ν_{10}	CD_3 d-stretch	2235 B	2235	ia	
	ν_{11}	CD_3 d-deform	1081 B	1080.9	ia	
	ν_{12}	CD_3 rock	594 A	594.4	ia	

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[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
[2] IR. G. E. Hansen and D. M. Dennison, J. Chem. Phys. **20**, 313 (1952).
[3] IR.R. R. Van Riet, Bull. Roy. Acad. Belg. **1955**, 188.
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[5] IR. S. Weiss and G. E. Leroi, J. Chem. Phys. **48**, 962 (1968).
[6] IR I. Nakagawa and T. Shimanouchi, J. Mol. Spectrosc. **39**, 255 (1971).

Molecule: Hexafluoroethane CF_3CF_3 No. 157
Symmetry D_{3d} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	CC stretch	1228 D	ia	1228	OC.[a]
	ν_2	CF_3 s-stretch	807 C	ia	807 VS, p	
	ν_3	CF_3 s-deform	348 C	ia	348 W, p	
a_{1u}	ν_4	Torsion	68 D	ia	ia	CF[2]
a_{2u}	ν_5	CF_3 s-stretch	1117 B	1117 VS	ia	
	ν_6	CF_3 s-deform	714 B	714 VS	ia	
e_g	ν_7	CF_3 d-stretch	1250 C	ia	1250 VW, dp	
	ν_8	CF_3 d-deform	619 C	ia	619 W, dp	
	ν_9	CF_3 rock	372 C	ia	372 W, dp	
e_u	ν_{10}	CF_3 d-stretch	1251 B	1251 VS	ia	
	ν_{11}	CF_3 d-deform	520 C	520 S	ia	
	ν_{12}	CF_3 rock	220 C	220 S	ia	

[a] Mean value of frequencies obtained from six combination bands [2].

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[2] IR.R. R. A. Carney, Y. A. Piotrowski, A. G. Meister, J. H. Braun, and F. F. Cleveland, J. Mol. Spectrosc. **7**, 209 (1961).
[3] Th. T. Fujiyama and T. Shimanouchi, unpublished.

Molecule: Hexachloroethane CCl_3CCl_3 No. 158
Symmetry D_{3d} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Solid)	
a_{1g}	ν_1	CC stretch	975 C	ia	975 VW, p	
	ν_2	CCl_3 s-stretch	431 C	ia	431 VS, p	
	ν_3	CCl_3 s-deform	170 C	ia	170 W	
a_{1u}	ν_4	Torsion	61 D	ia	ia	OC ($\nu_4+\nu_{10}$, $\nu_4+\nu_{11}$).
a_{2u}	ν_5	CCl_3 s-stretch	675 C	675 S	ia	
	ν_6	CCl_3 s-deform	372 C	372 S	ia	
e_g	ν_7	CCl_3 d-stretch	859 C	ia	859 W	
	ν_8	CCl_3 d-deform	340 C	ia	340 M	
	ν_9	CCl_3 rock	223 C	ia	223 S	
e_u	ν_{10}	CCl_3 d-stretch	778 C	778 VS	ia	
	ν_{11}	CCl_3 d-deform	271 C	271 S	ia	
	ν_{12}	CCl_3 rock	114 C	114 W	ia	

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[1] IR.R. R. A. Carney, E. A. Piotrowski, A. G. Meister, J. H. Braun, and F. F. Cleveland, J. Mol. Spectrosc. **7**, 209 (1961).
[2] IR.R.Th. T. Fujiyama and T. Shimanouchi, unpublished.

Molecule: Hexabromoethane CBr_3CBr_3 No. 159
Symmetry D_{3d} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Solid)	
a_g	ν_1	CC stretch	940 C	ia	940 M	
	ν_2	CBr_3 s-stretch	255 C	ia	255 VS, p	
	ν_3	CBr_3 s-deform	120 C	ia	120 W	
a_{1u}	ν_4	Torsion	51 D	ia	ia	OC ($\nu_4+\nu_{10}$, $\nu_4+\nu_{11}$).
a_{2u}	ν_5	CBr_3 s-stretch	559 C	559 S	ia	
	ν_6	CBr_3 s-deform	254 C	254 S	ia	
e_g	ν_7	CBr_3 d-stretch	768 C	ia	768 M, dp	
	ν_8	CBr_3 d-deform	204 C	ia	204 S, dp	
	ν_9	CBr_3 rock	139 C	ia	139 M	
e_u	ν_{10}	CBr_3 d-stretch	656 C	656 VS	ia	
	ν_{11}	CBr_3 d-deform	168 C	168 S	ia	
	ν_{12}	CBr_3 rock	82 C	82 M	ia	

References

See No. 158.

Molecule: 1,2-Dichloroethane CH_2ClCH_2Cl (trans form) No. 160
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_g	ν_1	CH_2 s-stretch	2957 D	ia	2957 (10) p	
	ν_2	CH_2 scis	1445 C	ia	1445 (4b) dp	
	ν_3	CH_2 wag	1304 C	ia	1304 (6) p	
	ν_4	CC stretch	1052 C	ia	1052 (4) p	
	ν_5	CCl stretch	754 C	ia	754 (10b) p	
	ν_6	CCCl deform	300 C	ia	300 (8) p	
a_u	ν_7	CH_2 a-stretch	3005 D	3005 W (liquid)	ia	SF (gauche ν_1, gauche ν_{11}).
	ν_8	CH_2 twist	1123 B	1122.5 W	ia	
	ν_9	CH_2 rock	773 B	772.5 M	ia	
	ν_{10}	Torsion	123 C	123 M	ia	
b_g	ν_{11}	CH_2 a-stretch	3005 D	ia	3005 (8b) dp	
	ν_{12}	CH_2 twist	1264 C	ia	1264 (3) dp	
	ν_{13}	CH_2 rock	989 C	ia	989 (2) p	
b_u	ν_{14}	CH_2 s-stretch	2983 C	2983.3 M	ia	
	ν_{15}	CH_2 scis	1461 A	1460.6 S	ia	
	ν_{16}	CH_2 wag	1232 B	1232.3 S	ia	
	ν_{17}	CCl stretch	728 C	728.3 VS	ia	
	ν_{18}	CCCl deform	222 C	222.3 W	ia	

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[2] IR.R. S. Mizushima, Y. Morino, I. Watanabe, T. Shimanouchi, and S. Yamaguchi, J. Chem. Phys. 17, 591 (1949).
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[6] IR. I. Ichishima, H. Kamiyama, T. Shimanouchi, and S. Mizushima, J. Chem. Phys. 29, 1190 (1958).
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Molecule: 1,2-Dichloroethane CH_2ClCH_2Cl (gauche form) No. 161
Symmetry C_2 **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a	ν_1	CH_2 a-stretch	3005 D	3005 W (liquid)	3005 (8b) dp	SF (ν_{11}, trans ν_7).
	ν_2	CH_2 s-stretch	2957 D	2957 M (liquid)	2957 (10) p	SF (trans ν_1, trans ν_{14}).
	ν_3	CH_2 scis	1433 C	1433 M (liquid)	1429 (6) dp	OV (ν_{13}).
	ν_4	CH_2 wag	1315 C	1315 W	1304 (6)	
	ν_5	CH_2 twist	1207 C	.....	1207 (5) p	
	ν_6	CC stretch	1027 D	1027 W	1031 (2) dp	
	ν_7	CH_2 rock	948 B	947.7 M	943 (5) p	
	ν_8	CCl stretch	669 C	669 M	654 (8) p	
	ν_9	CCCl deform	272 D	272 VW (liquid)	265 (5) p	
	ν_{10}	Torsion	.....	.....	125 (5b)	
b	ν_{11}	CH_2 a-stretch	3005 D	3005 W	3005 (8b) dp	SF (ν_1, trans ν_7).
	ν_{12}	CH_2 s-stretch	2957 C	2957.2 W		
	ν_{13}	CH_2 scis	1436 B	1436.3 W		
	ν_{14}	CH_2 wag	1292 B	1292.1 S		
	ν_{15}	CH_2 twist	1146 D	1146 VW	1145 (3) dp	
	ν_{16}	CH_2 rock	890 B	890.3 M	881 (4) dp	
	ν_{17}	CCl stretch	693 B	692.5 W	677 (6b) dp	
	ν_{18}	CCCl deform	410 C	409.6 M	411 (5) dp	

References

See No. 160.

Molecule: 1,2-Dibromoethane CH_2BrCH_2Br (trans form) No. 162
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_g	ν_1	CH_2 s-stretch	2972 D	ia	2972 (10) p	
	ν_2	CH_2 scis	1440 C	ia	1440 (5) dp	
	ν_3	CH_2 wag	1255 C	ia	1255 (10b) p	SF (ν_{12}).
	ν_4	CC stretch	1053 C	ia	1053 (9) dp	
	ν_5	CBr stretch	660 C	ia	660 (10b) p	
	ν_6	CCBr deform	190 C	ia	190 (10) p	
a_u	ν_7	CH_2 a-stretch	3037 D	3037 S	ia	
	ν_8	CH_2 twist	1087 C	1087 M	ia	
	ν_9	CH_2 rock	753 C	753 S	ia	
	ν_{10}	Torsion	118 D	118 (gas)	132 (0)	
b_g	ν_{11}	CH_2 a-stretch	3013 D	ia	3013 (4b) dp	
	ν_{12}	CH_2 twist	1255 C	ia	1255 (10b) p	SF (ν_3).
	ν_{13}	CH_2 rock	933 C	ia	933 (2) p	
b_u	ν_{14}	CH_2 s-stretch	2974 D	2974 S	ia	
	ν_{15}	CH_2 scis	1441 D	1441 M	ia	
	ν_{16}	CH_2 wag	1186 C	1186 VS	1186 (0)	
	ν_{17}	CBr stretch	589 C	589 S	ia	
	ν_{18}	CCBr deform	193 D	193	ia	

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[2] IR.R. John T. Neu and Wm. D. Gwinn, J. Chem. Phys. 18, 1642 (1950).
[3] IR.R. J. K. Brown and N. Sheppard, Trans. Faraday Soc. 48, 128 (1952).
[4] IR. I. Ichishima, H. Kamiyama, T. Shimanouchi, and S. Mizushima, J. Chem. Phys. 29, 1190 (1958).

Molecule: 1,2-Dibromoethane CH_2BrCH_2Br (gauche form) No. 163
Symmetry C_2 **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a	ν_1	CH_2 a-stretch	3005 D	.....	3005 (5)	SF (ν_{11}).
	ν_2	CH_2 s-stretch	2953 D	2953 VS	2953 (8) p	SF (ν_{12}).
	ν_3	CH_2 scis	1420 C	1420 M	1419 (3) dp	SF (ν_{13}).
	ν_4	CH_2 wag	1278 C	1278 M	1276 (3)	
	ν_5	CH_2 twist	1104 C	1104 M	1104 (1) dp	SF (ν_{15}).
	ν_6	CC stretch	1019 C	1019 M	1019 (1)	
	ν_7	CH_2 rock	898 C	898 M	899 (3) p	
	ν_8	CBr stretch	550 C	550 M	551 (8)	
	ν_9	CCBr deform	231 C	.....	231 (3) p	
	ν_{10}	Torsion	91 D	.....	91 (2b) dp	
b	ν_{11}	CH_2 a-stretch	3005 D	.....	3005 (5)	SF (ν_1).
	ν_{12}	CH_2 s-stretch	2953 D	2953 VS	2953 (8) p	SF (ν_2).
	ν_{13}	CH_2 scis	1420 C	1420 M	1419 (3) dp	SF (ν_3).
	ν_{14}	CH_2 wag	1245 C	1245 S	1243 (1)	
	ν_{15}	CH_2 twist	1104 C	1104 W	1104 (1) dp	SF (ν_5).
	ν_{16}	CH_2 rock	836 C	836 S	836 (2) dp	
	ν_{17}	CBr stretch	589 C	589 S	583 (6b) dp	
	ν_{18}	CCBr deform	355 C	355	355 (5) dp	

References

See No. 162.

Molecule: 1-Bromo-2-chloroethane CH_2ClCH_2Br (trans form) No. 164
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Liquid)	
a'	ν_1	CH_2 s-stretch	2960 D	.....	2960 (10vb)	SF (ν_2, gauche ν_3, gauche ν_4).
	ν_2	CH_2 s-stretch	2960 D	.....	2960 (10vb)	SF (ν_1, gauche ν_3, gauche ν_4).
	ν_3	CH_2 scis	1446 D	1446 S		
	ν_4	CH_2 scis	1444 C	.....	1444 (3b)	
	ν_5	CH_2 wag	1284 C	1284 M	1284 (7) p	
	ν_6	CH_2 wag	1203 C	1203 S	1203 (3)	
	ν_7	CC stretch	1052 C	1056 M	1052 (4) dp	
	ν_8	CCl stretch	726 C	722 S	726 (10b) p	
	ν_9	CBr stretch	630 C	630 S	630 (9)	
	ν_{10}	CCCl deform	251 C	.....	251 (10) p	SF (gauche ν_{17}).
	ν_{11}	CCBr deform	202 C	202.0 (CCl_4 soln.)	210 (2b)	
a''	ν_{12}	CH_2 a-stretch	3010 D	.....	3010 (3vb)	SF (ν_{13}, gauche ν_1, gauche ν_2).
	ν_{13}	CH_2 a-stretch	3010 D	.....	3010 (3vb)	SF (ν_{12}, gauche ν_1, gauche ν_2).
	ν_{14}	CH_2 twist	1259 C	1258 VW	1259 (3)	
	ν_{15}	CH_2 twist	1111 D	1111 M		
	ν_{16}	CH_2 rock	961 C	961 VW	961 (1b)	
	ν_{17}	CH_2 rock	763 D	763 M		
	ν_{18}	Torsion	123 C	123 (CCl_4 soln.)		

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[2] IR.R. J. K. Brown and N. Sheppard, Trans. Faraday Soc. 48, 128 (1952).
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Molecule: 1-Bromo-2-chloroethane CH_2ClCH_2Br (gauche form) No. 165
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a	ν_1	CH_2 a-stretch	3010 D	.....	3010 (3vb)	SF (ν_2, trans ν_{12}, trans ν_{13}).
	ν_2	CH_2 a-stretch	3010 D	.....	3010 (3vb)	SF (ν_1, trans ν_{12}, trans ν_{13}).
	ν_3	CH_2 s-stretch	2960 D	.....	2960 (10vb)	SF (ν_4, trans ν_1, trans ν_2).
	ν_4	CH_2 s-stretch	2960 D	.....	2960 (10vb)	SF (ν_3, trans ν_1, trans ν_2).
	ν_5	CH_2 scis	1428 D	1428 S	1421 (3b)	OV (ν_6).
	ν_6	CH_2 scis	1428 D	1428 S	1421 (3b)	OV (ν_5).
	ν_7	CH_2 wag	1299 C	1299 S	1299 (1)	
	ν_8	CH_2 wag	1260 C	1260 S	1259 (3)	
	ν_9	CH_2 twist	1190 D	1190 M	1189 (2) p	
	ν_{10}	CH_2 twist	1127 C	1127 M	1128 (1) dp	
	ν_{11}	CC stretch	1025 C	1025 M	1023 (1)	
	ν_{12}	CH_2 rock	923 C	923 S	919 (3) p	
	ν_{13}	CH_2 rock	856 C	856 S	852 (2)	
	ν_{14}	CCl stretch	664 C	664 S	665 (6)	
	ν_{15}	CBr stretch	571 C	571 S	568 (9) p	
	ν_{16}	CCCl deform	385 C	.....	385 (3) dp	
	ν_{17}	CCBr deform	251 D	.....	251 (10)	SF (trans ν_{10}).
	ν_{18}	Torsion	107 D	.....	107 (2b)	

References

See No. 164.

Molecule: Fluoroethane CH_3CH_2F No. 166
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch	3003 D	3003 VS	2986 VS, dp	OV (ν_{12}, ν_{13}).
	ν_2	CH_2 s-stretch	2941 D	2941	2941 VS, p	
	ν_3	CH_3 s-stretch	2915 D	2915 S	2921 M	
	ν_4	CH_2 scis	1479 C	1479 M	1480 W, b, dp	
	ν_5	CH_3 d-deform	1449 D	1449 S	1458 M, b, dp	OV (ν_{14}).
	ν_6	CH_3 s-deform	1395 C	1395 S	1393 W, p	
	ν_7	CH_2 wag	1365 D	1365 M (liquid)	1365 VW	
	ν_8	CH_3 rock	1108 C	1108 VS	1103 S, p	
	ν_9	CC stretch	1048 D	1048 VS	1041 M, b, dp	OV (ν_{16}).
	ν_{10}	CF stretch	880 B	880 VS	873 VS, p	
	ν_{11}	CCF deform	415 C	415	419 W, p	
a''	ν_{12}	CH_2 a-stretch	3003 D	3003 VS	2986 VS, dp	OV (ν_1, ν_{13}).
	ν_{13}	CH_3 d-stretch	3003 D	3003 VS	2986 VS, dp	OV (ν_1, ν_{12}).
	ν_{14}	CH_3 d-deform	1449 D	1449 S	1458 M, b, dp	OV (ν_5).
	ν_{15}	CH_2 twist	1277 C	1277	1276 W, b, dp	
	ν_{16}	CH_3 rock	1048 D	1048 VS	1041 M, b, dp	OV (ν_9).
	ν_{17}	CH_2 rock	810 C	810 W	815 WV	
	ν_{18}	Torsion	243 B	243		

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[2] IR. E. Catalano and K. S. Pitzer, J. Phys. Chem. **62**, 873 (1958).
[3] IR. G. Sage and W. Klemperer, J. Chem. Phys. **39**, 371 (1963).

Molecule: Chloroethane CH_3CH_2Cl No. 167
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_2 s-stretch	2967 D	2977 M (solid)	2967 M, p	
	ν_2	CH_3 d-stretch	2946 C	2946 S	2934 M, p	
	ν_3	CH_3 s-stretch	2881 C	2881 S	2883 W, p	
	ν_4	CH_3 d-deform	1463 D	1463 S (solid)		
	ν_5	CH_2 scis	1448 D	1448 S	1453 M, dp	OV (ν_{14}).
	ν_6	CH_3 s-deform	1385 C	1385 S	1383 W, dp	
	ν_7	CH_2 wag	1289 C	1289 VS	1283 W, p	
	ν_8	CH_3 rock	1081 D	1081 VW	1072 M, p	
	ν_9	CC stretch	974 D	974 VS	969 W, dp	OV (ν_{16}).
	ν_{10}	CCl stretch	677 C	677 VS	659 VS, p	
	ν_{11}	CCCl deform	336 C	336 M	337 S, p	
a''	ν_{12}	CH_2 a-stretch	3014 D	3014 VS	3013 W	
	ν_{13}	CH_3 d-stretch	2986 D	2986 VS	2978 W	
	ν_{14}	CH_3 d-deform	1448 D	1448 S	1453 M, dp	OV (ν_5).
	ν_{15}	CH_2 twist	1251 D	1251 VW	1248 W, dp	
	ν_{16}	CH_3 rock	974 D	974 VS	969 W, dp	OV (ν_9).
	ν_{17}	CH_2 rock	786 B	786 M		
	ν_{18}	Torsion	251 B	251 W	.....	MW: 251 [4].

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[8] Th. A. B. Dempster and G. Zerbi, J. Mol. Spectrosc. **39**, 1 (1971).

Molecule: **Bromoethane** CH_3CH_2Br No. 168
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch	2988 C	2988 S	2971 (2b) p	OV (ν_{13}).
	ν_2	CH_2 s-stretch	2937 B	2936.5 S	2924 (2) p	
	ν_3	CH_3 s-stretch	2880 B	2879.8 S		
	ν_4	CH_2 scis	1451 D	1451 M	1442 (2b) dp	OV (ν_5, ν_{14}).
	ν_5	CH_3 d-deform	1451 D	1451 M	1442 (2b) dp	OV (ν_4, ν_{14}).
	ν_6	CH_3 s-deform	1386 B	1386 M		
	ν_7	CH_2 wag	1252 E	1258 VS 1247 VS	1248 (2b) p	FR ($\nu_9 + \nu_{11}$).
	ν_8	CH_3 rock	1061 D	1061 VW	1069 (1) p	
	ν_9	CC stretch	964 B	964 S	960 (1b) dp	OV (ν_{16}).
	ν_{10}	CBr stretch	583 B	583 VS	560 (10) p	
	ν_{11}	CCBr deform	290 B	290 S	292 (3) p	
a''	ν_{12}	CH_2 a-stretch	3018 B	3018 S		
	ν_{13}	CH_3 d-stretch	2988 C	2988 S	2971 (2b) p	OV (ν_1).
	ν_{14}	CH_3 d-deform	1451 D	1451 M	1442 (2b) dp	OV (ν_4, ν_5).
	ν_{15}	CH_2 twist	1248 E	.....	.....	CF [7].
	ν_{16}	CH_3 rock	964 D	964 S	960 (1b) dp	OV (ν_9).
	ν_{17}	CH_2 rock	770 B	770 M		
	ν_{18}	Torsion	247 C	247	.....	MW: 247 [5, 6].

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Molecule: Ethylene imine C_2H_5N No. 169
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	NH stretch	3338 C	3338 W	3302 M, p	
	ν_2	CH_2 a-stretch	3079 D	3079 S	3059 M, dp	OV (ν_{11}).
	ν_3	CH_2 s-stretch	3015 D	3015 S	2999 VS, p	OV (ν_{12}).
	ν_4	CH_2 scis	1482 C	1482 W	1471 W, p	
	ν_5	Ring stretch	1211 C	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 deform	856 C	856 VS	855 M, dp	
	ν_{10}	CH_2 rock	773 C	773 S	787 W, dp	
a''	ν_{11}	CH_2 a-stretch	3079 D	3079 S	3059 M, dp	OV (ν_2).
	ν_{12}	CH_2 s-stretch	3015 D	3015 S	2999 VS, p	OV (ν_3).
	ν_{13}	CH_2 scis	1463 C	1463 W	1452 W, dp	
	ν_{14}	CH_2 twist	1268 C	1268 M	1276 VW	
	ν_{15}	NH bend	1237 C	1237 M	1297 W, p	
	ν_{16}	CH_2 wag	1131 C	1131 M	1130 VW	
	ν_{17}	Ring deform	904 C	904 S		
	ν_{18}	CH_2 rock	817 D	.....	817 M, dp	

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Molecule: Methyl formate $HCOOCH_3$ No. 170
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch	3045 D	3045 M	3030 (3b)	
	ν_2	CH_3 s-stretch	2969 D	2969 S	2955 (10) p	
	ν_3	CH stretch	2943 D	2943 S		
	ν_4	C=O stretch	1754 C	1754 VS	1717 (5b) p	
	ν_5	CH_3 d-deform	1454 D	1454 W (CCl_4 soln.)		
	ν_6	CH_3 s-deform	1445 D	1445 M		
	ν_7	CH bend	1371 D	1371 W	1379 (4b) p	
	ν_8	C–O stretch	1207 C	1207 VS	1207 (0.5b)	
	ν_9	CH_3 rock	1166 D	1166 VS	1157 (1b)	
	ν_{10}	O–CH_3 stretch	925 C	925 S	912 (10) p	
	ν_{11}	OCO deform	767 C	767 M	765 (2)	
	ν_{12}	COC deform	318 D	318 M		
a''	ν_{13}	CH_3 d-stretch	3012 D	3012 M		
	ν_{14}	CH_3 d-deform	1443 E	1443 W (CCl_4 soln.)	1440 (3b)	
	ν_{15}	CH_3 rock	1168 D	1168 M		
	ν_{16}	CH bend	1032 C	1032 M	1030 (0.5)	
	ν_{17}	C–O torsion	332 D	332 M	332 (3b) p	
	ν_{18}	CH_3 torsion	130 D	130 VW	.....	MW: 132 [3].

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[1] R. K. W. F. Kohlrausch, Ramanspektren, p. 263 (Edwards Bros., Inc., Ann Arbor, 1945).
[2] IR.R. J. K. Wilmshurst, J. Mol. Spectrosc. 1, 201 (1957).
[3] MW. R. F. Curl, J. Chem. Phys. 30, 1529 (1959).
[4] IR. W. G. Fateley and F. A. Miller, Spectrochim. Acta 17, 857 (1961).
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[6] IR.Th. S. Ichikawa, K. Toriyama, and T. Shimanouchi, unpublished.

Molecule: Methyl formate-d_1 $DCOOCH_3$ No. 171

Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_3 d-stretch	3041 C	3041 M		
	ν_2	CH_3 s-stretch	2967 C	2967 S		
	ν_3	CD stretch	2216 C	2216 S		
	ν_4	C=O stretch	1739 E	1755 VS 1716 VS	.....	FR ($2\nu_{16}$).
	ν_5	CH_3 d-deform	1448 E	1448 W (CCl_4 soln.)		
	ν_6	CH_3 s-deform	1441 D	1441 M		
	ν_7	CD bend	1048 D	1048 M		
	ν_8	C–O stretch	1213 C	1213 VS		
	ν_9	CH_3 rock	1157 D	1157 VS		
	ν_{10}	O–CH_3 stretch	878 C	878 S		
	ν_{11}	OCO deform	762 C	762 M		
	ν_{12}	COC deform	315 E	315 M		
a''	ν_{13}	CH_3 d-stretch	3007 D	3007 S		
	ν_{14}	CH_3 d-deform	1440 E	1440 W (CCl_4 soln.)		
	ν_{15}	CH_3 rock	1164 E	.....	.....	CF [2], OV (ν_9).
	ν_{16}	CD bend	870 E	.....	.....	CF [2], OV (ν_{10}).
	ν_{17}	C–O torsion	290 E	290 M		
	ν_{18}	CH_3 torsion	130 E	.....	.....	CF [2].

References

[1] IR. H. Susi and T. Zell, Spectrochim. Acta 19, 1933 (1963).
[2] IR.Th. S. Ichikawa, K. Toriyama, and T. Shimanouchi, unpublished.

Molecule: Methyl formate-d_3 $HCOOCD_3$ No. 172
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CD_3 d-stretch	2284 D	2284 M		
	ν_2	CD_3 s-stretch	2087 D	2087 M		
	ν_3	CH stretch	2931 D	2931 S		
	ν_4	C=O stretch	1754 C	1754 VS		
	ν_5	CD_3 d-deform	1060 E	1060 W	.....	OV (ν_{14}).
	ν_6	CD_3 s-deform	1102 E	1102 S		
	ν_7	CH ip-bend	1368 D	1368 M		
	ν_8	C–O stretch	1210 C	1210 VS		
	ν_9	CD_3 rock	985 D	985 M		
	ν_{10}	O–CD_3 stretch	877 C	877 M		
	ν_{11}	OCO deform	714 C	714 M		
	ν_{12}	COC deform	297 E	297 M		
a''	ν_{13}	CD_3 d-stretch	2258 D	2258 M		
	ν_{14}	CD_3 d-deform	1060 E	1060 W	.....	OV (ν_5).
	ν_{15}	CD_3 rock	905 D	905 W		
	ν_{16}	CH op-bend	1040 E	1040 W		
	ν_{17}	C–O torsion	312 E	312 M		
	ν_{18}	CD_3 torsion	96 E	.....	.....	CF [2].

References

See No. 171.

Molecule: Methyl formate-d_4 $DCOOCD_3$ No. 173
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CD_3 d-stretch	2291 D	2291 M		
	ν_2	CD_3 s-stretch	2100 D	2100 M		
	ν_3	CD stretch	2210 D	2210 S		
	ν_4	C=O stretch	1739 E	1749 VS 1719 VS	.....	FR ($2\nu_{16}$).
	ν_5	CD_3 d-deform	1060 E	1060 W	.....	OV (ν_{14}).
	ν_6	CD_3 s-deform	1107 D	1107 S		
	ν_7	CD bend	1041 E	1041 W		
	ν_8	C–O stretch	1203 D	1203 VS		
	ν_9	CD_3 rock	974 D	974 M		
	ν_{10}	O–CD_3 stretch	840 D	840 M		
	ν_{11}	OCO deform	708 D	708 M		
	ν_{12}	COC deform	295 E	295 M		
a''	ν_{13}	CD_3 d-stretch	2267 D	2267 M		
	ν_{14}	CD_3 d-deform	1060 D	1060 W	.....	OV (ν_4).
	ν_{15}	CD_3 rock	908 D	908 M		
	ν_{16}	CD op-bend	870 D	870 W		
	ν_{17}	C–O torsion	280 D	280 M		
	ν_{18}	CD_3 torsion	96 E	.....	.....	CF [1].

Reference

[1] IR.Th. S. Ichikawa, K. Toriyama, and T. Shimanouchi, unpublished.

Molecule: Acetic acid CH_3COOH No. 174
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	OH stretch	3583 B	3583 M		
	ν_2	CH_3 d-stretch	3051 B	3051 VW		
	ν_3	CH_3 s-stretch	2944 B	2944 VW		
	ν_4	C=O stretch	1788 B	1788 VS		
	ν_5	CH_3 d-deform	1430 C	1430 sh	.....	SF (ν_{14}).
	ν_6	CH_3 s-deform	1382 B	1382 M		
	ν_7	OH bend	1264 B	1264 M		
	ν_8	C–O stretch	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}	CCO deform	581 B	581 M		
a''	ν_{13}	CH_3 d-stretch	2996 B	2996 VW		
	ν_{14}	CH_3 d-deform	1430 C	1430 sh	.....	SF (ν_5).
	ν_{15}	CH_3 rock	1048 B	1048 W		
	ν_{16}	C=O op-bend	642 B	642 S		
	ν_{17}	C–O torsion	534 B	534 M		
	ν_{18}	CH_3 torsion	93 E	.....	.....	CF [3].

References

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[2] IR. J. K. Wilmshurst, J. Chem. Phys. 25, 1171 (1956).
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[4] IR. M. Ohara and T. Shimanouchi, unpublished.

Molecule: Acetic acid-d_1 CH_3COOD No. 175
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_3 d-stretch	3039 B	3039 VW		
	ν_2	CH_3 s-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 d-deform	1440 C	1440 sh	.....	SF (ν_{14}).
	ν_6	CH_3 s-deform	1383 B	1383 S		
	ν_7	C–O stretch	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}	CCO deform	543 B	543 M		
a''	ν_{13}	CH_3 d-stretch	2997 D	2997 VW		
	ν_{14}	CH_3 d-deform	1440 C	1440 sh	.....	SF (ν_5).
	ν_{15}	CH_3 rock	1052 B	1052 W		
	ν_{16}	C=O ip-bend	603 B	603 M		
	ν_{17}	C–O torsion	415 B	415 M		
	ν_{18}	CH_3 torsion	93 E	.....	.....	CF [3].

References

See No. 174.

Molecule: Dimethylether CH_3OCH_3 No. 176
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 d-stretch	2996 B	2996 S	2989 S	
	ν_2	CH_3 s-stretch	2817 B	2817 S	2815 VS, p	
	ν_3	CH_3 d-deform	1464 D	1464 M		
	ν_4	CH_3 s-deform	1452 D	1452 M	1452 S, dp	
	ν_5	CH_3 rock	1244 B	1244 W		
	ν_6	CO s-stretch	928 B	928 S	922 S, p	
	ν_7	COC deform	418 C	418 M	428 M, p	
a_2	ν_8	CH_3 d-stretch	2952 C	ia	2952 S	
	ν_9	CH_3 d-deform	1464 D	ia	.....	SF (ν_3).
	ν_{10}	CH_3 rock	1150 C	ia	1150 M, d	
	ν_{11}	Torsion	203 E	ia	.....	CF [3].
b_1	ν_{12}	CH_3 d-stretch	2996 B	2996 S	2989 S	OV (ν_1).
	ν_{13}	CH_3 s-stretch	2817 B	2817 S	2815 VS, p	OV (ν_2).
	ν_{14}	CH_3 d-deform	1464 D	1464 M	.....	OV (ν_3).
	ν_{15}	CH_3 s-deform	1452 D	1452 M	1452 S, dp	OV (ν_4).
	ν_{16}	CH_3 rock	1227 C	.....	1227 W	
	ν_{17}	CO a-stretch	1102 B	1102 VS	1104 M, dp	
b_2	ν_{18}	CH_3 d-stretch	2925 B	2925 S		
	ν_{19}	CH_3 d-deform	1464 D	1464 M	.....	OV (ν_3).
	ν_{20}	CH_3 rock	1179 B	1179 VS	1170 sh	
	ν_{21}	Torsion	242 C	242 W		

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[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] R. R. C. Taylor and G. L. Vidale, J. Chem. Phys. 26, 122 (1957).
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[5] IR. J.-P. Perchard, M.-T. Forel, and M.-L. Josien, J. Chim. Phys. 61, 632 (1964).
[6] Th. T. Shimanouchi and M. Oka, unpublished.

Molecule: Dimethylether-d_3 CH_3OCD_3 No. 177
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_3 d-stretch	2992 B	2992 S		
	ν_2	CH_3 s-stretch	2819 B	2819 S		
	ν_3	CD_3 d-stretch	2244 B	2244 S		
	ν_4	CD_3 s-stretch	2058 B	2058 S		
	ν_5	CH_3 d-deform	1465 C	1465 M		
	ν_6	CH_3 s-deform	1453 C	1453 M		
	ν_7	CH_3 rock	1212 B	1212 M		
	ν_8	CO a-stretch	1156 C	1156 VS	.....	SF (ν_{17}).
	ν_9	CD_3 s-deform	1111 B	1111 S		
	ν_{10}	CD_3 d-deform	1061 C	1061 M	.....	SF (ν_{18}).
	ν_{11}	CD_3 rock	947 C	947 W		
	ν_{12}	CO s-stretch	860 C	860 M		
	ν_{13}	COC deform	395 E	.....	.....	CF [2].
a''	ν_{14}	CH_3 d-stretch	2932 B	2932 S		
	ν_{15}	CD_3 d-stretch	2189 B	2189 S		
	ν_{16}	CH_3 d-deform	1462 D	1462 M		
	ν_{17}	CH_3 rock	1156 C	1156 VS	.....	SF (ν_8).
	ν_{18}	CD_3 d-deform	1061 C	1061 M	.....	SF (ν_{10}).
	ν_{19}	CD_3 rock	901 C	901 W		
	ν_{20}	Torsion	227 E	.....	.....	CF [2].
	ν_{21}	Torsion	164 E	.....	.....	CF [2].

References

[1] IR. J.-P. Perchard, M.-T. Forel, and M.-L. Josien, J. Chim. Phys. **61**, 632 (1964).
[2] Th. T. Shimanouchi and M. Oka, unpublished.

Molecule: Allene CH_2CCH_2 No. 178
Symmetry D_{2d} **Symmetry number** $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_2 s-stretch	3015 A	.....	3015.0	
	ν_2	CH_2 scis	1443 A	.....	1442.6	
	ν_3	CC stretch	1073 A	.....	1072.6	
b_1	ν_4	CH_2 twist	865 C	865	865 (liquid)	
b_2	ν_5	CH_2 s-stretch	3007 A	3006.7		
	ν_6	CC stretch	1957 C	1957	1960 (liquid)	
	ν_7	CH_2 scis	1398 C	1398	1421 (liquid)	
e	ν_8	CH_2 a-stretch	3086 A	3085.5		
	ν_9	CH_2 rock	999 A	999.1		
	ν_{10}	CH_2 wag	841 A	840.8		
	ν_{11}	CCC deform	355 A	355.3		

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[12] IR. I. M. Mills, W. L. Smith, and J. L. Duncan, J. Mol. Spectrosc, 16, 349 (1965).
[13] IR. A. G. Maki and R. A. Toth, J. Mol. Spectrosc. 17, 136 (1965).

Molecule: Methylacetylene CH_3CCH No. 179
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3334 C	3334	3305 M	
	ν_2	CH_3 s-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 s-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 d-stretch	3008 A	3008.3 M	2971 M	
	ν_7	CH_3 d-deform	1452 B	1452 M	1448 M	
	ν_8	CH_3 rock	1053 A	1052.5 W	1035 VW	
	ν_9	CH bend	633 C	633 S	643 S, dp	
	ν_{10}	CCC bend	328 C	328 W	336 VS, dp	

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[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-d_1 CH_3CCD No. 180
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 s-stretch	2920 E	2941.0 M 2881.0 M	.....	FR ($2\nu_7$) [1].
	ν_2	CD stretch	2617 B	2616.8 S		
	ν_3	C≡C stretch	2060 C	2060.3 W		
	ν_4	CH_3 s-deform	1378 E	1378 W	.....	OV (ν_7).
	ν_5	C–C stretch	886 E	.....	.....	CF [1].
e	ν_6	CH_3 d-stretch	3009 B	3008.9 M		
	ν_7	CH_3 deform	1454 B	1453.5 M		
	ν_8	CH_3 rock	1051 B	1051.0 W		
	ν_9	CD bend	498 B	497.5 S		
	ν_{10}	CCC bend	314 B	314 M		

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[2] Th. J. L. Duncan, Spectrochim. Acta **20**, 1197 (1964).

Molecule: Methyl-d_3-acetylene CD_3CCH No. 181
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH stretch	3336 A	3335.8 S		
	ν_2	CD_3 s-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 s-deform	1115 B	1115 M		
	ν_5	C–C stretch	830 B	830 W	.....	OV (ν_8).
e	ν_6	CD_3 d-stretch	2235 A	2234.9 M		
	ν_7	CD_3 d-deform	1048 A	1048.2 M		
	ν_8	CD_3 rock	835 A	835.4 W	.....	OV (ν_5).
	ν_9	CH bend	633 B	633 S		
	ν_{10}	CCC bend	305 B	304.5 M		

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[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. 182
Symmetry C_{3v} Symmetry number $\sigma = 3$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD stretch	2616 A	2616.3 VS		
	ν_2	CD_3 s-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 s-deform	1110 A	1110.1 M		
	ν_5	C–C stretch	810 E	.....	.....	CF [1].
e	ν_6	CD_3 d-stretch	2235 A	2234.8 M		
	ν_7	CD_3 d-deform	1048 A	1048.2 M		
	ν_8	CD_3 rock	834 A	834.4 W		
	ν_9	CD bend	492 B	492 VS		
	ν_{10}	CCC bend	294 B	294 M		

References

See No. 181.

Molecule: Malononitrile $NCCH_2CN$ No. 183
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 s-stretch	2935 C	2935 VS	2929 (5)	
	ν_2	CN s-stretch	2275 C	2275 M	2263 (7)	SF (ν_9).
	ν_3	CH_2 scis	1395 C	1395 VS	1386 (4)	
	ν_4	CC s-stretch	890 C	890 S	892 (5)	
	ν_5	CCC deform	582 C	582 M	574 (3b)	
	ν_6	CCN bend	167 C	.....	167 (10)	
a_2	ν_7	CH_2 twist	1220 C	ia, 1220 VW	1214 (3)	
	ν_8	CCN bend	367 C	ia, 371 M	367 (10)	SF (ν_{12}).
b_1	ν_9	CN a-stretch	2275 C	2275 M	2263 (7)	SF (ν_2).
	ν_{10}	CH_2 wag	1318 C	1318 W	1310 (2)	
	ν_{11}	CC a-stretch	982 C	982 S	975 (1)	
	ν_{12}	CCN bend	366 C	366 S	367 (10)	SF (ν_8).
b_2	ν_{13}	CH_2 a-stretch	2968 C	2968 VS	2960 (1)	
	ν_{14}	CH_2 rock	933 C	933 M		
	ν_{15}	CCN bend	337 C	337 S		

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Molecule: Malononitrile-d_2 $NCCD_2CN$ No. 184
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (D_2O soln.)	
a_1	ν_1	CD_2 s-stretch	2146 C	2146 S	2146 (4)	
	ν_2	CN s-stretch	2272 C	2272 M	2273 (8)	SF (ν_9).
	ν_3	CD_2 scis	1037 C	1037 S	1033 (3)	
	ν_4	CC s-stretch	858 C	858 M	854 (5)	
	ν_5	CCC deform	577 C	577 M	581 (2)	
	ν_6	CCN bend	163 C	.....	163 (4)	
a_2	ν_7	CD_2 twist	892 C	ia, 892 VW	892 (1)	
	ν_8	CCN bend	356 C	ia	356 (4)	SF (ν_{12}).
b_1	ν_9	CN a-stretch	2272 C	2272 M	2273 (8)	SF (ν_2).
	ν_{10}	CD_2 wag	1153 C	1165 M 1142 M	1162 (0.5) 1130 (0.5)	FR ($\nu_{12} + \nu_{14}$).
	ν_{11}	CC a-stretch	829 C	829 M	828 (1)	
	ν_{12}	CCN bend	356 C	356 S	356 (4)	SF (ν_8).
b_2	ν_{13}	CD_2 a-stretch	2230 C	2230 S	2228 (2)	
	ν_{14}	CD_2 rock	795 C	795 W		
	ν_{15}	CCN bend	302 C	.....	302 (1)	

Reference

[1] IR.R.Th. T. Fujiyama and T. Shimanouchi, Spectrochim. Acta 20, 829 (1964).

Molecule Propenal CH_2CHCHO[a] No. 185
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_2 a-stretch	3103 C	3103 M		
	ν_2	CH(β) stretch	3028 D	3028 M (solid)		
	ν_3	CH_2 s-stretch	3000 D	3000 M		
	ν_4	CH(α) stretch	2800 C	2800 S		
	ν_5	CO stretch	1724 C	1724 VS		
	ν_6	C=C stretch	1625 C	1625 M		
	ν_7	CH_2 scis	1420 C	1420 S		
	ν_8	CH(α) ip-bend	1360 C	1360 M		
	ν_9	CH(β) ip-bend	1275 C	1275 W		
	ν_{10}	C–C stretch	1158 C	1158 S		
	ν_{11}	CH_2 rock	912 C	912 S		
	ν_{12}	CCO deform	564 C	564 M		
	ν_{13}	CCC bend	327 C	327 M		
a''	ν_{14}	CH(β) op-bend	993 B	993 S		
	ν_{15}	CH(α) op-bend	980 E	.....	.....	CF [1, 2].
	ν_{16}	CH_2 wag	959 B	959 S		
	ν_{17}	CH_2 twist	593 C	593 S		
	ν_{18}	CC torsion	157 C	157 M		

[a] Numbering of atoms: $C^{\gamma}H_2C^{\beta}HC^{\alpha}HO$.

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[1] IR. J. C. D. Brand and D. G. Williamson, Disc. Faraday Soc. 35, 184 (1963).
[2] IR. R. K. Harris, Spectrochim. Acta 20, 1129 (1964).

Molecule: Cyclopropane C_3H_6 No. 186

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1'	ν_1	CH_2 s-stretch	3038 C	ia	3038 S, p	
	ν_2	CH_2 scis	1479 D	ia	1504 W, p 1453 W, p	FR ($2\nu_{14}$).
	ν_3	Ring stretch	1188 C	ia	1188 S, p	
a_1''	ν_4	CH_2 twist	1126 D	ia, 1126 VW	ia, 1133	
a_2'	ν_5	CH_2 wag	1070 D	ia, 1075 (solid)	ia	OC ($\nu_5 + \nu_{10}$).
a_2''	ν_6	CH_2 a-stretch	3103 C	3103 S	ia	
	ν_7	CH_2 rock	854 C	854 S	ia	
e'	ν_8	CH_2 s-stretch	3025 C	3025 VS	3020 VS, p	
	ν_9	CH_2 scis	1438 C	1438 M	1442 M, dp	
	ν_{10}	CH_2 wag	1029 C	1029 S	1023 VW (liquid)	
	ν_{11}	Ring deform	866 C	866 VS	866 S, dp	
e''	ν_{12}	CH_2 a-stretch	3082 C	ia	3082 S, dp	
	ν_{13}	CH_2 twist	1188 C	ia	1188 M	
	ν_{14}	CH_2 rock	739 C	ia	739 W, dp	

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[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
[2] IR.R. A. W. Baker and R. C. Lord, J. Chem. Phys. **23**, 1636 (1955).
[3] IR.Th. Hs. H. Günthard, R. C. Lord, and T. K. McCubbin, Jr., J. Chem. Phys. **25**, 768 (1956).
[4] R. P. M. Mathai, G. G. Shepherd, and H. L. Welsh, Can. J. Phys. **34**, 1448 (1956).
[5] IR. C. Brecher, E. Krikorian, J. Blanc, and R. S. Halford, J. Chem. Phys. **35**, 1097 (1961).
[6] IR. J. L. Duncan and D. C. McKean, J. Mol. Spectrosc. **27**, 117 (1968).

Molecule: Cyclopropane-d_6 C_3D_6 No. 187
Symmetry D_{3h} **Symmetry number** $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1'	ν_1	CD_2 s-stretch	2236 C	ia	2236 VS, p	
	ν_2	CD_2 scis	1274 D	ia	1274 S, p	
	ν_3	Ring stretch	956 C	ia	956 S, p	
a_1''	ν_4	CD_2 twist	800 D	ia, 800 VW	ia	CF [2].
a_2'	ν_5	CD_2 wag	870 D	ia, 875 (solid)	ia	CF [2], OC ($\nu_5 + \nu_{11}$).
a_2''	ν_6	CD_2 a-stretch	2336 C	2336 VS	ia	
	ν_7	CD_2 rock	614 C	614 W	ia	
e'	ν_8	CD_2 s-stretch	2211 C	2211 VS	2204 W, dp	
	ν_9	CD_2 scis	1072 C	1072 S	1068 W, dp	
	ν_{10}	CD_2 wag	885 C	885 M	884 M, dp	
	ν_{11}	Ring deform	717 C	717 VS	721 M, dp	
e''	ν_{12}	CD_2 a-stretch	2329 C	ia	2329 S, p	
	ν_{13}	CD_2 twist	940 E	ia	.....	CF [2], OC ($2\nu_{13}$).
	ν_{14}	CD_2 rock	528 C	ia	528 W, dp	

References

[1] IR.R. A. W. Baker and R. C. Lord, J. Chem. Phys. **23**, 1636 (1955).
[2] IR.Th. Hs. H. Günthard, R. C. Lord, and T. K. McCubbin, Jr., J. Chem. Phys. **25**, 768 (1956).
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Molecule: Ethylcyanide CH_3CH_2CN No. 188
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch	3001 C	3001 VS	2999 S	OV (ν_{14}).
	ν_2	CH_2 s-stretch	2955 C	2955 VS	2949 VS, p	
	ν_3	CH_3 s-stretch	2900 C	2900 S	2898 S, p	
	ν_4	CN stretch	2254 C	2254 VS	2251 VS, p	
	ν_5	CH_3 d-deform	1465 C	1465 S	1466 VS, p	SF (ν_{16}).
	ν_6	CH_2 scis	1433 C	1433 S	1436 M, p	
	ν_7	CH_3 s-deform	1387 C	1387 M	1374 VW, p	
	ν_8	CH_2 wag	1319 C	1319 M	1322 W, p	
	ν_9	C–CN stretch	1077 C	1077 S	1078 M, p	
	ν_{10}	CC stretch	1005 C	1005 M	1010 S, p	
	ν_{11}	CH_3 rock	836 C	836 W	838 S, p	
	ν_{12}	CCC deform	545 C	545 M	548 M, p	
	ν_{13}	CCN bend	226 C	226 M	226 M, p	
a''	ν_{14}	CH_3 d-stretch	3001 C	3001 VS	2999 S	OV (ν_1).
	ν_{15}	CH_2 a-stretch	2849 C	2849 S	2850 M	
	ν_{16}	CH_3 d-deform	1465 C	1465 S	1466 VS, dp	SF (ν_5).
	ν_{17}	CH_2 twist	1256 C	1256 VW	1270 VW, dp	
	ν_{18}	CH_3 rock	1022 E	.....	.....	CF [2].
	ν_{19}	CH_2 rock	786 C	786 M	784 VW, dp	
	ν_{20}	CCN bend	378 C	378 M	378 M, dp	
	ν_{21}	Torsion	222 C	.....	.....	MW [2].

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[2] MW. V. W. Laurie, J. Chem. Phys. 31, 1500 (1959).
[3] IR.R.Th. T. Fujiyama, Bull. Chem. Soc. Japan 44, 89 (1971).

Molecule: Acetone CH_3COCH_3 No. 189
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 d-stretch	3019 C	3018.5 S	3005.5 S	SF (ν_{13}).
	ν_2	CH_3 s-stretch	2937 D	2937 S	2922 VS, p	SF (ν_{14}).
	ν_3	CO stretch	1731 C	1731 VS	1710.5 S, p	
	ν_4	CH_3 d-deform	1435 C	1435 S	1430 S	
	ν_5	CH_3 s-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	777 C	777 W	787 VS, p	
	ν_8	CCC deform	385 C	385 W	393 W, dp	
a_2	ν_9	CH_3 d-stretch	2963 E	ia	.....	CF [4].
	ν_{10}	CH_3 d-deform	1426 E	ia	.....	CF [4].
	ν_{11}	CH_3 rock	877 E	ia	.....	CF [4].
	ν_{12}	Torsion	105 D	ia	.....	CF [4]; MW: 102 [1].
b_1	ν_{13}	CH_3 d-stretch	3019 C	3018.5 S	3005.5 S, dp	SF (ν_1).
	ν_{14}	CH_3 s-stretch	2937 D	2937 S	2922 VS	SF (ν_2).
	ν_{15}	CH_3 d-deform	1410 C	1410 S		
	ν_{16}	CH_3 s-deform	1364 C	1363.5 VS	.....	SF (ν_5).
	ν_{17}	CC stretch	1216 C	1215.5 VS	1221 M, dp	
	ν_{18}	CH_3 rock	891 C	891 M	902.5 W, dp	
	ν_{19}	CO ip-bend	530 C	530 S	531 M, dp	
b_2	ν_{20}	CH_3 d-stretch	2972 C	2972 S	2967 S	
	ν_{21}	CH_3 d-deform	1454 C	1454 S		
	ν_{22}	CH_3 rock	1091 C	1090.5 M		
	ν_{23}	CO op-bend	484 C	484 W	493 W, dp	
	ν_{24}	Torsion	109 D	109	.....	MW: 102. [1].

References

[1] MW. J. D. Swalen and C. C. Costain, J. Chem. Phys. **31**, 1562 (1959).
[2] IR. W. G. Fateley and F. A. Miller, Spectrochim. Acta **18**, 977 (1962).
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[4] IR.R.Th. G. Dellepiane and J. Overend, Spectrochim. Acta **22**, 593 (1966).
[5] IR.R.Th. M. Mikami, Ph.D. Thesis, (University of Tokyo, 1969).
[6] R. T. Fujiyama and T. Shimanouchi, Bull. Chem. Soc. Japan, in press.

Molecule: Acetone-α, α, α-d_3 CH_3COCD_3 No. 190
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch	3018 C	3017.5 S	3004.5 S	
	ν_2	CH_3 s-stretch	2922 C	.....	2921.5 VS, p	
	ν_3	CD_3 d-stretch	2265 C	2265 M	2256 S	
	ν_4	CD_3 s-stretch	2115 E	2150 VVW 2095 VW	2141.5 VS, p 2095.5 S, p	FR ($2\nu_9$).
	ν_5	CO stretch	1734 C	1734 VS	1706 S	
	ν_6	CH_3 d-deform	1430 C	1430 S	1427.5 M	
	ν_7	CH_3 s-deform	1360 C	1360 VS	1361.5 VW	
	ν_8	CC stretch	1225 C	1224.5 VS	1227.5 W	
	ν_9	CD_3 s-deform	1058 C	.....	1057.5 W	
	ν_{10}	CH_3 rock	1021 C	1021 S	1029.5 W	
	ν_{11}	CD_3 d-deform	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 ip-bend	502 C	501.5 S		
	ν_{15}	CCC deform	352 C	352 W	356.5 W	
a''	ν_{16}	CH_3 d-stretch	2968 C	2968 S	2965 S	
	ν_{17}	CD_3 d-stretch	2222 C	2222 M	2217.5 S	
	ν_{18}	CH_3 d-deform	1447 C	1447 S		
	ν_{19}	CH_3 rock	1035 C	1035 S		
	ν_{20}	CD_3 d-deform	999 C	999 S		
	ν_{21}	CD_3 rock	764 D	764 M (solid)		
	ν_{22}	CO op-bend	438 C	438	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, Ph.D. Thesis, (University of Tokyo, 1969).

Molecule: Acetone-d_6 CD_3COCD_3 No. 191
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_3 d-stretch	2264 C	2263.5 S	.....	SF (ν_{13}).
	ν_2	CD_3 s-stretch	2123 C	2123 W	2108.5 VS, p	SF (ν_{14}).
	ν_3	CO stretch	1732 C	1732 VS	1700.5 S	
	ν_4	CD_3 s-deform	1080 C	1080 M	1088 M, p	
	ν_5	CD_3 d-deform	1035 D	1035 M	1036 M	
	ν_6	CD_3 rock	887 C	887 W	889 M, p	
	ν_7	CC stretch	689 C	689 W	695.5 VS, p	
	ν_8	CCC deform	321 C	321 W	330 VW, dp	
a_2	ν_9	CD_3 d-stretch	2219 E	ia	.....	CF [3].
	ν_{10}	CD_3 d-deform	1021 E	ia	.....	CF [3].
	ν_{11}	CD_3 rock	669 E	ia	.....	CF [3].
	ν_{12}	Torsion	75 E	ia	.....	CF [3].
b_1	ν_{13}	CD_3 d-stretch	2264 C	2263.5 S	2256.5 S	SF (ν_1).
	ν_{14}	CD_3 s-stretch	2123 C	2123 W	.....	SF (ν_2).
	ν_{15}	CC stretch	1242 C	1241.7 VS	1248.5 VW	
	ν_{16}	CD_3 s-deform	1035 D	1035 M	1036 M	
	ν_{17}	CD_3 d-deform	1004 C	1004 M	1006 sh	
	ν_{18}	CD_3 rock	724 D	724 W (solid)		
	ν_{19}	CO ip-bend	475 C	475 S	478 W, dp	
b_2	ν_{20}	CD_3 d-stretch	2227 C	2226.5 S	2222 S	
	ν_{21}	CD_3 d-deform	1050 C	1050 S		
	ν_{22}	CD_3 rock	960 C	960 M		
	ν_{23}	CO op-bend	405 C	405 W	410 VW, dp	
	ν_{24}	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, Ph.D. Thesis (University of Tokyo, 1969).

Molecule: Propane $CH_3CH_2CH_3$ No. 192

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 d-stretch	2977 C	2977		
	ν_2	CH_3 s-stretch	2962 D	2962		
	ν_3	CH_2 s-stretch	2887 C	2887		
	ν_4	CH_3 d-deform	1476 C	1476		
	ν_5	CH_2 scis	1462 C	1462		
	ν_6	CH_3 s-deform	1392 C	1392		
	ν_7	CH_3 rock	1158 C	1158	1152 W	
	ν_8	CC stretch	869 C	869	867 S	
	ν_9	CCC deform	369 C	369	375 W	
a_2	ν_{10}	CH_3 d-stretch	2967 C	ia	2967 M	
	ν_{11}	CH_3 d-deform	1451 C	ia	1451 S	
	ν_{12}	CH_2 twist	1278 C	ia	1278 W	
	ν_{13}	CH_3 rock	940 D	ia	940 VW	
	ν_{14}	Torsion	[a]216 C	ia	.....	MW [10,11].
b_1	ν_{15}	CH_3 d-stretch	2968 C	2968		
	ν_{16}	CH_3 s-stretch	2887 C	2887	.....	OV (ν_3).
	ν_{17}	CH_3 d-deform	1464 C	1464		
	ν_{18}	CH_3 s-deform	1378 C	1378		
	ν_{19}	CH_2 wag	1338 C	1338	1338 M	
	ν_{20}	CC stretch	1054 C	1054	1054 M	
	ν_{21}	CH_3 rock	922 C	922		
b_2	ν_{22}	CH_3 d-stretch	2973 C	2973		
	ν_{23}	CH_2 a-stretch	2968 C	2968		
	ν_{24}	CH_3 d-deform	1472 C	1472		
	ν_{25}	CH_3 rock	1192 C	1192		
	ν_{26}	CH_2 rock	748 C	748		
	ν_{27}	Torsion	[a]268 C	.....	.....	MW [10,11].

[a] These values are in agreement with the results of neutron-inelastic scattering experiment (D. M. Grant, R. J. Pugmire, and R. C. Livingston, J. Chem. Phys. 52, 4424 (1970)).

References

[1] IR. D. M. Gates, J. Chem. Phys. 17, 393 (1949).
[2] IR. H. L. McMurry, V. Thornton, and F. E. Condon, J. Chem. Phys. 17, 918 (1949).
[3] IR. H. L. McMurry and V. Thornton, J. Chem. Phys. 19, 1014 (1951).
[4] IR. J. J. Comeford and J. H. Gould, J. Mol. Spectrosc. 5, 474 (1960).
[5] Th. H. Takahashi, Nippon Kagaku Zasshi 82, 1304 (1961).
[6] IR. R. G. Snyder and J. H. Schachtschneider, Spectrochim. Acta 19, 85 (1963).
[7] Th. J. H. Schachtschneider and R. G. Snyder, Spectrochim. Acta 19, 117 (1963).
[8] IR. J. N. Gayles, Jr. and W. T. King, Spectrochim. Acta 21, 543 (1965).
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[10] MW. E. Hirota, C. Matsumura, and Y. Morino, Bull. Chem. Soc. Japan 40, 1124 (1967).
[11] MW. J. R. Hoyland, J. Chem. Phys. 49, 1908 (1968).

Molecule: Propane-2,2-d_2 $CH_3CD_2CH_3$ No. 193
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_3 d-stretch	2974 C	2974		
	ν_2	CH_3 s-stretch	2883 C	2883		
	ν_3	CD_2 s-stretch	2141 C	2141		
	ν_4	CH_3 d-deform	1459 C	1459		
	ν_5	CH_3 s-deform	1392 C	1392		
	ν_6	CH_3 rock	1207 D	1207		
	ν_7	CD_2 scis	1064 C	1064		
	ν_8	CC stretch	843 C	843		
	ν_9	CCC deform	362 E	.....	.....	CF [5].
a_2	ν_{10}	CH_3 d-stretch	2956 E	ia	.....	OC ($\nu_{10} + \nu_{18}$) [4].
	ν_{11}	CH_3 d-deform	1453 E	ia	.....	CF [5].
	ν_{12}	CH_3 rock	1083 E	ia	.....	OC ($\nu_{12} + \nu_{16}$) [4].
	ν_{13}	CD_2 twist	777 E	ia	.....	CF [5].
	ν_{14}	Torsion	[a]208 E	ia	.....	OC ($\nu_{18} - \nu_{14}$) [4].
b_1	ν_{15}	CH_3 d-stretch	2974 C	2974	.....	SF (ν_1).
	ν_{16}	CH_3 s-stretch	2883 C	2883	.....	SF (ν_2).
	ν_{17}	CH_3 d-deform	1461 C	1461		
	ν_{18}	CH_3 s-deform	1374 C	1374		
	ν_{19}	CC stretch	1203 C	1203		
	ν_{20}	CH_3 rock	964 C	964		
	ν_{21}	CD_2 wag	829 C	829		
b_2	ν_{22}	CH_3 d-stretch	2963 C	2963		
	ν_{23}	CD_2 a-stretch	2182 C	2182		
	ν_{24}	CH_3 d-deform	1476 C	1476		
	ν_{25}	CH_3 rock	1146 C	1146		
	ν_{26}	CD_2 rock	622 C	622		
	ν_{27}	Torsion	[a]217 E	.....	.....	CF [4].

[a] Assigning frequencies higher than these by 10–20 percent may be more reasonable in view of the results for $CH_3CH_2CH_3$.

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[2] IR. H. L. McMurry and V. Thornton, J. Chem. Phys. **19**, 1014 (1951).
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[6] Th. J. N. Gayles, Jr., W. T. King, and J. H. Schachtschneider, Spectrochim. Acta **23A**, 703 (1967).

Molecule: Propane-1,1,1-d_3 $CH_3CH_2CD_3$
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_3 d-stretch	2966 C	2966		
	ν_2	CH_3 s-stretch	2934 D	2934		
	ν_3	CH_2 s-stretch	2882 C	2882		
	ν_4	CD_3 d-stretch	2225 C	2225		
	ν_5	CD_3 s-stretch	2075 C	2075		
	ν_6	CH_2 scis	1461 D	1461		
	ν_7	CH_3 d-deform	1460 D	1460		
	ν_8	CH_3 s-deform	1383 C	1383		
	ν_9	CH_2 wag	1332 C	1332		
	ν_{10}	CC stretch	1132 C	1132		
	ν_{11}	CH_3 rock	1101 C	1101		
	ν_{12}	CD_3 d-deform	1062 C	1062		
	ν_{13}	CD_3 s-deform	999 D	999		
	ν_{14}	CC stretch	846 C	846		
	ν_{15}	CD_3 rock	750 C	750		
	ν_{16}	CCC deform	339 E	.....	.....	CF [2].
a''	ν_{17}	CH_3 d-stretch	2966 C	2966	.....	SF (ν_1).
	ν_{18}	CD_2 a-stretch	2935 C	2935		
	ν_{19}	CD_3 d-stretch	2214 C	2214		
	ν_{20}	CH_3 d-deform	1461 D	1461	.....	SF (ν_6).
	ν_{21}	CH_2 twist	1285 D	1285		
	ν_{22}	CH_3 rock	1129 C	1129		
	ν_{23}	CD_3 d-deform	1063 C	1063		
	ν_{24}	CH_2 rock	831 C	831		
	ν_{25}	CD_3 rock	660 C	660		
	ν_{26}	CH_3 torsion	[a]216 E	.....	.....	CF [2].
	ν_{27}	CD_3 torsion	[a]161 E	.....	.....	CF [2].

[a] Assigning frequencies higher than these by 10–20 percent may be more reasonable in view of the results for $CH_3CH_2CH_3$.

References

[1] IR. J. N. Gayles, Jr. and W. T. King, Spectrochim. Acta. **21**, 543 (1965).
[2] Th. T. Shimanouchi and T. Ueda, unpublished.
[3] Th. J. N. Gayles, Jr., W. T. King, and J. H. Schachtschneider, Spectrochim. Acta **23A**, 703 (1967).

Molecule: Propane-1,1,1,3,3,3-d_6 $CD_3CH_2CD_3$ No. 105
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_2 s-stretch	2883 C	2883		
	ν_2	CD_3 d-stretch	2225 C	2225	.....	SF (ν_{23}).
	ν_3	CD_3 s-stretch	2091 C	2091	.....	SF (ν_{16}).
	ν_4	CH_2 scis	1467 C	1467		
	ν_5	CD_3 s-deform	1098 E	.....	.....	CF [4].
	ν_6	CD_3 d-deform	1066 C	1066	.....	SF (ν_{19}).
	ν_7	CD_3 rock	962 E	962		
	ν_8	CC stretch	711 D	711		
	ν_9	CCC deform	315 E	.....	.....	CF [4].
a_2	ν_{10}	CD_3 d-stretch	2222 E	ia	.....	CF [4].
	ν_{11}	CH_2 twist	1257 E	ia	.....	CF [4].
	ν_{12}	CD_3 d-deform	1052 E	ia	.....	CF [4].
	ν_{13}	CD_3 rock	700 E	ia	.....	CF [4].
	ν_{14}	Torsion	[a]142 E	ia	.....	OC ($\nu_{14} + \nu_{21}$, $\nu_{21} - 2\nu_{14}$) [3].
b_1	ν_{15}	CD_3 d-stretch	2227 C	2227		
	ν_{16}	CD_3 s-stretch	2091 C	2091	.....	SF (ν_3).
	ν_{17}	CH_2 wag	1331 C	1331		
	ν_{18}	CC stretch	1131 C	1131		
	ν_{19}	CD_3 d-deform	1066 C	1066	.....	SF (ν_6).
	ν_{20}	CD_3 s-deform	920 E	920		
	ν_{21}	CD_3 rock	725 C	725		
b_2	ν_{22}	CH_2 a-stretch	2929 C	2929		
	ν_{23}	CD_3 d-stretch	2225 C	2225	.....	SF (ν_2).
	ν_{24}	CD_3 d-deform	1087 C	1087		
	ν_{25}	CH_2 rock	1066 D	1066		
	ν_{26}	CD_3 rock	640 C	640		
	ν_{27}	Torsion	[a]173 E	.....	.....	OC ($\nu_{21} + \nu_{27} - \nu_{14}$) [3].

[a] Assigning frequencies higher than these by 10–20 percent may be more reasonable in view of the results for $CH_3CH_2CH_3$.

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.
[5] Th. J. N. Gayles, Jr., W. T. King, and J. H. Schachtschneider, Spectrochim. Acta 23A, 703 (1967).

Molecule: Propane-d_8 $CD_3CD_2CD_3$ No. 196
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 d-stretch	2225 C	2225		
	ν_2	CD_3 s-stretch	2122 C	2122		
	ν_3	CD_2 s-stretch	2081 C	2081		
	ν_4	CD_3 s-deform	1086 D	1086		
	ν_5	CD_2 scis	1064 D	1064		
	ν_6	CD_3 d-deform	1064 D	1064	.....	SF (ν_5).
	ν_7	CD_3 rock	959 C	959		
	ν_8	CC stretch	712 C	712		
	ν_9	CCC deform	332 E	.....	.....	CF [3].
a_2	ν_{10}	CD_3 d-stretch	2221 E	ia	.....	CF [4].
	ν_{11}	CD_3 d-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}	Torsion	[a]143 E	ia	.....	OC ($\nu_{14} + \nu_{22}$, $\nu_{14} + \nu_{24}$) [3].
b_1	ν_{15}	CD_3 d-stretch	2224 C	2224		
	ν_{16}	CD_3 s-stretch	2081 C	2081	.....	SF (ν_3).
	ν_{17}	CC stretch	1203 C	1203		
	ν_{18}	CD_3 d-deform	1086 D	1086	.....	SF (ν_4).
	ν_{19}	CD_3 s-deform	1068 D	1068		
	ν_{20}	CD_2 wag	862 D	862		
	ν_{21}	CD_3 rock	688 C	688		
b_2	ν_{22}	CD_3 d-stretch	2224 C	2224	.....	SF (ν_{15}).
	ν_{23}	CD_2 a-stretch	2149 D	2149		
	ν_{24}	CD_3 d-deform	1064 D	1064	.....	SF (ν_5, ν_6).
	ν_{25}	CD_3 rock	949 D	949		
	ν_{26}	CD_2 rock	544 D	544		
	ν_{27}	Torsion	[a]172 E	.....	.....	OC ($\nu_{25} + \nu_{27} - \nu_{21}$) [3.]

[a] Assigning frequencies higher than 10–20 percent may be more reasonable in view of the results for $CH_3CH_2CH_3$.

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.
[5] Th. J. N. Gayles, Jr., W. T. King, and J. H. Schachtschneider, Spectrochim. Acta **23A**, 703 (1967).

Molecule: Methyl acetate CH_3COOCH_3 No. 197
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3(O) d-stretch	3035 D	3035 M	3028 (3b)	
	ν_2	CH_3(C) d-stretch	3031 E	.....	.....	SF (ν_2 of CH_3COOCD_3).
	ν_3	CH_3(O) s-stretch	2966 D	2966 S	2954 (3) p	
	ν_4	CH_3(C) s-stretch	2964 E	.....	2942 (7b) p	SF (ν_4 of CH_3COOCD_3).
	ν_5	C=O stretch	1771 C	1771 VS	1738 (3b) p	
	ν_6	CH_3(O) d-deform	1460 E	1460 W, sh (CCl_4 soln.)	.....	OV (ν_{20}).
	ν_7	CH_3(O) s-deform	1440 D	1440 M		
	ν_8	CH_3(C) d-deform	1430 E	.....	.....	SF (ν_8 of CH_3COOCD_3).
	ν_9	CH_3(C) s-deform	1375 D	1375 S	1372 (0.5) p	
	ν_{10}	C–O stretch	1248 C	1248 VS	1254 (0)	
	ν_{11}	CH_3(O) rock	1159 E	1159 VW (liquid)		
	ν_{12}	O–CH_3 stretch	1060 C	1060 S	1044 (2b)	
	ν_{13}	CH_3(C) rock	980 C	980 W	980 (1b) p	
	ν_{14}	CC stretch	844 C	844 M	844 (8) p	
	ν_{15}	C=O ip-bend	639 C	639 M	640 (7) p	
	ν_{16}	CCO deform	429 C	429 M	433 (3) p	
	ν_{17}	COC deform	303 D	303 M	303 (1b) p	
a''	ν_{18}	CH_3(O) d-stretch	3005 D	3005 M	3002 (3b)	
	ν_{19}	CH_3(C) d-stretch	2994 D	2994 W		
	ν_{20}	CH_3(O) d-deform	1460 E	1460 W, sh (CCl_4 soln.)	1449 (4b) dp	OV (ν_6).
	ν_{21}	CH_3(C) d-deform	1430 E	1430 W		
	ν_{22}	CH_3(O) rock	1187 D	1187 W	1187 (0.5b)	
	ν_{23}	CH_3(C) rock	1036 E	1036 W (solid)		
	ν_{24}	C=O op-bend	607 D	607 M	610 (0) dp	
	ν_{25}	C–O torsion	187 D	187 W		
	ν_{26}	C–C torsion	136 E	136 VW (liquid)		
	ν_{27}	O–CH_3 torsion	110 E	110 VW (liquid)		

References

[1] R. K. W. F. Kohlrausch, Ramanspektren, p. 263 (Edwards Bros., Inc., Ann Arbor, 1945).
[2] IR. B. Nolin and R. N. Jones, Can. J. Chem. 34, 1382 (1956).
[3] IR.R. J. K. Wilmshurst, J. Mol. Spectrosc. 1, 201 (1957).
[4] IR.Th. S. Ichikawa, Y. Udagawa, and T. Shimanouchi, unpublished.

Molecule: Methyl acetate-d_3 CD_3COOCH_3 No. 198
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_3 d-stretch	3032 D	3032 M		
	ν_2	CD_3 d-stretch	2275 E	2275 W		
	ν_3	CH_3 s-stretch	2967 D	2967 S		
	ν_4	CD_3 s-stretch	2087 E	2087 W		
	ν_5	C=O stretch	1768 C	1768 VS		
	ν_6	CH_3 d-deform	1455 E	1455 W, sh (CCl_4 soln.)	.....	OV (ν_{20}).
	ν_7	CH_3 s-deform	1439 D	1439 M		
	ν_8	CD_3 d-deform	1007 D	1007 M		
	ν_9	CD_3 s-deform	1086 C	1086 S		
	ν_{10}	C–O stretch	1268 C	1268 VS		
	ν_{11}	CH_3 rock	1160 D	1160 W		
	ν_{12}	O–CH_3 stretch	1049 D	1049 W		
	ν_{13}	CD_3 rock	780 C	780 M		
	ν_{14}	CC stretch	860 C	860 M		
	ν_{15}	C=O ip-bend	599 C	599 M		
	ν_{16}	CCO deform	390 C	390 M		
	ν_{17}	COC deform	298 D	298 M		
a''	ν_{18}	CH_3 d-stretch	3004 D	3004 M		
	ν_{19}	CD_3 d-stretch	2253 D	2253 W		
	ν_{20}	CH_3 d-deform	1455 E	1455 W, sh (CCl_4 soln.)	.....	OV (ν_6).
	ν_{21}	CD_3 d-deform	1033 D	1033 W		
	ν_{22}	CH_3 rock	1181 E	1181 W		
	ν_{23}	CD_3 rock	918 C	918 M		
	ν_{24}	C=O op-bend	525 D	525 M		
	ν_{25}	C–O torsion	178 D	178 M		
	ν_{26}	C–C torsion	98 E	.....	.....	CF [2].
	ν_{27}	O–CH_3 torsion	110 E	.....	.....	CF [2].

References

[1] IR. B. Nolin and R. N. Jones, Can. J. Chem. 34, 1382 (1956).
[2] IR.Th. S. Ichikawa, Y. Udagawa, and T. Shimanouchi, unpublished.

Molecule: Methyl-d_3-acetate CH_3COOCD_3 No. 199
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CD_3 d-stretch	2288 D	2288 M		
	ν_2	CH_3 d-stretch	3031 D	3031 W		
	ν_3	CD_3 s-stretch	2104 D	2104 M		
	ν_4	CH_3 s-stretch	2964 D	2964 W		
	ν_5	C=O stretch	1769 C	1769 VS		
	ν_6	CD_3 d-deform	1050 E	1050 W	.....	OV (ν_{20}).
	ν_7	CD_3 s-deform	1106 C	1106 S		
	ν_8	CH_3 d-deform	1430 E	1430 W (CCl_4 soln.)	.....	OV (ν_{21}).
	ν_9	CH_3 s-deform	1375 D	1375 S		
	ν_{10}	C–O stretch	1268 C	1268 VS		
	ν_{11}	CD_3 rock	985 D	985 W		
	ν_{12}	O–CD_3 stretch	1043 D	1043 M		
	ν_{13}	CH_3 rock	947 C	947 M		
	ν_{14}	CC stretch	781 C	781 M		
	ν_{15}	C=O ip-bend	619 C	619 M		
	ν_{16}	CCO deform	420 C	420 M		
	ν_{17}	COC deform	270 D	270 M		
a''	ν_{18}	CD_3 d-stretch	2263 D	2263 M		
	ν_{19}	CH_3 d-stretch	2994 D	2994 W		
	ν_{20}	CD_3 d-deform	1050 D	1050 W	.....	OV (ν_6).
	ν_{21}	CH_3 d-deform	1430 E	1430 W (CCl_4 soln.)	.....	OV (ν_8).
	ν_{22}	CD_3 rock	908 E	908 VW		
	ν_{23}	CD_3 rock	1015 E	1015 W, sh		
	ν_{24}	C=O op-bend	600 D	600 W, sh		
	ν_{25}	C–O torsion	165 D	165 M		
	ν_{26}	C–C torsion	136 E	.....	.....	CF [2].
	ν_{27}	O–CD_3 torsion	81 E	.....	.....	CF [2].

References

See No. 198.

Molecule: Methyl acetate-d_6 CD_3COOCD_3 No. 200
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CD_3(O) d-stretch	2285 D	2285 M		
	ν_2	CD_3(C) d-stretch	2275 E	.....	.....	SF (ν_2 of CD_3COOCH_3).
	ν_3	CD_3(O) s-stretch	2099 D	2099 M		
	ν_4	CD_3(C) s-stretch	2087 E	.....	.....	SF (ν_4 of CD_3COOCH_3).
	ν_5	C=O stretch	1767 C	1767 VS		
	ν_6	CD_3(O) d-deform	1059 E	1059 W	.....	OV (ν_{20}).
	ν_7	CD_3(O) s-deform	1106 C	1106 S		
	ν_8	CD_3(C) d-deform	1003 E	1003 W		
	ν_9	CD_3(C) s-deform	1086 E	.....	.....	SF (ν_9 of CD_3COOCH_3).
	ν_{10}	C–O stretch	1282 C	1282 VS		
	ν_{11}	CD_3(O) rock	975 D	975 M		
	ν_{12}	O–CH_3 stretch	1045 E	1045 W		
	ν_{13}	CD_3(C) rock	828 E	828 W		
	ν_{14}	CC stretch	747 C	747 M		
	ν_{15}	C=O ip-bend	585 C	585 M		
	ν_{16}	CCO deform	334 C	334 M		
	ν_{17}	COC deform	266 D	266 M		
a''	ν_{18}	CD_3(O) d-stretch	2264 D	2264 M		
	ν_{19}	CD_3(C) d-stretch	2253 E	.....	.....	SF (ν_{19} of CD_3COOCH_3).
	ν_{20}	CD_3(O) d-deform	1059 D	1059 W	.....	OV (ν_6).
	ν_{21}	CD_3(C) d-deform	1038 E	1038 W		
	ν_{22}	CD_3(O) rock	908 E	.....	.....	SF (ν_{22} of CH_3COOCD_3).
	ν_{23}	CD_3(C) rock	925 D	925 M		
	ν_{24}	C=O op-bend	522 D	522 M		
	ν_{25}	C–O torsion	160 D	160 W		
	ν_{26}	C–C torsion	100 E	.....	.....	CF [2].
	ν_{27}	O–CH_3 torsion	80 E	.....	.....	CF [2].

References

See No. 198.

Molecule: Butadiyne HCCCCH No. 201
Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
σ_g^+	ν_1	CH stretch	3293 D	ia	3293 VW (liquid)	
	ν_2	C≡C stretch	2184 C	ia	2184 VS	
	ν_3	C–C stretch	874 C	ia	874 W	
σ_u^+	ν_4	CH stretch	3329 C	3329 VS	ia	
	ν_5	C≡C stretch	2020 C	2020 M	ia	
π_g	ν_6	CH bend	627 C	ia	627 M	
	ν_7	CCC bend	482 C	ia	482 S	
π_u	ν_8	CH bend	630 B	630 VS	ia	
	ν_9	CCC bend	231 E	ia	231 VW (liquid)	

Reference

[1] IR.R. A. V. Jones, Proc. Roy. Soc. (London), Ser. A, 211, 285 (1952).

Molecule: Furan C_4H_4O No. 202

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3154 D	.....	3154 VS, p	
	ν_2	CH stretch	3140 D	3140 sh		
	ν_3	ip-Ring II	1491 C	1491 VS	1483 VS, p	
	ν_4	ip-Ring III	1384 C	1384 M	1380 S, p	
	ν_5	ip-Ring IV	1140 D	1140 sh (liquid)	1137 VS, p	
	ν_6	CH ip-bend	1066 C	1066 S	1061 M, p	
	ν_7	CH ip-bend	995 C	995 VS	986 M, p	
	ν_8	ip-Ring VII	871 C	871 S		
a_2	ν_9	CH op-bend	863 C	ia	.....	OC ($\nu_9 + \nu_{16}$, $\nu_9 + \nu_{17}$, $\nu_9 + \nu_{19}$, $\nu_9 + \nu_2$).
	ν_{10}	CH op-bend	728 D	ia	728 W, dp	
	ν_{11}	op-Ring I	613 D	ia	613 VW, dp	
b_1	ν_{12}	CH stretch	3161 C	3161 M		
	ν_{13}	CH stretch	3129 C	3129 M	3121 S, dp	
	ν_{14}	ip-Ring I	1556 C	1556 W		
	ν_{15}	CH ip-bend	1267 C	1267 VW	1270 VW, dp	
	ν_{16}	CH ip-bend	1180 C	1180 VS	1171 W, dp	
	ν_{17}	ip-Ring V	1040 D	1040 sh (liquid)	1034 M, dp	
	ν_{18}	ip-Ring VI	873 D	.....	873 W, dp	
b_2	ν_{19}	CH op-bend	838 C	838 VW	839 W, dp	
	ν_{20}	CH op-bend	745 C	745 VS		
	ν_{21}	op-Ring II	603 C	603 S	601 W, dp	

References

[1] R. A. W. Reitz, Z. Phys. Chem. **B38**, 381 (1938).
[2] IR. H. W. Thompson and R. B. Temple, Trans. Faraday Soc. 41, 27 (1945).
[3] IR.R. G. B. Guthrie, D. W. Scott, W. N. Hubbard, C. Katz, J. P. McCullough, M. E. Gross, K. D. Williamson, and G. Waddington, J. Amer. Chem. Soc. 74, 4662 (1952).
[4] IR. B. Bak, S. Brodersen, and L. Hansen, Acta Chem. Scand. 9, 749 (1955).
[5] IR.R. M. Rico, M. Barrachina, and J. M. Orza, J. Mol. Spectrosc. 24, 133 (1967).

Molecule: Thiophene C_4H_4S No. 203
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch	3126 C	3126 M	3107 (10) p	
	ν_2	CH stretch	3098 C	3098 S	3084 (5sh)	
	ν_3	ip-Ring II	1409 C	1409 S	1407 (7) p	
	ν_4	ip-Ring III	1360 C	1360 VW	1358 (5) p	
	ν_5	CH ip-bend	1083 C	1083 S	1081 (5) p	
	ν_6	CH ip-bend	1036 C	1036 S	1035	
	ν_7	ip-Ring IV	839 C	839 VS	832 (5) p	
	ν_8	ip-Ring VII	608 C	608 W	606 (2) p	
a_2	ν_9	CH op-bend	903 D	ia, 900 VW (solid)	903 (0) dp	
	ν_{10}	CH op-bend	688 D	ia	688 (0) dp	
	ν_{11}	op-Ring I	567 D	ia, 565 VW (liquid)	567 (0) dp	
b_1	ν_{12}	CH stretch	[a]3125 E			
	ν_{13}	CH stretch	3086 C	3086 S	3076 (sh)	
	ν_{14}	ip-Ring I	1504 D	1504 VW (liquid)	1502 (0) dp	
	ν_{15}	CH ip-bend	1256 C	1256 S	1257 (0)	
	ν_{16}	CH ip-bend	[a]1085 E	.....	.....	OV (ν_5).
	ν_{17}	ip-Ring V	872 C	872 M	869 (4) dp	
	ν_{18}	ip-Ring VI	751 D	763 VW	751 (1) dp	
b_2	ν_{19}	CH op-bend	867 E	.....	.....	OC ($\nu_9 + \nu_{19}$, $2\nu_{19}$).
	ν_{20}	CH op-bend	712 C	712 VS		
	ν_{21}	op-Ring II	452 C	452 W	453 (0) dp	

[a] These frequencies were estimated from isotopic rule [3].

References

[1] IR. H. W. Thompson and R. B. Temple, Trans. Faraday Soc. 41, 27 (1945).
[2] R. K. W. Kohlrausch and H. Schreiner, Acta Phys. Austriaca 1, 373 (1948).
[3] IR.R. M. Rico, J. M. Orza, and J. Morcillo, Spectrochim. Acta 21, 689 (1965).
[4] IR.R. V. T. Aleksanyan, Ya. M. Kimelfeld, N. N. Magdesieva, and Yu. K. Yurev, Opt. Spectrosc. 22, 116 (1967).

Molecule: Thiophene-d_4 C_4D_4S No. 204
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD stretch	2343 C	2343 M	2326 (6)	
	ν_2	CD stretch	2290 C	2290 M		
	ν_3	ip-Ring II	1376 C	1376 S	1372 (10) p	
	ν_4	ip-Ring III	1248 C	1248 W	1240 (5)	
	ν_5	CD ip-bend	896 C	896 M	891 (10) p	
	ν_6	CD ip-bend	785 C	785 M	780 (3) dp	
	ν_7	ip-Ring IV	731 C	731 VS	723 (3)	
	ν_8	ip-Ring VII	585 D	585 VW	582 (2) p	
a_2	ν_9	CD op-bend	752 E	ia, 756 (solid)	752 (3) dp	SF (ν_{17}).
	ν_{10}	CD op-bend	532 D	ia	532 (2) dp	
	ν_{11}	op-Ring I	488 D	ia	488	
b_1	ν_{12}	CD stretch	[a]2340 E			
	ν_{13}	CD stretch	2305 C	2305 M	2286 (4) dp	
	ν_{14}	ip-Ring I	1459 C	1459 M		
	ν_{15}	CD ip-bend	1034 C	1034 S		
	ν_{16}	CD ip-bend	846 C	846 S	847 (2)	
	ν_{17}	ip-Ring V	752 D	756 (solid)	752 (3) dp	
	ν_{18}	ip-Ring VI	712 C	712 W		
b_2	ν_{19}	CD op-bend	684 C	684 VW	682 (1)	
	ν_{20}	CD op-bend	531 C	531 VS		
	ν_{21}	op-Ring II	414 C	414 VW	411	

[a] This frequency was estimated from isotopic rule [2].

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Molecule: 1,3-Butadiene $CH_2CHCHCH_2$ No. 205
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Solid)	
a_g	ν_1	CH_2 a-stretch	3087 D	ia	3087 M	
	ν_2	CH stretch	3003 D	ia	3003 M	
	ν_3	CH_2 s-stretch	2992 D	ia	2992 S	
	ν_4	C=C stretch	1630 D	ia	1630 VS	
	ν_5	CH_2 scis	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 a-stretch	3101 B	3100.6 S	ia	
	ν_{18}	CH stretch	3055 B	3054.9 S	ia	
	ν_{19}	CH_2 s-stretch	2984 B	2984.3 S	ia	
	ν_{20}	C=C stretch	1596 B	1596.0 S	ia	
	ν_{21}	CH_2 scis	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	

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[3] IR. R. K. Harris, Spectrochim. Acta **20**, 1129 (1964).
[4] IR.R.Th. K. Abe, Ph.D. Thesis (University of Tokyo, 1970).

Molecule: 1,3-Butadiene-1-d_1 (trans) $CH_2CHCHCHD$ No. 206
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Solid)	
a'	ν_1	CH_2 a-stretch	3100 C	3100.4 S	3090 M	
	ν_2	CH stretch	3075 D	.....	3075 W	
	ν_3	CH stretch	3048 C	3047.9 S		
	ν_4	CH stretch	3021 C	3020.5 S		
	ν_5	CH_2 s-stretch	3003 D	.....	3003 M	
	ν_6	CD stretch	2286 C	2285.9 M	2276 M	
	ν_7	C=C stretch	1631 D	.....	1631 VS	
	ν_8	C=C stretch	1580 B	1579.7 S	1572 M	
	ν_9	CH_2 scis	1409 D	.....	1409 VW	
	ν_{10}	CH ip-bend	1304 E	.....	.....	CF [1].
	ν_{11}	CH ip-bend	1288 D	.....	1288 S	
	ν_{12}	CH ip-bend	1270 C	1270 M	1272 VW	
	ν_{13}	C–C stretch	1183 D	1185 W	1183 S	
	ν_{14}	CH_2 rock	964 D	964 W (solid)		
	ν_{15}	CD ip-bend	793 D	.....	793 W	
	ν_{16}	CCC deform	511 D	.....	511 M	
	ν_{17}	CCC deform	288 C	288 VW		
a''	ν_{18}	CH op-bend	1008 B	1008.0 VS		
	ν_{19}	CH op-bend	960 B	959.9 S		
	ν_{20}	CH_2 wag	909 B	908.6 VS	921 M	
	ν_{21}	CH op-bend	849 B	849.2 S	862 M	
	ν_{22}	CD op-bend	674 C	673.9 VW		
	ν_{23}	CH_2 twist	464 C	464.0 W		
	ν_{24}	C–C torsion	161 E	.....	.....	CF [1].

Reference

[1] IR.R.Th. K. Abe, Ph.D. Thesis (University of Tokyo, 1970).

Molecule: 1,3-Butadiene-1,1,2-d_3 $CH_2CHCDCD_2$ No. 207
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_2 a-stretch	3099 C	3099.1 S		
	ν_2	CH stretch	3016 C	3016.4 S		
	ν_3	CH_2 s-stretch	2995 C	2995.4 S		
	ν_4	CD_2 a-stretch	2342 C	2341.9 S		
	ν_5	CD stretch	2268 C	2267.9 S		
	ν_6	CD_2 s-stretch	2217 C	2217.1 S		
	ν_7	C=C stretch	1630 C	1630.4 M		
	ν_8	C=C stretch	1549 B	1548.5 S		
	ν_9	CH_2 scis	1425 C	1425 M		
	ν_{10}	CH ip-bend	1298 C	1298 W		
	ν_{11}	C–C stretch	1185 C	1185 W		
	ν_{12}	CD_2 scis	1080 C	1080 W		
	ν_{13}	CD ip-bend	992 D	991.8 W (solid)		
	ν_{14}	CH_2 rock	880 D	879.9 M (solid)		
	ν_{15}	CD_2 rock	757 E	.....	.....	CF [1].
	ν_{16}	CCC deform	476 E	.....	.....	CF [1].
	ν_{17}	CCC deform	280 D	280 W		
a''	ν_{18}	CH op-bend	991 B	990.6 VS		
	ν_{19}	CH_2 wag	909 B	909.2 VS		
	ν_{20}	CD op-bend	791 B	791.3 W		
	ν_{21}	CD_2 wag	715 E	734.0 S 710.1 VS	.....	FR ($\nu_{17} + \nu_{23}$).
	ν_{22}	CH_2 twist	674 B	673.8 S		
	ν_{23}	CD_2 twist	439 C	439.0 M		
	ν_{24}	C–C torsion	153 E	.....	.....	CF [1].

Reference

[1] IR.Th. K. Abe, Ph.D. Thesis (University of Tokyo, 1970).

Molecule: 1,3-Butadiene-1,1,4,4-d_4 $CD_2CHCHCD_2$ No. 208
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Solid)	
a_g	ν_1	CH stretch	3010 D	ia	3010 M	
	ν_2	CD_2 a-stretch	2315 D	ia	2315 S	
	ν_3	CD_2 s-stretch	2212 D	ia	2212 S	
	ν_4	C=C stretch	1610 D	ia	1610 VS	
	ν_5	CH ip-bend	1296 D	ia	1296 S	
	ν_6	C–C stretch	1170 D	ia	1170 S	
	ν_7	CD_2 scis	1040 D	ia	1040 S	
	ν_8	CD_2 rock	740 D	ia	740 W	
	ν_9	CCC deform	457 D	ia	457 S	
a_u	ν_{10}	CH op-bend	955 B	955.1 S	ia	
	ν_{11}	CD_2 wag	728 B	728.0 VS	ia	
	ν_{12}	CD_2 twist	397 C	397 W	ia	
	ν_{13}	C–C torsion	149 E	.....	ia	CF [1].
b_g	ν_{14}	CH op-bend	948 D	ia	948 M	
	ν_{15}	CD_2 wag	728 D	ia	728 S	
	ν_{16}	CD_2 twist	610 D	ia	610 VW	
b_u	ν_{17}	CH stretch	3041 C	3040.8 S	ia	
	ν_{18}	CD_2 a-stretch	2350 D	2350 S	ia	
	ν_{19}	CD_2 s-stretch	2228 C	2228 S	ia	
	ν_{20}	C=C stretch	1535 B	1535.0 S	ia	
	ν_{21}	CH ip-bend	1335 C	1335.2 M	ia	
	ν_{22}	CD_2 scis	1031 C	1031.3 S	ia	
	ν_{23}	CD_2 rock	817 C	816.5 M	ia	
	ν_{24}	CCC deform	258 C	258 W	ia	

Reference

[1] IR.R.Th. K. Abe, Ph.D. Thesis (University of Tokyo, 1970).

Molecule: 1,3-Butadiene-d_6 $CD_2CDCDCD_2$ No. 209
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Solid)	
a_g	ν_1	CD_2 a-stretch	2320 D	ia	2320 M	
	ν_2	CD stretch	2250 D	ia	2250 M	
	ν_3	CD_2 s-stretch	2210 D	ia	2210 M	
	ν_4	C=C stretch	1580 D	ia	1580 VS	
	ν_5	C–C stretch	1196 D	ia	1196 M	
	ν_6	CD_2 scis	1045 D	ia	1045 W	
	ν_7	CD ip-bend	918 D	ia	918 S	
	ν_8	CD_2 rock	746 D	ia	746 M	
	ν_9	CCC deform	439 D	ia	439 S	
a_u	ν_{10}	CD op-bend	741 B	741.4 W	ia	
	ν_{11}	CD_2 wag	718 B	718.4 S	ia	
	ν_{12}	CD_2 twist	381 C	381.1 W	ia	
	ν_{13}	C–C torsion	140 C	140 VW	ia	
b_g	ν_{14}	CD op-bend	799 D	ia	799 S	
	ν_{15}	CD_2 wag	705 D	ia	705 S	
	ν_{16}	CD_2 twist	603 D	ia	603 VW	
b_u	ν_{17}	CD_2 a-stretch	2320 D	2320.3 M	ia	
	ν_{18}	CD stretch	2266 C	2265.9 M	ia	
	ν_{19}	CD_2 s-stretch	2218 C	2218.0 M	ia	
	ν_{20}	C=C stretch	1520 B	1519.6 S	ia	
	ν_{21}	CD_2 scis	1048 C	1048.0 W	ia	
	ν_{22}	CD ip-bend	1005 C	1005.4 M	ia	
	ν_{23}	CD_2 rock	769 D	768.9 W (solid)	ia	
	ν_{24}	CCC deform	250 C	250 W	ia	

Reference

[1] IR.R.Th. K. Abe, Ph.D. Thesis (University of Tokyo, 1970).

Molecule: 2-Butyne CH_3CCCH_3 No. 210
Symmetry $^aD'_{3h}$ **Symmetry number** $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'_1	ν_1	CH_3 s-stretch	2916 C	ia	2916 S p	
	ν_2	C≡C stretch	2240 E	ia	2310 S p	FR ($2\nu_8$).
				ia	2233 S p	
	ν_3	CH_3 s-deform	1380 C	ia	1380 S	
	ν_4	C–C stretch	725 E	ia	774 M p	FR ($2\nu_{16}$).
				ia	693 M p	
a''_1	ν_5	CH_3 torsion[a]	.....	ia	ia	
a''_2	ν_6	CH_3 s-stretch	2938 B	2938 S	ia	
	ν_7	CH_3 s-deform	1382 B	1382 M	ia	
	ν_8	C–C stretch	1152 B	1152 W	ia	
e'	ν_9	CH_3 d-stretch	2973 B	2973 S		
	ν_{10}	CH_3 d-deform	1456 B	1456 S		
	ν_{11}	CH_3 rock	1054 B	1054 M		
	ν_{12}	CCC deform	213 C	.....	213 VW	
e''	ν_{13}	CH_3 d-stretch	2966 D	ia	2966 W	
	ν_{14}	CH_3 d-deform	1448 C	ia	1448 M dp	
	ν_{15}	CH_3 rock	1029 C	ia	1029 M dp	
	ν_{16}	CCC deform	371 C	ia	371 S dp	

[a] Free rotation [5].

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[6] Th. J. T. Hougen, Can. J. Phys. **42**, 1920 (1964).
[7] Th. P. R. Bunker, J. Chem. Phys. **47**, 718 (1967).

Molecule: Cyclobutane C_4H_8 No. 211
Symmetry D_{2d} **Symmetry number** $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 s-stretch	2895 D	ia	2916 p 2866 p	FR ($2\nu_2$, $2\nu_{13}$).
	ν_2	CH_2 scis	1443 C	ia	1443 p	SF (ν_{13}).
	ν_3	Ring stretch	1001 C	ia	1001 p	SF (ν_{14}).
	ν_4	CH_2 a-stretch	2975 E	ia	.....	CF [3].
	ν_5	CH_2 rock	741 C	ia	741 dp	
	ν_6	Ring puckering	197 C	ia	197	CF [3].
a_2	ν_7	CH_2 wag	1260 E	ia	ia	CF [3].
	ν_8	CH_2 twist	1257 E	ia	ia	CF [3].
b_1	ν_9	CH_2 wag	1219 C	ia	1219 dp	
	ν_{10}	Ring deform	926 C	ia	926 dp	
	ν_{11}	CH_2 twist	1222 E	ia	.....	CF [3].
b_2	ν_{12}	CH_2 s-stretch	2893 E	.....	.....	CF [3].
	ν_{13}	CH_2 scis	1443 C	.....	1443 dp	SF (ν_2).
	ν_{14}	Ring deform	1001 D	.....	1001 p	SF (ν_3).
	ν_{15}	CH_2 a-stretch	2987 C	2987 S		
	ν_{16}	CH_2 rock	627 C	627 S		
e	ν_{17}	CH_2 a-stretch	2952 C	.....	2952	
	ν_{18}	CH_2 twist	1223 C	1223 W		
	ν_{19}	CH_2 rock	749 C	749 W		
	ν_{20}	CH_2 s-stretch	2887 D	2897 S 2878 S		
	ν_{21}	CH_2 scis	1447 C	1447 S		
	ν_{22}	CH_2 wag	1257 C	1257 S		
	ν_{23}	Ring deform	898 C	898 S		

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Molecule: Cyclobutane-d_8 C_4D_8 No. 212
Symmetry D_{2d} **Symmetry number** $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_2 s-stretch	2124 E	ia	.....	CF [2].
	ν_2	CD_2 scis	1160 C	ia	1160 p	
	ν_3	Ring stretch	882 C	ia	882 p	
	ν_4	CD_2 a-stretch	2224 E	ia	.....	CF [2].
	ν_5	CD_2 rock	632 E	ia	.....	CF [2].
	ν_6	Ring puckering	158 D	ia	.....	RP [3].
a_2	ν_7	CD_2 wag	1010 E	ia	ia	CF [2].
	ν_8	CD_2 twist	889 E	ia	ia	CF [2].
b_1	ν_9	CD_2 wag	1078 C	ia	1078 dp	
	ν_{10}	Ring deform	746 C	ia	746 dp	
	ν_{11}	CD_2 twist	864 E	ia	.....	CF [2].
b_2	ν_{12}	CD_2 s-stretch	2115 E	.....	.....	CF [2].
	ν_{13}	CD_2 scis	1040 D	.....	1040 dp	
	ν_{14}	Ring deform	938 D	.....	938 dp	SF (ν_{18}).
	ν_{15}	CD_2 a-stretch	2242 C	2242 S		
	ν_{16}	CD rock	483 C	483 S		
e	ν_{17}	CD_2 a-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		
	ν_{20}	CD_2 s-stretch	2103 E	.....	.....	CF [2].
	ν_{21}	CD_2 scis	1078 C	1078 S		
	ν_{22}	CD_2 wag	1048 C	1048 S		
	ν_{23}	Ring deform	734 C	734 S		

References

[1] IR.R. D. G. Rea, Ph.D. Thesis (Massachusetts Institute of Technology, 1954).
[2] Th. R. C. Lord and I. Nakagawa, J. Chem. Phys. 39, 2951 (1963).
[3] IR.R. J. M. R. Stone and I. M. Mills, Mol. Phys. 18, 653 (1970).

Molecule: 2-Methylpropene $(CH_3)_2CCH_2$ No. 213
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 s-stretch	2989 D	2991 M (solid)	2989 S, p	
	ν_2	CH_3 d-stretch	2941 C	2940.8	2930 W, p	
	ν_3	CH_3 s-stretch	2911 D	2919 W	2911 S, p	
	ν_4	C=C stretch	1661 C	1661.1 S	1655 S, p	
	ν_5	CH_3 d-deform	1470 C	1469.6 S	1462 VW	
	ν_6	CH_2 scis	1416 D	1419 W (solid)	1416 S, p	
	ν_7	CH_3 s-deform	1366 D	.....	1366 VW, p	
	ν_8	CH_3 rock	1064 C	1063.9 S	1058 W, p	
	ν_9	C–C stretch	801 C	801 W	803 VS, p	
	ν_{10}	$C=CC_2$ ip-deform	383 D	384 W (solid)	383 W	
a_2	ν_{11}	CH_3 d-stretch	2970 D	ia	2970 W, p	OV (ν_{17}).
	ν_{12}	CH_3 d-deform	1459 D	ia	1459 VW	
	ν_{13}	CH_3 rock	1076 E	ia	.....	CF [4].
	ν_{14}	CH_2 twist	981 E	ia	.....	CF [4].
	ν_{15}	CH_3 torsion	193 E	ia	.....	CF [3].
b_1	ν_{16}	CH_2 a-stretch	3086 C	3086.0 S	3079 W, dp	
	ν_{17}	CH_3 d-stretch	2980 C	2980.4	2970 W, dp	OV (ν_{11}).
	ν_{18}	CH_3 s-stretch	2893 C	2892.9 W	2892 W, dp	
	ν_{19}	CH_3 d-deform	1458 C	1458.4 S		
	ν_{20}	CH_3 s-deform	1381 C	1381.2 S	1386 W	
	ν_{21}	C–C stretch	1282 C	1281.9 S	1281 W	
	ν_{22}	CH_3 rock	1043 E	.....	.....	CF [4].
	ν_{23}	CH_2 rock	974 C	973.7 W	972 VW	
	ν_{24}	$C=CC_2$ ip-deform	430 D	430 sh (solid)		
b_2	ν_{25}	CH_3 d-stretch	2945 C	2944.9 S		
	ν_{26}	CH_3 d-deform	1444 C	1443.7 S	1439 VW	
	ν_{27}	CH_3 rock	1079 C	1079.0 S		
	ν_{28}	CH_2 wag	890 C	889.7 VS	883 W, dp	
	ν_{29}	$C=CC_2$ op-deform	429 C	429.1 S	431 W, dp	
	ν_{30}	CH_3 torsion	196 C	196 VW		

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[1] IR. D. R. Smith, B. K. McKenna, and K. D. Möller, J. Chem. Phys. 45, 1904 (1966).
[2] IR.R. W. Lüttke and S. Braun, Ber. Bunsenges. Phys. Chem. 71, 34 (1967).
[3] IR.Th. Y. Abe, Ph.D. Thesis (University of Tokyo, 1968).
[4] IR.R. C. M. Pathak and W. H. Fletcher, J. Mol. Spectrosc. 31, 32 (1969).

Molecule: 2-Methyl-d_3-propene-3,3,3-d_3 $(CD_3)_2CCH_2$ No. 214
Symmetry C_{2v} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CH_2 s-stretch	2996 C	2996 M		
	ν_2	CD_3 d-stretch	2166 D	2166 W (solid)		
	ν_3	CD_3 s-stretch	2111 C	2111 W		
	ν_4	C=C stretch	1650 C	1650 S		
	ν_5	CH_2 scis	1410 C	1410 W		
	ν_6	CD_3 s-deform	1092 D	1092 W (solid)		
	ν_7	CD_3 d-deform	1056 D	1056 M (solid)		
	ν_8	CD_3 rock	850 E	.....	.....	CF [1].
	ν_9	C–C stretch	718 D	718 W (solid)		
	ν_{10}	$C=CC_2$ ip-deform	319 C	319 W		
a_2	ν_{11}	CD_3 d-stretch	2208 E	ia	.....	CF [1].
	ν_{12}	CD_3 d-deform	1054 E	ia	.....	CF [1].
	ν_{13}	CD_3 rock	731 E	ia	.....	CF [1].
	ν_{14}	CH_2 twist	664 E	ia	.....	CF [1].
	ν_{15}	CD_3 torsion	138 E	ia	.....	CF [1].
b_1	ν_{16}	CH_2 a-stretch	3085 C	3085 S		
	ν_{17}	CD_3 d-stretch	2236 C	2236 S		
	ν_{18}	CD_3 s-stretch	2072 C	2072 M		
	ν_{19}	C–C stretch	1294 C	1294 M		
	ν_{20}	CD_3 d-deform	1074 C	1074 W		
	ν_{21}	CD_3 s-deform	1052 D	1052 M (solid)		
	ν_{22}	CH_2 rock	880 E	.....	.....	CF [1].
	ν_{23}	CD_3 rock	745 C	745 W		
	ν_{24}	$C=CC_2$ ip-deform	400 C	400 M		
b_2	ν_{25}	CD_3 d-stretch	2204 C	2204 S		
	ν_{26}	CD_3 d-deform	1055 C	1055 S		
	ν_{27}	CD_3 rock	923 C	923 M		
	ν_{28}	CH_2 wag	884 C	884 VS		
	ν_{29}	$C=CC_2$ op-deform	369 C	369 S		
	ν_{30}	CD_3 torsion	143 E	.....	.....	CF [1].

Reference

[1] IR.Th. Y. Abe, Ph.D. Thesis (University of Tokyo, 1968).

Molecule: 2-Butanone $CH_3COCH_2CH_3$ (trans form) No. 215
Symmetry C_s **Symmetry number** $\sigma = 1$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Liquid)	
a'	ν_1	CH_3(1) d-stretch	2983 D	2983 S (liquid)	2983 M	OV (ν_2, ν_{21}, ν_{22}).
	ν_2	CH_3(4) d-stretch	2983 D	2983 S (liquid)	2983 M	OV (ν_1, ν_{21}, ν_{22}).
	ν_3	CH_3(1) s-stretch	2910 D	2910 S (liquid)	2924 S, p	OV (ν_4).
	ν_4	CH_3(4) s-stretch	2910 D	2910 S (liquid)	2924 S, p	OV (ν_3).
	ν_5	CH_2 s-stretch	2884 D	2884 S (liquid)		
	ν_6	CO stretch	1716 C	1716 S	1715 M, p	
	ν_7	CH_3(4) d-deform	1460 D	1460 M	1450 M	OV (ν_{24}).
	ν_8	CH_2 scis	1422 C	1422 S	1419 M	
	ν_9	CH_3(1) d-deform	1413 D	1413 S	.....	OV (ν_{25}).
	ν_{10}	CH_3(4) s-deform	1373 C	1373 S		
	ν_{11}	CH_3(1) s-deform	1346 C	1346 S	1345 W	
	ν_{12}	CH_2 wag	1263 D	1263 W	1258 W	OV (ν_{26}).
	ν_{13}	CC(12) stretch	1182 C	1182 S	1169 W	
	ν_{14}	CH_3(4) rock	1089 C	1089 M	1087 M, p	
	ν_{15}	CC(34) stretch	997 C	997	999 W	
	ν_{16}	CH_3(1) rock	939 C	939	951 W	
	ν_{17}	CC(23) stretch	760 D	760 S (liquid)	760 M, p	
	ν_{18}	CO ip-bend	590 C	590 S	591 W	
	ν_{19}	CCC(123) deform	413 C	413 S	410 W	
	ν_{20}	CCC(234) deform	260 C	260 S	264 W	
a''	ν_{21}	CH_3(1) d-stretch	2983 D	2983 S (liquid)	2983	OV (ν_1, ν_2, ν_{22}).
	ν_{22}	CH_3(4) d-stretch	2983 D	2983 S (liquid)	2983	OV (ν_1, ν_2, ν_{21}).
	ν_{23}	CH_2 d-stretch	2941 D	2941 S (liquid)		
	ν_{24}	CH_3(4) d-deform	1460 D	1460 M	1450 M	OV (ν_7).
	ν_{25}	CH_3(1) d-deform	1413 D	1413 S	.....	OV (ν_9).
	ν_{26}	CH_2 twist	1263 D	1263 W	1258 W	OV (ν_{12}).
	ν_{27}	CH_3(4) rock	1108 C	1108 W		
	ν_{28}	CH_3(1) rock	952 C	952 sh	951 W	
	ν_{29}	CH_2 rock	768 D	768 S (liquid)		
	ν_{30}	CO op-bend	460 C	460 VW		
	ν_{31}	CC(34) torsion	201 E	.....	.....	CF [4].
	ν_{32}	CC(12) torsion	106 E	.....	.....	CF [4].
	ν_{33}	CC(23) torsion	87 C	87 W		

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[2] IR.R. J. E. Katon and F. F. Bentley, Spectrochim. Acta **19**, 639 (1963).
[3] IR.Th. T. Shimanouchi, Y. Abe, and M. Mikami, Spectrochim. Acta, **24A**, 1037 (1968).
[4] IR.R.Th. M. Mikami, Ph.D. Thesis (University of Tokyo, 1969).

Molecule: n-Butane $CH_3CH_2CH_2CH_3$ (trans form) No. 216
Symmetry C_{2h} **Symmetry number** $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Matrix isolation)	cm^{-1} (Solid)	
a_g	ν_1	CH_3 d-stretch	2965 C	ia	2965 (9)	SF (ν_{20}).
	ν_2	CH_3 s-stretch	2872 C	ia	2872 (8)	
	ν_3	CH_2 s-stretch	2853 D	ia	2853 (8)	
	ν_4	CH_3 d-deform	1460 C	ia	1460 (2)	SF (ν_{22}).
	ν_5	CH_2 scis	1442 D	ia	1442 (3)	
	ν_6	CH_3 s-deform	1382 C	ia	.....	CF [9].
	ν_7	CH_2 wag	1361 D	ia	.....	CF [9].
	ν_8	CH_3 rock	1151 C	ia	1151 (4)	
	ν_9	CC stretch	1059 C	ia	1059 (5)	
	ν_{10}	CC stretch	837 C	ia	837 (6)	
	ν_{11}	CCC deform	425 C	ia	425 (4)	
a_u	ν_{12}	CH_3 d-stretch	2968 C	2968 S	ia	SF (ν_{27}).
	ν_{13}	CH_2 a-stretch	2930 C	2930 S	ia	
	ν_{14}	CH_3 d-deform	1461 C	1461 S	ia	SF (ν_{30}), OV (ν_{30}, ν_{31})
	ν_{15}	CH_2 twist	1257 C	1257 W (solid)	ia	
	ν_{16}	CH_3 rock	948 B	948 M	ia	
	ν_{17}	CH_2 rock	731 B	731 S	ia	
	ν_{18}	CH_3-CH_2 torsion	194 E	.....	ia	CF [9].
	ν_{19}	CH_2-CH_2 torsion	102 E	.....	ia	CF [9].
b_g	ν_{20}	CH_3 d-stretch	2965 C	ia	2965 (9)	SF (ν_1).
	ν_{21}	CH_2 a-stretch	2912 C	ia	2912 (4)	
	ν_{22}	CH_3 d-deform	1460 C	ia	1460 (2)	SF (ν_4).
	ν_{23}	CH_2 twist	1300 C	ia	1300 (4)	
	ν_{24}	CH_3 rock	1180 D	ia	.....	CF [9].
	ν_{25}	CH_2 rock	803 D	ia	.....	CF [9].
	ν_{26}	CH_3-CH_2 torsion	225 E	ia	.....	CF [9].
b_u	ν_{27}	CH_3 d-stretch	2968 C	2968 S	ia	SF (ν_{12}).
	ν_{28}	CH_3 s-stretch	2870 C	2870 S	ia	
	ν_{29}	CH_2 s-stretch	2853 E	.....	ia	SF (ν_3).
	ν_{30}	CH_3 d-deform	1461 C	1461 S	ia	SF (ν_{14}), OV (ν_{14}, ν_{31}).
	ν_{31}	CH_2 scis	1461 C	1461 S	ia	OV (ν_{14}, ν_{30}).
	ν_{32}	CH_3 s-deform	1379 B	1379 M	ia	
	ν_{33}	CH_2 wag	1290 B	1290 W	ia	
	ν_{34}	CC stretch	1009 C	1009 W (solid)	ia	
	ν_{35}	CH_3 rock	964 B	964 M	ia	
	ν_{36}	CCC deform	271 E		ia	CF [9].

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[2] IR. D. W. E. Axford and D. H. Rank, J. Chem. Phys. 17, 430 (1949).
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Molecule: n-Butane $CH_3CH_2CH_2CH_3$ (gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a	ν_1	CH_3 d-stretch	[a]2968 C			
	ν_2	CH_3 d-stretch	[a]2968 C			
	ν_3	CH_2 a-stretch	[a]2920 D			
	ν_4	CH_3 s-stretch	[a]2870 C			
	ν_5	CH_2 s-stretch	[a]2860 D			
	ν_6	CH_3 d-deform	[a]1460 C			
	ν_7	CH_3 d-deform	[a]1460 C			
	ν_8	CH_2 scis	[a]1450 D			
	ν_9	CH_3 s-deform	[a]1380 C			
	ν_{10}	CH_2 wag	1350 C	1350 W		
	ν_{11}	CH_2 twist	1281 C	.....	1281 (0)	
	ν_{12}	CH_3 rock	1168 D	.....	1168 (0)	
	ν_{13}	CC stretch	1077 D	.....	1077 (1)	
	ν_{14}	CH_3 rock	980 D	.....	980 (2)	OV (ν_{32}).
	ν_{15}	CC stretch	827 D	.....	827 (6)	
	ν_{16}	CH_2 rock	788 C	788 M	789 (2)	
	ν_{17}	CCC deform	320 C	.....	320 (1)	
	ν_{18}	CH_3-CH_2 torsion	201 E	.....	.....	CF [5].
	ν_{19}	CH_2-CH_2 torsion	101 E	.....	.....	CF [5].
b	ν_{20}	CH_3 d-stretch	[a]2968 C			
	ν_{21}	CH_3 d-stretch	[a]2968 C			
	ν_{22}	CH_2 a-stretch	[a]2920 D			
	ν_{23}	CH_3 s-stretch	[a]2870 C			
	ν_{24}	CH_2 s-stretch	[a]2860 D			
	ν_{25}	CH_3 d-deform	[a]1460 C			
	ν_{26}	CH_3 d-deform	[a]1460 C			
	ν_{27}	CH_2 scis	[a]1450 D			
	ν_{28}	CH_3 s-deform	[a]1380 C			
	ν_{29}	CH_2 wag	1370 D	.....	1370 VW	
	ν_{30}	CH_2 twist	1233 C	1233 W		
	ν_{31}	CC stretch	1133 D	1133 M		
	ν_{32}	CH_3 rock	980 D	.....	980 (2)	OV (ν_{14}).
	ν_{33}	CH_3 rock	955 C	.....	955 (1b)	
	ν_{34}	CH_2 rock	747 C	747 S		
	ν_{35}	CCC deform	469 D	.....	.....	CF [5].
	ν_{36}	CH_3-CH_2 torsion	197 E	.....	.....	CF [5].

[a] Deduced from the corresponding frequencies of the trans form.

References

[1] R. N. Sheppard and G. J. Szasz, J. Chem. Phys. 17, 86 (1949).
[2] IR. D. W. E. Axford and D. H. Rank, J. Chem. Phys. 17, 430 (1949).
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Molecule: **Benzene** C_6H_6 No. 218
Symmetry D_{6h} **Symmetry number** $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	CH stretch	3062 C	ia	3061.9 VS, p	
	ν_2	Ring stretch	992 C	ia	991.6 VS, p	
a_{2g}	ν_3	CH bend	1326 E	ia	1326 VW	
a_{2u}	ν_4	CH bend	673 B	673 S	ia	
b_{1u}	ν_5	CH stretch	3068 C	3067.57 VW (solid)	ia	
	ν_6	Ring deform	1010 C	1010 W (solid)	ia	
b_{2g}	ν_7	CH bend	995 E	ia	ia	OC ($\nu_{19}+\nu_7$, $\nu_{20}+\nu_7$).
	ν_8	Ring deform	703 E	ia	ia	OC ($\nu_{19}+\nu_8$, $\nu_{20}+\nu_8$).
b_{2u}	ν_9	Ring stretch	1310 C	1310 W (liquid)	ia	
	ν_{10}	CH bend	1150 C	1150 W (liquid)	ia	
e_{1g}	ν_{11}	CH bend	849 C	ia	848.9 M, dp	
e_{1u}	ν_{12}	CH stretch	3063 E	3080 S 3030 S (liquid)	ia	FR ($\nu_{13} + \nu_{16}$).
	ν_{13}	Ring stretch + deform	1486 B	1486 S	ia	
	ν_{14}	CH bend	1038 B	1038 S	ia	
e_{2g}	ν_{15}	CH stretch	3047 C	ia	3046.8 S, dp	
	ν_{16}	Ring stretch	1596 E	ia	1606.4 S, dp 1584.6 S, dp	FR ($\nu_2 + \nu_{18}$).
	ν_{17}	CH bend	1178 C	ia	1178.0 S, dp	
	ν_{18}	Ring deform	606 C	ia	605.6 S, dp	
e_{2u}	ν_{19}	CH bend	975 C	975 W (liquid)	ia	
	ν_{20}	Ring deform	410 C	417.7 403.0 (solid)	ia	

References

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[4] Th. S. Califano and B. Crawford, Jr., Spectrochim. Acta 16, 889 (1960).
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Molecule: Benzene-d_6 C_6D_6 No. 219
Symmetry D_{6h} **Symmetry number** $\sigma = 12$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	CD stretch	2293 C	ia	2292.6 VS, p	
	ν_2	Ring stretch	943 C	ia	943.2 VS, p	
a_{2g}	ν_3	CD bend	1037 E	ia	ia	OC ($\nu_3+\nu_{14}$, $\nu_3+\nu_{16}$).
a_{2u}	ν_4	CD bend	497 C	496.5 S (liquid)	ia	
b_{1u}	ν_5	CD stretch	2292 E	2292 VW (solid)	ia	
	ν_6	Ring deform	969 C	970.48 969.77 966.76 (solid)	ia	
b_{2g}	ν_7	CD bend	827 E	ia	ia	OC ($\nu_7+\nu_{19}$).
	ν_8	Ring deform	601 E	ia	ia	OC ($\nu_8+\nu_{10}$).
b_{2u}	ν_9	Ring stretch	1286 C	1287.51 1286.41 1285.14 (solid)	ia	
	ν_{10}	CD bend	824 C	825.2 822.57 (solid)	ia	
e_{1g}	ν_{11}	CD bend	662 C	ia	661.7 M, dp	
e_{1u}	ν_{12}	CD stretch	2287 C	2287 S	ia	
	ν_{13}	Ring stretch + deform	1335 B	1335 M	ia	
	ν_{14}	CD bend	814 B	814 S	ia	
e_{2g}	ν_{15}	CD stretch	2265 C	ia	2264.9 S, dp	
	ν_{16}	Ring stretch	1552 C	ia	1551.5 S, dp	
	ν_{17}	CD bend	867 C	ia	867.3 S, dp	
	ν_{18}	Ring deform	577 C	ia	577.4 M, dp	
e_{2u}	ν_{19}	CD bend	795 C	799.91 797.37 794.64 790.9 790.3 (solid)	ia	
	ν_{20}	Ring deform	352 E	ia	ia	OC ($\nu_4+\nu_{20}$, $\nu_{14}+\nu_{20}$).

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Molecule: Cyclohexane C_6H_{12} No. 220
Symmetry D_{3d} Symmetry number $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	CH_2 a-stretch	2930 E	ia	2938 VS, p 2923 VS, p	FR ($2\nu_3$).
	ν_2	CH_2 s-stretch	2852 C	ia	2852 VS, p	
	ν_3	CH_2 scis	1465 C	ia	1465 M, p	
	ν_4	CH_2 rock	1157 C	ia	1157 S, p	
	ν_5	CC stretch	802 C	ia	802 VS, p	
	ν_6	CCC deform + CC torsion	383 C	ia	383 M, p	
a_{1u}	ν_7	CH_2 twist	1383 C	[a]1383	ia	
	ν_8	CH_2 wag	1157 C	[a]1157	ia	
	ν_9	CC stretch + CC torsion	1057 C	[a]1057	ia	
a_{2g}	ν_{10}	CH_2 wag	1437 C	[a]1437	ia	
	ν_{11}	CH_2 twist	1090 C	[a]1090	ia	
a_{2u}	ν_{12}	CH_2 a-stretch	2915 E	2915 M	ia	
	ν_{13}	CH_2 s-stretch	2860 E	.....	ia	SF (ν_2, ν_{18}, ν_{26}).
	ν_{14}	CH_2 scis	1437 C	1437 M	ia	
	ν_{15}	CH_2 rock	1030 D	1040 M 1016 M	ia	FR ($\nu_{23} + \nu_{32}$).
	ν_{16}	CCC deform	523 A	523 W	ia	
e_g	ν_{17}	CH_2 a-stretch	2930 E	ia	.....	SF (ν_1, ν_{12}, ν_{25}).
	ν_{18}	CH_2 s-stretch	2897 E	ia	2897 M, vb	
	ν_{19}	CH_2 scis	1443 C	ia	1443 S, dp	
	ν_{20}	CH_2 wag	1347 C	ia	1347 S, dp	
	ν_{21}	CH_2 twist	1266 C	ia	1266 VS, dp	
	ν_{22}	CC stretch	1027 C	ia	1027 VS, dp	
	ν_{23}	CH_2 rock	785 C	[a]785	785 VW, dp	
	ν_{24}	CCC deform + CC torsion	426 C	ia	426 S, dp	
e_u	ν_{25}	CH_2 a-stretch	2933 A	2933 VS	ia	
	ν_{26}	CH_2 s-stretch	2863 A	2863 VS	ia	
	ν_{27}	CH_2 scis	1457 A	1457 VS	ia	
	ν_{28}	CH_2 wag	1355 B	1355 W	ia	
	ν_{29}	CH_2 twist	1261 A	1261 S	ia	
	ν_{30}	CH_2 rock	907 B	907 S	ia	
	ν_{31}	CC stretch	863 A	863 S	ia	
	ν_{32}	CCC deform. + CC torsion	248 C	248 VW (liquid)	ia	

[a] Observed in the crystalline state at about 90 K [8].

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Molecule: Cyclohexane-d_{12} C_6D_{12} No. 221
Symmetry D_{3d} **Symmetry number** $\sigma = 6$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_{1g}	ν_1	CD_2 a-stretch	2152 C	ia	2152 VS, p	
	ν_2	CD_2 s-stretch	2082 C	ia	2082 VS, p	
	ν_3	CD_2 scis	1117 C	ia	1117 M, p	
	ν_4	CD_2 rock	1012 C	ia	1012 W, p	
	ν_5	CC stretch	723 C	ia	723 VS, p	
	ν_6	CCC deform. + CC torsion	298 C	ia	298 W, p	
a_{1u}	ν_7	CD_2 twist	864 E	ia	ia	CF [4].
	ν_8	CD_2 wag	842 E	ia	ia	CF [4].
	ν_9	CC stretch. + CC torsion	1187 E	ia	ia	CF [4].
a_{2g}	ν_{10}	CD_2 wag	1126 E	ia	ia	CF [4].
	ν_{11}	CD_2 twist	778 E	ia	ia	CF [4].
a_{2u}	ν_{12}	CD_2 a-stretch	2206 C	2206 VS	ia	OV (ν_{25}).
	ν_{13}	CD_2 s-stretch	2108 C	2108 VS	ia	OV (ν_{26}).
	ν_{14}	CD_2 scis	1091 B	1091 VS	ia	
	ν_{15}	CD_2 rock	917 A	917 VS	ia	
	ν_{16}	CCC deform	395 B	395 S	ia	
e_g	ν_{17}	CD_2 a-stretch	2199 C	ia	2199 VS, dp	
	ν_{18}	CD s-stretch	2104 C	ia	2104 VS, dp	
	ν_{19}	CD_2 scis	1071 C	ia	1071 M, dp	
	ν_{20}	CD_2 wag	1212 C	ia	1212 M, dp	
	ν_{21}	CD_2 twist	937 C	ia	937 S, dp	
	ν_{22}	CC stretch	795 C	ia	795 S, dp	
	ν_{23}	CD_2 rock	637 C	ia	637 W, dp	
	ν_{24}	CCC deform. + CC torsion	373 C	ia	373 M, dp	
e_u	ν_{25}	CD_2 a-stretch	2206 C	2206 VS	ia	OV (ν_{12}).
	ν_{26}	CD_2 s-stretch	2108 C	2108 VS	ia	OV (ν_{13}).
	ν_{27}	CD_2 scis	1069 C	1069 M (liquid)	ia	
	ν_{28}	CD_2 wag	1165 A	1165 VS	ia	
	ν_{29}	CD_2 twist	991 A	991 VS	ia	
	ν_{30}	CD_2 rock	687 B	687 S	ia	
	ν_{31}	CC stretch	720 A	720 S	ia	
	ν_{32}	CCC deform. + CC torsion	203 C	.....	ia	CF [4].

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Molecule: Poly(methylene) $(CH_2)_n$ No. 222
Symmetry D_{2h} **Symmetry number** $\sigma = 4$

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Solid)	
a_g	ν_1	CH_2 s-stretch	2848 C	ia	2848 S	
	ν_2	CH_2 scis	1440 C	ia	1440 M	
	ν_3	CC stretch	1131 C	ia	1131 M	
a_u	ν_4	CH_2 twist	[a]1050 D	ia, 1050 VW	ia	
b_{1g}	ν_5	CH_2 wag	1370 D	ia	1370 VW	
	ν_6	CC stretch	1061 C	ia	1061 M	
b_{1u}	ν_7	CH_2 a-stretch	2919 C	2919 S	ia	
	ν_8	CH_2 rock	725 C	[b] 731 S, 720 S	ia	
b_{2g}	ν_9	CH_2 twist	1295 C	ia	1295 M	
b_{2u}	ν_{10}	CH_2 s-stretch	2851 C	2851 S	ia	
	ν_{11}	CH_2 scis	1468 C	[b] 1473 S, 1463 S	ia	
b_{3g}	ν_{12}	CH_2 a-stretch	2883 C	ia	2883 S	
	ν_{13}	CH_2 rock	1168 C	ia	1168 W	
b_{3u}	ν_{14}	CH_2 wag	1176 C	1176 VW	ia	

[a] 1063 cm^{-1} is given to this mode in ref. 6.
[b] Doublet due to the crystal field effect [1, 8].

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Molecule: **Poly(methylene-d_2)$_n$ (CD_2)** No. 223
Symmetry D_{2h} Symmetry number $\sigma = 4$

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

In this index molecules are divided into two groups: (a) those containing no carbon atoms, which are arranged with the elemental symbols of the empirical formulas in alphabetical order and are listed alphabetically, and in ascending order of the empirical formula subscripts; (b) molecules containing carbon, which are ordered in the same way except that carbon is listed first and hydrogen second. No distinction is made for isotpic species in the empirical formula; this deuterium is listed as H.

Compounds Not Containing Carbon

Empirical formula	Name	Molecule No.
AsH_3	Arsine	21
AsH_3	Arsine-d_3	22
B_2H_6	Diborane-$^{11}B_2H_6$	55
B_2H_6	Diborane-$^{10}B_2H_6$	56
B_2H_6	Diborane-$^{10}B_2D_6$	57
$BrCl_3Si$	Bromotrichlorosilane	45
BrH_3Si	Silyl bromide	44
Br_2Cl_2Si	Dibromodichlorosilane	49
Br_3ClSi	Tribromochlorosilane	47
Br_4Ge	Germanium tetrabromide	39
Br_4Si	Silicon tetrabromide	31
Br_4Sn	Tin tetrabromide	41
ClH_3Si	Silyl chloride	43
ClI_3Si	Chlorotriiodosilane	48
Cl_2O	Oxygen dichloride	8
Cl_3ISi	Trichloroiodosilane	46
Cl_3P	Phosphorus trichloride	20
Cl_4Ge	Germanium tetrachloride	38
Cl_4Si	Silicon tetrachloride	30
Cl_4Sn	Tin tetrachloride	40
FH_3Si	Silyl fluoride	42
F_2O	Oxygen difluoride	7
F_3N	Nitrogen trifluoride	16
F_3P	Phosphorus trifluoride	19
F_4Si	Silicon tetrafluoride	29
F_6Mo	Molybdenum hexafluoride	52
F_6S	Sulfur hexafluoride	50
F_6Se	Selenium hexafluoride	51
F_6U	Uranium hexafluoride	54
F_6W	Tungsten hexa fluoride	53
GeH_4	Germane	33
GeH_4	Germane-d_1	34
GeH_4	Germane-d_2	35
GeH_4	Germane-d_3	36
GeH_4	Germane-d_4	37
H_2O	Water	4
H_2O	Water-d_1	5
H_2O	Water-d_2	6
H_2S	Hydrogen sulfide	9
H_2S	Deuterium sulfide	10
H_2Se	Hydrogen selenide	12
H_2Se	Hydrogen deuterium selenide	13
H_3N	Ammonia	14
H_3N	Ammonia-d_3	15
H_3P	Phosphine	17
H_3P	Phosphine-d_3	18
H_3Sb	Stibine	23
H_3Sb	Stibine-d_3	24
H_4Si	Silane	25
H_4Si	Silane-d_2	26
H_4Si	Silane-d_3	27
H_4Si	Silane-d_4	28
I_4Si	Silicon tetraiodide	32
N_2O	Nitrous oxide	1
N_2O	Nitrous oxide-$^{14}N^{15}NO$	2
N_2O	Nitrous oxide-$^{15}N_2O$	3
O_2S	Sulfur dioxide	11

Compounds Containing Carbon

Empirical formula	Name	Molecule No.
$CBrCl_3$	Bromotrichloromethane	93
$CBrN$	Cyanogen bromide-$^{79}BrCN$	66
$CBrN$	Cyanogen bromide-$^{81}BrCN$	67
CBr_2Cl_2	Dibromodichloromethane	101
CBr_3Cl	Tribromochloromethane	94
CBr_4	Carbon tetrabromide	78
$CClN$	Cyanogen chloride-$^{35}ClCN$	64
$CClN$	Cyanogen chloride-$^{37}ClCN$	65
CCl_4	Carbon tetrachloride	77
CF_4	Carbon tetrafluoride	76
CI_4	Carbon tetraiodide	79
COS	Carbonyl sulfide	61
CO_2	Carbon dioxide	58
CO_2	Carbon dioxide-$^{13}CO_2$	59
CS_2	Carbon disulfide	60
$CHBr_3$	Tribromomethane	91
$CHBr_3$	Tribromomethane-d_1	92
$CHCl_3$	Trichloromethane	89
$CHCl_3$	Trichloromethane-d_1	90
CHF_3	Trifluoromethane	88
CHN	Hydrogen cyanide	62
CHN	Deuterium cyanide	63
CH_3BrCl	Bromochloromethane	102
CH_2BrCl	Bromochloromethane-d_1	103
CH_2BrCl	Bromochloromethane-d_2	104
CH_2Br_2	Dibromomethane	98
CH_2Br_2	Dibromomethane-d_1	99
CH_2Br_2	Dibromomethane-d_2	100
CH_2Cl_2	Dichloromethane	95
CH_2Cl_2	Dichloromethane-d_1	96
CH_2Cl_2	Dichloromethane-d_2	97
CH_2O	Formaldehyde	68

Empirical formula	Name	Molecule No.
CH_2O	Formaldehyde-d_1	69
CH_2O	Formaldehyde-d_2	70
CH_2O_2	Formic acid	105
CH_2O_2	Formic acid-d_2	106
CH_3Br	Methyl bromide	84
CH_3Br	Methyl bromide-d_3	85
CH_3Cl	Methyl chloride	82
CH_3Cl	Methyl chloride-d_3	83
CH_3F	Methyl fluoride	80
CH_3F	Methyl fluoride-d_3	81
CH_3I	Methyl iodide	86
CH_3I	Methyl iodide-d_3	87
CH_4	Methane	71
CH_4	Methane-d_1	72
CH_4	Methane-d_2	73
CH_4	Methane-d_3	74
CH_4	Methane-d_4	75
CH_4O (Gas)	Methanol	107
CH_4O (Liquid)	Methanol	108
CH_4O (Gas)	Methanol-d_1	109
CH_4O (Liquid)	Methanol-d_1	110
CH_4O (Gas)	Methanol-d_3	111
CH_4O (Liquid)	Methanol-d_3	112
CH_4O (Gas)	Methanol-d_4	113
CH_5N	Methylamine	114
CH_5N	Methylamine-d_2	115
CH_5N	Methylamine-d_3	116
CH_5N	Methylamine-d_5	117
C_2Br_4	Tetrabromoethylene	128
C_2Br_6	Hexabromoethane	159
$C_2Cl_2F_2$	Trans-1,2-Dichloro-1,2-difluoroethylene	138
$C_2Cl_2F_2$	1,1-Dichloro-2,2-difluoroethylene	142
C_2Cl_4	Tetrachloroethylene	127
C_2Cl_6	Hexachloroethane	158
C_2F_4	Tetrafluoroethylene	126
C_2F_6	Hexafluoroethane	157
C_2HBr	Bromoacetylene	123
C_2HCl	Chloroacetylene	122
C_2HF	Fluoroacetylene	121
C_2H_2	Acetylene	118
C_2H_2	Acetylene-d_1	119
C_2H_2	Acetylene-d_2	120
$C_2H_2Cl_2$	Trans-1,2-Dichloroethylene	132
$C_2H_2Cl_2$	Trans-1,2-Dichloroethylene-d_1	133
$C_2H_2Cl_2$	Trans-1,2-Dichloroethylene-d_2	134
$C_2H_2Cl_2$	Cis-1,2-Dichloroethylene	135
$C_2H_2Cl_2$	Cis-1,2-Dichloroethylene-d_1	136
$C_2H_2Cl_2$	Cis-1,2-Dichloroethylene-d_2	137
$C_2H_2Cl_2$	1,1-Dichloroethylene	139
$C_2H_2Cl_2$	1,1-Dichloroethylene-d_1	140
$C_2H_2Cl_2$	1,1-Dichloroethylene-d_2	141
$C_2H_2F_2$	Cis-1,2-Difluoroethylene	129
$C_2H_2F_2$	Cis-1,2-Difluoroethylene-d_1	130
$C_2H_2F_2$	Cis-1,2-Difluoroethylene-d_2	131
$C_2H_2N_2O$	1,2,5-Oxadiazole	147
C_2H_3N	Methyl cyanide	143
C_2H_3N	Methyl cyanide-d_3	144
C_2H_3N	Methyl isocyanide	145
C_2H_3N	Methyl isocyanide-d_3	146
C_2H_4	Ethylene	124
C_2H_4	Ethylene-d_4	125
C_2H_4BrCl	1-Bromo-2-chloroethane, trans form	164
C_2H_4BrCl	1-Bromo-2-chloroethane, gauche form	165
$C_2H_4Br_2$	1,2-Dibromoethane, trans form	162
$C_2H_4Br_2$	1,2-Dibromoethane, gauche form	163
$C_2H_4Cl_2$	1,2-Dichloroethane, trans form	160
$C_2H_4Cl_2$	1,2-Dichloroethane, gauche form	161
C_2H_4O	Ethylene oxide	149
C_2H_4O	Ethylene oxide-d_4	150
C_2H_4O	Acetaldehyde	151
C_2H_4O	Acetaldehyde-d_1	152
C_2H_4O	Acetaldehyde-d_4	153
$C_2H_4O_2$	Methyl formate	170
$C_2H_4O_2$	Methyl formate-d_1	171
$C_2H_4O_2$	Methyl formate-d_3	172
$C_2H_4O_2$	Methyl formate-d_4	173
$C_2H_4O_2$	Acetic acid	174
$C_2H_4O_2$	Acetic acid-d_1	175
C_2H_4Si	Silylacetylene	148
C_2H_5Br	Bromoethane	168
C_2H_5Cl	Chloroethane	167
C_2H_5F	Fluoroethane	166
C_2H_5N	Ethylene imine	169
C_2H_6	Ethane	154
C_2H_6	Ethane-d_3	155
C_2H_6	Ethane-d_6	156
C_2H_6O	Dimethylether	176
C_2H_6O	Dimethylether-d_3	177
$C_3H_2N_2$	Malononitrile	183
$C_3H_2N_2$	Malononitrile-d_2	184
C_3H_4	Allene	178
C_3H_4	Methylacetylene	179
C_3H_4	Methylacetylene-d_1	180
C_3H_4	Methylacetylene-d_3	181
C_3H_4	Methylacetylene-d_4	182
C_3H_4O	Propenal	185
C_3H_5N	Ethylcyanide	188
C_3H_6	Cyclopropane	186
C_3H_6	Cyclopropane-d_6	187
C_3H_6O	Acetone	189
C_3H_6O	Acetone-d_3	190
C_3H_6O	Acetone-d_6	191
$C_3H_6O_2$	Methyl acetate	197
$C_3H_6O_2$	Methyl-d_3-acetate	198
$C_3H_6O_2$	Methyl acetate-d_3	199
$C_3H_6O_2$	Methyl acetate-d_6	200
C_3H_8	Propane	192
C_3H_8	Propane-d_3	193
C_3H_8	Propane-d_2	194
C_3H_8	Propane-d_6	195
C_3H_8	Propane-d_8	196
C_4H_2	Butadiyne	201
C_4H_4O	Furan	202
C_4H_4S	Thiophene	203
C_4H_4S	Thiophene-d_4	204
C_4H_6	1,3-Butadiene	205
C_4H_6	1,3-Butadiene-d_1, trans	206
C_4H_6	1,3-Butadiene-1,1,2-d_3	207
C_4H_6	1,3-Butadiene-1,1,4,4-d_4	208
C_4H_6	1,3-Butadiene-d_6	209

Empirical formula	Name	Molecule No.
C_4H_6	2-Butyne	210
C_4H_8	Cyclobutane	211
C_4H_8	Cyclobutane-d_8	212
C_4H_8	2-Methylpropene	213
C_4H_8	2-Methyl-d_3-propene-3,3,3-d_3	214
C_4H_8O	2-Butanone, trans form	215
C_4H_{10}	n-Butane, trans form	216
C_4H_{10}	n-Butane, gauche form	127
C_6H_6	Benzene	218
C_6H_6	Benzene-d_6	219
C_6H_{12}	Cyclohexane	220
C_6H_{12}	Cyclohexane-d_{12}	221
$(CH_2)n$	Poly(methylene)	222
$(CH_2)n$	Poly(methylene-d_2)	223