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**Tables of
Molecular Vibrational Frequencies
Consolidated Volume I**

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Supersedes and extends the data contained in Tables of Molecular Vibrational
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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 investiga-

tors. 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 follow-

ing rules:

- (a) Number of carbon atoms.
- (b) Total number of atoms.
- (c) Molecular shape: linear, planar, and non-planar.
- (d) Molecular symmetry, in descending order of the number 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_{2v} 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 $G(v_i = 1, \text{ all other } v_j = 0)$ and $G(v_i = 0, \text{ and other } v_j = 0)$ expressed in cm^{-1} . Fundamental frequencies rather than harmonic frequencies (ω_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.

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4. Tables of Vibrational Frequencies

C₀-triatomic molecules

		Page		Page	
1	Nitrous oxide, $^{14}\text{N}_2\text{O}$	9	3	Nitrous oxide, $^{15}\text{N}_2\text{O}$	10
2	Nitrous oxide, $^{14}\text{N}^{15}\text{NO}$	9	4	Water, H_2O	10
			5	Water-d ₁ , HDO.....	10

	Page
6 Water-d ₂ , D ₂ O	11
7 Oxygen difluoride, F ₂ O	11
8 Oxygen dichloride, ³⁵ Cl ₂ ¹⁶ O	12
9 Hydrogen sulfide, H ₂ S	12
10 Deuterium sulfide, D ₂ S	13
11 Sulfur dioxide, ³² S ¹⁶ O ₂	13
12 Hydrogen selenide, H ₂ Se	14
13 Hydrogen deuterium selenide, HDSe	14

C₀-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

C₀-five-atomic molecules

25 Silane, SiH ₄	20
26 Silane-d ₂ , SiH ₂ D 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 ₃ D	25
35 Germane-d ₂ , GeH ₂ D 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 ₃ F	29
43 Silyl chloride, SiH ₃ Cl	29
44 Silyl bromide, SiH ₃ Br	30
45 Bromotrichlorosilane, SiBrCl ₃	30
46 Trichloriodosilane, SiCl ₃ I	31
47 Tribromochlorosilane, SiBr ₃ Cl	31
48 Chlorotriiodosilane, SiClI ₃	32
49 Dichromodichlorosilane, SiBr ₂ Cl ₂	32

C₀-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

C₀-eight-atomic molecules

	Page
55 Diborane, ¹⁰ B ₂ H ₆	36
56 Diborane, ¹¹ B ₂ H ₆	37
57 Diborane-d ₆ , ¹⁰ B ₂ D ₆	38

C₁-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

C₁-four-atomic molecules

68 Formaldehyde, H ₂ CO	44
69 Formaldehyde-d ₁ , HDCO	44
70 Formaldehyde-d ₂ , D ₂ CO	45

C₁-five-atomic molecules

71 Methane, CH ₄	45
72 Methane-d ₁ , CH ₃ D	46
73 Methane-d ₂ , CH ₂ D 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 ₃ F	50
81 Methyl fluoride-d ₃ , CD ₃ F	50
82 Methyl chloride, CH ₃ Cl	51
83 Methyl chloride-d ₃ , CD ₃ Cl	51
84 Methyl bromide, CH ₃ Br	52
85 Methyl bromide-d ₃ , CD ₃ Br	52
86 Methyl iodide, CH ₃ I	53
87 Methyl iodide-d ₃ , CD ₃ I	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 ₃ Cl	57
95 Dichloromethane, CH ₂ Cl ₂	57
96 Dichloromethane-d ₁ , CHDCl ₂	58
97 Dichloromethane-d ₂ , CD ₂ Cl ₂	58
98 Dibromomethane, CH ₂ Br ₂	59
99 Dibromomethane-d ₁ , CHDBr ₂	59
100 Dibromomethane-d ₂ , CD ₂ Br ₂	60
101 Dibromodichloromethane, CBr ₂ Cl ₂	60
102 Bromochloromethane, CH ₂ BrCl	61
103 Bromochloromethane-d ₁ , CHDBrCl	61
104 Bromochloromethane-d ₂ , CD ₂ BrCl	62

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105 Formic acid, HCOOH	62	149 Ethylene oxide, C ₂ H ₄ O	87
106 Formic acid-d ₂ , DCOOD	63	150 Ethylene oxide-d ₄ , C ₂ D ₄ O	88
C₁-six-atomic molecules			
107 Methanol, CH ₃ OH (Gas)	63	151 Acetaldehyde, CH ₃ CHO	89
108 Methanol, CH ₃ OH (Liquid)	64	152 Acetaldehyde-d ₁ , CH ₃ CDO	90
109 Methanol-d ₁ , CH ₃ OD (Gas)	64	153 Acetaldehyde-d ₄ , CD ₃ CDO	91
110 Methanol-d ₃ , CH ₃ OD (liquid)	65	C₂-eight-atomic molecules	
111 Methanol-d ₃ , CD ₃ OH (gas)	65	154 Ethane, CH ₃ CH ₃	92
112 Methanol-d ₃ , CD ₃ OH (liquid)	66	155 Ethane-1, 1, 1-d ₃ , CH ₃ CD ₃	93
113 Methanol-d ₄ , CD ₃ OD (gas)	66	156 Ethane-d ₆ , CD ₃ CD ₃	94
C₁-seven-atomic molecules			
114 Methylamine, CH ₃ NH ₂	67	157 Hexafluoroethane, CF ₃ CF ₃	95
115 Methylamine-d ₂ , CH ₃ ND ₂	68	158 Hexachloroethane, CCl ₃ CCl ₃	95
116 Methylamine-d ₃ , CD ₃ NH ₂	69	159 Hexabromoethane, CBr ₃ CBr ₃	96
117 Methylamine-d ₅ , CD ₃ ND ₂	70	160 1,2-Dichloroethane, CH ₂ ClCH ₂ Cl (trans form)	97
C₂-four-atomic molecules			
118 Acetylene, CHCH	71	161 1,2-Dichloroethane, CH ₂ ClCH ₂ Cl (gauche form)	98
119 Acetylene-d ₁ , CHCD	71	162 1,2-Dibromoethane, CH ₂ BrCH ₂ Br (trans form)	99
120 Acetylene-d ₂ , CDCD	72	163 1,2-Dibromoethane, CH ₂ BrCH ₂ Br (gauche form)	100
121 Fluoroacetylene, CHCF	72	164 1-Bromo-2-chloroethane, CH ₂ ClCH ₂ Br (trans form)	101
122 Chloroacetylene, CHCCL	73	165 1-Bromo-2-chloroethane, CH ₂ ClCH ₂ Br (gauche form)	102
123 Bromoacetylene, CHCBr	73	166 Fluoroethane, CH ₃ CH ₂ F	103
C₂-six-atomic molecules			
124 Ethylene, CH ₂ CH ₂	74	167 Chloroethane, CH ₃ CH ₂ Cl	104
125 Ethylene-d ₄ , C ₂ D ₄	75	168 Bromoethane, CH ₃ CH ₂ Br	105
126 Tetrafluoroethylene, CF ₂ CF ₂	75	169 Ethylene imine, C ₂ H ₃ N	106
127 Tetrachloroethylene, CCl ₂ CCl ₂	76	170 Methyl formate, HCOOCH ₃	107
128 Tetrabromoethylene, CBr ₂ CBr ₂	76	171 Methyl formate-d ₁ , DCOOCH ₃	108
129 cis-1, 2-Difluoroethylene, CHFCHF	77	172 Methyl formate-d ₃ , HCOOCD ₃	109
130 cis-1, 2-Difluoroethylene-d ₁ , CHFCDF	77	173 Methyl formate-d ₄ , DCOOCD ₃	110
131 cis-1, 2-Difluoroethylene-d ₂ , CDFCDF	78	174 Acetic acid, CH ₃ COOH	111
132 trans-1, 2-Dichloroethylene, CHClCHCl	78	175 Acetic acid-d ₁ , CH ₃ COOD	112
133 trans-1, 2-Dichloroethylene-d ₁ , CHClCDCl	79	C₂-nine-atomic molecules	
134 trans-1, 2-Dichloroethylene-d ₂ , CDClCDCl	79	176 Dimethylether, CH ₃ OCH ₃	113
135 cis-1, 2-Dichloroethylene, CHClCHCl	80	177 Dimethylether-d ₃ , CH ₃ OCD ₃	114
136 cis-1, 2-Dichloroethylene-d ₁ , CHClCDCl	80	C₃-seven-atomic molecules	
137 cis-1, 2-Dichloroethylene-d ₂ , CDClCDCl	81	178 Allene, CH ₂ CCH ₂	115
138 trans-1, 2-Dichloro-1, 2-difluoroethylene, CFClCFCl	81	179 Methylacetylene, CH ₃ CCH	116
139 1, 1-Dichloroethylene, CH ₂ CCl ₂	82	180 Methylacetylene-d ₁ , CH ₃ CCD	116
140 1, 1-Dichloroethylene-d ₁ , CHDCCl ₂	82	181 Methyl-d ₃ -acetylene, CD ₃ CCH	117
141 1, 1-Dichloroethylene-d ₂ , CD ₂ CCl ₂	83	182 Methylacetylene-d ₄ , CD ₃ CCD	117
142 1, 1-Dichloro-2, 2-difluoroethylene, CF ₂ CCl ₂	83	183 Malononitrile, NCCCH ₂ CN	118
143 Methyl cyanide, CH ₃ CN	84	184 Malononitrile-d ₂ , NCCD ₂ CN	118
144 Methyl cyanide-d ₃ , CD ₃ CN	84	C₃-eight-atomic molecules	
145 Methylisocyanide, CH ₃ NC	85	185 Propenal, CH ₂ CHCHO	119
146 Methylisocyanide-d ₃ , CD ₃ NC	85	C₃-nine-atomic molecules	
C₂-seven-atomic molecules			
147 1, 2, 5-Oxadiazole, C ₂ H ₂ N ₂ O	86	186 Cyclopropane, C ₃ H ₆	120
148 Silylacetylene, SiH ₃ CCH	86	187 Cyclopropane-d ₆ , C ₃ D ₆	121
		188 Ethylcyanide, CH ₃ CH ₂ CN	122

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C₃-ten-atomic molecules			
189	Acetone,	CH ₃ COCH ₃	123
190	Acetone- α, α, α -d ₃ ,	CH ₃ COCD ₃	124
191	Acetone-d ₆ ,	CD ₃ COCD ₃	125
C₃-11-atomic molecules			
192	Propane,	CH ₃ CH ₂ CH ₃	126
193	Propane-2, 2-d ₂ ,	CH ₃ CD ₂ CH ₃	127
194	Propane-1, 1, 1-d ₃ ,	CH ₃ CH ₂ CD ₃	128
195	Propane-1, 1, 1, 3, 3, 3-d ₆ ,	CD ₃ CH ₂ CD ₃	129
196	Propane-d ₈ ,	CD ₃ CD ₂ CD ₃	130
197	Methyl acetate,	CH ₃ COOCH ₃	131
198	Methyl acetate-d ₃ ,	CD ₃ COOCH ₃	132
199	Methyl-d ₃ -acetate,	CH ₃ COOCD ₃	133
200	Methyl acetate-d ₆ ,	CD ₃ COOCD ₃	134
C₄-six-atomic molecules			
201	Butadiyne,	HCCCCH.....	135
C₄-nine-atomic molecules			
202	Furan,	C ₄ H ₄ O.....	136
203	Thiophene,	C ₄ H ₄ S.....	137
204	Thiophene-d ₄ ,	C ₄ D ₄ S.....	138
C₄-ten-atomic molecules			
205	1, 3-Butadiene,	CH ₂ CHCHCH ₂	139
206	1, 3-Butadiene-1-d ₁ (trans),	CH ₂ CHCHCHD... ..	140
207	1, 3-Butadiene-1, 1, 2-d ₃ ,	CH ₂ CHCD ₂ CD ₂	141
208	1, 3-Butadiene-1, 1, 4, 4-d ₄ ,	CD ₂ CHCHCD ₂	142
209	1, 3-Butadiene-d ₆ ,	CD ₂ CD ₂ CD ₂	143
210	2-Butyne,	CH ₃ CCCH ₃	144
C₄-12-atomic molecules			
211	Cyclobutane,	C ₄ H ₈	145
212	Cyclobutane-d ₈ ,	C ₄ D ₈	146
213	2-Methylpropene,	(CH ₃) ₂ CCH ₂	147
214	2-Methyl-d ₃ -propene-3, 3, 3-d ₃ ,	(CD ₃) ₂ CCH ₂	148
C₄-13-atomic molecules			
215	2-Butanone	CH ₃ COCH ₂ CH ₃ (trans form).....	149
C₄-14-atomic molecules			
216	n-Butane,	CH ₂ CH ₂ CH ₂ CH ₂ (trans form).....	150
217	n-Butane,	CH ₃ CH ₂ CH ₂ CH ₃ (gauche form).....	151
C₆-12-atomic molecules			
218	Benzene,	C ₆ H ₆	152
219	Benzene-d ₆ ,	C ₆ D ₆	153
C₆-18-atomic molecules			
220	Cyclohexane,	C ₆ H ₁₂	154
221	Cyclohexane-d ₁₂ ,	C ₆ D 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	Point group	Symmetry species
C ₂	A, B	D _{3h}	A ₁ ', A ₁ '', A ₂ ', A ₂ '', E', E''
C _s	A', A''	D _{3h}	A ₁ ', A ₁ '', A ₂ ', A ₂ '', E ₁ ', E ₁ '', E ₂ ', E ₂ ''
C _i	A _g , A _u	D _{4h}	A _{1g} , A _{1u} , A _{2g} , A _{2u} , B _{1g} , B _{1u} , B _{2g} , B _{2u} , E _g , E _u
C _{2v}	A ₁ , A ₂ , B ₁ , B ₂	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}
C _{2h}	A _g , A _u , B _g , B _u	D _{∞h}	Σ _g ⁺ , Σ _u ⁺ , Σ _g ⁻ , Σ _u ⁻ , π _g , π _u , Δ _g , Δ _u , Φ _g , Φ _u , ...
D ₂	A, B ₁ , B ₂ , B ₃	C ₃	A, E
D _{2h}	A _g , A _u , B _{1g} , B _{1u} , B _{2g} , B _{2u} , B _{3g} , B _{3u}	C ₆	A, B, E ₁ , E ₂
C _{3v}	A ₁ , A ₂ , E	S ₆	A _g , A _u , E _g , E _u
D ₃	A ₁ , A ₂ , E	C _{3h}	A, A', E', E''
C _{3v}	A ₁ , A ₂ , E	C _{4h}	A _g , A _u , B _g , B _u , E _g , E _u
C _{∞v}	Σ ⁺ , Σ ⁻ , π, Δ, Φ, ...	C _{6h}	A _g , A _u , B _g , B _u , E _{1g} , E _{1u} , E _{2g} , E _{2u}
C _{4v} , D ₄ , D _{2d}	A ₁ , A ₂ , B ₁ , B ₂ , E	T _d , O	A ₁ , A ₂ , E, F ₁ , F ₂
C _{6v} , D ₆	A ₁ , A ₂ , B ₁ , B ₂ , E ₁ , E ₂	O _h	A _{1g} , A _{1u} , A _{2g} , A _{2u} , E _g , E _u , F _{1g} , F _{1u} , F _{2g} , F _{2u}
D _{3d}	A _{1g} , A _{1u} , A _{2g} , A _{2u} , E _g , E _u	T	A, E, F
D _{4d}	A ₁ , A ₂ , B ₁ , B ₂ , E ₁ , E ₂ , E ₃		

TABLE II. Definition of local symmetry coordinates

<p>(a) Local symmetry coordinates for the CH₃ group (see fig. 1a)</p> <p>CH₃ symmetrical stretching: $(\Delta r_1 + \Delta r_2 + \Delta r_3)/\sqrt{3}$</p> <p>CH₃ degenerate stretching: $(2\Delta r_1 - \Delta r_2 - \Delta r_3)/\sqrt{6}$ $(\Delta r_2 - \Delta r_3)/\sqrt{2}$</p> <p>CH₃ symmetrical deformation: $(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12} - \Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3)/\sqrt{6}$</p> <p>CH₃ degenerate deformation: $(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{6}$ $(\Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{2}$</p> <p>CH₃ rocking: $(2\Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3)/\sqrt{6}$ $(\Delta\beta_2 - \Delta\beta_3)/\sqrt{2}$.</p> <p>(b) Local symmetry coordinates for the CH₂ group (see fig. 1b)</p> <p>CH₂ symmetrical stretching: $(\Delta r_1 + \Delta r_2)/\sqrt{2}$</p> <p>antisymmetrical stretching: $(\Delta r_1 - \Delta r_2)/\sqrt{2}$</p> <p>CH₂ scissors: $(4\Delta\alpha - \Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y})/\sqrt{20}$</p> <p>CH₂ wagging: $(\Delta\beta_{1X} + \Delta\beta_{2X} - \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$</p> <p>CH₂ twisting: $(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y})/2$</p> <p>CH₂ rocking: $(\Delta\beta_{1X} - \Delta\beta_{2X} + \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$.</p>	<p>(c) Local symmetry coordinates for the CH group (see fig. 1c)</p> <p>CH stretching: Δr_{CH}</p> <p>CH bending: $(2\Delta\beta_{HX} - \Delta\beta_{HY} - \Delta\beta_{HZ})/\sqrt{6}$ $(\Delta\beta_{HY} - \Delta\beta_{HZ})/\sqrt{2}$</p> <p>(d) Local symmetry coordinates for the planar CH₂ group (see fig. 1d)</p> <p>CH₂ symmetrical stretching: $(\Delta r_1 + \Delta r_2)/\sqrt{2}$</p> <p>CH₂ antisymmetrical stretching: $(\Delta r_1 - \Delta r_2)/\sqrt{2}$</p> <p>CH₂ scissors: $(2\Delta\alpha - \Delta\beta_1 - \Delta\beta_2)/\sqrt{6}$</p> <p>CH₂ rocking: $(\Delta\beta_1 - \Delta\beta_2)/\sqrt{2}$</p> <p>CH₂ wagging: $\Delta\theta \cdot \sin \alpha$.</p> <p>(e) Local symmetry coordinates for the planar CH group (see fig. 1e)</p> <p>CH stretching: Δr_{CH}</p> <p>in-plane CH bending: $(\Delta\beta_{HX} - \Delta\beta_{HY})/\sqrt{2}$</p> <p>out-of-plane CH bending: $\Delta\theta \cdot \sin \gamma_{XY}$.</p>
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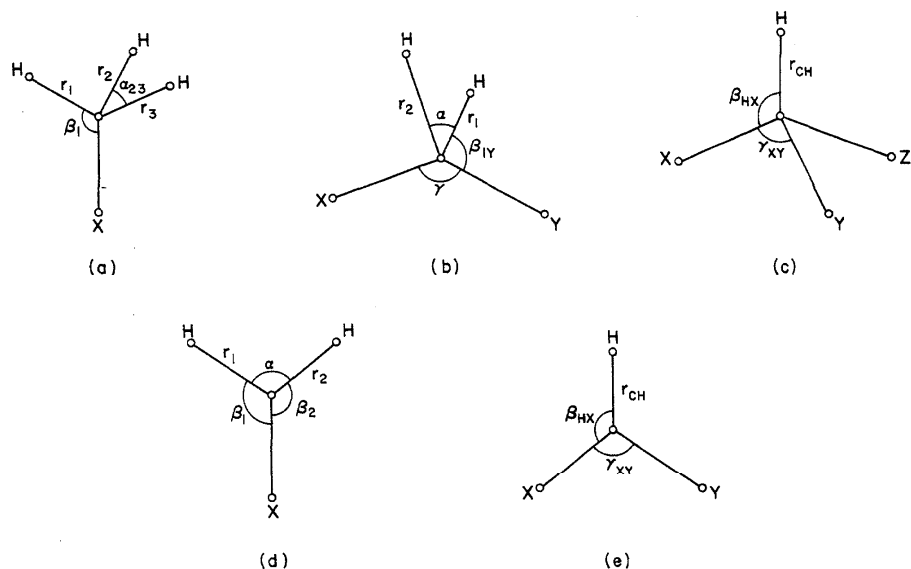


FIGURE 1. Parameters of methyl, methylene, and methin groups.

TABLE III. Uncertainty code for the selected values of frequencies

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

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

Molecule: Nitrous oxide $^{14}\text{N}_2\text{O}$
 Symmetry $\text{C}_{\infty v}$ Symmetry number $\delta = 1$

No. 1

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	NN stretch.....	2224 A	cm^{-1} (Gas) 2223.7 VW	cm^{-1} (Gas) 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	

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

Molecule: Nitrous oxide $^{14}\text{N}^{15}\text{NO}$
 Symmetry $\text{C}_{\infty v}$ Symmetry number $\delta = 1$

No. 2

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

References

- [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 $^{15}\text{N}_2\text{O}$
 Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

No. 3

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	NN stretch.....	2155 A	cm^{-1} (Gas) 2154.7	cm^{-1}	
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
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 4

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

References

- [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
 Symmetry C_s Symmetry number $\sigma = 1$

No. 5

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

References

- [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).
 [3] IR. N. Gailar and F. P. Dickey, J. Mol. Spectrosc. 4, 1 (1960).

Molecule: Water-d₂ D₂O
 Symmetry C_{2v} Symmetry number σ = 2

No. 6

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	Sym. stretch.....	2671 A	cm ⁻¹ (Gas) 2671.46	cm ⁻¹ (Gas) 2666	
	ν ₂	Bend.....	1178 A	1178.33		
b ₁	ν ₃	Antisym. stretch.....	2788 A	2788.05		

References

- [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: Oxygen difluoride F₂O
 Symmetry C_{2v} Symmetry number σ = 2

No. 7

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	Sym. stretch.....	928 B	cm ⁻¹ (Gas) 928 S	cm ⁻¹	
	ν ₂	Bend.....	461 B	461 S		
b ₁	ν ₃	Antisym. stretch.....	831 B	831 VS		

References

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

Molecule: Oxygen dichloride $^{35}\text{Cl}_2^{16}\text{O}$
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 8

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

References

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 [2] IR.Th. K. Hedberg, J. Chem. Phys. 19, 509 (1951).
 [3] IR.Th. M. M. Rochkind and G. C. Pimentel, J. Chem. Phys. 42, 1361 (1965).

Molecule: Hydrogen sulfide H_2S
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 9

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

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. B. Lohman, F. P. Reding, and D. F. Hornig, J. Chem. Phys. 19, 252 (1951).
 [3] IR. H. C. Allen, Jr., L. R. Blaine, E. K. Plyler, and P. C. Cross, J. Chem. Phys. 24, 35 (1956).
 [4] IR. H. C. Allen, Jr., and E. K. Plyler, J. Chem. Phys. 25, 1132 (1956).

Molecule: Deuterium sulfide D_2S
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 10

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

References

- [1] IR. A. H. Nielsen and H. H. Nielsen, J. Chem. Phys. 5, 277 (1937).
 [2] R. G. M. Murphy and J. E. Vance, J. Chem. Phys. 6, 426 (1938).
 [3] R. R. E. Miller and D. F. Eggers, Jr., J. Chem. Phys. 45, 3028 (1966).

Molecule Sulfur dioxide $^{32}S^{16}O_2$
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 11

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	1151 B	cm^{-1} (Gas) 1151.4 S	cm^{-1} (Gas) 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)	

References

- [1] IR.R. C. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
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 [3] IR. S. R. Polo and M. K. Wilson, J. Chem. Phys. 22, 900 (1954).

Molecule: Hydrogen selenide H_2Se
 Symmetry C_{2v} Symmetry number $\delta = 2$

No. 12

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

References

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

Molecule: Hydrogen deuterium selenide HDSe
 Symmetry C_s Symmetry number $\delta = 1$

No. 13

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

References

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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).

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

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

References

- [1] IR.R. C. 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] IR. J. S. Garing, H. H. Nielsen, and K. N. Rao, *J. Mol. Spectrosc.* 3, 496 (1959).
- [4] IR. W. S. Benedict, E. K. Plyler, and E. D. Tidwell, *J. Chem. Phys.* 32, 32 (1960).
- [5] Th. J. L. Duncan and I. M. Mills, *Spectrochim. Acta* 20, 523 (1964).

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

^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
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 16

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	

References

- [1] IR. C. R. Bailey, S. C. Carson, and J. W. Thompson, J. Chem. Phys. 5, 274 (1937).
- [2] IR. M. K. Wilson and S. R. Polo, J. Chem. Phys. 20, 1716 (1952).
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- [5] Th. P. N. Schatz, J. Chem. Phys. 29, 481 (1958).
- [6] IR. I. W. Levin and S. Abramowitz, J. Chem. Phys. 44, 2562 (1966).

Molecule: Phosphine PH_3
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 17

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	

References

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- [2] IR. L. W. Fung and E. F. Barker, Phys. Rev. 45, 238 (1934).
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- [6] IR. J. M. Hoffman, H. H. Nielsen, and K. N. Rao, Z. Elektrochem. 64, 606 (1960).
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Molecule: Phosphine-d₃ PD₃
 Symmetry C_{3v} Symmetry number σ = 3

No. 18

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	Sym. stretch.....	1694 B	cm ⁻¹ (Gas) 1694	cm ⁻¹	CF [2].
e	ν ₂	Sym. deform.....	730 B	730		
	ν ₃	Deg. stretch.....	1687 D			
	ν ₄	Deg. deform.....	806 B	806		

References

- [1] IR. E. Lee and C. K. Wu, Trans. Faraday Soc. 35, 1366 (1939).
 [2] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta 20, 523 (1964).

Molecule: Phosphorus trifluoride PF₃
 Symmetry C_{3v} Symmetry number σ = 3

No. 19

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	Sym. stretch.....	892 B	cm ⁻¹ (Gas) 892 S	cm ⁻¹ (Liquid) 890 (10)	
e	ν ₂	Sym. deform.....	487 B	487 M	486 (3)	
	ν ₃	Deg. stretch.....	860 C	860 S	840 (10)	
	ν ₄	Deg. deform.....	344 B	344 M		

References

- [1] R. D. M. Yost and T. F. Anderson, J. Chem. Phys. 2, 624 (1934).
 [2] IR. H. S. Gutowsky and A. D. Liehr, J. Chem. Phys. 20, 1652 (1952).
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 [5] IR. I. W. Levin and S. Abramowitz, J. Chem. Phys. 44, 2562 (1966).

Molecule: Phosphorus trichloride PCl_3
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 20

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

References

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Molecule Arsine AsH_3
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 21

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

References

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 [4] IR. H. H. Nielsen, J. Chem. Phys. 20, 759 (1952).
 [5] IR. H. H. Nielsen, J. Chem. Phys. 20, 1955 (1952).
 [6] Th. J. L. Ducau and I. M. Mills, Spectrochim. Acta 20, 523 (1964).

Molecule: **Arsine-d₃** **AsD₃**
 Symmetry **C_{3v}** Symmetry number **$\sigma = 3$**

No. 22

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	1523 B	cm^{-1} (Gas) 1523.1	cm^{-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		

References

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

Molecule: **Stibine** **SbH₃**
 Symmetry **C_{3v}** Symmetry number **$\sigma = 3$**

No. 23

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	1891 B	cm^{-1} (Gas) 1890.9	cm^{-1}	
	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-d₃ SbD₃
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 24

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	Sym. stretch.....	1359 B	<i>cm</i> ⁻¹ (Gas) 1358.8	<i>cm</i> ⁻¹	
	ν_2	Sym. deform.....	561 C	561.1		
<i>e</i>	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 SiH₄
 Symmetry T_d Symmetry number $\sigma = 12$

No. 25

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	Sym. stretch.....	2187 B	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 2187.0 S	
<i>e</i>	ν_2	Deg. deform.....	975 C	ia, ^a 974.6	978 W	
<i>f</i> 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-d₂ SiH₂D₂
 Symmetry C_{2v} Symmetry number δ = 2

No. 26

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		CF [1].
	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		
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-d₃ SiHD₃
 Symmetry C_{3v} Symmetry number δ = 3

No. 27

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		SF (ν ₆) [1].
	ν ₂	SiD ₃ s-stretch.....	1573 C	1573 S		
	ν ₃	SiD ₃ s-deform.....	683 C	683 S		
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		

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-d₄ SiD₄
 Symmetry T_d Symmetry number $\sigma = 12$

No. 28

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	Sym. stretch.....	1558 E	<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	CF [4].
<i>e</i>	ν_2	Deg. deform.....	700 E	CF [4].
<i>f</i> 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 SiF₄
 Symmetry T_d Symmetry number $\sigma = 12$

No. 29

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	Sym. stretch.....	800 C	<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>e</i>	ν_2	Deg. deform.....	268 C	ia	800 S	
<i>f</i> ₂	ν_3	Deg. stretch.....	1032 B	1031.8 S	268 W	
	ν_4	Deg. deform.....	389 B	389.35 S	1010 W	
					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
 Symmetry T_d Symmetry number $\delta = 12$

No. 30

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	424 C	cm^{-1} (Gas) ia	cm^{-1} (Liquid) 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. Delwaille, 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. Radhakrishnan, Z. Phys. Chem. (Frankfurt am Main) 41, 197 (1964).

Molecule: Silicon tetrabromide SiBr_4
 Symmetry T_d Symmetry number $\delta = 12$

No. 31

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	249 C	cm^{-1} (Gas) ia	cm^{-1} (Liquid) 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. Delwaille, 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
 Symmetry T_d Symmetry number $\sigma = 12$

No. 32

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	168 C	cm^{-1} ia	cm^{-1} (Liquid) 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
 Symmetry T_d Symmetry number $\sigma = 12$

No. 33

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	2106 B	cm^{-1} (Gas) ia	cm^{-1} (Gas) 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-d₁ GeH₃D
Symmetry C_{3v} Symmetry number σ = 3

No. 34

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	GeH ₃ s-stretch.....	2106 C	cm ⁻¹ (Gas)	cm ⁻¹ (Gas) 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-d₂ GeH₂D₂
Symmetry C_{2v} Symmetry number σ = 2

No. 35

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	GeH ₂ s-stretch.....	2112 C	cm ⁻¹ (Gas)	cm ⁻¹	
	ν ₂	GeD ₂ s-stretch.....	1512 C	2112		
	ν ₃	GeH ₂ scis.....	881 B	1512		
	ν ₄	GeD ₂ scis.....	620 C	881		
a ₂	ν ₅	GeH ₂ twist.....	807 E	620		
b ₁	ν ₆	GeH ₂ a-stretch.....	2112 C	807		
	ν ₇	GeH ₂ rock.....	657 C	2112		
b ₂	ν ₈	GeD ₂ a-stretch.....	1522 C	657		
	ν ₉	GeH ₂ wag.....	770 C	1522		

Reference

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

Molecule: Germane-d₃ GeHD₃
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 36

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν_1	GeH stretch.....	2112 B	cm ⁻¹ (Gas) 2112.4	cm ⁻¹ (Gas)	
	ν_2	GeD ₃ s-stretch.....	1504 B	1504	
e	ν_3	GeD ₃ s-deform.....	595 C	595		
	ν_4	GeD ₃ 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-d₄ GeD₄
 Symmetry T_d Symmetry number $\delta = 12$

No. 37

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν_1	Sym. stretch.....	1504 C	cm ⁻¹ (Gas) ia	cm ⁻¹ (Gas) 1504	
e	ν_2	Deg. deform.....	665 D	ia, *665 W		
f ₂	ν_3	Deg. stretch.....	1522 B	1522.2 S		
	ν_4	Deg. deform.....	596 C	596 S		

* 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
 Symmetry T_d Symmetry number $\delta = 12$

No. 38

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. 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
 Symmetry T_d Symmetry number $\delta = 12$

No. 39

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
 Symmetry T_d Symmetry number $\delta = 12$

No. 40

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	Sym. stretch.....	366 C	ia	(Liquid) 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
 Symmetry T_d Symmetry number $\delta = 12$

No. 41

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	Sym. stretch.....	220 C	ia	(Liquid) 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. 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
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 42

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	SiH_3 s-stretch.....	2206 D	cm^{-1} (Gas) 2206	cm^{-1}	OV (ν_4).
	ν_2	SiH_3 s-deform.....	990 C	990 S		
e	ν_3	SiF stretch.....	872 B	872 M		
	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
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 43

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

No. 44

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	SiH_3 s-stretch	2200 D	cm^{-1} (Gas) 2200	cm^{-1}	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
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 45

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a_1	ν_1	SiCl_3 s-stretch	545 C	cm^{-1}	cm^{-1} (Liquid) 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. Delwaille, M. B. Buisset, and M. Delhay, J. Amer. Chem. Soc. **74**, 5768 (1952).
 [2] R. M. L. Delwaille, J. Phys. Chem. **56**, 355 (1952).
 [3] Th. Y. Kakiuchi, Bull. Chem. Soc. Japan **26**, 260 (1953).

Molecule: Trichloriodosilane SiCl_3I
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 46

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

No. 47

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

No. 48

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

No. 49

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 SF₆
 Symmetry O_h Symmetry number $\sigma = 24$

No. 50

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> _{1g}	ν_1	Sym. stretch.....	774 B	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 773.5 VS	
<i>e</i> _g	ν_2	Deg. stretch.....	642 B	ia	641.7 W	
<i>f</i> _{1u}	ν_3	Deg. stretch.....	948 C	947.5	ia	
	ν_4	Deg. deform.....	616 C	615.5	ia	
<i>f</i> _{2g}	ν_5	Deg. deform.....	525 C	ia	525 W	
<i>f</i> _{2u}	ν_6	Deg. deform.....	347 E	ia	ia	OC (2 ν_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 SeF₆
 Symmetry O_h Symmetry number $\sigma = 24$

No. 51

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> _{1g}	ν_1	Sym. stretch.....	707 B	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 706.9 VS	
<i>e</i> _g	ν_2	Deg. stretch.....	659 B	ia	658.7 W	
<i>f</i> _{1u}	ν_3	Deg. stretch.....	780 C	780	ia	
	ν_4	Deg. deform.....	437 C	437	ia	
<i>f</i> _{2g}	ν_5	Deg. deform.....	405 C	ia	405 W	
<i>f</i> _{2u}	ν_6	Deg. deform.....	264 E	ia	ia	OC (2 ν_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 MoF₆
 Symmetry O_h Symmetry number σ = 24

No. 52

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> _{1g}	<i>ν</i> ₁	Sym. stretch.....	742 B	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 741.5 VS, p	OC (2 <i>ν</i> ₆) [3].
<i>e</i> _g	<i>ν</i> ₂	Deg. stretch.....	652 B	ia	651.6 W, dp	
<i>f</i> _{1u}	<i>ν</i> ₃	Deg. stretch.....	741 C	741 VS	ia	
	<i>ν</i> ₄	Deg. deform.....	264 C	264 S	ia	
<i>f</i> _{2g}	<i>ν</i> ₅	Deg. deform.....	318 C	ia	318 W, dp	
<i>f</i> _{2u}	<i>ν</i> ₆	Deg. deform.....	116 E	ia	ia	

References

- [1] IR.R. H. H. Claassen, H. Selig, and J. G. Malm, J. Chem. Phys. 36, 2888 (1962).
 [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: Tungsten hexafluoride WF₆
 Symmetry O_h Symmetry number σ = 24

No. 53

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> _{1g}	<i>ν</i> ₁	Sym. stretch.....	771 B	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 771.0 VS, p	OC (2 <i>ν</i> ₆) [3].
<i>e</i> _g	<i>ν</i> ₂	Deg. stretch.....	677 B	ia	677.2 W, dp	
<i>f</i> _{1u}	<i>ν</i> ₃	Deg. stretch.....	712 C	712 VS	ia	
	<i>ν</i> ₄	Deg. deform.....	258 C	258 S	ia	
<i>f</i> _{2g}	<i>ν</i> ₅	Deg. deform.....	320 C	ia	320 W, dp	
<i>f</i> _{2u}	<i>ν</i> ₆	Deg. deform.....	127 E	ia	ia	

References

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

Molecule: Uranium hexafluoride UF_6
 Symmetry O_h Symmetry number $\sigma = 24$

No. 54

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_{1g}	ν_1	Sym. stretch	667 B	cm^{-1} (Gas) ia	cm^{-1} (Gas) 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. Fricke 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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_g	ν_1	BH ₂ s-stretch.....	2537 C	cm^{-1} (Gas) ia	cm^{-1} (Gas) 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].
b_{2g}	ν_{10}	Ring puckering.....	368 C	368 S	ia	
	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
	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 $^{11}\text{B}_2\text{H}_6$.

References

- [1] R. T. F. Anderson and A. B. Burg, J. Chem. Phys. 6, 586 (1938).
- [2] I.R.R. F. Stitt, J. Chem. Phys. 9, 780 (1941).
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- [5] I.R.R. A. N. Webb, J. T. Neu, and K. S. Pitzer, J. Chem. Phys. 17, 1007 (1949).
- [6] I.R.R. R. C. Lord and E. Nielsen, J. Chem. Phys. 19, 1 (1951).
- [7] I.R. W. J. Lehman, J. F. Ditter, and J. Shapiro, J. Chem. Phys. 29, 1248 (1958).
- [8] R. R. C. Taylor and A. R. Emery, Spectrochim. Acta 10, 419 (1958).
- [9] I.R. J. T. Kaufman, W. S. Koski, and R. Anacron, J. Mol. Spectrosc. 11, 1 (1963).
- [10] Th. T. Ogawa and T. Miyazawa, Spectrochim. Acta 20, 557 (1964).
- [11] I.R. W. L. Smith and I. M. Mills, J. Chem. Phys. 41, 1479 (1964).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_g	ν_1	BH_2 s-stretch.....	2524 C	cm^{-1} (Gas) ia	cm^{-1} (Liquid) 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	
	ν_6	Ring stretch.....	1768 E	ia	{ 1788 (1) dp 1747 (1) dp }	FR ($\nu_5 + \nu_9$).
b_{1u}	ν_7	BH_2 wag.....	850 E	ia	OC ($\nu_7 + \nu_{10}$).
	ν_8	BH_2 a-stretch.....	2612 C	2612 VS	ia	{ OC ($\nu_5 + \nu_9$). OC ($\nu_9 + \nu_{10}$).
	ν_9	BH_2 rock.....	950 E	ia	
b_{2g}	ν_{10}	Ring puckering.....	368 C	368 S	ia	OC ($\nu_{10} + \nu_{12}$).
	ν_{11}	BH_2 a-stretch.....	2591 C	ia	2591 (9) dp	
b_{2u}	ν_{12}	BH_2 rock.....	915 E	ia	OC ($\nu_{10} + \nu_{12}$).
	ν_{13}	Ring stretch.....	1915 E	{ 1887 M (1999 W) }	ia	
b_{3g}	ν_{14}	BH_2 wag.....	973 C	973 S	ia	1012 (5) dp
	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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a_g</i>	<i>ν</i> ₁	BD ₂ s-stretch	1860 E	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Liquid) {1880 VS, p 1833 S, p	FR (2 <i>ν</i> ₃).
	<i>ν</i> ₂	Ring stretch	1511 C	ia	1511 VS, p	
	<i>ν</i> ₃	BD ₂ scis	929 C	ia	929 p	
	<i>ν</i> ₄	Ring deform	726 C	ia	726 VS, p	
<i>a_u</i>	<i>ν</i> ₅	BD ₂ twist	592 D	*592 VW	ia	
	<i>ν</i> ₆	Ring stretch	1273 C	ia	1273 (2) dp	
<i>b_{1g}</i>	<i>ν</i> ₇	BD ₂ wag	870 E	ia		OC (<i>ν</i> ₅ + <i>ν</i> ₇).
	<i>ν</i> ₈	BD ₂ a-stretch	1999 C	1999 VS	ia	
<i>b_{1u}</i>	<i>ν</i> ₉	BD ₂ rock	705 E		ia	OC (<i>ν</i> ₉ + <i>ν</i> ₁₀).
	<i>ν</i> ₁₀	Ring puckering	262 C	262 M	ia	
<i>b_{2g}</i>	<i>ν</i> ₁₁	BD ₂ a-stretch	1980 E	ia	{1975 (9) dp (2000 (5)) dp	
	<i>ν</i> ₁₂	BD ₂ rock	740 E	ia		OC (<i>ν</i> ₁₀ + <i>ν</i> ₁₂). FR (<i>ν</i> ₅ + <i>ν</i> ₇).
<i>b_{2u}</i>	<i>ν</i> ₁₃	Ring stretch	1465 E	{1491 M 1459 MS	ia	
	<i>ν</i> ₁₄	BD ₂ wag	728 C	728 S	ia	
<i>b_{3g}</i>	<i>ν</i> ₁₅	BD ₂ twist	730 C	ia	730 (4) dp	FR (<i>ν</i> ₃ + <i>ν</i> ₁₃).
	<i>ν</i> ₁₆	BD ₂ s-stretch	1845 C	{1857 VS (1799 S)	ia	
<i>b_{3u}</i>	<i>ν</i> ₁₇	Ring deform	1205 C	1205 VS	ia	
	<i>ν</i> 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).
- [2] IR.R. R. C. Lord and E. Nielsen, J. Chem. Phys. 19, 1 (1951).
- [3] R. R. C. Taylor and A. R. Emery, Spectrochim. Acta 10, 419 (1958).
- [4] Th. T. Ogawa and T. Miyazawa, Spectrochim. Acta 20, 557 (1964).

Molecule: Carbon dioxide $^{12}\text{C}^{16}\text{O}_2$
 Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

No. 58

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ_g^+	ν_1	Sym. stretch.....	1333 C	cm^{-1} (Gas) ia	cm^{-1} (Gas) {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 $^{13}\text{C}^{16}\text{O}_2$
 Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

No. 59

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ_g^+	ν_1	Sym. stretch.....	1334 C	cm^{-1} (Gas) ia	cm^{-1} (Gas) {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 $^{12}\text{C}^{32}\text{S}_2$
 Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

No. 60

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

References

- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
 [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 $^{12}\text{C}^{16}\text{O}^{32}\text{S}$
 Symmetry $C_{\infty v}$ Symmetry number $\sigma = 1$

No. 61

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	CO stretch.....	2062 A	cm^{-1} (Gas) 2062.22	cm^{-1} (Liquid) 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
 Symmetry $C_{\infty v}$ Symmetry number $\delta = 1$

No. 62

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	CH stretch	3311 A	cm^{-1} (Gas) 3311.47 S	cm^{-1} (Liquid) 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).
- [2] IR. H. C. Allen, Jr., E. D. Tidwell, and E. K. Plyler, J. Chem. Phys. 25, 302 (1956).
- [3] IR. A. G. Maki and L. R. Blaine, J. Mol. Spectrosc. 12, 45 (1964).

Molecule: Deuterium cyanide DCN
 Symmetry $C_{\infty v}$ Symmetry number $\delta = 1$

No. 63

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	CD stretch	2630 A	cm^{-1} (Gas) 2630.30 S	cm^{-1} (Liquid) 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 ³⁵CICN
 Symmetry C_{∞v} Symmetry number δ = 1

No. 64

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ ⁺	ν ₁	CN stretch.....	2216 A	cm ⁻¹ (Gas) 2215.6 VS	cm ⁻¹ (Liquid) 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 (2ν 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 ³⁷CICN
 Symmetry C_{∞v} Symmetry number δ = 1

No. 65

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ ⁺	ν ₁	CN stretch.....	2215 A	cm ⁻¹ (Gas) 2215.3 VS	cm ⁻¹ (Liquid) 2206 (10)	
π	ν ₂	Bend.....	378 A	380 S	394 (3)	RP [2].
σ ⁺	ν ₃	CCl stretch.....	736 C	730 (5)	FR (2ν ₂) [2].

References

See No. 64.

Molecule: Cyanogen bromide ⁷⁹BrCN
 Symmetry C_{∞v} Symmetry number σ = 1

No. 66

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ ⁺	ν ₁	CN stretch.....	2198 A	cm ⁻¹ (Gas) 2198.3	cm ⁻¹ (Liquid) 2191	RP [2].
π	ν ₂	Bend.....	342 A	341.5	357	
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 ⁸¹BrCN
 Symmetry C_{∞v} Symmetry number σ = 1

No. 67

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ ⁺	ν ₁	CN stretch.....	2198 A	cm ⁻¹ (Gas) 2198.3	cm ⁻¹ (Liquid) 2191	RP [2].
π	ν ₂	Bend.....	342 A	341.5	357	
σ ⁺	ν ₃	CBr stretch.....	575 C	575	568	

References

See No. 66.

Molecule: Formaldehyde H₂CO
Symmetry C_{2v} Symmetry number $\delta = 2$

No. 68

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Gas)	
<i>a</i> ₁	ν_1	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	
<i>b</i> ₁	ν_4	CH ₂ a-stretch.....	2843 A	2843.1 VS	2866 W	
	ν_5	CH ₂ rock.....	1249 A	1249.1 S		
<i>b</i> ₂	ν_6	CH ₂ wag.....	1167 A	1167.3 S		

References

- [1] R. D. W. Davidson, B. P. Stoicheff, and H. J. Bernstein, J. Chem. Phys. 22, 289 (1954).
 [2] IR. H. H. Blau, Jr. and H. H. Nielsen, J. Mol. Spectrosc. 1, 124 (1957).
 [3] IR. K. B. Harvey and J. F. Ogilvie, Can. J. Chem. 40, 85 (1962).
 [4] IR.Th. T. Nakagawa, H. Kashiwagi, H. Kurihara, and Y. Morino, J. Mol. Spectrosc., 31, 436 (1969).

Molecule: Formaldehyde-d₁ HDCO
Symmetry C_s Symmetry number $\delta = 1$

No. 69

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Gas)	
<i>a</i> '	ν_1	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		
<i>a</i> ''	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-d₂ D₂CO
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 70

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 ν_2).
	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 CH₄
 Symmetry T_d Symmetry number $\sigma = 12$

No. 71

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].

References

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 [5] IR. J. Herranz, J. Morcillo, and A. Gómez, J. Mol. Spectrosc. 19, 266 (1966).

Molecule: Methane-d₁ CH₃D
 Symmetry C_{3v} Symmetry number σ = 3

No. 72

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	CH ₃ s-stretch.....	2945 E	cm ⁻¹ (Gas) 2973 M 2914 M	cm ⁻¹ (Gas)	FR (2ν ₅).
	ν ₂	CD stretch.....	2200 A			
e	ν ₃	CH ₃ s-deform.....	1300 C	1300 M	1306	
	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	

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. Wilmhurst and H. J. Bernstein, Can. J. Chem. 35, 226 (1957).
 [3] IR. H. C. Allen, and E. K. Plyler, J. Res. NBS 63, 145 (1959).
 [4] IR. L. H. Jones, J. Mol. Spectrosc. 4, 86 (1960).

Molecule: Methane-d₂ CH₂D₂
 Symmetry C_{2v} Symmetry number σ = 2

No. 73

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a ₁	ν ₁	CH ₂ s-stretch.....	2974 C	cm ⁻¹ (Gas) 2976 M 2202 W 1436 W 1033 S	cm ⁻¹ (Gas) 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
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			
b ₂	ν ₇	CH ₂ rock.....	1090 C	1090 S	1090		
	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 ν₃.

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. Wilmhurst and H. J. Bernstein, Can. J. Chem. 35, 226 (1957).

Molecule: Methane-d₃ CHD₃
 Symmetry C_{3v} Symmetry number δ = 3

No. 74

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-d₄ CD₄
 Symmetry T_d Symmetry number δ = 12

No. 75

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 ν₄ [5].

References

- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
- [2] IR. H. M. Kaylor and A. H. Nielsen, J. Chem. Phys. 23, 2139 (1955).
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- [5] IR. H. Herranz, J. Morcillo, and A. Gómez, J. Mol. Spectrosc. 19, 266 (1966).

Molecule: Carbon tetrafluoride CF_4
 Symmetry T_d Symmetry number $\delta = 12$

No. 76

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	909 B	cm^{-1} (Gas) ia	cm^{-1} (Gas) 908.5 S	FR ($2\nu_4$).
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	
	ν_4	Deg. deform.....	632 B	631.73 VS	631.2 S	

References

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- [3] IR.Th. E. K. Plyler and W. S. Benedict, J. Res. NBS 47, 202 (1951), RP 2245.
- [4] IR. P. J. H. Woltz and A. H. Nielsen, J. Chem. Phys. 20, 307 (1952).
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Molecule: Carbon tetrachloride CCl_4
 Symmetry T_d Symmetry number $\delta = 12$

No. 77

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	459 C	cm^{-1} (Gas) ia	cm^{-1} (Liquid) 458.7 (10) p	FR ($\nu_1 + \nu_4$).
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	
	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).
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- [7] R. M. Ito, Spectrochim. Acta 21, 731 (1965).

Molecule: Carbon tetrabromide CBr_4
 Symmetry T_d Symmetry number $\sigma = 12$

No. 78

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

- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
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- [3] IR.R. E. K. Plyler, W. H. Smith, and N. Acquista, J. Res. NBS 44, 503 (1950), RP2097.
- [4] R. D. A. Long, D. C. Milner, and A. G. Thomas, Proc. Roy. Soc. (London), Ser. A, 240, 499 (1957).

Molecule: Carbon tetraiodide CI_4
 Symmetry T_d Symmetry number $\sigma = 12$

No. 79

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	123 (5)	
	ν_4	Deg. deform.....	125 E	^a { 123 W 127 W }		

^a Crystal field splitting.

Reference

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CH ₃ s-stretch.....	2930 E	cm^{-1} (Gas) { 2964 VS } { 2863 S } { 1464 S } { 1048.6 S } { 3005.8 S } { 1466.5 M } { 1182.4 M }	cm^{-1}	FR (2 <i>ν</i> ₆).
	<i>ν</i> ₂	CH ₃ s-deform.....	1464 A			
<i>e</i>	<i>ν</i> ₃	CF stretch.....	1049 A			
	<i>ν</i> ₄	CH ₃ d-stretch.....	3006 A			
	<i>ν</i> ₅	CH ₃ d-deform.....	1467 A			
	<i>ν</i> ₆	CH ₃ rock.....	1182 A			

References

- [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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 [5] IR. E. W. Jones, E. J. L. Poplewell, and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 290, 490 (1966).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CD ₃ s-stretch.....	2110 E	cm^{-1} (Gas) { 2090 } { 2150 } { 1136 } { 991 } { 2258 } { 1072 } { 903 }	cm^{-1}	FR (2 <i>ν</i> ₆).
	<i>ν</i> ₂	CD ₃ s-deform.....	1136 A			
<i>e</i>	<i>ν</i> ₃	CF stretch.....	991 A			
	<i>ν</i> ₄	CD ₃ d-stretch.....	2258 A			
	<i>ν</i> ₅	CD ₃ d-deform.....	1072 A			
	<i>ν</i> ₆	CD ₃ rock.....	903 A			

References

- [1] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 222, 443 (1954).
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 [3] IR. E. W. Jones, E. J. L. Poplewell, and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 290, 490 (1966).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_3 s-stretch.....	2937 E	cm^{-1} (Gas)	cm^{-1} (Liquid)	} FR ($2\nu_6$).
	ν_2	CH_3 s-deform.....	1355 A	2967.78 M	2955 VS, p	
e	ν_3	CCl stretch.....	732 A	2879.28 M	2861 M	} FR ($3\nu_6$) [6, 8].
	ν_4	CH_3 d-stretch.....	3039 B	1354.9 S	1370 VW, p	
	ν_5	CH_3 d-deform.....	1452 A	732.1 S	709 VS, p	
	ν_6	CH_3 rock.....	1017 A	3039.31 S	3036 M, dp	
				3042.75 S	1446 W, dp	
				1452.1 M	1016 W, dp	
				1017.3 M		

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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- [8] IR. M. Morillon-Chapey, Ph.D. Thesis (University of Paris, 1970).

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

References

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- [2] IR. W. T. King, I. M. Mills, and B. L. Crawford, Jr., J. Chem. Phys. 27, 455 (1964).
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Molecule: Methylbromide CH_3Br
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 84

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

References

- [1] R. H. L. Welsh, M. F. Crawford, T. R. Thomas, and G. R. Love, *Can. J. Phys.* **30**, 577 (1952).
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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
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 85

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

References

- [1] IR. H. B. Weissman, R. B. Bernstein, S. E. Roser, A. G. Meister, and F. F. Cleveland, *J. Chem. Phys.* **23**, 544 (1955).
- [2] IR. Y. Morino and J. Nakamura, *Bull. Chem. Soc. Japan* **38**, 443 (1965).
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Molecule: Methyl iodide CH_3I
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 86

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

References

- [1] Th. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. 27, 455 (1957).
- [2] IR. E. W. Jones and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 288, 50 (1965).
- [3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan 38, 443 (1965).
- [4] IR. Y. Morino, J. Nakamura, and S. Yamamoto, J. Mol. Spectrosc. 22, 34 (1967).
- [5] IR. T. L. Barnett and T. H. Edwards, J. Mol. Spectrosc. 23, 302 (1967).

Molecule: Methyl iodide- d_3 CD_3I
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 87

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CD_3 s-stretch	2130 E	cm^{-1} (Gas) { 2155.1 { 2081.0 { 950.7 { 501.4 { 2298 { 1049.3 { 655.9	cm^{-1}	FR ($2\nu_5$).
	ν_2	CD_3 s-deform	951 A			
e	ν_3	CI stretch	501 A			
	ν_4	CD_3 d-stretch	2298 A			
	ν_5	CD_3 d-deform	1049 A			
	ν_6	CD_3 rock	656 A			

References

- [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).
- [3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan 38, 443 (1965).
- [4] IR. R. W. Peterson and T. H. Edwards, J. Mol. Spectrosc. 38, 1 (1971).

Molecule: Trifluoromethane CHF_3
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 88

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH stretch	3036 C	cm^{-1} (Gas) 3036 S	cm^{-1} (Liquid) 3062 S, p	
	ν_2	CF_3 s-stretch	1117 C	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	

References

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

Molecule: Trichloromethane CHCl_3
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 89

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH stretch	3034 B	cm^{-1} (Gas) 3034.1 M	cm^{-1} (Gas) 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	

References

- [1] R. J. R. Nielsen and N. E. Ward, J. Chem. Phys. 10, 81 (1942).
 [2] IR.R. J. R. Madigan and F. F. Cleveland, J. Chem. Phys. 19, 119 (1951).
 [3] IR. T. G. Gibian and D. S. McKinney, J. Amer. Chem. Soc. 73, 1431 (1951).
 [4] IR. A. E. Stanevich and N. G. Yaroslavskii, Opt. Spectrosc. 9, 31 (1961).
 [5] IR. I. Suzuki, unpublished.

Molecule: Trichloromethane-d₁ CCl₃
 Symmetry C_{3v} Symmetry number σ = 3

No. 90

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	CD stretch	2266 C	2266 W <i>cm</i> ⁻¹ (Gas)	2255 (2) p <i>cm</i> ⁻¹ (Liquid)	
	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	

References

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

Molecule: Tribromomethane CHBr₃
 Symmetry C_{3v} Symmetry number σ = 3

No. 91

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	CH stretch	3042 B	3042 M <i>cm</i> ⁻¹ (Gas)	3017 (6) p <i>cm</i> ⁻¹ (Liquid)	
	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-d₁ CDBr₃
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 92

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	CD stretch	2251 C	<i>cm</i> ⁻¹ (Liquid) 2251 M	<i>cm</i> ⁻¹ (Liquid) 2247 (4)	} FR ($\nu_3 + \nu_5$).
	ν_2	CBr ₃ s-stretch	521 C	521 M	519.3 (7)	
<i>e</i>	ν_3	CBr ₃ s-deform	222 C	221.6 (10)	
	ν_4	CD bend	850 D	{ 858 VS	856.5 (3)	
	ν_5	CBr ₃ d-stretch	632 C	844 VS	840 (3)	
	ν_6	CBr ₃ d-deform	153 C	632 VS	628.5 (5)	
				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 CBrCl₃
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 93

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	CCl ₃ s-stretch	716 C	<i>cm</i> ⁻¹ (Liquid) 719 VS	<i>cm</i> ⁻¹ (Liquid) 716.3 (2) p	
	ν_2	CBr stretch	422 C	420 W	422.3 (10) p	
<i>e</i>	ν_3	CCl ₃ s-deform	247 C	247.3 (5) p	
	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
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 94

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CCl stretch.....	747 C	cm^{-1} (CS_2 , C_7H_{14} soln.) 747 S	cm^{-1} (C_6H_6 , CCl_4 soln.) 748 (1)	CF [1].
	ν_2	CBr_3 s-stretch.....	329 C	(CS_2 soln.) 329 W (C_7H_{14} soln.)	326 (10) p	
e	ν_3	CBr_3 s-deform.....	210 C	210 (10) p	
	ν_4	CBr_3 d-stretch.....	675 C	675 S (CS_2 soln.)	677 (4) dp	
	ν_5	CCl bend.....	211 E	
	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. Delwaille, 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
 Symmetry C_{2v} Symmetry number $\delta = 2$

No. 95

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_2 s-stretch.....	2999 B	cm^{-1} (Gas) 2999 M	cm^{-1} (Gas) 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	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-d₁ CHDCl₂
 Symmetry C_s Symmetry number $\sigma = 1$

No. 96

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	CH stretch.....	3024 B	cm^{-1} (Gas) 3024	cm^{-1} (Liquid) 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	
<i>a''</i>	ν_5	CCl ₂ s-stretch.....	692 B	692	682 S, p	
	ν_6	CCl ₂ scis.....	283 B	283 M, p	
	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-d₂ CD₂Cl₂
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 97

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	CD ₂ s-stretch.....	2205 B	cm^{-1} (Gas) 2205 W	cm^{-1} (Liquid) 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	
<i>a</i> ₂	ν_5	CD ₂ twist.....	826 C	ia	826 VW	
<i>b</i> ₁	ν_6	CD ₂ a-stretch.....	2304 C	2304 (liquid)	2304 VW	
	ν_7	CD ₂ rock.....	^a 712 D	OV (ν_9).
<i>b</i> 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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_2 s-stretch.....	3009 C	cm^{-1} (Gas) 3009 W	cm^{-1} (Gas) 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. Delwaille 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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH stretch.....	3040 C	cm^{-1} (Gas) 3040 W	cm^{-1} (Liquid) 3028 VW, p	
	ν_2	CD stretch.....	2249 D	2249 W (liquid)	2245 W, p	
a''	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	
	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-d₂ CD₂Br₂**
 Symmetry **C_{2v}** Symmetry number **$\delta = 2$**

No. 100

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	CD ₂ s-stretch.....	2214 C	<i>cm</i> ⁻¹ (Gas) 2214 W	<i>cm</i> ⁻¹ (Liquid) 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	
<i>a</i> ₂	ν_5	CD ₂ twist.....	782 D	ia	782 W, p	
<i>b</i> 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	
<i>b</i> 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 CBr₂Cl₂**
 Symmetry **C_{2v}** Symmetry number **$\delta = 2$**

No. 101

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	CCl ₂ s-stretch.....	733 C	<i>cm</i> ⁻¹ (Liquid) 733 VS	<i>cm</i> ⁻¹ (Liquid) 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	
<i>a</i> ₂	ν_5	CCl ₂ twist.....	175 C	ia	175 (2) dp	
<i>b</i> ₁	ν_6	CBr ₂ a-stretch.....	683 C	683 VS	684 (3) dp	
	ν_7	CCl ₂ wag.....	229 C	229 (2) dp	
<i>b</i> 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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	CH ₂ s-stretch.....	3003 A	cm^{-1} (Gas) 3003 S	cm^{-1} (Liquid) 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	
<i>a''</i>	ν_6	CBrCl scis.....	229 C	229 S, p	
	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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i>	ν_1	CH stretch.....	3031 C	cm^{-1} (Gas) 3031 S	cm^{-1} (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-d₂ CD₂BrCl
Symmetry C_s Symmetry number $\sigma = 1$

No. 104

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a'</i>	ν_1	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	
<i>a''</i>	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
Symmetry C_s Symmetry number $\sigma = 1$

No. 105

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	ν_1	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		
<i>a''</i>	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-Thomae, 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-d₂ DCOOD
 Symmetry C_s Symmetry number δ = 1

No. 106

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν ₁	OD stretch	2632 C	2632 W	cm ⁻¹ (Gas)	
	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 CH₃OH (gas)
 Symmetry C_s Symmetry number δ = 1

No. 107

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments		
a'	ν ₁	OH stretch	3681 A	3681 M	cm ⁻¹ (Gas)			
	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				
	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				
a''	ν ₈	CO stretch	1033 A	1033 VS			1032 (2)	OV (ν ₈)
	ν ₉	CH ₃ d-stretch	2960 C	2960 S			2955 (4)	OV (ν ₄)
	ν ₁₀	CH ₃ d-deform	1477 B	1477 M	1165 (1) (liquid)			
	ν ₁₁	CH ₃ rock	1165 C					
	ν ₁₂	Torsion	{ 295 (A) 200 (E) }	80~300		{ MW: ^a 295 (A) 200 (E) }		

^a The value of ν₁₂ 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].

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- [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 CH₃OH (liquid)
Symmetry C_s Symmetry number $\sigma = 1$

No. 108

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	OH stretch	3328 D	cm^{-1} (Liquid) 3328 νb	cm^{-1} (Liquid) 3270 3480	OV (ν_{10}).
	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)	
	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)	
<i>a''</i>	ν_8	CO stretch	1030 C	1030 VS	1033 (6)	OV (ν_4).
	ν_9	CH ₃ d-stretch	2946 C	2946 S	2940 (9)	
	ν_{10}	CH ₃ d-deform	1480 C	1480 M	1464 (5b)	
	ν_{11}	CH ₃ rock	1165 C	1165	1165 (1)	
	ν_{12}	Torsion	655 D	655 νb		

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- [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).
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 [4] IR.Th. C. Tanaka and T. Shimanouchi, unpublished.

Molecule: Methanol-d₁ CH₃OD (gas)
Symmetry C_s Symmetry number $\sigma = 1$

No. 109

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	OD stretch	2718 A	cm^{-1} (Gas) 2718 M	cm^{-1}	SF (ν_2 of CH ₃ OH). OV (ν_{10}).
	ν_2	CH ₃ d-stretch	3000 C	3000 M		
	ν_3	CH ₃ s-stretch	2843 A	2843 S		
	ν_4	CH ₃ d-deform	1473 B	1473 M		
	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		
<i>a''</i>	ν_8	CO stretch	1040 A	1040 VS		SF (ν_9 of CH ₃ OH). OV (ν_4). CF [5, 6].
	ν_9	CH ₃ d-stretch	2960 C	2960 S		
	ν_{10}	CH ₃ d-deform	1473 B	1473 M		
	ν_{11}	CH ₃ rock	1160 C	1160 VW		
	ν_{12}	Torsion	213 E			

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- [1] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
 [2] IR. C. Tanaka, K. Kuratani, and S. Mizushima, Spectrochim. Acta 9, 265 (1957).
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 [4] IR. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961) and references cited there.
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 [6] IR.Th. C. Tanaka and T. Shimanouchi, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments		
a'	ν ₁	OD stretch	2467 D	cm ⁻¹ (Liquid) 2467 vb	cm ⁻¹ (Liquid) 2420- 2560	OV (ν ₁₀).		
	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)			
	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)	OV (ν ₄).
		ν ₁₀	CH ₃ d-deform	1469 C	1469 M		1463 (5b)	
		ν ₁₁	CH ₃ rock	1163 C		1163 (1)	
		ν ₁₂	Torsion	475 D	475 vb			

References

- [1] R. S. Mizushima, Y. Morino, and G. Okamoto, Bull. Chem. Soc. Japan 11, 698 (1936).
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- [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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments		
a'	ν ₁	OH stretch	3690 D	cm ⁻¹ (Gas) 3690 S	cm ⁻¹	CF [1, 3].		
	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				

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- [1] Th. M. Margottin-Maclou, J. Phys. Radium 21, 634 (1960).
- [2] IR. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961), and references cited there.
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- [4] Th. C. Tanaka and T. Shimanouchi, unpublished.

Molecule: Methanol-d₃ CD₃OH (liquid)
Symmetry C_s Symmetry number δ = 1

No. 112

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν ₁	OH stretch.....	3310 D	3310 S, vb	3350 W, vb	OV (ν ₁₀).
	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	
	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	
a''	ν ₈	CO stretch.....	982 C	982 VS	986 VS, p	OV (ν ₄).
	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	
	ν ₁₁	CD ₃ rock.....	882 D	882 M	894 M, dp	
	ν ₁₂	Torsion.....	665 D	665 S, vb		

^a The value obtained in the vitreous solid (-180 °C).

References

- [1] IR.R. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961), and references cited there.
[2] Th. C. Tanaka and T. Shimanouchi, unpublished.

Molecule: Methanol-d₄ CD₃OD (gas)
Symmetry C_s Symmetry number δ = 1

No. 113

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν ₁	OD stretch.....	2724 D	2724 S	cm ⁻¹	SF (ν ₂ of CD ₃ OH).
	ν ₂	CD ₃ d-stretch.....	2260 E	2260		
	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		
a''	ν ₈	CO stretch.....	983 C	983 VS	cm ⁻¹	CF [1, 3].
	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			

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- [1] Th. M. Margottin-Maclou, J. Phys. Radium 21, 634 (1960).
[2] IR. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961).
[3] Th. C. Tanaka and T. Shimanouchi, unpublished.

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	
a''	ν_9	NH_2 wag.....	780 A	780 VS	781 W	
	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	MW: 272 (A).
	ν_{15}	Torsion.....	268 B	268	265 (E).

^a Estimated from RQ branch frequency.

References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	ND ₂ s-stretch.....	2479 B	cm^{-1} (Gas) 2479 W	cm^{-1} (Gas) 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	
<i>a''</i>	ν_9	ND ₂ wag.....	625 A	625 VS		
	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.

References

- [1] R. J. T. Edsall and H. Schinberg, J. Chem. Phys. 8, 520 (1940).
- [2] IR. A. P. Gray and R. C. Lord, J. Chem. Phys. 26, 690 (1957).
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- [7] IR.R. J. R. Durig, S. F. Bush, and F. G. Baglin, J. Chem. Phys. 49, 2106 (1968).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	<i>ν</i> ₁	NH ₂ s-stretch.....	3361 B	3361 W		
	<i>ν</i> ₂	CD ₃ d-stretch.....	2203 B	2203 VS		
	<i>ν</i> ₃	CD ₃ s-stretch.....	2077 A	2077 VS		
	<i>ν</i> ₄	NH ₂ scis.....	1624 B	1624 S		
	<i>ν</i> ₅	CD ₃ d-deform.....	1065 D	CF [3].
	<i>ν</i> ₆	CD ₃ s-deform.....	1142 A	1142 S		
	<i>ν</i> ₇	CD ₃ rock.....	913 A	913 S		
	<i>ν</i> ₈	CN stretch.....	973 B	973 M		
<i>a''</i>	<i>ν</i> ₉	NH ₂ wag.....	740 A	740 VS		
	<i>ν</i> ₁₀	NH ₂ a-stretch.....	3427 C	3427 W		
	<i>ν</i> ₁₁	CD ₃ d-stretch.....	2236 C	2236 VS		
	<i>ν</i> ₁₂	CD ₃ d-deform.....	1077 C	1077 W		
	<i>ν</i> ₁₃	NH ₂ twist.....	1416 C	1416 W		
	<i>ν</i> ₁₄	CD ₃ rock.....	926 D	CF [3].
	<i>ν</i> ₁₅	Torsion.....	247 D	CF [3].

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- [3] Th. A. Y. Hirakawa, unpublished.
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	<i>ν</i> ₁	ND ₂ s-stretch.....	2477 B	2477 W		
	<i>ν</i> ₂	CD ₃ d-stretch.....	2202 B	2202 VS		
	<i>ν</i> ₃	CD ₃ s-stretch.....	2073 B	2073 VS		
	<i>ν</i> ₄	ND ₂ scis.....	1227 B	1227 S		
	<i>ν</i> ₅	CD ₃ d-deform.....	1065 D			CF [2.]
	<i>ν</i> ₆	CD ₃ s-deform.....	1123 B	1123 M		
	<i>ν</i> ₇	CD ₃ rock.....	880 B	880 M		
	<i>ν</i> ₈	CN stretch.....	942 A	942 S		
<i>a''</i>	<i>ν</i> ₉	ND ₂ wag.....	601 A	601 VS		
	<i>ν</i> ₁₀	ND ₂ a-stretch.....	2556 C	2556 W		
	<i>ν</i> ₁₁	CD ₃ d-stretch.....	2238 C	2238 VS		
	<i>ν</i> ₁₂	CD ₃ d-deform.....	1077 C	1077 W		
	<i>ν</i> ₁₃	ND ₂ twist.....	1072 D			CF [2.]
	<i>ν</i> ₁₄	CD ₃ rock.....	910 B	910 M		
	<i>ν</i> ₁₅	Torsion.....	201 C			CF [2]. MW: 200 (A). 203 (E).

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- [1] IR. A. P. Gray and R. C. Lord, J. Chem. Phys. 26, 690 (1957).
- [2] Th. A. Y. Hirakawa, unpublished.
- [3] IR.R. J. R. Durig, S. F. Bush, and F. G. Baglin, J. Chem. Phys. 49, 2106 (1968).
- [4] MW. D. R. Lide, J. Chem. Phys. 27, 343 (1957).

Molecule: Acetylene CHCH
Symmetry $D_{\infty h}$ Symmetry number $\delta = 2$

No. 118

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ_g^+	ν_1	CH stretch	3374 C	cm^{-1} (Gas) ia	cm^{-1} (Gas) 3373.7 S	FR ($\nu_2 + \nu_4 + \nu_5$).
	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	
π_g	ν_4	CH bend	612 C		ia	
π_u	ν_5	CH bend	730 A	730.3 VS	ia	

References

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Molecule: Acetylene- d_1 CHCD
Symmetry $C_{\infty v}$ Symmetry number $\delta = 1$

No. 119

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	CH stretch	3336 A	cm^{-1} (Gas) 3335.6 S	cm^{-1} (Gas) 3335 S	RP [4]. RP [4].
	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		
	ν_5	CD bend	678 A	677.8 S		

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- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
- [2] IR. J. Overend and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 234, 306 (1955).
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Molecule: Acetylene-d₂ CDCD
 Symmetry D_{∞h} Symmetry number δ = 2

No. 120

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ_g^+	ν_1	CD stretch.....	2701 C	cm^{-1} (Gas) ia	cm^{-1} (Gas) 2700.5 S	OC ($\nu_4 + \nu_5$) [1].
	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	
π_u	ν_5	CD bend.....	537 A	536.9 VS	ia	

References

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Molecule: Fluoroacetylene CHCF
 Symmetry C_{∞v} Symmetry number δ = 1

No. 121

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	CH stretch.....	3355 B	cm^{-1} (Gas) 3355 VS	cm^{-1}	
	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		

References

- [1] IR. W. J. Middleton and W. H. Sharkey, J. Amer. Chem. Soc. 81, 803 (1959).
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Molecule: Chloroacetylene CHCl
 Symmetry $C_{\infty v}$ Symmetry number $\delta = 1$

No. 122

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	ν_1	CH stretch	3340 B	cm^{-1} (Gas) 3340 VS	cm^{-1}	
	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
 Symmetry $C_{\infty v}$ Symmetry number $\delta = 1$

No. 123

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

References

See No. 121.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_g	ν_1	CH_2 s-stretch.....	3026 B	cm^{-1} (Gas) ia	cm^{-1} (Gas) 3026.4 (10)p	FR ($2\nu_{10}$). OC ($\nu_4 + \nu_6$) [7].
	ν_2	CC stretch.....	1623 D	ia	1622.6 (8)p	
	ν_3	CH_2 scis.....	1342 B	ia	1342.2 (10)p	
a_u	ν_4	CH_2 twist.....	1023 E	ia	ia	
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	

References

- [1] I.R.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
- [2] R. H. Rank, E. R. Shull, and D. W. E. Axford, J. Chem. Phys. 18, 116 (1950).
- [3] I.R. R. L. Arnett and B. L. Crawford, Jr., J. Chem. Phys. 18, 118 (1950).
- [4] R. T. Feldman, J. Romanko, and H. L. Welsh, Can. J. Phys. 34, 737 (1956).
- [5] I.R. H. C. Allen, Jr., and E. K. Plyler, J. Amer. Chem. Soc. 80, 2673 (1958).
- [6] I.R. D. A. Dows, J. Chem. Phys. 36, 2833 (1962).
- [7] I.R. W. L. Smith and I. M. Mills, J. Chem. Phys. 40, 2095 (1963).

Molecule: Ethylene-d₄ C₂D₄
 Symmetry D_{2h} Symmetry number σ = 4

No. 125

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 (ν ₆ + ν 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.

References

- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
- [2] IR. R. L. Arnett and B. L. Crawford, Jr., J. Chem. Phys. 18, 118 (1950).
- [3] Th B. N. Cyvin and S. J. Cyvin, Acta Chem. Scand. 17, 1831 (1963).
- [4] Th. J. Hiraishi and T. Shimanouchi, unpublished.

Molecule: Tetrafluoroethylene CF₂CF₂
 Symmetry D_{2h} Symmetry number σ = 4

No. 126

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	

References

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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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_g	ν_1	CC stretch	1571 D	cm^{-1} (Liquid) ia	cm^{-1} (Liquid) 1571 (7)p	OC ($2\nu_4$) [2].
	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	
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	ia	
	ν_{12}	CCl_2 scis	310 C	(CS_2 soln.) 310 W	ia	

References

- [1] IR.R. G. Herzberg, *Infrared and Raman Spectra of Polyatomic Molecules* (Van Nostrand, New York, 1945), and references cited there.
 [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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_g	ν_1	CC stretch	1535 E	cm^{-1} (Liquid) ia	cm^{-1} (Liquid) {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	}CF [2].
a_u	ν_4	CBr_2 twist	66 E	ia	ia	
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	
	ν_9	CBr_2 a-stretch	766 C	766 S	ia	
b_{3u}	ν_{10}	CBr_2 rock	119 C	119 M	ia	
	ν_{11}	CBr_2 s-stretch	635 C	635 S	ia	
	ν_{12}	CBr_2 scis	188 C	188 M	ia	

References

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

No. 129

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 CF. ^b
	ν_7	Torsion	482 E	ia	
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		
b_2	ν_{11}	CCF deform	768 B	768 S		
	ν_{12}	CH bend	756 B	756 S		

^a From product rule.

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

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-d₁** **CHFCD_F**
 Symmetry C_s Symmetry number $\sigma = 1$

No. 130

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		
a''	ν_8	CCF deform	757 B	757 S		
	ν_9	CCF deform	255 D	255 W		
	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-d₂** CDFCDF
 Symmetry C_{2v} Symmetry number δ = 2

No. 131

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 $\frac{\nu_{12}(cis-d_1)}{\nu_{10}(trans-d_1)} = \frac{\nu_7(cis-d_2)}{\nu_7(trans-d_2)}$.

Reference

See No. 130.

Molecule: **trans-1,2-Dichloroethylene** CHClCHCl
 Symmetry C_{2h} Symmetry number δ = 2

No. 132

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] IR. J. M. Dowling, J. Chem. Phys. 25, 284 (1956).
- [6] IR. T. Shimanouchi and T. Shimanouchi, unpublished.

Molecule: **trans-1,2-Dichloroethylene-d₁** CHClCDCl
 Symmetry C_s Symmetry number $\delta = 1$

No. 133

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	CH stretch.....	3087 C	<i>cm</i> ⁻¹ (Gas) 3087 S	<i>cm</i> ⁻¹ (Liquid) 3074 M	CF [6].
	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	
<i>a''</i>	ν_7	CCl stretch.....	775 B	775 VS	775 M	
	ν_8	CCCl deform.....	348 C	348 VS	
	ν_9	CCCl deform.....	245 E	
	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	

References

See No. 132.

Molecule: **trans-1,2-Dichloroethylene-d₂** CDClCDCl
 Symmetry C_{2h} Symmetry number $\delta = 2$

No. 134

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a_g</i>	ν_1	CD stretch.....	2325 C	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Liquid) 2325 S	CF [5, 6].
	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	
<i>a_u</i>	ν_6	CD bend.....	660 B	660 S	ia	
	ν_7	Torsion.....	221 E	ia	
<i>b_g</i>	ν_8	CD bend.....	657 C	ia	657 M	
	<i>b_u</i>	ν_9	CD stretch.....	2290 C	2290 S	
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	

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
<i>a</i> ₁	ν_1	CH stretch	3077 C	<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
	ν_2	CC stretch	1587 C	3077	3077	
	ν_3	CH bend	1179 C	1590 S (liquid)	1587 S, p	
	ν_4	CCl stretch	711 C	1183 W (liquid)	1179 S, p	
<i>a</i> ₂	ν_5	CCCl deform	173 C	714 S (liquid)	711 S, p	
	ν_6	CH bend	876 C	173 C	173 S, p	
	ν_7	Torsion	406 C	ia	876 W, dp	
<i>b</i> ₁	ν_8	CH stretch	3072 C	ia	406 S, dp	
	ν_9	CH bend	1303 C	3072		
<i>b</i> ₂	ν_{10}	CCl stretch	857 B	1303		
	ν_{11}	CCCl deform	571 B	857		
	ν_{12}	CH bend	697 B	571	563 M, dp	
				697		

References

See No. 132.

Molecule: **cis-1,2-Dichloroethylene-d₁** **CHClCDCI**
 Symmetry **C_s** Symmetry number **$\sigma = 1$**

No. 136

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

References

See No. 132.

Molecule: **cis-1,2-Dichloroethylene-d₂** CDCICDCI
 Symmetry C_{2v} Symmetry number δ = 2

No. 137

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	CF [6].
	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	
	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	
b ₂	ν ₁₁	CCCl deform.....	558 C	558 S	
	ν ₁₂	CD bend.....	540 C	540 S	

References

See No. 132.

Molecule: **trans-1,2-Dichloro-1,2-difluoroethylene** CCIFCCIF
 Symmetry C_{2h} Symmetry number δ = 2

No. 138

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	CF [2]. FR (ν ₅ + ν ₁₀).
	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	
b _g	ν ₈	CFCl wag.....	529 C	ia	529 M, dp	
	ν ₉	CF stretch.....	1190 E	{ 1214 VS 1167 VS }	ia	
b _u	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	

References

- [1] IR.R. D. E. Mann and E. K. Plyler, J. Chem. Phys. 26, 773 (1957).
 [2] Th. D. E. Mann, L. Fano, J. H. Meal, and T. Shimanouchi, J. Chem. Phys. 27, 51 (1957).

Molecule: 1,1-Dichloroethylene CH_2CCl_2
 Symmetry C_{2v} Symmetry number $\delta = 2$

No. 139

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).
 [2] R. P. Joyner and G. Glocker, J. Chem. Phys. 20, 302 (1952).
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Molecule: 1,1-Dichloroethylene- d_1 CHDCCl_2
 Symmetry C_s Symmetry number $\delta = 1$

No. 140

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	
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		CF [1].

^a CCl_4 solution.

Reference

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

Molecule: 1,1-Dichloroethylene-d₂ CD₂CCl₂
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 141

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		CF [1].
	ν_2	CC stretch.....	1565 C	1565 VS		
	ν_3	CD ₂ scis.....	1039 E			CF [1]. CF [1].
	ν_4	CCl ₂ s-stretch.....	580 C	580 VS		
	ν_5	CCl ₂ scis.....	305 E			CF [1]. CF [1].
a ₂	ν_6	Torsion.....	488 E	ia		
b ₁	ν_7	CD ₂ a-stretch.....	2380 D	^a 2380 W		SF (ν_{11}).
	ν_8	CD ₂ rock.....	998 C	998 VS		
	ν_9	CCl ₂ a-stretch.....	697 C	697 S		SF (ν_9).
	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 CCl₄ solution.

Reference

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

Molecule: 1,1-Dichloro 2,2-difluoroethylene CF₂CCl₂
 Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 142

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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 [2] IR. D. E. Mann and E. K. Plyler, J. Chem. Phys. 23, 1989 (1955).
 [3] Th. D. E. Mann, L. Fano, J. H. Meal, and T. Shimanouchi, J. Chem. Phys. 27, 51 (1957).

Molecule: Methyleyanide CH_3CN
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 143

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

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- [1] R. A. Dadiou, Monatsh. Chem. 57, 437 (1931).
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- [3] IR.R. P. Venkateswarlu, J. Chem. Phys. 19, 293 (1951).
- [4] IR.R. H. W. Thompson and R. L. Williams, Trans Faraday Soc. 48, 502 (1952).
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- [7] Th. J. L. Duncan, Spectrochim. Acta 20, 1197 (1964).
- [8] Th. G. Amat and H. H. Nielsen, Molecular Orbitals in Chemistry, Physics and Biology p. 293 (Academic Press, New York, 1964).
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- [10] IR. H. Matsuura, Bull. Chem. Soc. Japan 44, 2379 (1971).

Molecule: Methyleyanide- d_3 CD_3CN
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 144

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CD_3 s-stretch	2126 A	cm^{-1} (Gas) 2125.6	cm^{-1} (Liquid) 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	340 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
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 145

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_3 s-stretch.....	2966 B	cm^{-1} (Gas) 2965.8 M	cm^{-1} (Liquid) 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).
- [4] Th. W. H. Fletcher and C. S. Shoup, Proceedings of the International Symposium on Molecular Structure and Spectroscopy, C204 (Tokyo, 1962).
- [5] Th. J. L. Duncan, Spectrochim. Acta 20, 1197 (1964).

Molecule: Methyl isocyanide- d_3 CD_3NC
 Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 146

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CD_3 s-stretch.....	2251 B	cm^{-1} (Gas) 2250.6 W	cm^{-1}	
	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).
- [3] Th. J. L. Duncan, Spectrochim. Acta 20, 1197 (1964).

Molecule: 1,2,5-Oxadiazole $C_2H_2N_2O$
 Symmetry C_{2v} Symmetry number $\delta = 2$

No. 147

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH stretch	3140 C	cm^{-1} (Gas) 3140 VW	cm^{-1} (Liquid) 3144 VS, p	OC ($2\nu_8, \nu_4 + \nu_8, \nu_8 + \nu_{12}$).
	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) ia	824 VW, dp	
	ν_8	op-Ring I	635 E			
b_1	ν_9	CH stretch	3133 D	3133 sh (liquid)		
	ν_{10}	ip-Ring I	1546 D	1546 VW (liquid)		
b_2	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		
	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
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 148

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH stretch	3311 B	cm^{-1} (Gas) 3311.4 M	cm^{-1}	
	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 $\nu_5, \nu_7, \nu_8,$ 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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 [2] IR. R. B. Reeves, R. E. Wilde, and D. W. Robinson, J. Chem. Phys. 40, 125 (1964).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH ₂ s-stretch.....	3006 C	cm^{-1} (Gas) 3006 S	cm^{-1} (Liquid) 3005 S, p	OV (ν_{13}). OV (ν_1).
	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	
a_2	ν_5	Ring deform.....	877 B	877 VS	867 M, dp	
	ν_6	CH ₂ a-stretch.....	3063 D	ia	3063 W, dp	
	ν_7	CH ₂ twist.....	1300 E	ia		
b_1	ν_8	CH ₂ rock.....	860 E	ia		
	ν_9	CH ₂ s-stretch.....	3006 C	3006 S	3005 S, p	
b_2	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		
	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).
- [3] IR.R. H. W. Thompson and W. T. Cave, Trans. Faraday Soc. 47, 946 (1951).
- [4] IR. R. C. Lord and B. Nolin, J. Chem. Phys. 24, 656 (1956).
- [5] IR.R. W. J. Potts, Spectrochim. Acta 21, 511 (1965).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	<i>ν</i> ₁	CD ₂ s-stretch.....	2204 C	2204 S	
	<i>ν</i> ₂	CD ₂ scis.....	1311 C	1311 M	1301 VS	
	<i>ν</i> ₃	Ring stretch.....	1013 C	1014 W	1013 S	
	<i>ν</i> ₄	CD ₂ wag.....	970 C	970 VS	952 M	
	<i>ν</i> ₅	Ring deform.....	755 C	755 VS	755 M	
<i>a</i> ₂	<i>ν</i> ₆	CD ₂ a-stretch.....	2250 D	ia	2250 W	
	<i>ν</i> ₇	CD ₂ twist.....	1083 D	ia	1083 VW	
<i>b</i> ₁	<i>ν</i> ₈	CD ₂ rock.....	581 D	ia	581 W	
	<i>ν</i> ₉	CD ₂ s-stretch.....	2174 C	2174 VS	2157 M	
	<i>ν</i> ₁₀	CD ₂ scis.....	1145 D	1145 VW		
	<i>ν</i> ₁₁	CD ₂ wag.....	952 D	952 M	
<i>b</i> ₂	<i>ν</i> ₁₂	Ring deform.....	809 C	809 S	786 M	
	<i>ν</i> ₁₃	CD ₂ a-stretch.....	2317 C	2317 VS	2319 S	
	<i>ν</i> ₁₄	CD ₂ twist.....	896 C	896 S	896 W	
	<i>ν</i> ₁₅	CD ₂ rock.....	577 C	577 W		

References

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 [2] IR.R. R. C. Lord and B. Nolin, J. Chem. Phys. 24, 656 (1956).

Molecule: Acetaldehyde CH_3CHO
 Symmetry C_s Symmetry number $\sigma = 1$

No. 151

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH_3 d-stretch.....	3005 C	cm^{-1} (Gas) 3005 M	cm^{-1} (Liquid) 3001 W	
	ν_2	CH_3 s-stretch.....	2917 D	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

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- [4] IR.R.Th. P. Cossee and J. H. Schachtschneider, J. Chem. Phys. 44, 97 (1966).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a'</i>	ν_1	CH ₃ d-stretch.....	3028 C	3028 M	2998 W	
	ν_2	CH ₃ s-stretch.....	2917 D	2917 S, p	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	
<i>a''</i>	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		

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- [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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	CD ₃ d-stretch.....	2265 C	<i>cm</i> ⁻¹ (Gas) 2265 W	<i>cm</i> ⁻¹ (Liquid) 2128	
	ν_2	CD ₃ s-stretch.....	2130 C	2130 W	2072	
	ν_3	CO stretch.....	2060 C	2060 M	1706	
	ν_4	CO stretch.....	1737 C	1737 VS	1090	
	ν_5	CD ₃ d-deform.....	1045 C	1045 M		
	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	
<i>a''</i>	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 C	670 D		CF [5].
	ν_{15}	Torsion.....	116 C	116 W		MW [3].

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- [5] IR.R.Th. P. Cossee and J. H. Schachtschneider, J. Chem. Phys. 44, 97 (1966).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a _{1g}	ν ₁	CH ₃ s-stretch	2954 B	cm ⁻¹ (Gas) ia	cm ⁻¹ (Gas) 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		
e _u	ν ₉	CH ₃ rock	1190 E	ia		OC [2, 3].
	ν ₁₀	CH ₃ d-stretch	2985 A	2985.4	ia		
	ν ₁₁	CH ₃ d-deform	1469 C	1469	ia		FR (ν ₄ + ν ₁₂).
	ν ₁₂	CH ₃ rock	822 A	821.6	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. L. G. Smith, *J. Chem. Phys.* 17, 139 (1949).
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>v</i> ₁	CH ₃ s-stretch.....	2912 E	<i>cm</i> ⁻¹ (Gas) 2955.1 S 2897.4 S	<i>cm</i> ⁻¹ (Gas) 2955.5 2898.2	} FR (2 <i>v</i> ₉).
	<i>v</i> ₂	CD ₃ s-stretch.....	2098 E	2139.6 S 2089.7 S	
	<i>v</i> ₃	CH ₃ s-deform.....	1387 B	1386.6 W		
	<i>v</i> ₄	CD ₃ s-deform.....	1122 B	1122.0 W		
	<i>v</i> ₅	CC stretch.....	904 A	903.8 VW	904.7	
<i>a</i> ₂	<i>v</i> ₆	Torsion.....	253 B	253 VW		
<i>e</i>	<i>v</i> ₇	CH ₃ d-stretch.....	2977 D	2976.5 S	2976.6	
	<i>v</i> ₈	CD ₃ d-stretch.....	2240 E	2240 S		
	<i>v</i> ₉	CH ₃ d-deform.....	1471 A	1471.1 M		
	<i>v</i> ₁₀	CH ₃ rock.....	1115 B	1115.0 W		
	<i>v</i> ₁₁	CD ₃ d-deform.....	1066 B	1065.7 M	1062.6	
	<i>v</i> ₁₂	CD ₃ rock.....	678 A	678.4 M		

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- [4] IR.Th. I. Nakagawa and T. Shimanouchi, J. Mol. Spectrosc. 39, 255 (1971).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Gas)	
<i>a</i> _{1g}	<i>v</i> ₁	CD ₃ s-stretch	2083 B	ia	2083.0	
	<i>v</i> ₂	CD ₃ s-deform	1155 A	ia	1154.5	
	<i>v</i> ₃	CC stretch	843 A	ia	843.0	
<i>a</i> _{1u}	<i>v</i> ₄	Torsion	208 B	208	ia	
<i>a</i> _{2u}	<i>v</i> ₅	CD ₃ s-stretch	2087 B	2087.4	ia	
	<i>v</i> ₆	CD ₃ s-deform	1077 B	1077.1	ia	
<i>e</i> _g	<i>v</i> ₇	CD ₃ d-stretch	2226 A	ia	2225.6	
	<i>v</i> ₈	CD ₃ d-deform	1041 B	ia	1041	
	<i>v</i> ₉	CD ₃ rock	970 C	ia	970 (liquid)	
<i>e</i> _u	<i>v</i> ₁₀	CD ₃ d-stretch	2235 B	2235	ia	
	<i>v</i> ₁₁	CD ₃ d-deform	1081 B	1080.9	ia	
	<i>v</i> ₁₂	CD ₃ rock	594 A	594.4	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_{1g}	ν_1	CC stretch	1228 D	cm^{-1} (Gas) ia	cm^{-1} (Gas) 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	
e_g	ν_6	CF_3 s-deform	714 B	714 VS	ia	
	ν_7	CF_3 d-stretch	1250 C	ia	1250 VW, dp	
	ν_8	CF_3 d-deform	619 C	ia	619 W, dp	
e_u	ν_9	CF_3 rock	372 C	ia	372 W, dp	
	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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- [3] Th. T. Fujiyama and T. Shimanouchi, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_{1g}	ν_1	CC stretch	975 C	cm^{-1} (Solid) ia	cm^{-1} (Solid) 975 VW, p	OC ($\nu_4 + \nu_{10}$, $\nu_4 + \nu_{11}$).
	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	
a_{2u}	ν_5	CCl_3 s-stretch	675 C	675 S	ia	
e_g	ν_6	CCl_3 s-deform	372 C	372 S	ia	
	ν_7	CCl_3 d-stretch	859 C	ia	859 W	
	ν_8	CCl_3 d-deform	340 C	ia	340 M	
e_u	ν_9	CCl_3 rock	223 C	ia	223 S	
	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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- [2] IR.R.Th. T. Fujiyama and T. Shimanouchi, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_g	ν_1	CC stretch	940 C	cm^{-1} (Solid) ia	cm^{-1} (Solid) 940 M	OC ($\nu_4 + \nu_{10}, \nu_4 + \nu_{11}$).
	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	
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	
e_u	ν_9	CBr_3 rock	139 C	ia	139 M	
	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.

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	SF (gauche ν_1 , gauche ν_{11}).
	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	
	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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- [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: 1,2-Dichloroethane $\text{CH}_2\text{ClCH}_2\text{Cl}$ (gauche form)
 Symmetry C_2 Symmetry number $\sigma = 2$

No. 161

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i>	ν_1	CH_2 a-stretch.....	3005 D	cm^{-1} (Gas) 3005 W (liquid)	cm^{-1} (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	
<i>b</i>	ν_{10}	Torsion.....	125 (5b)	
	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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a_g</i>	ν_1	CH ₂ s-stretch	2972 D	<i>cm</i> ⁻¹ (Liquid) ia	<i>cm</i> ⁻¹ (Liquid) 2972 (10) p	SF (ν_{12}).
	ν_2	CH ₂ scis	1440 C	ia	1440 (5) dp	
	ν_3	CH ₂ wag	1255 C	ia	1255 (10b) p	
	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	
<i>a_u</i>	ν_7	CH ₂ a-stretch	3037 D	3037 S	ia	SF (ν_3).
	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)	
<i>b_g</i>	ν_{11}	CH ₂ a-stretch	3013 D	ia	3013 (4b) dp	SF (ν_3).
	ν_{12}	CH ₂ twist	1255 C	ia	1255 (10b) p	
<i>b_u</i>	ν_{13}	CH ₂ rock	933 C	ia	933 (2) p	SF (ν_3).
	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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- [1] IR.R. S. Mizushima, Y. Morino, I. Watanabe, T. Shimanouchi, and S. Yamaguchi, J. Chem. Phys. 17, 591 (1949).
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- [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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i>	ν_1	CH ₂ a-stretch.....	3005 D	<i>cm</i> ⁻¹ (Liquid)	<i>cm</i> ⁻¹ (Liquid)	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 dform.....	231 C	231 (3) p	
	ν_{10}	Torsion.....	91 D	91 (2b) dp	
<i>b</i>	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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH_2 s-stretch	2960 D	cm^{-1} (Solid)	cm^{-1} (Liquid)	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i>	ν_1	CH_2 a-stretch	3010 D	cm^{-1} (Liquid)	cm^{-1} (Liquid)	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.

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

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH_2 s-stretch.....	2967 D	cm^{-1} (Gas) 2977 M (solid)	cm^{-1} (Liquid) 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	
a''	ν_{11}	CCCl deform.....	336 C	336 M	337 S, p	
	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH_3 d-stretch.....	2988 C	cm^{-1} (Gas) 2988 S	cm^{-1} (Liquid) 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	
	a''	ν_{11}	CCBr deform.....	290 B	290 S	292 (3) p
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_6).
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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	NH stretch	3338 C	cm^{-1} (Gas) 3338 W	cm^{-1} (Liquid) 3302 M, p	OV (ν_{11}). OV (ν_{12}).
	ν_2	CH ₂ a-stretch	3079 D	3079 S	3059 M, dp	
	ν_3	CH ₂ s-stretch	3015 D	3015 S	2999 VS, p	
	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). OV (ν_3).
	ν_{12}	CH ₂ s-stretch	3015 D	3015 S	2999 VS, p	
	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH_3 d-stretch.....	3045 D	cm^{-1} (Gas) 3045 M	cm^{-1} (Liquid) 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)	
a''	ν_{12}	COC deform.....	318 D	318 M		
	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		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν ₁	CH ₃ d-stretch.....	3041 C	3041 M	} FR (2ν ₁₆).	
	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		
	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	} CF [2], OV (ν ₉). CF [2], OV (ν ₁₀). CF [2].	
	ν ₁₄	CH ₃ d-deform.....	1440 E	1440 W (CCl ₄ soln.)		
	ν ₁₅	CH ₃ rock.....	1164 E		
	ν ₁₆	CD bend.....	870 E		
	ν ₁₇	C-O torsion.....	290 E	290 M		
	ν ₁₈	CH ₃ torsion.....	130 E		

References

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	ν_1	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		
<i>a''</i>	ν_{11}	OCO deform.....	714 C	714 M		
	ν_{12}	COC deform.....	297 E	297 M		
	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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments		
<i>a'</i>	ν_1	CD ₃ d-stretch.....	2291 D	cm^{-1} (Gas) 2291 M	cm^{-1}			
	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			}.....	FR (2 ν_{16}).
				1719 VS				
	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					
<i>a''</i>	ν_{12}	COC deform.....	295 E	295 M				
	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.

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		
a''	ν_{12}	CCO deform.....	581 B	581 M		
	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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Molecule: Acetic acid-d₁ CH₃COOD
 Symmetry C_s Symmetry number δ = 1

No. 175

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	<i>ν</i> ₁	CH ₃ d-stretch.....	3039 B	3039 VW		
	<i>ν</i> ₂	CH ₃ s-stretch.....	2952 B	2952 VW		
	<i>ν</i> ₃	OD stretch.....	2642 B	2642 M		
	<i>ν</i> ₄	C=O stretch.....	1775 B	1775 VS		
	<i>ν</i> ₅	CH ₃ d-deform.....	1440 C	1440 sh	SF (<i>ν</i> ₁₄).
	<i>ν</i> ₆	CH ₃ s-deform.....	1383 B	1383 S		
	<i>ν</i> ₇	C-O stretch.....	1270 B	1270 S		
	<i>ν</i> ₈	CH ₃ rock.....	990 D	990 sh		
	<i>ν</i> ₉	OD bend.....	955 B	955 S		
	<i>ν</i> ₁₀	CC stretch.....	840 B	840 W		
<i>a''</i>	<i>ν</i> ₁₁	OCO deform.....	609 B	609 M		
	<i>ν</i> ₁₂	CCO deform.....	543 B	543 M		
	<i>ν</i> ₁₃	CH ₃ d-stretch.....	2997 D	2997 VW		
	<i>ν</i> ₁₄	CH ₃ d-deform.....	1440 C	1440 sh	SF (<i>ν</i> ₅).
	<i>ν</i> ₁₅	CH ₃ rock.....	1052 B	1052 W		
	<i>ν</i> ₁₆	C=O ip-bend.....	603 B	603 M		
	<i>ν</i> ₁₇	C-O torsion.....	415 B	415 M		
	<i>ν</i> ₁₈	CH ₃ torsion.....	93 E	CF [3].

References

See No. 174.

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	
a_2	ν_7	COC deform.....	418 C	418 M	428 M, p	
	ν_8	CH_3 d-stretch.....	2952 C	ia	2952 S	
b_1	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	
b_2	ν_{17}	CO a-stretch.....	1102 B	1102 VS	1104 M, dp	
	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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- [6] Th. T. Shimanouchi and M. Oka, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	ν_1	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		
<i>a''</i>	ν_{12}	CO s-stretch.....	860 C	860 M		
	ν_{13}	COC deform.....	395 E		CF [2].
	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

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 [2] Th. T. Shimanouchi and M. Oka, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_2 s-stretch	3015 A	cm^{-1} (Gas)	cm^{-1} (Gas)	
	ν_2	CH_2 scis	1443 A		3015.0	
	ν_3	CC stretch	1073 A		1442.6	
b_1	ν_4	CH_2 twist	865 C	865	1072.6	
					865 (liquid)	
b_2	ν_5	CH_2 s-stretch	3007 A	3006.7	1960	
	ν_6	CC stretch	1957 C	1957	(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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Molecule: Methylacetylene CH_3CCH
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 179

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH stretch	3334 C	cm^{-1} (Gas) 3334	cm^{-1} (Liquid) 3305 M	FR ($\nu_2 + 2\nu_7$) [2].
	ν_2	CH_3 s-stretch	2918 E	(2941 M 2881	2941 VS, p	
	ν_3	$\text{C}\equiv\text{C}$ 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
 Symmetry C_{3v} Symmetry number $\delta = 3$

No. 180

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_3 s-stretch	2920 E	cm^{-1} (Gas) 2941.0 M 2881.0 M	cm^{-1} }	FR ($2\nu_7$) [1].
	ν_2	CD stretch	2617 B	2616.8 S		
	ν_3	$\text{C}\equiv\text{C}$ stretch	2060 C	2060.3 W		
	ν_4	CH_3 s-deform	1378 E	1378 W		
e	ν_5	C-C stretch	886 E			OV (ν_7). CF [1].
	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		

References

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

Molecule: Methyl-d₃-acetylene CD₃CCH
 Symmetry C_{3v} Symmetry number δ = 3

No. 181

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	CH stretch	3336 A	cm^{-1} (Gas) 3335.8 S { 2121.0 M 2077.0 M } 2142.0 M 1115 M 830 W 2234.9 M 1048.2 M 835.4 W 633 S 304.5 M	cm^{-1}	FR (ν ₂ + 2ν ₇) [2].
	ν ₂	CD ₃ s-stretch	2110 E			
e	ν ₃	C≡C stretch	2142 A			
	ν ₄	CD ₃ s-deform	1115 B			
	ν ₅	C-C stretch	830 B			
	ν ₆	CD ₃ d-stretch	2235 A			
	ν ₇	CD ₃ d-deform	1048 A			
	ν ₈	CD ₃ rock	835 A			
	ν ₉	CH bend	633 B			
	ν ₁₀	CCC bend	305 B			

References

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

Molecule: Methylacetylene-d₄ CD₃CCD
 Symmetry C_{3v} Symmetry number δ = 3

No. 182

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	CD stretch	2616 A	cm^{-1} (Gas) 2616.3 VS { 2121 M 2077 M } 2008.4 W 1110.1 M 810 E 2234.8 M 1048.2 M 834.4 W 492 VS 294 M	cm^{-1}	FR (ν ₂ + 2ν ₇) [2].
	ν ₂	CD ₃ s-stretch	2110 E			
e	ν ₃	C≡C stretch	2008 A			
	ν ₄	CD ₃ s-deform	1110 A			
	ν ₅	C-C stretch	810 E			
	ν ₆	CD ₃ d-stretch	2235 A			
	ν ₇	CD ₃ d-deform	1048 A			
	ν ₈	CD ₃ rock	834 A			
	ν ₉	CD bend	492 B			
	ν ₁₀	CCC bend	294 B			

References

See No. 181.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_2 s-stretch.....	2935 C	cm^{-1} (Liquid) 2935 VS	cm^{-1} (Liquid) 2929 (5)	SF (ν_9).
	ν_2	CN s-stretch.....	2275 C	2275 M	2263 (7)	
	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)	SF (ν_{12}).
	ν_8	CCN bend.....	367 C	ia, 371 M	367 (10)	
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)	
b_2	ν_{11}	CC a-stretch.....	982 C	982 S	975 (1)	SF (ν_8).
	ν_{12}	CCN bend.....	366 C	366 S	367 (10)	
	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		

References

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 [2] IR.Th. F. Halverson and R. J. Francel, J. Chem. Phys. 17, 694 (1949).
 [3] IR.R.Th. T. Fujiyama and T. Shimanouchi, Spectrochim. Acta 20, 829 (1964).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CD_2 s-stretch.....	2146 C	cm^{-1} (Liquid) 2146 S	cm^{-1} (D_2O soln.) 2146 (4)	SF (ν_9).
	ν_2	CN s-stretch.....	2272 C	2272 M	2273 (8)	
	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)	SF (ν_{12}).
	ν_8	CCN bend.....	356 C	ia	356 (4)	
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 ($\nu_{12} + \nu_{14}$).
b_2	ν_{11}	CC a-stretch.....	829 C	829 M	828 (1)	SF (ν_8).
	ν_{12}	CCN bend.....	356 C	356 S	356 (4)	
	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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH_2 a-stretch.....	3103 C	cm^{-1} (Gas) 3103 M	cm^{-1}	
	ν_2	$\text{CH}(\beta)$ stretch.....	3028 D	3028 M (solid)		
	ν_3	CH_2 s-stretch.....	3000 D	3000 M		
	ν_4	$\text{CH}(\alpha)$ 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	$\text{CH}(\alpha)$ ip-bend.....	1360 C	1360 M		
	ν_9	$\text{CH}(\beta)$ 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		
	a''	ν_{13}	CCC bend.....	327 C		
ν_{14}		$\text{CH}(\beta)$ op-bend.....	993 B	993 S		
ν_{15}		$\text{CH}(\alpha)$ op-bend.....	980 E		
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: $\text{C}^{\gamma}\text{H}_2\text{C}^{\beta}\text{HC}^{\alpha}\text{HO}$.

References

- [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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1'	ν_1	CH_2 s-stretch	3038 C	cm^{-1} (Gas) ia	cm^{-1} (Gas) 3038 S, p	} FR ($2\nu_{14}$).
	ν_2	CH_2 scis	1479 D	ia	{1504 W, p 1453 W, p	
a_1''	ν_3	Ring stretch	1188 C	ia	1188 S, p	
	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)	
e''	ν_{11}	Ring deform	866 C	866 VS	866 S, dp	
	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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 [2] IR.R. A. W. Baker and R. C. Lord, J. Chem. Phys. 23, 1636 (1955).
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 [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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁ '	ν ₁	CD ₂ s-stretch	2236 C	cm ⁻¹ (Gas) ia	cm ⁻¹ (Liquid) 2236 VS, p	CF [2]. CF [2], OC (ν ₅ + ν ₁₁). CF [2], OC (2ν ₁₃).
	ν ₂	CD ₂ scis	1274 D	ia	1274 S, p	
a ₁ ''	ν ₃	Ring stretch	956 C	ia	956 S, p	
	ν ₄	CD ₂ twist	800 D	ia, 800 VW	ia	
a ₂ '	ν ₅	CD ₂ wag	870 D	ia, 875 (solid)	ia	
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	
e''	ν ₁₁	Ring deform	717 C	717 VS	721 M, dp	
	ν ₁₂	CD ₂ a-stretch	2329 C	ia	2329 S, p	
	ν ₁₃	CD ₂ twist	940 E	ia	
	ν ₁₄	CD ₂ rock	528 C	ia	528 W, dp	

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[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).
 [3] IR. J. L. Duncan and D. C. McKean, J. Mol. Spectrosc. 27, 117 (1968).

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	
	a''	ν_{13}	CCN bend.....	226 C	226 M	226 M, p
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].

References

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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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
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	
a_2	ν_8	CCC deform	385 C	385 W	393 W, dp	
	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].
b_1	ν_{12}	Torsion	105 D	ia	CF [4]; MW: 102 [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	
b_2	ν_{19}	CO ip-bend	530 C	530 S	531 M, dp	
	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].

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- [6] R. T. Fujiyama and T. Shimanouchi, Bull. Chem. Soc. Japan, in press.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH_3 d-stretch.....	3018 C	cm^{-1} (Gas) 3017.5 S	cm^{-1} (Liquid) 3004.5 S	} FR ($2\nu_9$).
	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	
	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		
a''	ν_{15}	CCC deform.....	352 C	352 W	356.5 W	
	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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
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].
b ₁	ν ₁₂	Torsion.....	75 E	ia	CF [3].
	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		
b ₂	ν ₁₉	CO ip-bend.....	475 C	475 S	478 W, dp	
	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).

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	
b_1	ν_{14}	Torsion.....	*216 C	ia	MW [10,11].
	ν_{15}	CH_3 d-stretch.....	2968 C	2968		
	ν_{16}	CH_3 s-stretch.....	2887 C	2887		
	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.....	*268 C	MW [10,11].

* 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)).

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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			
a ₂	ν ₁₀	CH ₃ d-stretch.....	2956 E	ia		CF [5]. OC (ν ₁₀ + ν ₁₈) [4].
	ν ₁₁	CH ₃ d-deform.....	1453 E	ia		CF [5].
	ν ₁₂	CH ₃ rock.....	1083 E	ia		OC (ν ₁₂ + ν ₁₆) [4].
	ν ₁₃	CD ₂ twist.....	777 E	ia		CF [5].
	ν ₁₄	Torsion.....	*208 E	ia		OC (ν ₁₈ - ν 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		
	ν ₂₂	CH ₃ d-stretch.....	2963 C	2963		
b ₂	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.....	*217 E			CF [4].

* Assigning frequencies higher than these by 10-20 percent may be more reasonable in view of the results for CH₃CH₂CH₃.

References

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- [2] IR. H. L. McMurry and V. Thornton, J. Chem. Phys. 19, 1014 (1951).
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- [4] IR. J. N. Gayles, Jr. and W. T. King, Spectrochim. Acta 21, 543 (1965).
- [5] Th. T. Shimanouchi and T. Ueda, unpublished.
- [6] Th. J. N. Gayles, Jr., W. T. King, and J. H. Schachtschneider, Spectrochim. Acta 23A, 703 (1967).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	ν_1	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		
<i>a''</i>	ν_{16}	CCC deform.....	339 E	CF [2].
	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 CH₃CH₂CH₃.

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).

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		
a ₂	ν ₉	CCC deform	315 E			CF [4].
	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	*142 E	ia		OC (ν ₁₄ + ν ₂₁ , ν ₂₁ - 2ν 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).
b ₂	ν ₂₀	CD ₃ s-deform	920 E	920		
	ν ₂₁	CD ₃ rock	725 C	725		
	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	*173 E			OC (ν ₂₁ + ν ₂₇ - ν ₁₄) [3].

* Assigning frequencies higher than these by 10-20 percent may be more reasonable in view of the results for CH₃CH₂CH₃.

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).

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 ₆).
	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 (ν ₁₄ + ν ₂₅ , ν ₁₄ + ν ₂₄) [3].
	ν ₁₅	CD ₃ d-stretch.....	2224 C	2224		
b ₁	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		
b ₂	ν ₂₁	CD ₃ rock.....	688 C	688		
	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 (ν ₂₅ + ν ₂₇ - ν ₂₁) [3.]

^a Assigning frequencies higher than 10-20 percent may be more reasonable in view of the results for CH₃CH₂CH₃.

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	$\text{CH}_3(\text{O})$ d-stretch.....	3035 D	cm^{-1} (Gas) 3035 M	cm^{-1} (Liquid) 3028 (3b)	SF (ν_2 of $\text{CH}_3\text{COOCD}_3$).
	ν_2	$\text{CH}_3(\text{C})$ d-stretch.....	3031 E			
	ν_3	$\text{CH}_3(\text{O})$ s-stretch.....	2966 D	2966 S	2954 (3) p	SF (ν_4 of $\text{CH}_3\text{COOCD}_3$).
	ν_4	$\text{CH}_3(\text{C})$ s-stretch.....	2964 E		2942 (7b) p	
	ν_5	C=O stretch.....	1771 C	1771 VS	1738 (3b) p	OV (ν_{20}).
	ν_6	$\text{CH}_3(\text{O})$ d-deform.....	1460 E	1460 W, sh (CCl_4 soln.)		
	ν_7	$\text{CH}_3(\text{O})$ s-deform.....	1440 D	1440 M		SF (ν_8 of $\text{CH}_3\text{COOCD}_3$).
	ν_8	$\text{CH}_3(\text{C})$ d-deform.....	1430 E			
	ν_9	$\text{CH}_3(\text{C})$ s-deform.....	1375 D	1375 S	1372 (0.5) p	OV (ν_6).
	ν_{10}	C-O stretch.....	1248 C	1248 VS	1254 (0)	
	ν_{11}	$\text{CH}_3(\text{O})$ rock.....	1159 E	1159 VW (liquid)		
ν_{12}	O- CH_3 stretch.....	1060 C	1060 S	1044 (2b)		
ν_{13}	$\text{CH}_3(\text{C})$ rock.....	980 C	980 W	900 (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}	$\text{CH}_3(\text{O})$ d-stretch.....	3005 D	3005 M	3002 (3b)	
	ν_{19}	$\text{CH}_3(\text{C})$ d-stretch.....	2994 D	2994 W		
	ν_{20}	$\text{CH}_3(\text{O})$ d-deform.....	1460 E	1460 W, sh (CCl_4 soln.)	1449 (4b) dp	
	ν_{21}	$\text{CH}_3(\text{C})$ d-deform.....	1430 E	1430 W		
	ν_{22}	$\text{CH}_3(\text{O})$ rock.....	1187 D	1187 W	1187 (0.5b)	
	ν_{23}	$\text{CH}_3(\text{C})$ 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).
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- [3] IR.R. J. K. Wilmshurst, J. Mol. Spectrosc. 1, 201 (1957).
- [4] IR.Th. S. Ichikawa, Y. Udagawa, and T. Shimanouchi, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	ν_1	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		
	<i>a''</i>	ν_{17}	COC deform.....	298 D	298 M	
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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
<i>a'</i>	<i>ν</i> ₁	CD ₃ d-stretch.....	2288 D	2288 M		
	<i>ν</i> ₂	CH ₃ d-stretch.....	3031 D	3031 W		
	<i>ν</i> ₃	CD ₃ s-stretch.....	2104 D	2104 M		
	<i>ν</i> ₄	CH ₃ s-stretch.....	2964 D	2964 W		
	<i>ν</i> ₅	C=O stretch.....	1769 C	1769 VS		
	<i>ν</i> ₆	CD ₃ d-deform.....	1050 E	1050 W	OV (<i>ν</i> ₂₀).
	<i>ν</i> ₇	CD ₃ s-deform.....	1106 C	1106 S		
	<i>ν</i> ₈	CH ₃ d-deform.....	1430 E	1430 W	OV (<i>ν</i> ₂₁).
	<i>ν</i> ₉	CH ₃ s-deform.....	1375 D	1375 S	(CCl ₄ soln.)	
	<i>ν</i> ₁₀	C-O stretch.....	1268 C	1268 VS		
<i>a''</i>	<i>ν</i> ₁₁	CD ₃ rock.....	985 D	985 W		
	<i>ν</i> ₁₂	O-CD ₃ stretch.....	1043 D	1043 M		
	<i>ν</i> ₁₃	CH ₃ rock.....	947 C	947 M		
	<i>ν</i> ₁₄	CC stretch.....	781 C	781 M		
	<i>ν</i> ₁₅	C=O ip-bend.....	619 C	619 M		
	<i>ν</i> ₁₆	CCO deform.....	420 C	420 M		
	<i>ν</i> ₁₇	COC deform.....	270 D	270 M		
	<i>ν</i> ₁₈	CD ₃ d-stretch.....	2263 D	2263 M		
	<i>ν</i> ₁₉	CH ₃ d-stretch.....	2994 D	2994 W		
	<i>ν</i> ₂₀	CD ₃ d-deform.....	1050 D	1050 W	OV (<i>ν</i> ₆).
	<i>ν</i> ₂₁	CH ₃ d-deform.....	1430 E	1430 W	OV (<i>ν</i> ₈).
	<i>ν</i> ₂₂	CD ₃ rock.....	908 E	908 VW	(CCl ₄ soln.)	
	<i>ν</i> ₂₃	CD ₃ rock.....	1015 E	1015 W, sh		
	<i>ν</i> ₂₄	C=O op-bend.....	600 D	600 W, sh		
	<i>ν</i> ₂₅	C-O torsion.....	165 D	165 M		
	<i>ν</i> ₂₆	C-C torsion.....	136 E			CF [2].
	<i>ν</i> ₂₇	O-CD ₃ torsion.....	81 E			CF [2].

References

See No. 198.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	CD ₃ (O) d-stretch	2285 D	<i>cm</i> ⁻¹ (Gas) 2285 M	<i>cm</i> ⁻¹	SF (ν_2 of CD ₃ COOCH ₃).
	ν_2	CD ₃ (C) d-stretch	2275 E			
	ν_3	CD ₃ (O) s-stretch	2099 D	2099 M		SF (ν_4 of CD ₃ COOCH ₃).
	ν_4	CD ₃ (C) s-stretch	2087 E			
	ν_5	C=O stretch	1767 C	1767 VS		OV (ν_{20}).
	ν_6	CD ₃ (O) d-deform	1059 E			
	ν_7	CD ₃ (O) s-deform	1106 C	1106 S		
	ν_8	CD ₃ (C) d-deform	1003 E			
	ν_9	CD ₃ (C) s-deform	1086 E	1003 W		SF (ν_9 of CD ₃ COOCH ₃).
	ν_{10}	C-O stretch	1282 C			
ν_{11}	CD ₃ (O) rock	975 D	1282 VS			
ν_{12}	O-CH ₃ stretch	1045 E				
ν_{13}	CD ₃ (C) rock	828 E	975 M			
ν_{14}	CC stretch	747 C				
ν_{15}	C=O ip-bend	585 C	828 W			
ν_{16}	CCO deform	334 C				
<i>a''</i>	ν_{17}	COC deform	266 D	334 M		
	ν_{18}	CD ₃ (O) d-stretch	2264 D			
	ν_{19}	CD ₃ (C) d-stretch	2253 E	266 M		SF (ν_{19} of CD ₃ COOCH ₃).
	ν_{20}	CD ₃ (O) d-deform	1059 D			
	ν_{21}	CD ₃ (C) d-deform	1038 E	1059 W		OV (ν_6).
	ν_{22}	CD ₃ (O) rock	908 E			
	ν_{23}	CD ₃ (C) rock	925 D	908 W		SF (ν_{22} of CH ₃ COOCD ₃).
	ν_{24}	C=O op-bend	522 D			
	ν_{25}	C-O torsion	160 D	522 M		
	ν_{26}	C-C torsion	100 E			
	ν_{27}	O-CH ₃ torsion	80 E	160 W		CF [2]. CF [2].

References

See No. 198.

Molecule: Butadiyne HCCCCH
 Symmetry $D_{\infty h}$ Symmetry number $\sigma = 2$

No. 201

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a_1	ν_1	CH stretch.....	3154 D	cm^{-1} (Gas)	cm^{-1} (Liquid)	OC ($\nu_9 + \nu_{16}$, $\nu_9 + \nu_{17}$, $\nu_9 + \nu_{19}$, $\nu_9 + \nu_2$).	
	ν_2	CH stretch.....	3140 D	3140 sh	3154 VS, p		
	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		
	a_2	ν_8	ip-Ring VII.....	871 C	871 S		
		ν_9	CH op-bend.....	863 C	ia		
b_1	ν_{10}	CH op-bend.....	728 D	ia	728 W, dp		
	ν_{11}	op-Ring I.....	613 D	ia	613 VW, dp		
	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		
b_2	ν_{17}	ip-Ring V.....	1040 D	1040 sh (liquid)	1034 M, dp		
	ν_{18}	ip-Ring VI.....	873 D		873 W, dp		
	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		

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- [2] IR. H. W. Thompson and R. B. Temple, Trans. Faraday Soc. 41, 27 (1945).
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- [5] IR.R. M. Rico, M. Barrachina, and J. M. Orza, J. Mol. Spectrosc. 24, 133 (1967).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	<i>v</i> ₁	CH stretch	3126 C	3126 M	3107 (10) p	
	<i>v</i> ₂	CH stretch	3098 C	3098 S	3084 (5sh)	
	<i>v</i> ₃	ip-Ring II	1409 C	1409 S	1407 (7) p	
	<i>v</i> ₄	ip-Ring III	1360 C	1360 VW	1358 (5) p	
	<i>v</i> ₅	CH ip-bend	1083 C	1083 S	1081 (5) p	
	<i>v</i> ₆	CH ip-bend	1036 C	1036 S	1035	
	<i>v</i> ₇	ip-Ring IV	839 C	839 VS	832 (5) p	
	<i>v</i> ₈	ip-Ring VII	608 C	608 W	606 (2) p	
<i>a</i> ₂	<i>v</i> ₉	CH op-bend	903 D	ia, 900 VW (solid)	903 (0) dp	
	<i>v</i> ₁₀	CH op-bend	688 D	ia	688 (0) dp	
	<i>v</i> ₁₁	op-Ring I	567 D	ia, 565 VW (liquid)	567 (0) dp	
<i>b</i> ₁	<i>v</i> ₁₂	CH stretch	^a 3125 E			
	<i>v</i> ₁₃	CH stretch	3086 C	3086 S	3076 (sh)	
	<i>v</i> ₁₄	ip-Ring I	1504 D	1504 VW (liquid)	1502 (0) dp	
	<i>v</i> ₁₅	CH ip-bend	1256 C	1256 S	1257 (0)	
	<i>v</i> ₁₆	CH ip-bend	^a 1085 E			OV (<i>v</i> ₅).
<i>b</i> ₂	<i>v</i> ₁₇	ip-Ring V	872 C	872 M	869 (4) dp	
	<i>v</i> ₁₈	ip-Ring VI	751 D	763 VW	751 (1) dp	
	<i>v</i> ₁₉	CH op-bend	867 E			OC (<i>v</i> ₉ + <i>v</i> ₁₉ , 2 <i>v</i> ₁₉).
	<i>v</i> ₂₀	CH op-bend	712 C	712 VS		
	<i>v</i> ₂₁	op-Ring II	452 C	452 W	453 (0) dp	

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

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[1] IR. H. W. Thompson and R. B. Temple, *Trans. Faraday Soc.* **41**, 27 (1945).
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 [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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	CD stretch.....	2343 C	cm ⁻¹ (Gas) 2343 M	cm ⁻¹ (Liquid) 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	
b ₁	ν ₁₁	op-Ring I.....	488 D	ia	488	
	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	
b ₂	ν ₁₈	ip-Ring VI.....	712 C	712 W		
	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].

References

- [1] R. K. W. Kohlrausch and H. Schreiner, *Acta Phys. Austriaca* **1**, 373 (1948).
- [2] IR.R. M. Rico, J. M. Orza, and J. Morcillo, *Spectrochim. Acta* **21**, 689 (1965).
- [3] IR.R. V. T. Aleksanyan, Ya. M. Kimelfeld, N. N. Magdesieva, and Yu. K. Yurev, *Opt. Spectrosc.* **22**, 116 (1967).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a_g</i>	<i>ν</i> ₁	CH ₂ a-stretch.....	3087 D	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Solid) 3087 M	
	<i>ν</i> ₂	CH stretch.....	3003 D	ia	3003 M	
	<i>ν</i> ₃	CH ₂ s-stretch.....	2992 D	ia	2992 S	
	<i>ν</i> ₄	C=C stretch.....	1630 D	ia	1630 VS	
	<i>ν</i> ₅	CH ₂ scis.....	1438 D	ia	1438 S	
	<i>ν</i> ₆	CH bend.....	1280 D	ia	1280 S	
	<i>ν</i> ₇	C-C stretch.....	1196 D	ia	1196 S	
	<i>ν</i> ₈	CH ₂ rock.....	894 D	ia	894 W	
	<i>ν</i> ₉	CCC deform.....	512 D	ia	512 S	
<i>a_u</i>	<i>ν</i> ₁₀	CH bend.....	1013 B	1013.4 VS	ia	
	<i>ν</i> ₁₁	CH ₂ wag.....	908 B	907.8 VS	ia	
	<i>ν</i> ₁₂	CH ₂ twist.....	522 B	522.2 M	ia	
<i>b_g</i>	<i>ν</i> ₁₃	C-C torsion.....	162 B	162.3 VW	ia	
	<i>ν</i> ₁₄	CH bend.....	976 D	ia	976 W	
	<i>ν</i> ₁₅	CH ₂ wag.....	912 D	ia	912 S	
<i>b_u</i>	<i>ν</i> ₁₆	CH ₂ twist.....	770 D	ia	770 VW	
	<i>ν</i> ₁₇	CH ₂ a-stretch.....	3101 B	3100.6 S	ia	
	<i>ν</i> ₁₈	CH stretch.....	3055 B	3054.9 S	ia	
	<i>ν</i> ₁₉	CH ₂ s-stretch.....	2984 B	2984.3 S	ia	
	<i>ν</i> ₂₀	C=C stretch.....	1596 B	1596.0 S	ia	
	<i>ν</i> ₂₁	CH ₂ scis.....	1381 B	1380.7 W	ia	
	<i>ν</i> ₂₂	CH bend.....	1294 B	1294.3 W	ia	
	<i>ν</i> ₂₃	CH ₂ rock.....	990 B	989.7 M	ia	
	<i>ν</i> ₂₄	CCC deform.....	301 B	300.6 VW	ia	

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	CH ₂ a-stretch.....	3100 C	3100.4 S	3090 M	CF [1].
	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	
	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)		
<i>a''</i>	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		
	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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a'</i>	<i>ν</i> ₁	CH ₂ a-stretch.....	3099 C	3099.1 S		
	<i>ν</i> ₂	CH stretch.....	3016 C	3016.4 S		
	<i>ν</i> ₃	CH ₂ s-stretch.....	2995 C	2995.4 S		
	<i>ν</i> ₄	CD ₂ a-stretch.....	2342 C	2341.9 S		
	<i>ν</i> ₅	CD stretch.....	2268 C	2267.9 S		
	<i>ν</i> ₆	CD ₂ s-stretch.....	2217 C	2217.1 S		
	<i>ν</i> ₇	C=C stretch.....	1630 C	1630.4 M		
	<i>ν</i> ₈	C=C stretch.....	1549 B	1548.5 S		
	<i>ν</i> ₉	CH ₂ scis.....	1425 C	1425 M		
	<i>ν</i> ₁₀	CH ip-bend.....	1298 C	1298 W		
	<i>ν</i> ₁₁	C-C stretch.....	1185 C	1185 W		
	<i>ν</i> ₁₂	CD ₂ scis.....	1080 C	1080 W		
	<i>ν</i> ₁₃	CD ip-bend.....	992 D	991.8 W (solid)		
<i>ν</i> ₁₄	CH ₂ rock.....	880 D	879.9 M (solid)			
<i>ν</i> ₁₅	CD ₂ rock.....	757 E		CF [1].	
<i>ν</i> ₁₆	CCC deform.....	476 E		CF [1].	
<i>a''</i>	<i>ν</i> ₁₇	CCC deform.....	280 D	280 W		
	<i>ν</i> ₁₈	CH op-bend.....	991 B	990.6 VS		
	<i>ν</i> ₁₉	CH ₂ wag.....	909 B	909.2 VS		
	<i>ν</i> ₂₀	CD op-bend.....	791 B	791.3 W		
	<i>ν</i> ₂₁	CD ₂ wag.....	715 E	{ 734.0 S 710.1 VS }		FR (<i>ν</i> ₁₇ + <i>ν</i> ₂₃).
	<i>ν</i> ₂₂	CH ₂ twist.....	674 B	673.8 S		
	<i>ν</i> ₂₃	CD ₂ twist.....	439 C	439.0 M		
	<i>ν</i> ₂₄	C-C torsion.....	153 E		CF [1].

Reference

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a_g</i>	<i>ν</i> ₁	CH stretch	3010 D	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Solid) 3010 M	CF [1].
	<i>ν</i> ₂	CD ₂ a-stretch	2315 D	ia	2315 S	
	<i>ν</i> ₃	CD ₂ s-stretch	2212 D	ia	2212 S	
	<i>ν</i> ₄	C = C stretch	1610 D	ia	1610 VS	
	<i>ν</i> ₅	CH ip-bend	1296 D	ia	1296 S	
	<i>ν</i> ₆	C-C stretch	1170 D	ia	1170 S	
	<i>ν</i> ₇	CD ₂ scis	1040 D	ia	1040 S	
	<i>ν</i> ₈	CD ₂ rock	740 D	ia	740 W	
	<i>ν</i> ₉	CCC deform	457 D	ia	457 S	
	<i>a_u</i>	<i>ν</i> ₁₀	CH op-bend	955 B	955.1 S	
<i>ν</i> ₁₁		CD ₂ wag	728 B	728.0 VS	ia	
<i>ν</i> ₁₂		CD ₂ twist	397 C	397 W	ia	
<i>b_g</i>	<i>ν</i> ₁₃	C-C torsion	149 E	ia	
	<i>ν</i> ₁₄	CH op-bend	948 D	ia	948 M	
	<i>ν</i> ₁₅	CD ₂ wag	728 D	ia	728 S	
<i>b_u</i>	<i>ν</i> ₁₆	CD ₂ twist	610 D	ia	610 VW	
	<i>ν</i> ₁₇	CH stretch	3041 C	3040.8 S	ia	
	<i>ν</i> ₁₈	CD ₂ a-stretch	2350 D	2350 S	ia	
	<i>ν</i> ₁₉	CD ₂ s-stretch	2228 C	2228 S	ia	
	<i>ν</i> ₂₀	C = C stretch	1535 B	1535.0 S	ia	
	<i>ν</i> ₂₁	CH ip-bend	1335 C	1335.2 M	ia	
	<i>ν</i> ₂₂	CD ₂ scis	1031 C	1031.3 S	ia	
	<i>ν</i> ₂₃	CD ₂ rock	817 C	816.5 M	ia	
	<i>ν</i> ₂₄	CCC deform	258 C	258 W	ia	

Reference

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a_g</i>	<i>ν</i> ₁	CD ₂ a-stretch.....	2320 D	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Solid) 2320 M	
	<i>ν</i> ₂	CD stretch.....	2250 D	ia	2250 M	
	<i>ν</i> ₃	CD ₂ s-stretch.....	2210 D	ia	2210 M	
	<i>ν</i> ₄	C=C stretch.....	1580 D	ia	1580 VS	
	<i>ν</i> ₅	C-C stretch.....	1196 D	ia	1196 M	
	<i>ν</i> ₆	CD ₂ scis.....	1045 D	ia	1045 W	
	<i>ν</i> ₇	CD ip-bend.....	918 D	ia	918 S	
	<i>ν</i> ₈	CD ₂ rock.....	746 D	ia	746 M	
	<i>ν</i> ₉	CCC deform.....	439 D	ia	439 S	
<i>a_u</i>	<i>ν</i> ₁₀	CD op-bend.....	741 B	741.4 W	ia	
	<i>ν</i> ₁₁	CD ₂ wag.....	718 B	718.4 S	ia	
	<i>ν</i> ₁₂	CD ₂ twist.....	381 C	381.1 W	ia	
<i>b_g</i>	<i>ν</i> ₁₃	C-C torsion.....	140 C	140 VW	ia	
	<i>ν</i> ₁₄	CD op-bend.....	799 D	ia	799 S	
	<i>ν</i> ₁₅	CD ₂ wag.....	705 D	ia	705 S	
<i>b_u</i>	<i>ν</i> ₁₆	CD ₂ twist.....	603 D	ia	603 VW	
	<i>ν</i> ₁₇	CD ₂ a-stretch.....	2320 D	2320.3 M	ia	
	<i>ν</i> ₁₈	CD stretch.....	2266 C	2265.9 M	ia	
	<i>ν</i> ₁₉	CD ₂ s-stretch.....	2218 C	2218.0 M	ia	
	<i>ν</i> ₂₀	C=C stretch.....	1520 B	1519.6 S	ia	
	<i>ν</i> ₂₁	CD ₂ scis.....	1048 C	1048.0 W	ia	
	<i>ν</i> ₂₂	CD ip-bend.....	1005 C	1005.4 M	ia	
	<i>ν</i> ₂₃	CD ₂ rock.....	769 D	768.9 W	ia	
	<i>ν</i> ₂₄	CCC deform.....	250 C	(solid) 250 W	ia	

Reference

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'_1	ν_1	CH_3 s-stretch	2916 C	cm^{-1} (Gas) ia	cm^{-1} (Liquid) 2916 S p	} FR ($2\nu_8$).
	ν_2	$\text{C}\equiv\text{C}$ stretch	2240 E	ia	{ 2310 S p	
	ν_3	CH_3 s-deform	1380 C	ia	{ 2233 S p	
	ν_4	C-C stretch	725 E	ia	{ 1380 S	} FR ($2\nu_{16}$).
a''_1	ν_5	CH_3 torsion ^a		ia	{ 774 M p	
a''_2	ν_6	CH_3 s-stretch	2938 B	2938 S	ia	
	ν_7	CH_3 s-deform	1382 B	1382 M	ia	
e'	ν_8	C-C stretch	1152 B	1152 W	ia	
	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		
e''	ν_{12}	CCC deform	213 C	213 VW	
	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].

References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν_1	CH ₂ s-stretch	2895 D	cm ⁻¹ (Gas) ia	cm ⁻¹ (Liquid) 2916 p 2866 p	} FR (2 ν_2 , 2 ν_{13}).
	ν_2	CH ₂ scis	1443 C	ia	1443 p	
	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	
a ₂	ν_6	Ring puckering	197 C	ia	197	CF [3].
	ν_7	CH ₂ wag	1260 E	ia	ia	CF [3].
b ₁	ν_8	CH ₂ twist	1257 E	ia	ia	CF [3].
	ν_9	CH ₂ wag	1219 C	ia	1219 dp	
	ν_{10}	Ring deform	926 C	ia	926 dp	
b ₂	ν_{11}	CH ₂ twist	1222 E	ia	CF [3].
	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).
e	ν_{15}	CH ₂ a-stretch	2987 C	2987 S		
	ν_{16}	CH ₂ rock	627 C	627 S		
	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	
	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a ₁	ν ₁	CD ₂ s-stretch	2124 E	cm ⁻¹ (Gas) ia	cm ⁻¹ (Liquid)	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	
b ₂	ν ₁₁	CD ₂ twist	864 E	ia	CF [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	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	CH ₂ s-stretch.....	2989 D	<i>cm</i> ⁻¹ (Gas) 2991 M (solid)	<i>cm</i> ⁻¹ (Liquid) 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	
<i>a</i> 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].
<i>b</i> ₁	ν_{15}	CH ₃ torsion.....	193 E	ia	CF [3].
	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)	
<i>b</i> 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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹	
<i>a</i> ₁	<i>ν</i> ₁	CH ₂ s-stretch.....	2996 C	2996 M		
	<i>ν</i> ₂	CD ₃ d-stretch.....	2166 D	2166 W (solid)		
	<i>ν</i> ₃	CD ₃ s-stretch.....	2111 C	2111 W		
	<i>ν</i> ₄	C=C stretch.....	1650 C	1650 S		
	<i>ν</i> ₅	CH ₂ scis.....	1410 C	1410 W		
	<i>ν</i> ₆	CD ₃ s-deform.....	1092 D	1092 W (solid)		
	<i>ν</i> ₇	CD ₃ d-deform.....	1056 D	1056 M (solid)		
	<i>ν</i> ₈	CD ₃ rock.....	850 E		CF [1].
	<i>ν</i> ₉	C-C stretch.....	718 D	718 W (solid)		
<i>a</i> ₂	<i>ν</i> ₁₀	C=CC ₂ ip-deform.....	319 C	319 W		
	<i>ν</i> ₁₁	CD ₃ d-stretch.....	2208 E	ia		CF [1].
	<i>ν</i> ₁₂	CD ₃ d-deform.....	1054 E	ia		CF [1].
	<i>ν</i> ₁₃	CD ₃ rock.....	731 E	ia		CF [1].
	<i>ν</i> ₁₄	CH ₂ twist.....	664 E	ia		CF [1].
<i>b</i> ₁	<i>ν</i> ₁₅	CD ₃ torsion.....	138 E	ia		CF [1].
	<i>ν</i> ₁₆	CH ₂ a-stretch.....	3085 C	3085 S		
	<i>ν</i> ₁₇	CD ₃ d-stretch.....	2236 C	2236 S		
	<i>ν</i> ₁₈	CD ₃ s-stretch.....	2072 C	2072 M		
	<i>ν</i> ₁₉	C-C stretch.....	1294 C	1294 M		
	<i>ν</i> ₂₀	CD ₃ d-deform.....	1074 C	1074 W		
	<i>ν</i> ₂₁	CD ₃ s-deform.....	1052 D	1052 M (solid)		
	<i>ν</i> ₂₂	CH ₂ rock.....	880 E		CF [1].
	<i>ν</i> ₂₃	CD ₃ rock.....	745 C	745 W		
	<i>ν</i> ₂₄	C=CC ₂ ip-deform.....	400 C	400 M		
<i>b</i> ₂	<i>ν</i> ₂₅	CD ₃ d-stretch.....	2204 C	2204 S		
	<i>ν</i> ₂₆	CD ₃ d-deform.....	1055 C	1055 S		
	<i>ν</i> ₂₇	CD ₃ rock.....	923 C	923 M		
	<i>ν</i> ₂₈	CH ₂ wag.....	884 C	884 VS		
	<i>ν</i> ₂₉	C=CC ₂ op-deform.....	369 C	369 S		
	<i>ν</i> ₃₀	CD ₃ torsion.....	143 E		CF [1].

Reference

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	$\text{CH}_3(1)$ d-stretch	2983 D	cm^{-1} (Solid) 2983 S	cm^{-1} (Liquid) 2983 M	OV ($\nu_2, \nu_{21}, \nu_{22}$).
	ν_2	$\text{CH}_3(4)$ d-stretch	2983 D	2983 S (liquid)	2983 M	OV ($\nu_1, \nu_{21}, \nu_{22}$).
	ν_3	$\text{CH}_3(1)$ s-stretch	2910 D	2910 S (liquid)	2924 S, p	OV (ν_4).
	ν_4	$\text{CH}_3(4)$ 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	$\text{CH}_3(4)$ d-deform	1460 D	1460 M	1450 M	OV (ν_{24}).
	ν_8	CH_2 scis	1422 C	1422 S	1419 M	
	ν_9	$\text{CH}_3(1)$ d-deform	1413 D	1413 S		OV (ν_{25}).
	ν_{10}	$\text{CH}_3(4)$ s-deform	1373 C	1373 S		
	ν_{11}	$\text{CH}_3(1)$ 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}	$\text{CH}_3(4)$ rock	1089 C	1089 M	1087 M, p	
	ν_{15}	CC(34) stretch	997 C	997 S	999 W	
	ν_{16}	$\text{CH}_3(1)$ rock	939 C	939 S	951 W	
	ν_{17}	CC(23) stretch	760 D	760 S (liquid)	760 M, p	
a''	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	
	ν_{21}	$\text{CH}_3(1)$ d-stretch	2983 D	2983 S (liquid)	2983	OV (ν_1, ν_2, ν_{22}).
	ν_{22}	$\text{CH}_3(4)$ 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}	$\text{CH}_3(4)$ d-deform	1460 D	1460 M	1450 M	OV (ν_7).
	ν_{25}	$\text{CH}_3(1)$ 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}	$\text{CH}_3(4)$ rock	1108 C	1108 W		
	ν_{28}	$\text{CH}_3(1)$ 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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
				<i>cm</i> ⁻¹ (Matrix isolation)	<i>cm</i> ⁻¹ (Solid)		
<i>a_g</i>	<i>v</i> ₁	CH ₃ d-stretch.....	2965 C	ia	2965 (9)	SF (<i>v</i> ₂₀).	
	<i>v</i> ₂	CH ₃ s-stretch.....	2872 C	ia	2872 (8)		
	<i>v</i> ₃	CH ₂ s-stretch.....	2853 D	ia	2853 (8)	SF (<i>v</i> ₂₂).	
	<i>v</i> ₄	CH ₃ d-deform.....	1460 C	ia	1460 (2)		
	<i>v</i> ₅	CH ₂ scis.....	1442 D	ia	1442 (3)		
	<i>v</i> ₆	CH ₃ s-deform.....	1382 C	ia	CF [9].	
	<i>v</i> ₇	CH ₂ wag.....	1361 D	ia		
	<i>v</i> ₈	CH ₃ rock.....	1151 C	ia	1151 (4)	CF [9].	
	<i>v</i> ₉	CC stretch.....	1059 C	ia	1059 (5)		
	<i>v</i> ₁₀	CC stretch.....	837 C	ia	837 (6)	SF (<i>v</i> ₂₇).	
	<i>v</i> ₁₁	CCC deform.....	425 C	ia	425 (4)		
<i>a_u</i>	<i>v</i> ₁₂	CH ₃ d-stretch.....	2968 C	2968 S	ia	SF (<i>v</i> ₂₇).	
	<i>v</i> ₁₃	CH ₂ a-stretch.....	2930 C	2930 S	ia		
	<i>v</i> ₁₄	CH ₃ d-deform.....	1461 C	1461 S	ia	SF (<i>v</i> ₃₀), OV (<i>v</i> ₃₀ , <i>v</i> ₃₁)	
	<i>v</i> ₁₅	CH ₂ twist.....	1257 C	1257 W (solid)	ia		
	<i>v</i> ₁₆	CH ₃ rock.....	948 B	948 M	ia	CF [9].	
	<i>v</i> ₁₇	CH ₂ rock.....	731 B	731 S	ia		
	<i>v</i> ₁₈	CH ₃ -CH ₂ torsion.....	194 E	ia	CF [9].	
	<i>v</i> ₁₉	CH ₂ -CH ₂ torsion.....	102 E	ia		
	<i>b_g</i>	<i>v</i> ₂₀	CH ₃ d-stretch.....	2965 C	ia	2965 (9)	SF (<i>v</i> ₁).
		<i>v</i> ₂₁	CH ₂ a-stretch.....	2912 C	ia	2912 (4)	
		<i>v</i> ₂₂	CH ₃ d-deform.....	1460 C	ia	1460 (2)	SF (<i>v</i> ₄).
		<i>v</i> ₂₃	CH ₂ twist.....	1300 C	ia	1300 (4)	
		<i>v</i> ₂₄	CH ₃ rock.....	1180 D	ia	CF [9].
		<i>v</i> ₂₅	CH ₂ rock.....	803 D	ia	CF [9].
		<i>v</i> ₂₆	CH ₃ -CH ₂ torsion.....	225 E	ia	CF [9].
<i>b_u</i>	<i>v</i> ₂₇	CH ₃ d-stretch.....	2968 C	2968 S	ia	SF (<i>v</i> ₁₂).	
	<i>v</i> ₂₈	CH ₃ s-stretch.....	2870 C	2870 S	ia	SF (<i>v</i> ₃).	
	<i>v</i> ₂₉	CH ₂ s-stretch.....	2853 E	ia		
	<i>v</i> ₃₀	CH ₃ d-deform.....	1461 C	1461 S	ia	SF (<i>v</i> ₁₄),	
	<i>v</i> ₃₁	CH ₂ scis.....	1461 C	1461 S	ia	OV (<i>v</i> ₁₄ , <i>v</i> ₃₁).	
	<i>v</i> ₃₂	CH ₃ s-deform.....	1379 B	1379 M	ia	OV (<i>v</i> ₁₄ , <i>v</i> ₃₀).	
	<i>v</i> ₃₃	CH ₂ wag.....	1290 B	1290 W	ia	CF [9].	
	<i>v</i> ₃₄	CC stretch.....	1009 C	1009 W (solid)	ia		
	<i>v</i> ₃₅	CH ₃ rock.....	964 B	964 M	ia	CF [9].	
	<i>v</i> ₃₆	CCC deform.....	271 E	ia		

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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 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (gauche form)
 Symmetry C_2 Symmetry number $\delta = 2$

No. 217

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
<i>a</i>	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].
<i>b</i>	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).
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments	
a_{1g}	ν_1	CH stretch.....	3062 C	cm^{-1} (Gas) ia	cm^{-1} (Liquid) 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		
h_{2g}	ν_7	CH bend.....	995 E	ia	ia		OC ($\nu_{10} + \nu_7, \nu_{20} + \nu_7$).
	ν_8	Ring deform.....	703 E	ia	ia		
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		FR ($\nu_{13} + \nu_{16}$).
e_{1u}	ν_{12}	CH stretch.....	3063 E	{ 3080 S 3030 S (liquid)	ia		
	ν_{13}	Ring stretch + deform.....	1486 B	1486 S	ia		
e_{2g}	ν_{14}	CH bend.....	1038 B	1038 S	ia		} FR ($\nu_2 + \nu_{18}$).
	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		
e_{2u}	ν_{17}	CH bend.....	1178 C	ia	1178.0 S, dp		
	ν_{18}	Ring deform.....	606 C	ia	605.6 S, dp		
	ν_{19}	CH bend.....	975 C	975 W (liquid)	ia		
	ν_{20}	Ring deform.....	410 C	{ 417.7 403.0 (solid)	ia		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> _{1g}	<i>ν</i> ₁	CD stretch.....	2293 C	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Liquid) 2292.6 VS, p 943.2 VS, p	OC (<i>ν</i> ₃ + <i>ν</i> ₁₄ , <i>ν</i> ₃ + <i>ν</i> ₁₆).
	<i>ν</i> ₂	Ring stretch.....	943 C	ia		
<i>a</i> _{2g}	<i>ν</i> ₃	CD bend.....	1037 E	ia	ia	
<i>a</i> _{2u}	<i>ν</i> ₄	CD bend.....	497 C	496.5 S (liquid)	ia	
<i>b</i> _{1u}	<i>ν</i> ₅	CD stretch.....	2292 E	2292 VW (solid)	ia	
	<i>ν</i> ₆	Ring deform.....	969 C	{ 970.48 969.77 966.76 (solid)	ia	
<i>b</i> _{2g}	<i>ν</i> ₇	CD bend.....	827 E	ia	ia	OC (<i>ν</i> ₇ + <i>ν</i> ₁₉). OC (<i>ν</i> ₈ + <i>ν</i> ₁₀).
	<i>ν</i> ₈	Ring deform.....	601 E	ia	ia	
<i>b</i> _{2u}	<i>ν</i> ₉	Ring stretch.....	1286 C	{ 1287.51 1286.41 1285.14 (solid)	ia	
	<i>ν</i> ₁₀	CD bend.....	824 C	{ 825.2 822.57 (solid)	ia	
<i>e</i> _{1g}	<i>ν</i> ₁₁	CD bend.....	662 C	ia	661.7 M, dp	
<i>e</i> _{1u}	<i>ν</i> ₁₂	CD stretch.....	2287 C	2287 S		ia
	<i>ν</i> ₁₃	Ring stretch + deform.....	1335 B	1335 M		ia
<i>e</i> _{2g}	<i>ν</i> ₁₄	CD bend.....	814 B	814 S	ia	
	<i>ν</i> ₁₅	CD stretch.....	2265 C	ia	2264.9 S, dp	
	<i>ν</i> ₁₆	Ring stretch.....	1552 C	ia	1551.5 S, dp	
	<i>ν</i> ₁₇	CD bend.....	867 C	ia	867.3 S, dp	
	<i>ν</i> ₁₈	Ring deform.....	577 C	ia	577.4 M, dp	
<i>e</i> _{2u}	<i>ν</i> ₁₉	CD bend.....	795 C	{ 799.91 797.37 794.64 790.9 790.3 (solid)	ia	
	<i>ν</i> ₂₀	Ring deform.....	352 E	ia	ia	OC (<i>ν</i> ₄ + <i>ν</i> ₂₀ , <i>ν</i> ₁₄ + <i>ν</i> ₂₀).

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_{1g}	ν_1	CH ₂ a-stretch	2930 E	cm^{-1} (Gas) ia	cm^{-1} (Liquid) {2938 VS, p 2923 VS, p 2852 VS, p 1465 M, p 1157 S, p 802 VS, p 383 M, p	FR ($2\nu_8$).
	ν_2	CH ₂ s-stretch	2852 C	ia		
	ν_3	CH ₂ scis.	1465 C	ia		
	ν_4	CH ₂ rock	1157 C	ia		
	ν_5	CC stretch	802 C	ia		
	ν_6	CCC deform + CC torsion	383 C	ia		
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 ($\nu_2, \nu_{18}, \nu_{26}$).
	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 ($\nu_1, \nu_{12}, \nu_{25}$).
	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a_{1g}</i>	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	
<i>a_{1u}</i>	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].
<i>a_{2g}</i>	ν_{10}	CD ₂ wag.....	1126 E	ia	ia	CF [4].
	ν_{11}	CD ₂ twist.....	778 F	ia	ia	CF [4].
<i>a_{2u}</i>	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	
<i>e_g</i>	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	
<i>e_u</i>	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Solid)	<i>cm</i> ⁻¹ (Solid)	
<i>a_g</i>	<i>v</i> ₁	CH ₂ s-stretch.....	2848 C	ia	2848 S	
	<i>v</i> ₂	CH ₂ scis.....	1440 C	ia	1440 M	
	<i>v</i> ₃	CC stretch.....	1131 C	ia	1131 M	
<i>a_u</i>	<i>v</i> ₄	CH ₂ twist.....	^a 1050 D	ia, 1050 VW	ia	
<i>b</i> _{1<i>g</i>}	<i>v</i> ₅	CH ₂ wag.....	1370 D	ia	1370 VW	
	<i>v</i> ₆	CC stretch.....	1061 C	ia	1061 M	
<i>b</i> _{1<i>u</i>}	<i>v</i> ₇	CH ₂ a-stretch.....	2919 C	2919 S	ia	
	<i>v</i> ₈	CH ₂ rock.....	725 C	^b { 731 S 720 S }	ia	
<i>b</i> _{2<i>g</i>}	<i>v</i> ₉	CH ₂ twist.....	1295 C	ia	1295 M	
<i>b</i> _{2<i>u</i>}	<i>v</i> ₁₀	CH ₂ s-stretch.....	2851 C	2851 S	ia	
	<i>v</i> ₁₁	CH ₂ scis.....	1468 C	^b { 1473 S 1463 S }	ia	
<i>b</i> _{3<i>g</i>}	<i>v</i> ₁₂	CH ₂ a-stretch.....	2883 C	ia	2883 S	
	<i>v</i> ₁₃	CH ₂ rock.....	1168 C	ia	1168 W	
<i>b</i> _{3<i>u</i>}	<i>v</i> 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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a_g</i>	<i>ν</i> ₁	CD ₂ s-stretch	2102 C	<i>cm</i> ⁻¹ (Solid) ia	<i>cm</i> ⁻¹ (Solid) 2102 S	CF [5].
	<i>ν</i> ₂	CD ₂ scis	1146 C	ia	1146 M	
	<i>ν</i> ₃	CC stretch	966 E	ia	966 VW	
<i>a_u</i>	<i>ν</i> ₄	CD ₂ twist	743 E	ia	ia	
<i>b_{1g}</i>	<i>ν</i> ₅	CD ₂ wag	1249 C	ia	1249 W	
	<i>ν</i> ₆	CC stretch	820 E	ia	
<i>b_{1u}</i>	<i>ν</i> ₇	CD ₂ a-stretch	2192 C	2192 S	ia	
	<i>ν</i> ₈	CD ₂ rock	526 C	^a { 528 M 522 M }	ia	
<i>b_{2g}</i>	<i>ν</i> ₉	CD ₂ twist	916 C	ia	916 M	
<i>b_{2u}</i>	<i>ν</i> ₁₀	CD ₂ s-stretch	2088 C	2088 S	ia	
	<i>ν</i> ₁₁	CD ₂ scis	1090 C	^a { 1092 S 1087 S }	ia	
<i>b_{3g}</i>	<i>ν</i> ₁₂	CD ₂ a-stretch	2197 C	ia	2197 M	
	<i>ν</i> ₁₃	CD ₂ rock	991 C	ia	991 M	
<i>b_{3u}</i>	<i>ν</i> ₁₄	CD ₂ wag	889 E	ia	

^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 isotopic species in the empirical formula; this deuterium is listed as H.

Compounds Not Containing Carbon

Empirical formula	Name	Molecule No.	Empirical formula	Name	Molecule No.
AsH ₃	Arsine	21	F ₆ W	Tungsten hexa fluoride	53
AsH ₃	Arsine-d ₃	22	GeH ₄	Germane	33
B ₂ H ₆	Diborane- ¹¹ B ₂ H ₆	55	GeH ₄	Germane-d ₁	34
B ₂ H ₆	Diborane- ¹⁰ B ₂ H ₆	56	GeH ₄	Germane-d ₂	35
B ₂ H ₆	Diborane- ¹⁰ B ₂ D ₆	57	GeH ₄	Germane-d ₃	36
BrCl ₃ Si	Bromotrichlorosilane	45	GeH ₄	Germane-d ₄	37
BrH ₃ Si	Silyl bromide	44	H ₂ O	Water	4
Br ₂ Cl ₂ Si	Dibromodichlorosilane	49	H ₂ O	Water-d ₁	5
Br ₃ ClSi	Tribromochlorosilane	47	H ₂ O	Water-d ₂	6
Br ₄ Ge	Germanium tetrabromide	39	H ₂ S	Hydrogen sulfide	9
Br ₄ Si	Silicon tetrabromide	31	H ₂ S	Deuterium sulfide	10
Br ₄ Sn	Tin tetrabromide	41	H ₂ Se	Hydrogen selenide	12
ClH ₃ Si	Silyl chloride	43	H ₂ Se	Hydrogen deuterium selenide	13
ClH ₃ Si	Chlorotriiodosilane	48	H ₃ N	Ammonia	14
Cl ₂ O	Oxygen dichloride	8	H ₃ N	Ammonia-d ₃	15
Cl ₃ ISi	Trichloroiodosilane	46	H ₃ P	Phosphine	17
Cl ₃ P	Phosphorus trichloride	20	H ₃ P	Phosphine-d ₃	18
Cl ₄ Ge	Germanium tetrachloride	38	H ₃ Sb	Stibine	23
Cl ₄ Si	Silicon tetrachloride	30	H ₃ Sb	Stibine-d ₃	24
Cl ₄ Sn	Tin tetrachloride	40	H ₄ Si	Silane	25
FH ₃ Si	Silyl fluoride	42	H ₄ Si	Silane-d ₂	26
F ₂ O	Oxygen difluoride	7	H ₄ Si	Silane-d ₃	27
F ₃ N	Nitrogen trifluoride	16	H ₄ Si	Silane-d ₄	28
F ₃ P	Phosphorus trifluoride	19	I ₄ Si	Silicon tetraiodide	32
F ₄ Si	Silicon tetrafluoride	29	N ₂ O	Nitrous oxide	1
F ₆ Mo	Molybdenum hexafluoride	52	N ₂ O	Nitrous oxide- ¹⁴ N ¹⁵ NO	2
F ₆ S	Sulfur hexafluoride	50	N ₂ O	Nitrous oxide- ¹⁵ N ₂ O	3
F ₆ Se	Selenium hexafluoride	51	O ₂ S	Sulfur dioxide	11
F ₆ U	Uranium hexafluoride	54			

Compounds Containing Carbon

Empirical formula	Name	Molecule No.	Empirical formula	Name	Molecule No.
CBrCl ₃	Bromotrichloromethane	93	CHBr ₃	Tribromomethane-d ₁	92
CBrN	Cyanogen bromide- ⁷⁹ BrCN	66	CHCl ₃	Trichloromethane	89
CBrN	Cyanogen bromide- ⁸¹ BrCN	67	CHCl ₃	Trichloromethane-d ₁	90
CBr ₂ Cl ₂	Dibromodichloromethane	101	CHF ₃	Trifluoromethane	88
CBr ₃ Cl	Tribromochloromethane	94	CHN	Hydrogen cyanide	62
CBr ₄	Carbon tetrabromide	78	CHN	Deuterium cyanide	63
CClN	Cyanogen chloride- ³⁵ ClCN	64	CH ₂ BrCl	Bromochloromethane	102
CClN	Cyanogen chloride- ³⁷ ClCN	65	CH ₂ BrCl	Bromochloromethane-d ₁	103
CCl ₄	Carbon tetrachloride	77	CH ₂ BrCl	Bromochloromethane-d ₂	104
CF ₄	Carbon tetrafluoride	76	CH ₂ Br ₂	Dibromomethane	98
Cl ₄	Carbon tetraiodide	79	CH ₂ Br ₂	Dibromomethane-d ₁	99
COS	Carbonyl sulfide	61	CH ₂ Br ₂	Dibromomethane-d ₂	100
CO ₂	Carbon dioxide	58	CH ₂ Cl ₂	Dichloromethane	95
CO ₂	Carbon dioxide- ¹³ CO ₂	59	CH ₂ Cl ₂	Dichloromethane-d ₁	96
CS ₂	Carbon disulfide	60	CH ₂ Cl ₂	Dichloromethane-d ₂	97
CHBr ₃	Tribromomethane	91	CH ₂ O	Formaldehyde	68

Empirical formula	Name	Molecule No.	Empirical formula	Name	Molecule No.
CH ₂ O	Formaldehyde-d ₁	69	C ₂ H ₃ N	Methyl isocyanide-d ₃	146
CH ₂ O	Formaldehyde-d ₂	70	C ₂ H ₄	Ethylene	124
CH ₂ O ₂	Formic acid	105	C ₂ H ₄	Ethylene-d ₄	125
CH ₂ O ₂	Formic acid-d ₂	106	C ₂ H ₄ BrCl	1-Bromo-2-chloroethane, trans form	164
CH ₃ Br	Methyl bromide	84	C ₂ H ₄ BrCl	1-Bromo-2-chloroethane, gauche form	165
CH ₃ Br	Methyl bromide-d ₃	85	C ₂ H ₄ Br ₂	1,2-Dibromoethane, trans form	162
CH ₃ Cl	Methyl chloride	82	C ₂ H ₄ Br ₂	1,2-Dibromoethane, gauche form	163
CH ₃ Cl	Methyl chloride-d ₃	83	C ₂ H ₄ Cl ₂	1,2-Dichloroethane, trans form	160
CH ₃ F	Methyl fluoride	80	C ₂ H ₄ Cl ₂	1,2-Dichloroethane, gauche form	161
CH ₃ F	Methyl fluoride-d ₃	81	C ₂ H ₄ O	Ethylene oxide	149
CH ₃ I	Methyl iodide	86	C ₂ H ₄ O	Ethylene oxide-d ₄	150
CH ₃ I	Methyl iodide-d ₃	87	C ₂ H ₄ O	Acetaldehyde	151
CH ₄	Methane	71	C ₂ H ₄ O	Acetaldehyde-d ₁	152
CH ₄	Methane-d ₁	72	C ₂ H ₄ O	Acetaldehyde-d ₄	153
CH ₄	Methane-d ₂	73	C ₂ H ₄ O ₂	Methyl formate	170
CH ₄	Methane-d ₃	74	C ₂ H ₄ O ₂	Methyl formate-d ₁	171
CH ₄	Methane-d ₄	75	C ₂ H ₄ O ₂	Methyl formate-d ₃	172
CH ₄ O (Gas)	Methanol	107	C ₂ H ₄ O ₂	Methyl formate-d ₄	173
CH ₄ O	Methanol	108	C ₂ H ₄ O ₂	Acetic acid	174
(Liquid)			C ₂ H ₄ O ₂	Acetic acid-d ₁	175
CH ₄ O (Gas)	Methanol-d ₁	109	C ₂ H ₄ Si	Silylacetylene	148
CH ₄ O	Methanol-d ₁	110	C ₂ H ₅ Br	Bromoethane	168
(Liquid)			C ₂ H ₅ Cl	Chloroethane	167
CH ₄ O (Gas)	Methanol-d ₃	111	C ₂ H ₅ F	Fluoroethane	166
CH ₄ O	Methanol-d ₃	112	C ₂ H ₅ N	Ethylene imine	169
(Liquid)			C ₂ H ₆	Ethane	154
CH ₄ O (Gas)	Methanol-d ₄	113	C ₂ H ₆	Ethane-d ₃	155
CH ₅ N	Methylamine	114	C ₂ H ₆	Ethane-d ₆	156
CH ₅ N	Methylamine-d ₂	115	C ₂ H ₆ O	Dimethylether	176
CH ₅ N	Methylamine-d ₃	116	C ₂ H ₆ O	Dimethylether-d ₃	177
CH ₅ N	Methylamine-d ₅	117	C ₃ H ₅ N ₂	Malononitrile	183
C ₂ Br ₄	Tetrabromoethylene	128	C ₃ H ₅ N ₂	Malononitrile-d ₂	184
C ₂ Br ₆	Hexabromoethane	159	C ₃ H ₄	Allene	178
C ₂ Cl ₂ F ₂	Trans-1,2-Dichloro-1,2-difluoroethylene	138	C ₃ H ₄	Methylacetylene	179
C ₂ Cl ₂ F ₂	1,1-Dichloro-2,2-difluoroethylene	142	C ₃ H ₄	Methylacetylene-d ₁	180
C ₂ Cl ₄	Tetrachloroethylene	127	C ₃ H ₄	Methylacetylene-d ₃	181
C ₂ Cl ₆	Hexachloroethane	158	C ₃ H ₄	Methylacetylene-d ₄	182
C ₂ F ₄	Tetrafluoroethylene	126	C ₃ H ₄ O	Propenal	185
C ₂ F ₆	Hexafluoroethane	157	C ₃ H ₅ N	Ethylcyanide	188
C ₂ HBr	Bromoacetylene	123	C ₃ H ₆	Cyclopropane	186
C ₂ HCl	Chloroacetylene	122	C ₃ H ₆	Cyclopropane-d ₆	187
C ₂ HF	Fluoroacetylene	121	C ₃ H ₆ O	Acetone	189
C ₂ H ₂	Acetylene	118	C ₃ H ₆ O	Acetone-d ₃	190
C ₂ H ₂	Acetylene-d ₁	119	C ₃ H ₆ O	Acetone-d ₆	191
C ₂ H ₂	Acetylene-d ₂	120	C ₃ H ₆ O ₂	Methyl acetate	197
C ₂ H ₂ Cl ₂	Trans-1,2-Dichloroethylene	132	C ₃ H ₆ O ₂	Methyl-d ₃ -acetate	198
C ₂ H ₂ Cl ₂	Trans-1,2-Dichloroethylene-d ₁	133	C ₃ H ₆ O ₂	Methyl acetate-d ₃	199
C ₂ H ₂ Cl ₂	Trans-1,2-Dichloroethylene-d ₂	134	C ₃ H ₆ O ₂	Methyl acetate-d ₆	200
C ₂ H ₂ Cl ₂	Cis-1,2-Dichloroethylene	135	C ₃ H ₈	Propane	192
C ₂ H ₂ Cl ₂	Cis-1,2-Dichloroethylene-d ₁	136	C ₃ H ₈	Propane-d ₃	193
C ₂ H ₂ Cl ₂	Cis-1,2-Dichloroethylene-d ₂	137	C ₃ H ₈	Propane-d ₂	194
C ₂ H ₂ Cl ₂	1,1-Dichloroethylene	139	C ₃ H ₈	Propane-d ₆	195
C ₂ H ₂ Cl ₂	1,1-Dichloroethylene-d ₁	140	C ₃ H ₈	Propane-d ₃	196
C ₂ H ₂ Cl ₂	1,1-Dichloroethylene-d ₂	141	C ₄ H ₂	Butadiyne	201
C ₂ H ₂ F ₂	Cis-1,2-Difluoroethylene	129	C ₄ H ₂ O	Furan	202
C ₂ H ₂ F ₂	Cis-1,2-Difluoroethylene-d ₁	130	C ₄ H ₄ S	Thiophene	203
C ₂ H ₂ F ₂	Cis-1,2-Difluoroethylene-d ₂	131	C ₄ H ₄ S	Thiophene-d ₄	204
C ₂ H ₂ N ₂ O	1,2,5-Oxadiazole	147	C ₄ H ₆	1,3-Butadiene	205
C ₂ H ₃ N	Methyl cyanide	143	C ₄ H ₆	1,3-Butadiene-d ₁ , trans	206
C ₂ H ₃ N	Methyl cyanide-d ₃	144	C ₄ H ₆	1,3-Butadiene-1,1,2-d ₃	207
C ₂ H ₃ N	Methyl isocyanide	145	C ₄ H ₆	1,3-Butadiene-1,1,4,4-d ₄	208
C ₂ H ₃ N			C ₄ H ₆	1,3-Butadiene-d ₆	209

Empirical formula	Name	Molecule No.	Empirical formula	Name	Molecule No.
C ₄ H ₆	2-Butyne	210	C ₄ H ₁₀	n-Butane, gauche form	127
C ₄ H ₈	Cyclobutane	211	C ₆ H ₆	Benzene	218
C ₄ H ₈	Cyclobutane-d ₈	212	C ₆ H ₆	Benzene-d ₆	219
C ₄ H ₈	2-Methylpropene	213	C ₆ H ₁₂	Cyclohexane	220
C ₄ H ₈	2-Methyl-d ₃ -propene-3,3,3-d ₃	214	C ₆ H ₁₂	Cyclohexane-d ₁₂	221
C ₄ H ₈ O	2-Butanone, trans form	215	(CH ₂) _n	Poly(methylene)	222
C ₄ H ₁₀	n-Butane, trans form	216	(CH ₂) _n	Poly(methylene-d ₂)	223