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Tables of Molecular
Vibrational Frequencies
Consolidated Volume I

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Tables of Molecular Vibrational Frequencies Consolidated Volume I

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NSRDS-NBS 39

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

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Foreword

The National Standard Reference Data System provides effective access to the quantitative data of physical science, critically evaluated and compiled for convenience, and readily accessible through a variety of distribution channels. The System was established in 1963 by action of the President's Office of Science and Technology and the Federal Council for Science and Technology, with responsibility to administer it assigned to the National Bureau of Standards.

The System now comprises a complex of data centers and other activities, carried on in academic institutions and other laboratories both in and out of government. The independent operational status of existing critical data projects is maintained and encouraged. Data centers that are components of the NSRDS produce compilations of critically evaluated data, critical reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data. In addition, the centers and projects establish criteria for evaluation and compilation of data and make recommendations on needed improvements in experimental techniques. They are normally closely associated with active research in the relevant field.

The technical scope of the NSRDS is indicated by the principal categories of data compilation projects now active or being planned: nuclear properties, atomic and molecular properties, solid state properties, thermodynamic and transport properties, chemical kinetics, and colloid and surface properties.

The NSRDS receives advice and planning assistance from the National Research Council of the National Academy of Sciences-National Academy of Engineering. An overall Review Committee considers the program as a whole and makes recommendations on policy, long-term planning, and international collaboration. Advisory Panels, each concerned with a single technical area, meet regularly to examine major portions of the program, assign relative priorities, and identify specific key problems in need of further attention. For selected specific topics, the Advisory Panels sponsor subpanels which make detailed studies of users' needs, the present state of knowledge, and existing data resources as a basis for recommending one or more data compilation activities. This assembly of advisory services contributes greatly to the guidance of NSRDS activities.

The NSRDS-NBS series of publications is intended primarily to include evaluated reference data and critical reviews of long-term interest to the scientific and technical community.

LAWRENCE M. KUSHNER, *Acting Director*

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Tables of Molecular Vibrational Frequencies

Consolidated Volume I

T. Shimanouchi

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_2X_6 type of molecule we adopt the numbering given in ref. [4], although it is based on D_{3h} symmetry. For some deuterated compounds the frequencies are arranged so that the same ν_i numbering is given to the corresponding vibrational modes of deuterated and normal compounds.

3.5. Approximate Type of Mode

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

The following abbreviations are used for the type

of mode:

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

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

3.6. Selected Value of Frequency

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

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

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

When the spectra in the gaseous state are not

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

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

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

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

3.7. Infrared and Raman Spectra

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

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

For some molecules the relative intensities of Raman lines are indicated by the numbers from one to ten in accordance with the tradition widely used. These

estimates of intensity are taken from the original references without any attempt at critical evaluation.

3.8. Comments

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

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

3.9. Footnotes and References

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

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

References

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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, HDS	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 Dibromodichlorosilane, 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, CHI ₃	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
106	Formic acid- d_2 , DCOOD	63

C₁-six-atomic molecules

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

C₁-seven-atomic molecules

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

C₂-four-atomic molecules

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

C₂-six-atomic molecules

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

C₂-seven-atomic molecules

147	1,2,5-Oxadiazole, $\text{C}_2\text{H}_2\text{N}_2\text{O}$	86
148	Silylacetylene, SiH_3CCH	86

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149	Ethylene oxide, $\text{C}_2\text{H}_4\text{O}$	87
150	Ethylene oxide- d_4 , $\text{C}_2\text{D}_4\text{O}$	88
151	Acetaldehyde, CH_3CHO	89
152	Acetaldehyde- d_1 , CH_3CDO	90
153	Acetaldehyde- d_4 , CD_3CDO	91

C₂-eight-atomic molecules

154	Ethane, CH_3CH_3	92
155	Ethane-1,1,1- d_3 , CH_3CD_3	93
156	Ethane- d_6 , CD_3CD_3	94
157	Hexafluoroethane, CF_3CF_3	95
158	Hexachloroethane, CCl_3CCl_3	95
159	Hexabromoethane, CBr_3CBr_3	96
160	1,2-Dichloroethane, $\text{CH}_2\text{ClCH}_2\text{Cl}$ (trans form).....	97
161	1,2-Dichloroethane, $\text{CH}_2\text{ClCH}_2\text{Cl}$ (gauche form).....	98
162	1,2-Dibromoethane, $\text{CH}_2\text{BrCH}_2\text{Br}$ (trans form).....	99
163	1,2-Dibromoethane, $\text{CH}_2\text{BrCH}_2\text{Br}$ (gauche form).....	100
164	1-Bromo-2-chloroethane, $\text{CH}_2\text{ClCH}_2\text{Br}$ (trans form).....	101
165	1-Bromo-2-chloroethane, $\text{CH}_2\text{ClCH}_2\text{Br}$ (gauche form).....	102
166	Fluoroethane, $\text{CH}_3\text{CH}_2\text{F}$	103
167	Chloroethane, $\text{CH}_3\text{CH}_2\text{Cl}$	104
168	Bromoethane, $\text{CH}_3\text{CH}_2\text{Br}$	105
169	Ethylene imine, $\text{C}_2\text{H}_5\text{N}$	106
170	Methyl formate, HCOOCH_3	107
171	Methyl formate- d_1 , DCOOCH_3	108
172	Methyl formate- d_3 , HCOOCD_3	109
173	Methyl formate- d_4 , DCOOCD_3	110
174	Acetic acid, CH_3COOH	111
175	Acetic acid- d_1 , CH_3COOD	112

C₂-nine-atomic molecules

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

C₃-seven-atomic molecules

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

C₃-eight-atomic molecules

185	Propenal, CH_2CHCHO	119
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C₃-nine-atomic molecules

186	Cyclopropane, C_3H_6	120
187	Cyclopropane- d_6 , C_3D_6	121
188	Ethylcyanide, $\text{CH}_3\text{CH}_2\text{CN}$	122

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C₃-ten-atomic molecules		209	1,3-Butadiene-d ₆ , CD ₂ CD ₂ CD ₂ 143
189	Acetone, CH ₃ COCH ₃ 123	210	2-Butyne, CH ₃ CCCH ₃ 144
190	Acetone-α,α,α-d ₃ , CH ₃ COCD ₃ 124	C₄-12-atomic molecules	
191	Acetone-d ₆ , CD ₃ COCD ₃ 125	211	Cyclobutane, C ₄ H ₈ 145
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192	Propane, CH ₃ CH ₂ CH ₃ 126	213	2-Methylpropene, (CH ₃) ₂ CCH ₂ 147
193	Propane-2,2-d ₂ , CH ₃ CD ₂ CH ₃ 127	214	2-Methyl-d ₃ -propene-3,3,3-d ₃ , (CD ₃) ₂ CCH ₂ ... 148
194	Propane-1,1,1-d ₃ , CH ₃ CH ₂ CD ₃ 128	C₄-13-atomic molecules	
195	Propane-1,1,1,3,3,3-d ₆ , CD ₃ CH ₂ CD ₃ 129	215	2-Butanone CH ₃ COCH ₂ CH ₃ (trans form)..... 149
196	Propane-d ₈ , CD ₃ CD ₂ CD ₃ 130	C₄-14-atomic molecules	
197	Methyl acetate, CH ₃ COOCH ₃ 131	216	n-Butane, CH ₃ CH ₂ CH ₂ CH ₃ (trans form)..... 150
198	Methyl acetate-d ₃ , CD ₃ COOCH ₃ 132	217	n-Butane, CH ₃ CH ₂ CH ₂ CH ₃ (gauche form).... 151
199	Methyl-d ₃ -acetate, CH ₃ COOCD ₃ 133	C₆-12-atomic molecules	
200	Methyl acetate-d ₆ , CD ₃ COOCD ₃ 134	218	Benzene, C ₆ H ₆ 152
C₄-six-atomic molecules		219	Benzene-d ₆ , C ₆ D ₆ 153
201	Butadiyne, HCCCCH..... 135	C₆-18-atomic molecules	
C₄-nine-atomic molecules		220	Cyclohexane, C ₆ H ₁₂ 154
202	Furan, C ₄ H ₄ O..... 136	221	Cyclohexane-d ₁₂ , C ₆ D ₁₂ 155
203	Thiophene, C ₄ H ₄ S..... 137	Polymer	
204	Thiophene-d ₄ , C ₄ D ₄ S..... 138	222	Poly (methylene), (CH ₂) _n 156
C₄-ten-atomic molecules		223	Poly (methylene-d ₂), (CD ₂) _n 157
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		

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 _{5h}	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 _{5v}	A ₁ , A ₂ , E ₁ , E ₂	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

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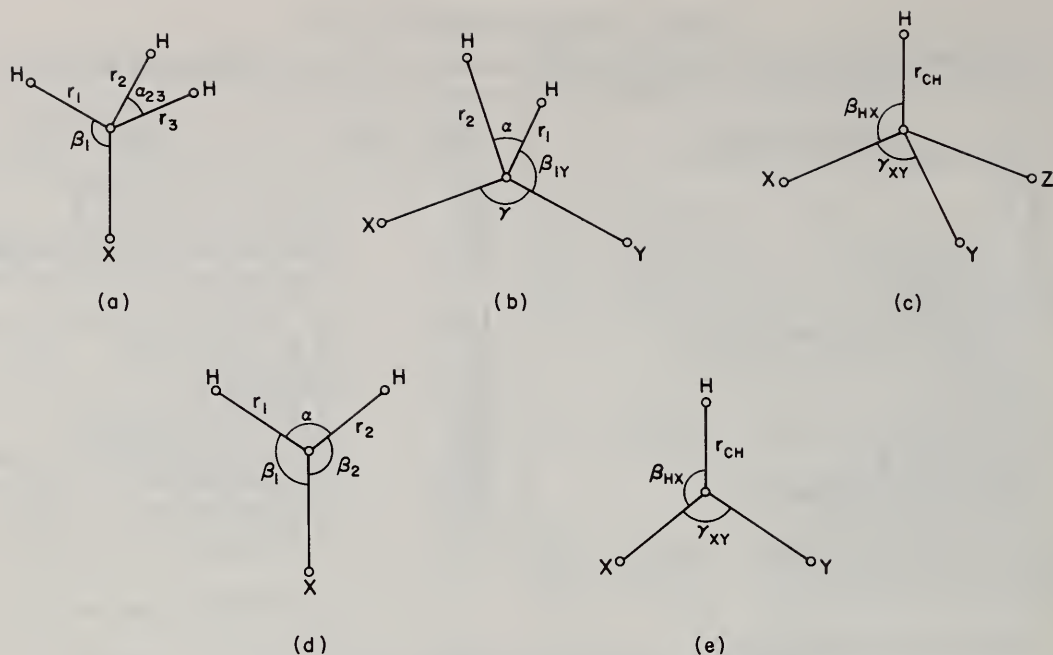


FIGURE 1. Parameters of methyl, methylene, and methin groups.

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

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

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 $\text{C}_{\infty v}$ 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
<i>a</i> ₁	<i>ν</i> ₁	Sym. stretch.....	2671 A	<i>cm</i> ⁻¹ (Gas) 2671.46	<i>cm</i> ⁻¹ (Gas) 2666	
	<i>ν</i> ₂	Bend.....	1178 A	1178.33		
<i>b</i> ₁	<i>ν</i> 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
<i>a</i> ₁	<i>ν</i> ₁	Sym. stretch.....	928 B	<i>cm</i> ⁻¹ (Gas) 928 S	<i>cm</i> ⁻¹	
	<i>ν</i> ₂	Bend.....	461 B	461 S		
<i>b</i> ₁	<i>ν</i> 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)	cm^{-1}	
	ν_2	Bend.....	296 C	296.4 W (solid)		
b_1	ν_3	Antisym. stretch.....	686 C	685.9 S		

References

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

Molecule: 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	cm^{-1}	
	ν_2	Bend.....	1183 A	1182.7		
b_1	ν_3	Antisym. stretch.....	2626 B	2626		

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).
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[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. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
[2] IR. R. D. Shelton, A. H. Nielsen, and W. H. Fletcher, J. Chem. Phys. 21, 2178 (1953).
[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 $\sigma = 2$

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

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

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

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

- [1] IR.R.Th. D. M. Cameron, W. C. Sears, and H. H. Nielsen, J. Chem. Phys. 7, 994 (1939).
 [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	cm^{-1}	
	ν_2	Sym. deform.....	950 C	932.5s 968.3a		
e	ν_3	Deg. stretch.....	3444 A	3443.6s 3443.9a		
	ν_4	Deg. deform.....	1627 A	1626.1s 1627.4a		

^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] 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	cm^{-1}	FR ($2\nu_4$).
	ν_2	Sym. deform.....	748 B	745.7s 749.4a		
e	ν_3	Deg. stretch.....	2564 A	2564.0		
	ν_4	Deg. deform.....	1191 B	1191		

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

References

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	1032 B	cm^{-1} (Gas) 1032 S	cm^{-1} (Liquid) 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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- [4] IR. P. N. Schatz and I. W. Levin, J. Chem. Phys. 29, 475 (1958).
- [5] Th. P. N. Schatz, J. Chem. Phys. 29, 481 (1958).
- [6] IR. I. W. Levin and S. Abramowitz, J. Chem. Phys. 44, 2562 (1966).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	2323 A	cm^{-1} (Gas) 2322.9	cm^{-1} (Liquid) 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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- [7] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta 20, 523 (1964).

Molecule: Phosphine-d₃ PD₃
 Symmetry C_{3v} Symmetry number $\sigma = 3$

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].
	ν_2	Sym. deform.....	730 B	730		
e	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 $\sigma = 3$

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)	
	ν_2	Sym. deform.....	487 B	487 M	486 (3)	
e	ν_3	Deg. stretch.....	860 C	860 S	840 (10)	
	ν_4	Deg. deform.....	344 B	344 M		

References

- [1] R. D. M. Yost and T. F. Anderson, J. Chem. Phys. 2, 624 (1934).
 [2] IR. H. S. Gutowsky and A. D. Liehr, J. Chem. Phys. 20, 1652 (1952).
 [3] IR. M. K. Wilson and S. R. Polo, J. Chem. Phys. 20, 1716 (1952).
 [4] Th. A. M. Mirri, F. Scappini, and P. G. Favero, Spectrochim. Acta 21, 965 (1965).
 [5] IR. I. W. Levin and S. Abramowitz, J. Chem. Phys. 44, 2562 (1966).

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	257 (6) p	
e	ν_3	Deg. stretch.....	482 C	482	480 (3) dp	
	ν_4	Deg. deform.....	198 C	198	190 (10) dp	

References

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

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	906.0		
e	ν_3	Deg. stretch.....	2123 B	2123.0		
	ν_4	Deg. deform.....	1003 B	1003		

References

- [1] IR. R. Robertson and J. J. Fox, Proc. Roy. Soc. (London), Ser. A, 120, 161 (1928).
- [2] IR. E. Lee and C. K. Wu, Trans. Faraday Soc. 35, 1366 (1939).
- [3] IR. V. M. McConaghie and H. H. Nielsen, Phys. Rev. 75, 633 (1949).
- [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. Duncan 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).

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

References

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

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

^a Observed in the infrared through Coriolis interaction with ν_4 .

References

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

Molecule: Silane-d₂ SiH₂D₂
Symmetry C_{2v} Symmetry number $\sigma = 2$

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		
	ν_2	SiD ₂ s-stretch.....	1587 C	1587 S		
	ν_3	SiH ₂ scis.....	944 B	944 W		
	ν_4	SiD ₂ scis.....	683 B	682.5 M		
a_2	ν_5	SiH ₂ twist.....	844 E	ia		CF [1].
b_1	ν_6	SiH ₂ a-stretch.....	2183 C	2183 S		
	ν_7	SiH ₂ rock.....	743 B	743 S		
b_2	ν_8	SiD ₂ a-stretch.....	1601 C	1601 S		
	ν_9	SiH ₂ wag.....	862 B	862 M		

Reference

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

Molecule: Silane-d₃ SiHD₃
Symmetry C_{3v} Symmetry number $\sigma = 3$

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		
	ν_2	SiD ₃ s-stretch.....	1573 C	1573 S		
	ν_3	SiD ₃ s-deform.....	683 C	683 S		SF (ν_6) [1].
e	ν_4	SiD ₃ d-stretch.....	1598 C	1598 S		
	ν_5	SiH bend.....	851 B	851 S		
	ν_6	SiD ₃ d-deform.....	683 C	683 S		SF (ν_3) [1].

References

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
a ₁	ν_1	Sym. stretch.....	1558 E			CF [4].
e	ν_2	Deg. deform.....	700 E			CF [4].
f ₂	ν_3	Deg. stretch.....	1597 B	1597 S		
	ν_4	Deg. deform.....	681 C	681 S		

References

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹ (Liquid)	
a ₁	ν_1	Sym. stretch.....	800 C	ia	800 S	
e	ν_2	Deg. deform.....	268 C	ia	268 W	
f ₂	ν_3	Deg. stretch.....	1032 B	1031.8 S	1010 W	
	ν_4	Deg. deform.....	389 B	389.35 S	390 W	

References

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

Molecule: Silicon tetrachloride SiCl_4
Symmetry T_d Symmetry number $\sigma = 12$

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. Delwaulle, J. Phys. Chem. 56, 355 (1952).
- [3] IR.R. A. L. Smith, J. Chem. Phys. 21, 1997 (1953).
- [4] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London), Ser. A, 240, 499 (1957).
- [5] Th. M. Radhakrishnan, Z. Phys. Chem. (Frankfurt am Main) 41, 197 (1964).

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

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. Delwaulle, J. Phys. Chem. 56, 355 (1952).
- [4] R. D. A. Long, T. V. Spencer, D. N. Waters, and L. A. Woodward, Proc. Roy. Soc. (London), Ser. A, 240, 499 (1957).
- [5] Th. M. Radhakrishnan, Z. Phys. Chem. (Frankfurt am Main) 35, 247 (1962).

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

Reference

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

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

^a Observed in the infrared through Coriolis interaction with ν_4 .

References

- [1] IR. J. W. Straley, C. H. Tindal, and H. H. Nielsen, Phys. Rev. 62, 161 (1942).
 [2] R. K. Schäfer and J. M. Gonzalez Barredo, Z. Phys. Chem. (Leipzig) 193, 334 (1944).
 [3] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
 [4] IR.R. L. P. Lindeman and M. K. Wilson, Z. Phys. Chem. (Frankfurt am Main) 9, 29 (1956).
 [5] IR. A. A. Chalmers and D. C. McKean, Spectrochim. Acta 21, 1941 (1965).

Molecule: Germane-d₁ GeH₃D
Symmetry C_{3v} Symmetry number $\sigma = 3$

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)	
	ν_2	GeD stretch.....	1520 B	1520.4 M	2106	
	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 $\sigma = 2$

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 σ = 3

No. 36

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	GeH stretch.....	2112 B	<i>cm</i> ⁻¹ (Gas) 2112.4	<i>cm</i> ⁻¹ (Gas) 1504	
	<i>ν</i> ₂	GeD ₃ s-stretch.....	1504 B			
	<i>ν</i> ₃	GeD ₃ s-deform.....	595 C	595		
<i>e</i>	<i>ν</i> ₄	GeD ₃ d-stretch.....	1522 C	1522		
	<i>ν</i> ₅	GeH bend.....	792 B	792.3		
	<i>ν</i> 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 σ = 12

No. 37

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	Sym. stretch.....	1504 C	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 1504	
<i>e</i>	<i>ν</i> ₂	Deg. deform.....	665 D	ia, ^a 665 W		
<i>f</i> ₂	<i>ν</i> ₃	Deg. stretch.....	1522 B	1522.2 S		
	<i>ν</i> ₄	Deg. deform.....	596 C	596 S		

^a Observed in the infrared through Coriolis interaction with *ν*₄.

Reference

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

Molecule: Germanium tetrachloride GeCl4
Symmetry T_d Symmetry number $\sigma = 12$

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 GeBr4
Symmetry T_d Symmetry number $\sigma = 12$

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 $\sigma = 12$

No. 40

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

No. 41

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	Sym. stretch.....	220 C	cm^{-1} ia	cm^{-1} (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. Trumphy, 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 $\sigma = 3$

No. 42

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

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

References

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

Molecule: Silyl chloride SiH_3Cl
Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 43

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

References

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

Molecule: **Silyl bromide** SiH_3Br
Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 44

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

References

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

Molecule: **Bromotrichlorosilane** SiBrCl_3
Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 45

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

References

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

Molecule: 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
a_1	ν_1	SiCl_3 s-stretch.....	519 C	cm^{-1}	cm^{-1} (Liquid)	
	ν_2	SiI stretch.....	333 C		519 W, p	
	ν_3	SiCl_3 s-deform.....	169 C		333 S, p	
e	ν_4	SiCl_3 d-stretch.....	600 C		169 M, p	
	ν_5	SiCl_3 rock.....	197 C		600 W, dp	
	ν_6	SiCl_3 d-deform.....	123 C		197 W, dp	
					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
a_1	ν_1	SiCl stretch.....	579 C	cm^{-1}	cm^{-1} (Liquid)	
	ν_2	SiBr_3 s-stretch.....	288 C		579 W, p	
	ν_3	SiBr_3 s-deform.....	159 C		288 S, p	
e	ν_4	SiBr_3 d-stretch.....	498 C		159 M, p	
	ν_5	SiBr_3 d-deform.....	173 C		498 M, dp	
	ν_6	SiCl bend.....	101 C		173 W, dp	
					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.

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	OC (2 ν_6) [3].
<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	

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).

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	OC (2 ν_6) [3].
<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	

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).

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

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).

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

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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_{1g}	ν_1	Sym. stretch.....	667 B	ia	667.1 VS	OC ($2\nu_6$) [3].
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	

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. Holloway, and H. Selig, J. Chem. Phys. 53, 341 (1970).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	BH_2 s-stretch.....	2537 C	ia	2537 VS	
	ν_2	Ring stretch.....	2110 C	ia	2110 S	
	ν_3	BH_2 scis.....	1186 C	ia	1186 M	
	ν_4	Ring deform.....	816 C	ia	816 S	
a_u	ν_5	BH_2 twist.....	833 C	ia, $^a 833.1$ VW	ia	
b_{1g}	ν_6	Ring stretch.....	1768 C	ia	1768 W	
	ν_7	BH_2 wag.....	850 E	ia		OC ($\nu_7 + \nu_{10}$).
b_{1u}	ν_8	BH_2 a-stretch.....	2625 C	2625 VS	ia	
	ν_9	BH_2 rock.....	955 E		ia	CF [9].
	ν_{10}	Ring puckering.....	368 C	368 S	ia	
b_{2g}	ν_{11}	BH_2 a-stretch.....	2640 E	ia	2640 W, b	
	ν_{12}	BH_2 rock.....	930 E	ia		OC ($\nu_{10} + \nu_{12}$) [6].
b_{2u}	ν_{13}	Ring stretch.....	1920 E	{ 1882 M (1992 W) }	ia	FR ($\nu_9 + \nu_{15}$).
	ν_{14}	BH_2 wag.....	977 C	977 S	ia	
b_{3g}	ν_{15}	BH_2 twist.....	1012 E	ia		CF. ^b
b_{3u}	ν_{16}	BH_2 s-stretch.....	2528 C	2528 VS	ia	
	ν_{17}	Ring deform.....	1606 C	1606 VS	ia	
	ν_{18}	BH_2 scis.....	1181 C	1181 VS	ia	

^a Observed very weakly and also confirmed by combination bands.

^b Estimated from ν_{15} of $^{11}\text{B}_2\text{H}_6$.

References

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- [6] IR.R. R. C. Lord and E. Nelsen, J. Chem. Phys. 19, 1 (1951).
- [7] IR. W. J. Lehman, J. F. Ditter, and J. Shapiro, J. Chem. Phys. 29, 1248 (1958).
- [8] R. R. C. Taylor and A. R. Emergy, Spectrochim. Acta 10, 419 (1958).
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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, $^{*}833.1$	ia	
				VW		
b_{1g}	ν_6	Ring stretch.....	1768 E	ia	{ 1788 (1) dp 1747 (1) dp }	FR ($\nu_5 + \nu_9$).
	ν_7	BH_2 wag.....	850 E	ia		OC ($\nu_7 + \nu_{10}$).
b_{1u}	ν_8	BH_2 a-stretch.....	2612 C	2612 VS	ia	
	ν_9	BH_2 rock.....	950 E		ia	{ OC ($\nu_5 + \nu_9$). OC ($\nu_9 + \nu_{10}$). }
	ν_{10}	Ring puckering.....	368 C	368 S	ia	
b_{2g}	ν_{11}	BH_2 a-stretch.....	2591 C	ia	2591 (9) dp	
	ν_{12}	BH_2 rock.....	915 E	ia		OC ($\nu_{10} + \nu_{12}$).
b_{2u}	ν_{13}	Ring stretch.....	1915 E	{ 1887 M (1999 W) }	ia	
	ν_{14}	BH_2 wag.....	973 C	973 S	ia	
b_{3g}	ν_{15}	BH_2 twist.....	1012 C	ia	1012 (5) dp	
b_{3u}	ν_{16}	BH_2 s-stretch.....	2525 C	2525 VS	ia	
	ν_{17}	Ring deform.....	1602 C	1602 VS	ia	
	ν_{18}	BH_2 scis.....	1177 C	1177 VS	ia	

^a Observed very weakly and also confirmed by combination bands.

References

See No. 55.

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	^a 592 VW	ia	
<i>b_{1g}</i>	<i>ν</i> ₆	Ring stretch	1273 C	ia	1273 (2) dp	OC (<i>ν</i> ₅ + <i>ν</i> ₇).
	<i>ν</i> ₇	BD ₂ wag	870 E	ia		
<i>b_{1u}</i>	<i>ν</i> ₈	BD ₂ a-stretch	1999 C	1999 VS	ia	OC (<i>ν</i> ₉ + <i>ν</i> ₁₀).
	<i>ν</i> ₉	BD ₂ rock	705 E		ia	
	<i>ν</i> ₁₀	Ring puckering	262 C	262 M	ia	{ 1975 (9) dp (2000 (5))dp
<i>b_{2g}</i>	<i>ν</i> ₁₁	BD ₂ a-stretch	1980 E	ia		
	<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	730 (4) dp
<i>b_{3g}</i>	<i>ν</i> ₁₅	BD ₂ twist	730 C	ia		
<i>b_{3u}</i>	<i>ν</i> ₁₆	BD ₂ s-stretch	1845 C	{ 1857 VS (1799 S)	ia	FR (<i>ν</i> ₃ + <i>ν</i> ₁₈).
	<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 $\text{D}_{\infty\text{h}}$ 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 ia ia	} FR ($2\nu_2$).
π_u	ν_2	Bend.....	667 A	667.38 S		
σ_u^+	ν_3	Antisym. stretch.....	2349 A	2349.16 VS		

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 $\text{D}_{\infty\text{h}}$ 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 ia ia	} FR ($2\nu_2$).
π_u	ν_2	Bend.....	649 A	648.91 S		
σ_u^+	ν_3	Antisym. stretch.....	2283 A	2283.48 VS		

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 $\sigma = 1$

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 $\sigma = 1$

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).
[2] IR. H. C. Allen, Jr., E. D. Tidwell, and E. K. Plyler, J. Chem. Phys. **25**, 302 (1956).
[3] IR. A. G. Maki, E. K. Plyler, and R. Thibault, J. Opt. Soc. Amer. **54**, 869 (1964).

Molecule: Cyanogen chloride $^{35}\text{ClCN}$
 Symmetry $\text{C}_{\infty v}$ Symmetry number $\sigma = 1$

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)	RP [2]. FR ($2\nu_2$) [2].
π	ν_2	Bend.....	378 A	380 S	394 (3)	
σ^+	ν_3	CCl stretch.....	744 C	{ 782.6 S 714.0 S }	{ 730 (5) }	

References

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

Molecule: Cyanogen chloride $^{37}\text{ClCN}$
 Symmetry $\text{C}_{\infty v}$ Symmetry number $\sigma = 1$

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)	RP [2]. FR ($2\nu_2$) [2].
π	ν_2	Bend.....	378 A	380 S	394 (3)	
σ^+	ν_3	CCl stretch.....	736 C		730 (5)	

References

See No. 64.

Molecule: Cyanogen bromide $^{79}\text{BrCN}$
 Symmetry $\text{C}_{\infty v}$ Symmetry number $\sigma = 1$

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 $^{81}\text{BrCN}$
 Symmetry $\text{C}_{\infty v}$ Symmetry number $\sigma = 1$

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 H_2CO
Symmetry C_{2v} Symmetry number $\sigma = 2$

No. 68

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_2 s-stretch.....	2783 A	2782.5 S	2781.6 S	
	ν_2	CO stretch.....	1746 A	1746.1 VS	1742.3 W	
	ν_3	CH_2 scis.....	1500 A	1500.1 S	1499.7 M	
b_1	ν_4	CH_2 a-stretch.....	2843 A	2843.1 VS	2866 W	
b_2	ν_5	CH_2 rock.....	1249 A	1249.1 S		
	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- d_1 HDCO
Symmetry C_s Symmetry number $\sigma = 1$

No. 69

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

Reference

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

Molecule: Formaldehyde-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
<i>a</i> ₁	ν_1	CD ₂ s-stretch.....	2056 D	<i>cm</i> ⁻¹ (Gas) 2056.4 S	<i>cm</i> ⁻¹	FR (2 ν_3).
	ν_2	CO stretch.....	1700 B	1700 VS		
	ν_3	CD ₂ scis.....	1106 C	1106.0 S		
<i>b</i> ₁	ν_4	CD ₂ a-stretch.....	2160 C	2160.3 VS		
	ν_5	CD ₂ rock.....	990 C	990.2 S		
<i>b</i> 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
<i>a</i> ₁	ν_1	Sym. stretch.....	2917 A	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 2917.0	
<i>e</i>	ν_2	Deg. deform.....	1534 A	ia, ^a 1533	1533.6	
<i>f</i> 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

- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
- [2] IR. H. C. Allen, Jr., and E. K. Plyler, J. Chem. Phys. 26, 972 (1957).
- [3] R. M. A. Thomas and H. L. Welsh, Can. J. Phys. 38, 1291 (1960).
- [4] R. J. Herranz and B. P. Stoicheff, J. Mol. Spectrosc. 10, 448 (1963).
- [5] IR. J. Herranz, J. Morcillo, and A. Gómez, J. Mol. Spectrosc. 19, 266 (1966).

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.....	2945 E	<i>cm</i> ⁻¹ (Gas) 2973 M 2914 M 2200.0 M	<i>cm</i> ⁻¹ (Gas)	FR (2 <i>ν</i> ₅).
	<i>ν</i> ₂	CD stretch.....	2200 A	2200.0 M		
	<i>ν</i> ₃	CH ₃ s-deform.....	1300 C	1300 M	1306	
<i>e</i>	<i>ν</i> ₄	CH ₃ d-stretch.....	3017 B	3016.9 S		
	<i>ν</i> ₅	CH ₃ d-deform.....	1471 C	1471 W		
	<i>ν</i> 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. Wilmshurst 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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CH ₂ s-stretch.....	2974 C	<i>cm</i> ⁻¹ (Gas) 2976 M	<i>cm</i> ⁻¹ (Gas) 2974	
	<i>ν</i> ₂	CD ₂ s-stretch.....	2202 C	2202 W		
	<i>ν</i> ₃	CH ₂ scis.....	1436 C	1436 W		
	<i>ν</i> ₄	CD ₂ scis.....	1033 C	1033 S	1034	
<i>a</i> ₂	<i>ν</i> ₅	CH ₂ twist.....	1333 C	ia, ^a 1329 W	1333	
<i>b</i> ₁	<i>ν</i> ₆	CH ₂ a-stretch.....	3013 C	3013 S		
	<i>ν</i> ₇	CH ₂ rock.....	1090 C	1090 S	1090	
<i>b</i> ₂	<i>ν</i> ₈	CD ₂ a-stretch.....	2234 C	2234 M		
	<i>ν</i> ₉	CH ₂ wag.....	1234 C	1234 M		

^a Observed in the infrared through Coriolis interaction with *ν*₉.

References

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

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

No. 74

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CH stretch	2993 C	<i>cm</i> ⁻¹ (Gas) 2993 M	<i>cm</i> ⁻¹ (Gas)	
	<i>ν</i> ₂	CD ₃ s-stretch	2142 C	2142 M	2141	
	<i>ν</i> ₃	CD ₃ s-deform	1003 C	1003 M		
<i>e</i>	<i>ν</i> ₄	CD ₃ d-stretch	2263 C	2263 M	2269	
	<i>ν</i> ₅	CD ₃ rock	1291 C	1291 M	1299	
	<i>ν</i> ₆	CD ₃ d-deform	1036 C	1036 S	1046	

References

See No. 73.

Molecule: Methane-d₄ CD₄
Symmetry T_d Symmetry number σ = 12

No. 75

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	Sym. stretch	2109 B	<i>cm</i> ⁻¹ (Gas) ia	<i>cm</i> ⁻¹ (Gas) 2108.9	
<i>e</i>	<i>ν</i> ₂	Deg. deform	1092 B	ia, ^a 1092	1091.9	
<i>f</i> ₂	<i>ν</i> ₃	Deg. stretch	2259 A	2259.3	2259.3	
	<i>ν</i> ₄	Deg. deform	996 B	996.0		

^a Observed in the infrared through Coriolis interaction with *ν*₄ [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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- [4] R. R. A. Olafson, M. A. Thomas, and H. L. Welsh, Can. J. Phys. 39, 419 (1961).
- [5] IR. H. Herranz, J. Morcillo, and A. Gómez, J. Mol. Spectrosc. 19, 266 (1966).

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

- [1] R. D. M. Yost, E. N. Lassetre, and S. T. Gross, J. Chem. Phys. 4, 325 (1936).
- [2] IR. C. R. Baeley, J. B. Hale, and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 167, 555 (1938).
- [3] IR.Th. E. K. Plyler and W. S. Benedict, J. Res. NBS 47, 202 (1951), RP 2245.
- [4] IR. P. J. H. Woltz and A. H. Nielsen, J. Chem. Phys. 20, 307 (1952).
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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).
- [2] R. J. P. Zietlow, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. 18, 1076 (1950).
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Molecule: Carbon tetrabromide CBr_4
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).
- [2] R. A. G. Meister, S. E. Rosser, and F. F. Cleveland, J. Chem. Phys. 18, 346 (1950).
- [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 $\left\{ \begin{matrix} 123 \text{ W} \\ 127 \text{ W} \end{matrix} \right\}$		

^a Crystal field splitting.

Reference

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

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

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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- [4] IR. W. L. Smith and I. M. Mills, J. Mol. Spectrosc. 11, 11 (1963).
- [5] IR. E. W. Jones, E. J. L. Popplewell, 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	CD_3 s-stretch	2110 E	cm^{-1} (Gas) 2090 2150	cm^{-1} }	FR ($2\nu_5$).
	ν_2	CD_3 s-deform	1136 A	1136		
	ν_3	CF stretch	991 A	991		
e	ν_4	CD_3 d-stretch	2258 A	2258		
	ν_5	CD_3 d-deform	1072 A	1072		
	ν_6	CD_3 rock	903 A	903		

References

- [1] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 222, 443 (1954).
- [2] IR. W. F. Edgell and L. Parts, J. Amer. Chem. Soc. 78, 2358 (1956).
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Molecule: Methylchloride CH_3Cl
Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 82

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) 2967.78 M 2879.28 M	cm^{-1} (Liquid) 2955 VS, p 2861 M	} FR ($2\nu_5$).
	ν_2	CH_3 s-deform	1355 A	1354.9 S	1370 VW, p	
e	ν_3	CCl stretch	732 A	732.1 S	709 VS, p	} FR ($3\nu_6$) [6, 8].
	ν_4	CH_3 d-stretch	3039 B	3039.31 S 3042.75 S	3036 M, dp	
	ν_5	CH_3 d-deform	1452 A	1452.1 M	1446 W, dp	
	ν_6	CH_3 rock	1017 A	1017.3 M	1016 W, dp	

References

- [1] R. J. Wagner, Z. Phys. Chem. B40, 439 (1938).
- [2] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, 222, 443 (1954).
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- [8] IR. M. Morillon-Chapey, Ph.D. Thesis (University of Paris, 1970).

Molecule: Methylchloride- d_3 CD_3Cl
Symmetry C_{3v} Symmetry number $\sigma = 3$

No. 83

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) 2160.28 S	cm^{-1}	
	ν_2	CD_3 s-deform	1029 A	1028.7 S		
e	ν_3	CCl stretch	701 A	701.4 S		
	ν_4	CD_3 d-stretch	2283 A	2283.3 S		
	ν_5	CD_3 d-deform	1060 A	1059.9 M		
	ν_6	CD_3 rock	768 A	767.6 M		

References

- [1] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) Ser. A, 222, 443 (1954).
- [2] IR. W. T. King, I. M. Mills, and B. L. Crawford, Jr., J. Chem. Phys. 27, 455 (1964).
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- [5] IR. C. Alamichel, C. R. B268, 483 (1969).

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) { 2972 M 2862.1 M	cm^{-1} (Liquid) 2972 VS 2862 W	} FR ($2\nu_5$).
	ν_2	CH_3 s-deform	1306 A	1305.9 S	1309 W	
	ν_3	CBr stretch	611 A	611.1 S	609 S	
e	ν_4	CH_3 d-stretch	3056 A	3056.35 S	3068 VS	
	ν_5	CH_3 d-deform	1443 A	1442.7 M	1456 M	
	ν_6	CH_3 rock	955 A	954.7 M	956 VW	

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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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) 2159.8 VS	cm^{-1}	
	ν_2	CD_3 s-deform	992 A	992.0 VS		
	ν_3	CBr stretch	577 A	576.7 S		
e	ν_4	CD_3 d-stretch	2297 A	2297.3 M		
	ν_5	CD_3 d-deform	1056 A	1055.6 S		
	ν_6	CD_3 rock	713 A	713.0 M		

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).
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- [3] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta 22, 639 (1966).

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 }	cm^{-1}	FR ($2\nu_5$).
e	ν_2	CH_3 s-deform.....	1252 A	1251.5 S		FR ($\nu_3 + \nu_6$).
	ν_3	CI stretch.....	533 A	532.8 S		
	ν_4	CH_3 d-stretch.....	3060 A	3060.06 S		
	ν_5	CH_3 d-deform.....	1436 C	1435.5 M		
	ν_6	CH_3 rock.....	882 A	882.4 M		

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- [1] Th. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1957).
- [2] IR. E. W. Jones and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, **288**, 50 (1965).
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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 }	cm^{-1}	FR ($2\nu_5$).
e	ν_2	CD_3 s-deform.....	951 A	950.7		
	ν_3	CI stretch.....	501 A	501.4		
	ν_4	CD_3 d-stretch.....	2298 A	2298		
	ν_5	CD_3 d-deform.....	1049 A	1049.3		
	ν_6	CD_3 rock.....	656 A	655.9		

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- [1] Th. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1957).
- [2] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Proc. Roy. Soc. (London), Ser. A, **288**, 39 (1965).
- [3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
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Molecule: Trifluoromethane CHF_3
Symmetry C_{3v} Symmetry number $\sigma = 3$

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 $\sigma = 3$

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).
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- [5] IR. I. Suzuki, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CD stretch	2266 C	<i>cm</i> ⁻¹ (Gas) 2266 W	<i>cm</i> ⁻¹ (Liquid) 2255 (2) p	
	<i>ν</i> ₂	CCl ₃ s-stretch	659 B	658.5 S	649 (7) p	
	<i>ν</i> ₃	CCl ₃ s-deform	369 C	366 W (liquid)	369 (9) p	
<i>e</i>	<i>ν</i> ₄	CD bend	914 B	913.9 VS	908 (1) dp	
	<i>ν</i> ₅	CCl ₃ d-stretch	749 B	748.5 VS	735 (2) dp	
	<i>ν</i> 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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CH stretch	3042 B	<i>cm</i> ⁻¹ (Gas) 3042 M	<i>cm</i> ⁻¹ (Liquid) 3017 (6) p	
	<i>ν</i> ₂	CBr ₃ s-stretch	541 B	541 M	540 (4) p	
	<i>ν</i> ₃	CBr ₃ s-deform	222 C		222 (10) p	
<i>e</i>	<i>ν</i> ₄	CH bend	1149 B	1149 VS	1143 (2) dp	
	<i>ν</i> ₅	CBr ₃ d-stretch	669 B	669 VS	655 (2) dp	
	<i>ν</i> 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).

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

References

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CCl ₃ s-stretch.	716 C	cm^{-1} (Liquid) 719 VS	cm^{-1} (Liquid) 716.3 (2) p	
	ν_2	CBr stretch.	422 C	420 W	422.3 (10) p	
	ν_3	CCl ₃ s-deform.	247 C		247.3 (5) p	
e	ν_4	CCl ₃ d-stretch.	775 C	773 VS	775.3 (1) dp	
	ν_5	CBr bend.	295 C	294 W	295.0 (3) dp	
	ν_6	CCl ₃ d-deform.	193 C		193.3 (4) dp	

References

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	ν_1	CCl stretch.....	747 C	cm^{-1} (CS ₂ , C ₇ H ₁₄ soln.) 747 S	cm^{-1} (C ₆ H ₆ , CCl ₄ soln.) 748 (1)	CF [1].
	ν_2	CBr ₃ s-stretch.....	329 C	(CS ₂ soln.) 329 W (C ₇ H ₁₄ soln.)	326 (10) p	
<i>e</i>	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. Delwaulle, M. B. Buisset, and M. Delhay, J. Amer. Chem. Soc. 74, 5768 (1952).
- [4] R. R. H. Krupp, S. M. Ferogle, and A. Weber, J. Chem. Phys. 24, 355 (1956).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> 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	
<i>a</i> ₂	ν_5	CH ₂ twist.....	1153 B	^a ia 1153	1153 VW	
<i>b</i> ₁	ν_6	CH ₂ a-stretch.....	3040 B	3045 (liquid)	3040 S, dp	
<i>b</i> ₂	ν_7	CH ₂ rock.....	898 B	897.7 M	893 VW	
	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 CH₂Cl₂, 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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	<i>ν</i> ₁	CH stretch.....	3024 B	cm ⁻¹ (Gas) 3024	cm ⁻¹ (Liquid) 3019 M, p	
	<i>ν</i> ₂	CD stretch.....	2249 B	2249	2246 M, p	
	<i>ν</i> ₃	CH bend.....	1282 B	1282	1276 VW	
	<i>ν</i> ₄	CD bend.....	778 C	778 (liquid)	779 W, p	
<i>a''</i>	<i>ν</i> ₅	CCl ₂ s-stretch.....	692 B	692	682 S, p	
	<i>ν</i> ₆	CCl ₂ scis.....	283 B		283 M, p	
	<i>ν</i> ₇	CH bend.....	1223 A	1222.9	1221 VW	
	<i>ν</i> ₈	CD bend.....	890 A	889.8	886 VW	
	<i>ν</i> 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).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CD ₂ s-stretch.....	2205 B	cm ⁻¹ (Gas) 2205 W	cm ⁻¹ (Liquid) 2198 M, p	
	<i>ν</i> ₂	CD ₂ scis.....	1052 D		1052 VW, p	
	<i>ν</i> ₃	CCl ₂ s-stretch.....	687 B	687 M	677 VS, p	
	<i>ν</i> ₄	CCl ₂ scis.....	282 C		282 S, p	
<i>a</i> ₂	<i>ν</i> ₅	CD ₂ twist.....	826 C	ia	826 VW	
<i>b</i> ₁	<i>ν</i> ₆	CD ₂ a-stretch.....	2304 C	2304 (liquid)	2304 VW	
<i>b</i> ₂	<i>ν</i> ₇	CD ₂ rock.....	^a 712 D			OV (<i>ν</i> ₉).
	<i>ν</i> ₈	CD ₂ wag.....	957 B	957 VS		
	<i>ν</i> 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. Delwaulle and F. Francois, J. Phys. Radium 7, 15 (1946).
- [3] IR. E. K. Plyler, W. A. Smith, and N. Acquista, J. Res. NBS 44, 503 (1950) RP2097.
- [4] IR.R. R. S. Dennen, E. A. Piotrowski, and F. F. Cleveland, J. Chem. Phys. 49, 4385 (1968).

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	
	ν_3	CH bend.....	1220 C	701 W	1239 W, p	
	ν_4	CD bend.....	701 C	1220 W	702 M, p	
	ν_5	CBr_2 s-stretch.....	565 C	565 VW	561 S, p	
	ν_6	CBr_2 scis.....	172 D		172 VS, p	
a''	ν_7	CH bend.....	1154 B	1154 VS		
	ν_8	CD bend.....	838 B	838 VS	835 VW, dp	
	ν_9	CBr_2 a-stretch.....	632 B	632 VS	623 W, dp	

References

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

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).

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	(liquid) 2252 M	2246 S, p	
	ν ₃	CH bend.....	1262 C	(liquid) 1262 S	1264 W, p	
	ν ₄	CH bend.....	1188 B	(liquid) 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>a'</i>	ν_1	CD ₂ s-stretch	2208 B	cm^{-1} (Gas) 2208 S	cm^{-1} (Liquid) 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	
<i>a''</i>	ν_6	CBrCl scis	226 C		226 S, p	
	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>a'</i>	ν_1	OH stretch	3570 D	cm^{-1} (Gas) 3570 M	cm^{-1}	
	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		
<i>a''</i>	ν_7	OCO deform	625 C	625 M		
	ν_8	CH bend	1033 C	1033 W		
	ν_9	Torsion	638 C	638 S		

References

- [1] IR. V. Z. Williams, J. Chem. Phys. 15, 232, 243 (1947).
- [2] IR. L. M. Sverdlov, Dokl. Akad. Nauk SSSR 91, 503 (1953).
- [3] IR. W. J. Orville-Thomas, Research 9, S15 (1956).
- [4] IR. J. K. Wilmshurst, J. Chem. Phys. 25, 478 (1956).
- [5] IR.Th. R. C. Millikan and K. S. Pitzer, J. Chem. Phys. 27, 1305 (1957).
- [6] IR.Th. T. Miyazawa and K. S. Pitzer, J. Chem. Phys. 30, 1076 (1959).
- [7] Th. K. Nakamoto and S. Kishida, J. Chem. Phys. 41, 1554 (1964).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	OD stretch.....	2632 C	cm^{-1} (Gas) 2632 W	cm^{-1}	
	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		
<i>a''</i>	ν_7	OCO deform.....	558 C	558 W		
	ν_8	CD bend.....	873 C	873 W		
	ν_9	Torsion.....	491 C	491 W		

References

See No. 105.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	OH stretch.....	3681 A	cm^{-1} (Gas) 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		OV (ν_{10})
	ν_5	CH ₃ s-deform.....	1455 A	1455 M		
	ν_6	OH bend.....	1345 B	1345 S		
	ν_7	CH ₃ rock.....	1060 D	1060 W		OV (ν_8)
<i>a''</i>	ν_8	CO stretch.....	1033 A	1033 VS	1032 (2)	
	ν_9	CH ₃ d-stretch.....	2960 C	2960 S	2955 (4)	
	ν_{10}	CH ₃ d-deform.....	1477 B	1477 M		OV (ν_4)
	ν_{11}	CH ₃ rock.....	1165 C		1165 (1) (liquid)	
	ν_{12}	Torsion.....	{ 295 (A) 200 (E) }	{ 80~300 }		{ MW: ^a 295 (A) 200 (E) }

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

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

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 vb	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 (1)	
	ν_{12}	Torsion	655 D	655 vb		

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

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		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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- [4] IR. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961) and references cited there.
- [5] Th. G. Zerbi, J. Overend, and B. Crawford, Jr., J. Chem. Phys. 38, 122 (1963).
- [6] IR.Th. C. Tanaka and T. Shimanouchi, unpublished.

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

No. 110

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	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)	
<i>a''</i>	ν_8	CO stretch	1038 C	1038 VS	1029 (6)	OV (ν_4).
	ν_9	CH ₃ d-stretch	2951 C	2951 S	2943 (9)	
	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

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- [2] R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
- [3] IR.R. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961), and references cited there.
- [4] IR.Th. C. Tanaka and T. Shimanouchi, unpublished.

Molecule: Methanol-d₃ CD₃OH (gas)
 Symmetry C_s Symmetry number $\sigma = 1$

No. 111

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	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		
<i>a''</i>	ν_8	CO stretch	988 C	988 VS		
	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).
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- [4] Th. C. Tanaka and T. Shimanouchi, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	OH stretch	3310 D	cm^{-1} (Liquid) 3310 S, vb	cm^{-1} (Liquid) 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	
<i>a''</i>	ν_8	CO stretch	982 C	982 VS	986 VS, p	OV (ν_{11}).
	ν_9	CD ₃ d-stretch	2213 D	^a 2213 M	2213 VW	OV (ν_4).
	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		OV (ν_7).

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

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- [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.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	OD stretch	2724 D	cm^{-1} (Gas) 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		
<i>a''</i>	ν_8	CO stretch	983 C	983 VS		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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[2] IR. M. Falk and E. Whalley, J. Chem. Phys. 34, 1554 (1961).
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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		
	ν_{15}	Torsion.....	268 B	268		MW: 272 (A). 265 (E).

^a Estimated from RQ branch frequency.

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- [2] IR. A. P. Gray and R. C. Lord, J. Chem. Phys. 26, 690 (1957).
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- [5] Th. A. Y. Hirakawa, unpublished.
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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	CF [5].
	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			
	ν ₁₄	CH ₃ rock.....	1187 C	1187 M		
	ν ₁₅	Torsion.....	228 C	228 S		

^a Estimated from RQ branch frequency.

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	<i>ν</i> ₁	NH ₂ s-stretch.....	3361 B	<i>cm</i> ⁻¹ (Gas) 3361 W	<i>cm</i> ⁻¹	CF [3].
	<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			
	<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].

References

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- [2] IR. M. Tsuboi, A. Y. Hirakawa, and K. Tamagake, J. Mol. Spectrosc. 22, 272 (1967).
- [3] Th. A. Y. Hirakawa, unpublished.
- [4] 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>a'</i>	<i>ν</i> ₁	ND ₂ s-stretch.....	2477 B	<i>cm</i> ⁻¹ (Gas) 2477 W	<i>cm</i> ⁻¹	CF [2.]
	<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			
	<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>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			
	<i>ν</i> ₁₄	CD ₃ rock.....	910 B	910 M		
	<i>ν</i> ₁₅	Torsion.....	201 C			
<i>a''</i>						CF [2].
						CF [2].
						MW: 200 (A).
						203 (E).

References

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- [2] Th. A. Y. Hirakawa, unpublished.
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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	
	ν_2	CC stretch	1974 C	ia	1973.8 VS	
σ_u^+	ν_3	CH stretch	3289 B	$\left\{ \begin{array}{l} 3294.9 \text{ S} \\ 3281.9 \text{ VS} \end{array} \right\}$	ia	FR ($\nu_2 + \nu_4 + \nu_5$).
π_g	ν_4	CH bend	612 C	ia	611.8 VW	
π_u	ν_5	CH bend	730 A	730.3 VS	ia	

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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	
	ν_2	CC stretch	1854 A	1853.8 M	1851 S	
	ν_3	CD stretch	2584 A	2583.6 S		
π	ν_4	CH bend	518 A	518.38 S		RP [4].
	ν_5	CD bend	678 A	677.8 S		RP [4].

References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ^+	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	

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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		

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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		SF (ν_4).
π	ν_4	CH bend.....	618 C	618 VS		SF (ν_3).
	ν_5	CCBr bend.....	295 B	295 W		

References

See No. 121.

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] IR.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] IR. 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).
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- [6] IR. D. A. Dows, J. Chem. Phys. 36, 2833 (1962).
- [7] IR. W. L. Smith and I. M. Mills, J. Chem. Phys. 40, 2095 (1963).

Molecule: Ethylene-d₄ C₂D₄
Symmetry D_{2h} Symmetry number $\sigma = 4$

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	CF [4]. OC ($\nu_6 + \nu_{10}$).
	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	
b_{1g}	ν_5	CD ₂ a-stretch.....	2304 C	ia	2304 W	
	ν_6	CD ₂ rock.....	1009 E	ia		
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	
b_{3u}	ν_{11}	CD ₂ a-stretch.....	2200 C	2200.2 S	ia	CF. ^a
	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).
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Molecule: Tetrafluoroethylene CF₂CF₂
Symmetry D_{2h} Symmetry number $\sigma = 4$

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	CF [3].
	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	
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

- [1] IR.R. J. R. Nielsen, H. H. Claassen, and D. C. Smith, J. Chem. Phys. 18, 812 (1950).
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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	
b_{3u}	ν_{10}	CCl_2 rock	176 C	176 S	ia	
	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]. CF [2].
	ν_2	CBr_2 s-stretch	265 D	ia	265 (10)p	
	ν_3	CBr_2 scis	144 D	ia	144 (1)p	
a_u	ν_4	CBr_2 twist	66 E	ia	ia	
b_{1g}	ν_5	CBr_2 a-stretch	880 D	ia	880 (1)dp	
	ν_6	CBr_2 rock	208 D	ia	208 (2)dp	
b_{1u}	ν_7	CBr_2 wag	245 C	245 S	ia	
b_{2g}	ν_8	CBr_2 wag	464 D	ia	464 (1)dp	
b_{2u}	ν_9	CBr_2 a-stretch	766 C	766 S	ia	
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

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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	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		
<i>a</i> ₂	ν_6	CH bend.....	866 E	ia		CF. ^a CF. ^b SF (ν_1).
	ν_7	Torsion.....	482 E	ia		
<i>b</i> ₁	ν_8	CH stretch.....	3135 D	3135 W		
	ν_9	CH bend.....	1376 C	1376 S		
	ν_{10}	CF stretch.....	1127 C	1127 VS		
<i>b</i> 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

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- [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).

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 stretch.....	3125 D	3125 W		
	ν_2	CD stretch.....	2364 D	2364 W		
	ν_3	CC stretch.....	1692 C	1692 S		
	ν_4	CH bend.....	1330 C	1330 S		
	ν_5	CF stretch.....	1167 C	1167 VS		
	ν_6	CF stretch.....	1033 C	1033 VS		
	ν_7	CD bend.....	889 B	889 M		
	ν_8	CCF deform.....	757 B	757 S		
<i>a</i> ''	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).

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	CD stretch.....	2320 D	2320 W		SF (<i>ν</i> ₈).
	<i>ν</i> ₂	CC stretch.....	1675 C	1675 S		
	<i>ν</i> ₃	CF stretch.....	1054 C	1054 S		
	<i>ν</i> ₄	CD bend.....	847 B	847 M		
	<i>ν</i> ₅	CCF deform.....	255 D	255 W		
<i>a</i> ₂	<i>ν</i> ₆	CD bend.....	656 E	ia		CF. ^a CF. ^b SF (<i>ν</i> ₁).
	<i>ν</i> ₇	Torsion.....	459 E	ia		
<i>b</i> ₁	<i>ν</i> ₈	CD stretch.....	2320 D	2320 W		
	<i>ν</i> ₉	CF stretch.....	1225 C	1225 VS		
	<i>ν</i> ₁₀	CD bend.....	937 B	937 M		
<i>b</i> ₂	<i>ν</i> ₁₁	CCF deform.....	748 B	748 S		
	<i>ν</i> ₁₂	CD bend.....	597 B	597 M		

^a From product rule.

^b Calculated by assuming $\frac{\nu_{12}(\text{cis-d}_1)}{\nu_{12}(\text{trans-d}_1)} = \frac{\nu_7(\text{cis-d}_2)}{\nu_7(\text{trans-d}_2)}$.

Reference

See No. 130.

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> _g	<i>ν</i> ₁	CH stretch.....	3073 C	ia	3073 S, p	
	<i>ν</i> ₂	CC stretch.....	1578 C	ia	1578 S, p	
	<i>ν</i> ₃	CH bend.....	1274 C	ia	1274 S, p	
	<i>ν</i> ₄	CCl stretch.....	846 C	ia	846 S, p	
	<i>ν</i> ₅	CCCl deform.....	350 C	ia	350 S, p	
<i>a</i> _u	<i>ν</i> ₆	CH bend.....	900 B	899.8 VS	ia	
	<i>ν</i> ₇	Torsion.....	227 C	227 M	ia	
<i>b</i> _g	<i>ν</i> ₈	CH bend.....	763 B	ia	763 M, dp	
<i>b</i> _u	<i>ν</i> ₉	CH stretch.....	3090 C	3090 S	ia	
	<i>ν</i> ₁₀	CH bend.....	1200 B	1200 S	ia	
	<i>ν</i> ₁₁	CCl stretch.....	828 B	828 VS	ia	
	<i>ν</i> 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).
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- [3] IR.R. H. J. Bernstein and A. D. E. Pullin, *Can. J. Chem.* 30, 963 (1952).
- [4] IR.R. K. S. Pitzer and J. L. Hollenberg, *J. Amer. Chem. Soc.* 76, 1493 (1954).
- [5] Th. J. M. Dowling, *J. Chem. Phys.* 25, 284 (1956).
- [6] Th. Y. Alaki and T. Shimanouchi, unpublished.

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

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			CF [5, 6].

References

See No. 132.

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

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	
<i>a_u</i>	ν_5	CCCl deform.....	346 C	ia	346 S	
	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	ia	
	ν_{10}	CD bend.....	916 C	916 VS	ia	
	ν_{11}	CCl stretch.....	791 C	791 VS	ia	
	ν_{12}	CCCl deform.....	240 E		ia	CF [6].

References

See No. 132.

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

No. 135

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a₁	ν_1	CH stretch.....	3077 C	cm^{-1} (Gas)	cm^{-1} (Liquid)	
	ν_2	CC stretch.....	1587 C		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	
a₂	ν_5	CCCl deform.....	173 C	714 S (liquid)	711 S, p	
	ν_6	CH bend.....	876 C		173 S, p	
b₁	ν_7	Torsion.....	406 C	ia	876 W, dp	
	ν_8	CH stretch.....	3072 C	ia	406 S, dp	
b₂	ν_9	CH bend.....	1303 C	3072		
	ν_{10}	CCl stretch.....	857 B	1303		
	ν_{11}	CCCl deform.....	571 B	857	563 M, dp	
	ν_{12}	CH bend.....	697 B	571		
				697		

References

See No. 132.

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

No. 136

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH stretch.....	3076 C	cm^{-1} (Gas)	cm^{-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	
	ν_9	CCl bend.....	175 D	558 S	561 S	
	ν_{10}	CH bend.....	822 C		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 **$\sigma = 2$**

No. 137

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Liquid)	
<i>a</i> ₁	ν_1	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	
<i>a</i> ₂	ν_6	CD bend.....	686 E	ia		
<i>b</i> ₁	ν_7	Torsion.....	368 C	ia	368 M	
	ν_8	CD stretch.....	2280 B	2280	2280 S	
	ν_9	CD bend.....	1051 B	1051	1040 VS	
<i>b</i> ₂	ν_{10}	CCl stretch.....	766 B	766	761 VS	
	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 **$\sigma = 2$**

No. 138

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> _g	ν_1	CC stretch.....	1707 C	ia	1707 VS, p	CF [2]. FR ($\nu_5 + \nu_{10}$).
	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	
<i>a</i> _u	ν_6	CFCl wag.....	333 C	333 M	ia	
	ν_7	Torsion.....	140 D		ia	
<i>b</i> _g	ν_8	CFCl wag.....	529 C	ia	529 M, dp	
<i>b</i> _u	ν_9	CF stretch.....	1190 E	{ 1214 VS 1167 VS }	ia	
	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

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 [2] Th. D. E. Mann, L. Fano, J. H. Meal, and T. Shimanouchi, J. Chem. Phys. **27**, 51 (1957).

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a_1	ν_1	CH_2 s-stretch.....	3035 D	cm^{-1} (Gas) $^a 3035$ W	cm^{-1} (Liquid) 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	
b_2	ν_{10}	CCl_2 rock.....	372 C	372 M	375 S, dp	
	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

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a'	ν_1	CH stretch.....	3082 D	cm^{-1} (Gas) ^a 3082 W	cm^{-1}	CF [1].
	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		
a''	ν_9	CCl ₂ scis.....	306 E			
	ν_{10}	CHD wag.....	819 B	819 S		
	ν_{11}	Torsion.....	555 C	555 W		
	ν_{12}	CCl ₂ wag.....	444 B	444 M		

^a CCl_4 solution.

Reference

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CD ₂ s-stretch.....	2262 D	<i>cm</i> ⁻¹ (Gas) ^a 2262 W	<i>cm</i> ⁻¹	
	<i>ν</i> ₂	CC stretch.....	1565 C	1565 VS		
	<i>ν</i> ₃	CD ₂ scis.....	1039 E			CF [1].
	<i>ν</i> ₄	CCl ₂ s-stretch.....	580 C	580 VS		
	<i>ν</i> ₅	CCl ₂ scis.....	305 E			CF [1].
<i>a</i> ₂	<i>ν</i> ₆	Torsion.....	488 E	ia		CF [1].
<i>b</i> ₁	<i>ν</i> ₇	CD ₂ a-stretch.....	2380 D	^a 2380 W		
	<i>ν</i> ₈	CD ₂ rock.....	998 C	998 VS		
	<i>ν</i> ₉	CCl ₂ a-stretch.....	697 C	697 S		SF (<i>ν</i> ₁₁).
	<i>ν</i> ₁₀	CCl ₂ rock.....	327 C	327 M		
<i>b</i> ₂	<i>ν</i> ₁₁	CD ₂ wag.....	697 C	697 S		SF (<i>ν</i> ₉).
	<i>ν</i> ₁₂	CCl ₂ wag.....	439 B	439 S		

^a CCl₄ solution.

Reference

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> ₁	<i>ν</i> ₁	CC stretch	1749 B	<i>cm</i> ⁻¹ (Gas) 1749 VS	<i>cm</i> ⁻¹ (Liquid) 1738.8 S	
	<i>ν</i> ₂	CF stretch.....	1032 B	1032 VS	1027.6 M	
	<i>ν</i> ₃	CCl stretch.....	622 C	622 M	623.0 S	
	<i>ν</i> ₄	CF ₂ scis.....	434 C	434	433.8 VS	
	<i>ν</i> ₅	CCl ₂ scis.....	258 C	258 S	258 VS	
<i>a</i> ₂	<i>ν</i> ₆	Torsion.....	167 D		167 VW	
<i>b</i> ₁	<i>ν</i> ₇	CF stretch.....	1327 B	1327 VS	1313 VW	
	<i>ν</i> ₈	CCl stretch.....	989 B	989 VS	986 VW	
	<i>ν</i> ₉	CF ₂ rock.....	459 C	459 VW	454 W	
	<i>ν</i> ₁₀	CCl ₂ rock.....	192 C	192	187.8 W	
<i>b</i> ₂	<i>ν</i> ₁₁	CF ₂ wag.....	564 C	564 S	560.8 VS	
	<i>ν</i> ₁₂	CCl ₂ wag.....	323 C	323 W		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 s-stretch	2954 A	2954.1 M	2942 VS	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CD_3 s-stretch	2126 A	2125.6	2112 S	
	ν_2	CN stretch	2278 A	2277.6	2258 S	
	ν_3	CD_3 s-deform	1110 B	1110	1103 W	
	ν_4	CC stretch	831 A	831.3	834 W	
e	ν_5	CD_3 d-stretch	2257 A	2256.6	2258 S	
	ν_6	CD_3 d-deform	1046 A	1046.4	1041 W	
	ν_7	CD_3 rock	847 A	846.6		
	ν_8	CCN bend	331 B	331.2	348 M	

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- [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
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 s-stretch.....	2966 B	2965.8 M	2951 S	
	ν_2	NC stretch.....	2166 B	2166.0 M	2161 S	
	ν_3	CH_3 s-deform.....	1429 D	1429	1414 M	
	ν_4	CN stretch.....	945 B	944.6 M	928 M	
e	ν_5	CH_3 d-stretch.....	3014 B	3014.3 S	3002 W	
	ν_6	CH_3 d-deform.....	1467 B	1466.9 S	1456 W	
	ν_7	CH_3 rock.....	1129 B	1129.3 S		
	ν_8	CNC bend.....	263 C	263 W	290 S	

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- [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
				cm^{-1} (Gas)	cm^{-1}	
a_1	ν_1	CD_3 s-stretch.....	2251 B	2250.6 W		
	ν_2	NC stretch.....	2165 B	2165.0 W		
	ν_3	CD_3 s-deform.....	1117 B	1117.4 W		
	ν_4	CN stretch.....	877 B	876.7 M		
e	ν_5	CD_3 d-stretch.....	2263 B	2262.9 S		
	ν_6	CD_3 d-deform.....	1058 B	1058.2 S		
	ν_7	CD_3 rock.....	900 B	900.1 S		
	ν_8	CNC bend.....	249 C			OC ($\nu_2 + \nu_8$)

References

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- [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).

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

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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 stretch.....	3311 B	3311.4 M		
	ν_2	SiH_3 s-stretch.....	2192 B	2192.4 VS		
	ν_3	CC stretch.....	2055 B	2054.9 S		
	ν_4	SiH_3 s-deform.....	935 B	935.3 VS		
	ν_5	SiC stretch.....	659 D	^a 659 S		
e	ν_6	SiH_3 d-stretch.....	2193 A	2192.9 VS		
	ν_7	SiH_3 d-deform.....	946 D	^a 946.4 VS		
	ν_8	SiH_3 rock.....	685 D	^a 685.4 VS		
	ν_9	CH bend.....	668 D	^a 668 VS		
	ν_{10}	SiCC deform.....	220 E	220		

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

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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		
	ν_8	CH_2 rock.....	860 E	ia		
b_1	ν_9	CH_2 s-stretch.....	3006 C	3006 S	3005 S, p	
	ν_{10}	CH_2 scis.....	1472 B	1472 W		
	ν_{11}	CH_2 wag.....	1151 D	1151 M	1150 W, dp	
	ν_{12}	Ring deform.....	892 D	892 VS		
b_2	ν_{13}	CH_2 a-stretch.....	3065 B	3065 S	3063 W, dp	
	ν_{14}	CH_2 twist.....	1142 D	1142 M	1150 W, dp	
	ν_{15}	CH_2 rock.....	822 B	822 M	807 M, dp	

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- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.
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- [3] IR.R. H. W. Thompson and W. T. Cave, *Trans. Faraday Soc.* 47, 946 (1951).
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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</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>ν</i> ₈	CD ₂ rock	581 D	ia	581 W	
<i>b</i> ₁	<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		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	CH_3 d-stretch.....	3005 C	3005 M	3001 W	
	ν_2	CH_3 s-stretch.....	2917 D		2917 S, p	
	ν_3	CH stretch.....	2822 C	2822 M	2843 W, p	
	ν_4	CO stretch.....	1743 C	1743 VS	1714 S, p	
	ν_5	CH_3 d-deform.....	1441 C	1441 S	1426 S	
	ν_6	CH bend.....	1400 C	1400 S	1391 S	
	ν_7	CH_3 s-deform.....	1352 C	1352 S	1342 M	
	ν_8	CC stretch.....	1113 C	1113 S	1109 M, p	
	ν_9	CH_3 rock.....	919 C	919 M	911 M	
a''	ν_{10}	CCO deform.....	509 C	509 S	512 S, p	
	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].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	<i>ν</i> ₁	CH ₃ d-stretch.....	3028 C	<i>cm</i> ⁻¹ (Gas) 3028 M	<i>cm</i> ⁻¹ (Liquid) 2998 W	
	<i>ν</i> ₂	CH ₃ s-stretch.....	2917 D		2917 S, p	
	<i>ν</i> ₃	CD stretch.....	2071 C	2071 W	2097 W, p	
	<i>ν</i> ₄	CO stretch.....	1743 C	1743 VS	1702 S, p	
	<i>ν</i> ₅	CH ₃ d-deform.....	1442 C	1442 S	1426 S	
	<i>ν</i> ₆	CD bend.....	1109 C	1109 S	1111 S, p	
	<i>ν</i> ₇	CD ₃ s-deform.....	1353 C	1353 S	1343 M	
	<i>ν</i> ₈	CC stretch.....	1043 C	1043 W	1080 W	
	<i>ν</i> ₉	CH ₃ rock.....	849 C	849 M	858 M	
	<i>ν</i> ₁₀	CCO deform.....	500 C	500 S	505 M, p	
<i>a''</i>	<i>ν</i> ₁₁	CH ₃ d-stretch.....	2970 C	2970 M	2965 W	
	<i>ν</i> ₁₂	CH ₃ d-deform.....	1420 C	1420 S	1426 S	
	<i>ν</i> ₁₃	CH ₃ rock.....	802 C	802 W	820 W, sh	
	<i>ν</i> ₁₄	CD bend.....	668 C	668 W	674 W, dp	
	<i>ν</i> ₁₅	Torsion.....	145 D	145		

References

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

Sym. species	No.	Approximate type of mode	Selected value o frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹ (Liquid)	
a'	ν ₁	CD ₃ d-stretch.....	2265 C	2265 W		
	ν ₂	CD ₃ s-stretch.....	2130 C	2130 W	2128	
	ν ₃	CD stretch.....	2060 C	2060 M	2072	
	ν ₄	CO stretch.....	1737 C	1737 VS	1706	
	ν ₅	CD ₃ d-deform.....	1045 C	1045 M	1090	
	ν ₆	CD bend.....	938 C	938 M		
	ν ₇	CD ₃ s-deform.....	1028 C	1028 M	1024	SF (ν ₁₂).
	ν ₈	CC stretch.....	1151 C	1151 S	1153	
	ν ₉	CD ₃ rock.....	747 C	747 W	762	
a''	ν ₁₀	CCO deform.....	436 C	436 S	422.4	
	ν ₁₁	CD ₃ d-stretch.....	2225 C	2225 W		
	ν ₁₂	CD ₃ d-deform.....	1028 C	1028 M	1024	SF (ν ₇).
	ν ₁₃	CD ₃ rock.....	573 C	573 W		
	ν ₁₄	CD bend.....	670 D			CF [5].
	ν ₁₅	Torsion.....	116 C	116 W		MW [3].

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

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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.....	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>ν</i> ₉). } FR (2 <i>ν</i> ₁₁).
	<i>ν</i> ₂	CD ₃ s-stretch.....	2098 E	{ 2139.6 S 2089.7 S		
	<i>ν</i> ₃	CH ₃ s-deform.....	1387 B	1386.6 W		
	<i>ν</i> ₄	CD ₃ s-deform.....	1122 B	1122.0 W		
<i>a</i> ₂ <i>e</i>	<i>ν</i> ₅	CC stretch.....	904 A	903.8 VW	904.7	
	<i>ν</i> ₆	Torsion.....	253 B	253 VW		
	<i>ν</i> ₇	CH ₃ d-stretch.....	2977 D	2976.5 S	2976.6	
	<i>ν</i> ₈	CD ₃ d-stretch.....	2240 E	2240 S		
	<i>ν</i> ₉	CH ₃ d-deform.....	1471 A	1471.1 M		
	<i>ν</i> ₁₀	CH ₃ rock.....	1115 B	1115.0 W		
	<i>ν</i> ₁₁	CD ₃ d-deform.....	1066 B	1065.7 M	1062.6	
	<i>ν</i> ₁₂	CD ₃ rock.....	678 A	678.4 M		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹ (Gas)	
<i>a_{1g}</i>	<i>ν</i> ₁	CD ₃ s-stretch.....	2083 B	ia	2083.0	
	<i>ν</i> ₂	CD ₃ s-deform.....	1155 A	ia	1154.5	
	<i>ν</i> ₃	CC stretch.....	843 A	ia	843.0	
<i>a_{1u}</i>	<i>ν</i> ₄	Torsion.....	208 B	208	ia	
<i>a_{2u}</i>	<i>ν</i> ₅	CD ₃ s-stretch.....	2087 B	2087.4	ia	
	<i>ν</i> ₆	CD ₃ s-deform.....	1077 B	1077.1	ia	
<i>e_g</i>	<i>ν</i> ₇	CD ₃ d-stretch.....	2226 A	ia	2225.6	
	<i>ν</i> ₈	CD ₃ d-deform.....	1041 B	ia	1041	
	<i>ν</i> ₉	CD ₃ rock.....	970 C	ia	970 (liquid)	
<i>e_u</i>	<i>ν</i> ₁₀	CD ₃ d-stretch.....	2235 B	2235	ia	
	<i>ν</i> ₁₁	CD ₃ d-deform.....	1081 B	1080.9	ia	
	<i>ν</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 CF[2]
	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	
a_{2u}	ν_5	CF_3 s-stretch	1117 B	1117 VS	ia	
	ν_6	CF_3 s-deform	714 B	714 VS	ia	
e_g	ν_7	CF_3 d-stretch	1250 C	ia	1250 VW, dp	
	ν_8	CF_3 d-deform	619 C	ia	619 W, dp	
	ν_9	CF_3 rock	372 C	ia	372 W, dp	
e_u	ν_{10}	CF_3 d-stretch	1251 B	1251 VS	ia	
	ν_{11}	CF_3 d-deform	520 C	520 S	ia	
	ν_{12}	CF_3 rock	220 C	220 S	ia	

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

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 [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	
	ν_6	CCl_3 s-deform	372 C	372 S	ia	
e_g	ν_7	CCl_3 d-stretch	859 C	ia	859 W	
	ν_8	CCl_3 d-deform	340 C	ia	340 M	
	ν_9	CCl_3 rock	223 C	ia	223 S	
e_u	ν_{10}	CCl_3 d-stretch	778 C	778 VS	ia	
	ν_{11}	CCl_3 d-deform	271 C	271 S	ia	
	ν_{12}	CCl_3 rock	114 C	114 W	ia	

References

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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
				cm^{-1} (Solid)	cm^{-1} (Solid)	
a_g	ν_1	CC stretch	940 C	ia	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	
	ν_9	CBr_3 rock	139 C	ia	139 M	
e_u	ν_{10}	CBr_3 d-stretch	656 C	656 VS	ia	
	ν_{11}	CBr_3 d-deform	168 C	168 S	ia	
	ν_{12}	CBr_3 rock	82 C	82 M	ia	

References

See No. 158.

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_g</i>	<i>ν</i> ₁	CH ₂ s-stretch	2957 D	ia	2957 (10) p	SF (gauche <i>ν</i> ₁ , gauche <i>ν</i> ₁₁).
	<i>ν</i> ₂	CH ₂ scis	1445 C	ia	1445 (4b) dp	
	<i>ν</i> ₃	CH ₂ wag	1304 C	ia	1304 (6) p	
	<i>ν</i> ₄	CC stretch	1052 C	ia	1052 (4) p	
	<i>ν</i> ₅	CCl stretch	754 C	ia	754 (10b) p	
	<i>ν</i> ₆	CCCl deform	300 C	ia	300 (8) p	
<i>a_u</i>	<i>ν</i> ₇	CH ₂ a-stretch	3005 D	3005 W (liquid)	ia	
	<i>ν</i> ₈	CH ₂ twist	1123 B	1122.5 W	ia	
	<i>ν</i> ₉	CH ₂ rock	773 B	772.5 M	ia	
<i>b_g</i>	<i>ν</i> ₁₀	Torsion	123 C	123 M	ia	
	<i>ν</i> ₁₁	CH ₂ a-stretch	3005 D	ia	3005 (8b) dp	
	<i>ν</i> ₁₂	CH ₂ twist	1264 C	ia	1264 (3) dp	
	<i>ν</i> ₁₃	CH ₂ rock	989 C	ia	989 (2) p	
<i>b_u</i>	<i>ν</i> ₁₄	CH ₂ s-stretch	2983 C	2983.3 M	ia	
	<i>ν</i> ₁₅	CH ₂ scis	1461 A	1460.6 S	ia	
	<i>ν</i> ₁₆	CH ₂ wag	1232 B	1232.3 S	ia	
	<i>ν</i> ₁₇	CCl stretch	728 C	728.3 VS	ia	
	<i>ν</i> ₁₈	CCCl deform	222 C	222.3 W	ia	

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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	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>	<i>ν</i> ₁	CH ₂ s-stretch	2972 D	<i>cm</i> ⁻¹ (Liquid) ia	<i>cm</i> ⁻¹ (Liquid) 2972 (10) p	SF (<i>ν</i> ₁₂).
	<i>ν</i> ₂	CH ₂ scis	1440 C	ia	1440 (5) dp	
	<i>ν</i> ₃	CH ₂ wag	1255 C	ia	1255 (10b) p	
	<i>ν</i> ₄	CC stretch	1053 C	ia	1053 (9) dp	
	<i>ν</i> ₅	CBr stretch	660 C	ia	660 (10b) p	
	<i>ν</i> ₆	CCBr deform	190 C	ia	190 (10) p	
<i>a_u</i>	<i>ν</i> ₇	CH ₂ a-stretch	3037 D	3037 S	ia	SF (<i>ν</i> ₃).
	<i>ν</i> ₈	CH ₂ twist	1087 C	1087 M	ia	
	<i>ν</i> ₉	CH ₂ rock	753 C	753 S	ia	
	<i>ν</i> ₁₀	Torsion	118 D	118 (gas)	132 (0)	
<i>b_g</i>	<i>ν</i> ₁₁	CH ₂ a-stretch	3013 D	ia	3013 (4b) dp	
	<i>ν</i> ₁₂	CH ₂ twist	1255 C	ia	1255 (10b) p	
<i>b_u</i>	<i>ν</i> ₁₃	CH ₂ rock	933 C	ia	933 (2) p	
	<i>ν</i> ₁₄	CH ₂ s-stretch	2974 D	2974 S	ia	
	<i>ν</i> ₁₅	CH ₂ scis	1441 D	1441 M	ia	
	<i>ν</i> ₁₆	CH ₂ wag	1186 C	1186 VS	1186 (0)	
	<i>ν</i> ₁₇	CBr stretch	589 C	589 S	ia	
	<i>ν</i> ₁₈	CCBr deform	193 D	193	ia	

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[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	cm^{-1} (Liquid)	cm^{-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 deform.....	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). SF (ν ₁ , gauche ν ₃ , gauche ν ₄). SF (gauche ν ₁₇).
	ν ₂	CH ₂ s-stretch.....	2960 D		2960 (10vb)	
	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	
	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). SF (ν ₁₂ , gauche ν ₁ , gauche ν ₂).
	ν ₁₃	CH ₂ a-stretch.....	3010 D		3010 (3vb)	
	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.)		

References

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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	
	ν_4	CH_2 scis.....	1479 C	1479 M	1480 W, b, dp	OV (ν_{14}).
	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	
				(liquid)		
	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	
a''	ν_{10}	CF stretch.....	880 B	880 VS	873 VS, p	OV (ν_1, ν_{13}).
	ν_{11}	CCF deform.....	415 C	415	419 W, p	
	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_{12}).
	ν_{14}	CH_3 d-deform.....	1449 D	1449 S	1458 M, b, dp	OV (ν_5).
	ν_{15}	CH_2 twist.....	1277 C	1277	1276 W, b, dp	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_{15}).
	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_5).
	ν_{15}	CH_2 twist.....	1248 E			CF [7].
	ν_{16}	CH_3 rock.....	964 D	964 S	960 (1b) dp	OV (ν_9).
	ν_{17}	CH_2 rock.....	770 B	770 M		
	ν_{18}	Torsion.....	247 C	247		MW: 247 [5, 6].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a'	ν_1	NH stretch.....	3338 C	3338 W	3302 M, p	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	
a''	ν_9	Ring deform.....	856 C	856 VS	855 M, dp	OV (ν_2). OV (ν_3).
	ν_{10}	CH ₂ rock.....	773 C	773 S	787 W, dp	
	ν_{11}	CH ₂ a-stretch.....	3079 D	3079 S	3059 M, dp	
	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)	
	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)	
a''	ν_{15}	CH_3 rock.....	1168 D	1168 M		
	ν_{16}	CH bend.....	1032 C	1032 M	1030 (0.5)	
	ν_{17}	C-O torsion.....	332 D	332 M	332 (3b) p	
	ν_{18}	CH_3 torsion.....	130 D	130 VW		MW: 132 [3].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν ₁	CH ₃ d-stretch.....	3041 C	<i>cm</i> ⁻¹ (Gas) 3041 M	<i>cm</i> ⁻¹	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		
	ν ₁₃	CH ₃ d-stretch.....	3007 D	3007 S		
	ν ₁₄	CH ₃ d-deform.....	1440 E	1440 W (CCl ₄ soln.)		
<i>a''</i>	ν ₁₅	CH ₃ rock.....	1164 E			CF [2], OV (ν ₉).
	ν ₁₆	CD bend.....	870 E			CF [2], OV (ν ₁₀).
	ν ₁₇	C-O torsion.....	290 E	290 M		
	ν ₁₈	CH ₃ torsion.....	130 E			CF [2].

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[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>a'</i>	<i>ν</i> ₁	CD ₃ d-stretch.....	2284 D	<i>cm</i> ⁻¹ (Gas) 2284 M	<i>cm</i> ⁻¹	
	<i>ν</i> ₂	CD ₃ s-stretch.....	2087 D	2087 M		
	<i>ν</i> ₃	CH stretch.....	2931 D	2931 S		
	<i>ν</i> ₄	C=O stretch.....	1754 C	1754 VS		
	<i>ν</i> ₅	CD ₃ d-deform.....	1060 E	1060 W		OV (<i>ν</i> ₁₄).
	<i>ν</i> ₆	CD ₃ s-deform.....	1102 E	1102 S		
	<i>ν</i> ₇	CH ip-bend.....	1368 D	1368 M		
	<i>ν</i> ₈	C-O stretch.....	1210 C	1210 VS		
	<i>ν</i> ₉	CD ₃ rock.....	985 D	985 M		
	<i>ν</i> ₁₀	O-CD ₃ stretch.....	877 C	877 M		
	<i>ν</i> ₁₁	OCO deform.....	714 C	714 M		
	<i>ν</i> ₁₂	COC deform.....	297 E	297 M		
<i>a''</i>	<i>ν</i> ₁₃	CD ₃ d-stretch.....	2258 D	2258 M		
	<i>ν</i> ₁₄	CD ₃ d-deform.....	1060 E	1060 W		OV (<i>ν</i> ₅).
	<i>ν</i> ₁₅	CD ₃ rock.....	905 D	905 W		
	<i>ν</i> ₁₆	CH op-bend.....	1040 E	1040 W		
	<i>ν</i> ₁₇	C-O torsion.....	312 E	312 M		
	<i>ν</i> 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>	<i>ν</i> ₁	CD ₃ d-stretch.....	2291 D	<i>cm</i> ⁻¹ (Gas) 2291 M	<i>cm</i> ⁻¹	FR (2 <i>ν</i> ₁₆).
	<i>ν</i> ₂	CD ₃ s-stretch.....	2100 D	2100 M		
	<i>ν</i> ₃	CD stretch.....	2210 D	2210 S		
	<i>ν</i> ₄	C=O stretch.....	1739 E	{ 1749 VS 1719 VS }	{ }	
	<i>ν</i> ₅	CD ₃ d-deform.....	1060 E	1060 W		OV (<i>ν</i> ₁₄).
	<i>ν</i> ₆	CD ₃ s-deform.....	1107 D	1107 S		
	<i>ν</i> ₇	CD bend.....	1041 E	1041 W		
	<i>ν</i> ₈	C-O stretch.....	1203 D	1203 VS		
	<i>ν</i> ₉	CD ₃ rock.....	974 D	974 M		OV (<i>ν</i> ₄).
	<i>ν</i> ₁₀	O-CD ₃ stretch.....	840 D	840 M		
	<i>ν</i> ₁₁	OCO deform.....	708 D	708 M		
	<i>ν</i> ₁₂	COC deform.....	295 E	295 M		
<i>a''</i>	<i>ν</i> ₁₃	CD ₃ d-stretch.....	2267 D	2267 M		OV (<i>ν</i> ₄).
	<i>ν</i> ₁₄	CD ₃ d-deform.....	1060 D	1060 W		
	<i>ν</i> ₁₅	CD ₃ rock.....	908 D	908 M		
	<i>ν</i> ₁₆	CD op-bend.....	870 D	870 W		
	<i>ν</i> ₁₇	C-O torsion.....	280 D	280 M		CF [1].
	<i>ν</i> ₁₈	CD ₃ torsion.....	96 E			

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
a'	ν_1	OH stretch.....	3583 B	cm^{-1} (Gas) 3583 M	cm^{-1}	SF (ν_{14}).
	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		
	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		
a''	ν_{11}	OCO deform.....	657 B	657 S		SF (ν_5).
	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		
	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].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	<i>ν</i> ₁	CH ₃ d-stretch.....	3039 B	<i>cm</i> ⁻¹ (Gas) 3039 VW	<i>cm</i> ⁻¹	SF (<i>ν</i> ₁₄).
	<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		
	<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>ν</i> ₁₁	OCO deform.....	609 B	609 M		
<i>a''</i>	<i>ν</i> ₁₂	CCO deform.....	543 B	543 M		SF (<i>ν</i> ₅).
	<i>ν</i> ₁₃	CH ₃ d-stretch.....	2997 D	2997 VW		
	<i>ν</i> ₁₄	CH ₃ d-deform.....	1440 C	1440 sh		
	<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	
	ν_9	CH_3 d-deform.....	1464 D	ia		SF (ν_3).
	ν_{10}	CH_3 rock.....	1150 C	ia	1150 M, d	
b_1	ν_{11}	Torsion.....	203 E	ia		CF [3].
	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>	<i>ν</i> ₁	CH ₃ d-stretch.....	2992 B	2992 S		
	<i>ν</i> ₂	CH ₃ s-stretch.....	2819 B	2819 S		
	<i>ν</i> ₃	CD ₃ d-stretch.....	2244 B	2244 S		
	<i>ν</i> ₄	CD ₃ s-stretch.....	2058 B	2058 S		
	<i>ν</i> ₅	CH ₃ d-deform.....	1465 C	1465 M		
	<i>ν</i> ₆	CH ₃ s-deform.....	1453 C	1453 M		
	<i>ν</i> ₇	CH ₃ rock.....	1212 B	1212 M		
	<i>ν</i> ₈	CO a-stretch.....	1156 C	1156 VS		SF (<i>ν</i> ₁₇).
	<i>ν</i> ₉	CD ₃ s-deform.....	1111 B	1111 S		
	<i>ν</i> ₁₀	CD ₃ d-deform.....	1061 C	1061 M		SF (<i>ν</i> ₁₈).
	<i>ν</i> ₁₁	CD ₃ rock.....	947 C	947 W		
	<i>ν</i> ₁₂	CO s-stretch.....	860 C	860 M		
<i>a''</i>	<i>ν</i> ₁₃	COC deform.....	395 E			CF [2].
	<i>ν</i> ₁₄	CH ₃ d-stretch.....	2932 B	2932 S		
	<i>ν</i> ₁₅	CD ₃ d-stretch.....	2189 B	2189 S		
	<i>ν</i> ₁₆	CH ₃ d-deform.....	1462 D	1462 M		
	<i>ν</i> ₁₇	CH ₃ rock.....	1156 C	1156 VS		SF (<i>ν</i> ₈).
	<i>ν</i> ₁₈	CD ₃ d-deform.....	1061 C	1061 M		SF (<i>ν</i> ₁₀).
	<i>ν</i> ₁₉	CD ₃ rock.....	901 C	901 W		
	<i>ν</i> ₂₀	Torsion.....	227 E			CF [2].
	<i>ν</i> ₂₁	Torsion.....	164 E			CF [2].

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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
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_1	ν_1	CH_2 s-stretch.....	3015 A		3015.0	
	ν_2	CH_2 scis.....	1443 A		1442.6	
	ν_3	CC stretch.....	1073 A		1072.6	
b_1	ν_4	CH_2 twist.....	865 C	865	865 (liquid)	
b_2	ν_5	CH_2 s-stretch.....	3007 A	3006.7		
	ν_6	CC stretch.....	1957 C	1957	1960 (liquid)	
	ν_7	CH_2 scis.....	1398 C	1398	1421 (liquid)	
e	ν_8	CH_2 a-stretch.....	3086 A	3085.5		
	ν_9	CH_2 rock.....	999 A	999.1		
	ν_{10}	CH_2 wag.....	841 A	840.8		
	ν_{11}	CCC deform.....	355 A	355.3		

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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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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		
	ν_5	C-C stretch	886 E			
e	ν_6	CH_3 d-stretch	3009 B	3008.9 M		OV (ν_7). CF [1].
	ν_7	CH_3 deform	1454 B	1453.5 M		
	ν_8	CH_3 rock	1051 B	1051.0 W		
	ν_9	CD bend	498 B	497.5 S		
	ν_{10}	CCC bend	314 B	314 M		

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

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	cm^{-1}	
	ν_2	CD ₃ s-stretch.....	2110 E	{ 2121.0 M 2077.0 M }		FR ($\nu_2 + 2\nu_7$) [2].
	ν_3	C $\equiv$ C stretch	2142 A	2142.0 M		
	ν_4	CD ₃ s-deform.....	1115 B	1115 M		
e	ν_5	C-C stretch.....	830 B	830 W		OV (ν_8).
	ν_6	CD ₃ d-stretch.....	2235 A	2234.9 M		
	ν_7	CD ₃ d-deform.....	1048 A	1048.2 M		
	ν_8	CD ₃ rock.....	835 A	835.4 W		OV (ν_5).
	ν_9	CH bend.....	633 B	633 S		
	ν_{10}	CCC bend.....	305 B	304.5 M		

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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	cm^{-1}	
	ν_2	CD ₃ s-stretch.....	2110 E	{ 2121 M 2077 M }		FR ($\nu_2 + 2\nu_7$) [2].
	ν_3	C $\equiv$ C stretch.....	2008 A	2008.4 W		
	ν_4	CD ₃ s-deform.....	1110 A	1110.1 M		
e	ν_5	C-C stretch.....	810 E			CF [1].
	ν_6	CD ₃ d-stretch.....	2235 A	2234.8 M		
	ν_7	CD ₃ d-deform.....	1048 A	1048.2 M		
	ν_8	CD ₃ rock.....	834 A	834.4 W		
	ν_9	CD bend.....	492 B	492 VS		
	ν_{10}	CCC bend.....	294 B	294 M		

References

See No. 181.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_1	ν_1	CH_2 s-stretch.....	2935 C	2935 VS	2929 (5)	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)	
	ν_{11}	CC a-stretch.....	982 C	982 S	975 (1)	
	ν_{12}	CCN bend.....	366 C	366 S	367 (10)	
b_2	ν_{13}	CH_2 a-stretch.....	2968 C	2968 VS	2960 (1)	SF (ν_8).
	ν_{14}	CH_2 rock.....	933 C	933 M		
	ν_{15}	CCN bend.....	337 C	337 S		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (D_2O soln.)	
a_1	ν_1	CD_2 s-stretch.....	2146 C	2146 S	2146 (4)	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) }	
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
				cm^{-1} (Gas)	cm^{-1}	
a'	ν_1	CH_2 a-stretch.....	3103 C	3103 M		
	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	$\text{C}=\text{C}$ 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		
a''	ν_{10}	$\text{C}-\text{C}$ stretch.....	1158 C	1158 S		
	ν_{11}	CH_2 rock.....	912 C	912 S		
	ν_{12}	CCO deform.....	564 C	564 M		
	ν_{13}	CCC bend.....	327 C	327 M		
	ν_{14}	$\text{CH}(\beta)$ op-bend.....	993 B	993 S		
	ν_{15}	$\text{CH}(\alpha)$ op-bend.....	980 E			CF [1, 2].
	ν_{16}	CH_2 wag.....	959 B	959 S		
	ν_{17}	CH_2 twist.....	593 C	593 S		
	ν_{18}	CC torsion.....	157 C	157 M		

^a Numbering of atoms: $\text{C}^{\gamma}\text{H}_2\text{C}^{\beta}\text{HC}^{\alpha}\text{HO}$.

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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	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	
	ν_3	Ring stretch	1188 C	ia	1188 S, p	
a_1''	ν_4	CH_2 twist	1126 D	ia, 1126 VW	ia, 1133	
a_2'	ν_5	CH_2 wag	1070 D	ia, 1075 (solid)	ia	OC ($\nu_5 + \nu_{10}$).
a_2''	ν_6	CH_2 a-stretch	3103 C	3103 S	ia	
	ν_7	CH_2 rock	854 C	854 S	ia	
e'	ν_8	CH_2 s-stretch	3025 C	3025 VS	3020 VS, p	
	ν_9	CH_2 scis	1438 C	1438 M	1442 M, dp	
	ν_{10}	CH_2 wag	1029 C	1029 S	1023 VW (liquid)	
	ν_{11}	Ring deform	866 C	866 VS	866 S, dp	
e''	ν_{12}	CH_2 a-stretch	3082 C	ia	3082 S, dp	
	ν_{13}	CH_2 twist	1188 C	ia	1188 M	
	ν_{14}	CH_2 rock	739 C	ia	739 W, dp	

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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].
	ν_2	CD ₂ scis.....	1274 D	ia	1274 S, p	
	ν_3	Ring stretch.....	956 C	ia	956 S, p	
a_1''	ν_4	CD ₂ twist.....	800 D	ia, 800 VW	ia	
a_2'	ν_5	CD ₂ wag.....	870 D	ia, 875 (solid)	ia	CF [2], OC ($\nu_5 + \nu_{11}$).
a_2''	ν_6	CD ₂ a-stretch.....	2336 C	2336 VS	ia	
	ν_7	CD ₂ rock.....	614 C	614 W	ia	
e'	ν_8	CD ₂ s-stretch.....	2211 C	2211 VS	2204 W, dp	
	ν_9	CD ₂ scis.....	1072 C	1072 S	1068 W, dp	CF [2], OC ($2\nu_{13}$).
	ν_{10}	CD ₂ wag.....	885 C	885 M	884 M, dp	
	ν_{11}	Ring deform.....	717 C	717 VS	721 M, dp	
e''	ν_{12}	CD ₂ a-stretch.....	2329 C	ia	2329 S, p	
	ν_{13}	CD ₂ twist.....	940 E	ia		
	ν_{14}	CD ₂ rock.....	528 C	ia	528 W, dp	

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- [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	SF (ν_{16}).
	ν_4	CN stretch.....	2254 C	2254 VS	2251 VS, p	
	ν_5	CH_3 d-deform.....	1465 C	1465 S	1466 VS, p	
	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	OV (ν_1).
	ν_{14}	CH_3 d-stretch.....	3001 C	3001 VS	2999 S	
	ν_{15}	CH_2 a-stretch.....	2849 C	2849 S	2850 M	SF (ν_5).
	ν_{16}	CH_3 d-deform.....	1465 C	1465 S	1466 VS, dp	
	ν_{17}	CH_2 twist.....	1256 C	1256 VW	1270 VW, dp	CF [2].
	ν_{18}	CH_3 rock.....	1022 E			
	ν_{19}	CH_2 rock.....	786 C	786 M	784 VW, dp	MW [2].
	ν_{20}	CCN bend.....	378 C	378 M	378 M, dp	
	ν_{21}	Torsion.....	222 C			

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 d-stretch.....	3019 C	3018.5 S	3005.5 S	SF (ν_{13}).
	ν_2	CH_3 s-stretch.....	2937 D	2937 S	2922 VS, p	SF (ν_{14}).
	ν_3	CO stretch.....	1731 C	1731 VS	1710.5 S, p	
	ν_4	CH_3 d-deform.....	1435 C	1435 S	1430 S	
	ν_5	CH_3 s-deform.....	1364 C	1363.5 VS	1356 W	SF (ν_{16}).
	ν_6	CH_3 rock.....	1066 C		1066 M, p	
	ν_7	CC stretch.....	777 C	777 W	787 VS, p	
	ν_8	CCC deform.....	385 C	385 W	393 W, dp	
a_2	ν_9	CH_3 d-stretch.....	2963 E	ia		CF [4].
	ν_{10}	CH_3 d-deform.....	1426 E	ia		CF [4].
	ν_{11}	CH_3 rock.....	877 E	ia		CF [4].
	ν_{12}	Torsion.....	105 D	ia		CF [4]; MW: 102 [1].
b_1	ν_{13}	CH_3 d-stretch.....	3019 C	3018.5 S	3005.5 S, dp	SF (ν_1).
	ν_{14}	CH_3 s-stretch.....	2937 D	2937 S	2922 VS	SF (ν_2).
	ν_{15}	CH_3 d-deform.....	1410 C	1410 S		
	ν_{16}	CH_3 s-deform.....	1364 C	1363.5 VS		SF (ν_5).
	ν_{17}	CC stretch.....	1216 C	1215.5 VS	1221 M, dp	
	ν_{18}	CH_3 rock.....	891 C	891 M	902.5 W, dp	
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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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 ν_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		
	ν_{15}	CCC deform.....	352 C	352 W	356.5 W	
a''	ν_{16}	CH ₃ d-stretch.....	2968 C	2968 S	2965 S	
	ν_{17}	CD ₃ d-stretch.....	2222 C	2222 M	2217.5 S	
	ν_{18}	CH ₃ d-deform.....	1447 C	1447 S		
	ν_{19}	CH ₃ rock.....	1035 C	1035 S		
	ν_{20}	CD ₃ d-deform.....	999 C	999 S		
	ν_{21}	CD ₃ rock.....	764 D	764 M (solid)		
	ν_{22}	CO op-bend.....	438 C	438	444 W	
	ν_{23}	CH ₃ torsion.....	106 E			CF [2].
	ν_{24}	CD ₃ torsion.....	78 E			CF [2].

References

- [1] IR.R.Th. G. Dellepiane and J. Overend, Spectrochim. Acta 22, 593 (1966).
 [2] IR.R.Th. M. Mikami, Ph.D. Thesis, (University of Tokyo, 1969).

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 ₃ d-stretch.....	2264 C	2263.5 S		SF (<i>ν</i> ₁₃).
	<i>ν</i> ₂	CD ₃ s-stretch.....	2123 C	2123 W	2108.5 VS, p	SF (<i>ν</i> ₁₄).
	<i>ν</i> ₃	CO stretch.....	1732 C	1732 VS	1700.5 S	
	<i>ν</i> ₄	CD ₃ s-deform.....	1080 C	1080 M	1088 M, p	
	<i>ν</i> ₅	CD ₃ d-deform.....	1035 D	1035 M	1036 M	
	<i>ν</i> ₆	CD ₃ rock.....	887 C	887 W	889 M, p	
	<i>ν</i> ₇	CC stretch.....	689 C	689 W	695.5 VS, p	
	<i>ν</i> ₈	CCC deform.....	321 C	321 W	330 VW, dp	
<i>a</i> ₂	<i>ν</i> ₉	CD ₃ d-stretch.....	2219 E	ia		CF [3].
	<i>ν</i> ₁₀	CD ₃ d-deform.....	1021 E	ia		CF [3].
	<i>ν</i> ₁₁	CD ₃ rock.....	669 E	ia		CF [3].
	<i>ν</i> ₁₂	Torsion.....	75 E	ia		CF [3].
<i>b</i> ₁	<i>ν</i> ₁₃	CD ₃ d-stretch.....	2264 C	2263.5 S	2256.5 S	SF (<i>ν</i> ₁).
	<i>ν</i> ₁₄	CD ₃ s-stretch.....	2123 C	2123 W		SF (<i>ν</i> ₂).
	<i>ν</i> ₁₅	CC stretch.....	1242 C	1241.7 VS	1248.5 VW	
	<i>ν</i> ₁₆	CD ₃ s-deform.....	1035 D	1035 M	1036 M	
	<i>ν</i> ₁₇	CD ₃ d-deform.....	1004 C	1004 M	1006 sh	
	<i>ν</i> ₁₈	CD ₃ rock.....	724 D	724 W		
<i>b</i> ₂	<i>ν</i> ₁₉	CO ip-bend.....	475 C	475 S	478 W, dp	
	<i>ν</i> ₂₀	CD ₃ d-stretch.....	2227 C	2226.5 S	2222 S	
	<i>ν</i> ₂₁	CD ₃ d-deform.....	1050 C	1050 S		
	<i>ν</i> ₂₂	CD ₃ rock.....	960 C	960 M		
	<i>ν</i> ₂₃	CO op-bend.....	405 C	405 W	410 VW, dp	
	<i>ν</i> ₂₄	Torsion.....	79 E			CF [3].

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

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

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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			CF [5].
a ₂	ν ₁₀	CH ₃ d-stretch.....	2956 E	ia		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	^a 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	^a 217 E			CF [4].

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

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
a'	ν ₁	CH ₃ d-stretch.....	2966 C	2966		
	ν ₂	CH ₃ s-stretch.....	2934 D	2934		
	ν ₃	CH ₂ s-stretch.....	2882 C	2882		
	ν ₄	CD ₃ d-stretch.....	2225 C	2225		
	ν ₅	CD ₃ s-stretch.....	2075 C	2075		
	ν ₆	CH ₂ scis.....	1461 D	1461		
	ν ₇	CH ₃ d-deform.....	1460 D	1460		
	ν ₈	CH ₃ s-deform.....	1383 C	1383		
	ν ₉	CH ₂ wag.....	1332 C	1332		
	ν ₁₀	CC stretch.....	1132 C	1132		
	ν ₁₁	CH ₃ rock.....	1101 C	1101		
	ν ₁₂	CD ₃ d-deform.....	1062 C	1062		
	ν ₁₃	CD ₃ s-deform.....	999 D	999		
	ν ₁₄	CC stretch.....	846 C	846		
	ν ₁₅	CD ₃ rock.....	750 C	750		
a''	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).
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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 ₂ s-stretch.....	2883 C	2883		
	ν ₂	CD ₃ d-stretch.....	2225 C	2225		SF (ν ₂₃).
	ν ₃	CD ₃ s-stretch.....	2091 C	2091		SF (ν ₁₆).
	ν ₄	CH ₂ scis.....	1467 C	1467		
	ν ₅	CD ₃ s-deform.....	1098 E			CF [4].
	ν ₆	CD ₃ d-deform.....	1066 C	1066		SF (ν ₁₉).
	ν ₇	CD ₃ rock.....	962 E	962		
	ν ₈	CC stretch.....	711 D	711		
	ν ₉	CCC deform.....	315 E			CF [4].
a ₂	ν ₁₀	CD ₃ d-stretch.....	2222 E	ia		CF [4].
	ν ₁₁	CH ₂ twist.....	1257 E	ia		CF [4].
	ν ₁₂	CD ₃ d-deform.....	1052 E	ia		CF [4].
	ν ₁₃	CD ₃ rock.....	700 E	ia		CF [4].
	ν ₁₄	Torsion.....	^a 142 E	ia		OC (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).
	ν ₂₀	CD ₃ s-deform.....	920 E	920		
b ₂	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.....	^a 173 E			OC (ν ₂₁ + ν ₂₇ - ν ₁₄) [3].

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

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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	CD ₃ d-stretch.....	2225 C	2225		
	ν ₂	CD ₃ s-stretch.....	2122 C	2122		
	ν ₃	CD ₂ s-stretch.....	2081 C	2081		
	ν ₄	CD ₃ s-deform.....	1086 D	1086		
	ν ₅	CD ₂ scis.....	1064 D	1064		
	ν ₆	CD ₃ d-deform.....	1064 D	1064		SF (ν ₅).
	ν ₇	CD ₃ rock.....	959 C	959		
	ν ₈	CC stretch.....	712 C	712		
	ν ₉	CCC deform.....	332 E			CF [3].
a ₂	ν ₁₀	CD ₃ d-stretch.....	2221 E	ia		CF [4].
	ν ₁₁	CD ₃ d-deform.....	1064 E	ia		CF [4].
	ν ₁₂	CD ₂ twist.....	945 E	ia		CF [4].
	ν ₁₃	CD ₃ rock.....	659 E	ia		CF [4].
	ν ₁₄	Torsion.....	^a 143 E	ia		OC (ν ₁₄ + ν ₂₂ , ν ₁₄ + ν ₂₄) [3].
b ₁	ν ₁₅	CD ₃ d-stretch.....	2224 C	2224		
	ν ₁₆	CD ₃ s-stretch.....	2081 C	2081		SF (ν ₃).
	ν ₁₇	CC stretch.....	1203 C	1203		
	ν ₁₈	CD ₃ d-deform.....	1086 D	1086		SF (ν ₄).
	ν ₁₉	CD ₃ s-deform.....	1068 D	1068		
	ν ₂₀	CD ₂ wag.....	862 D	862		
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

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- [2] Th. H. Takahashi, Nippon Kagaku Zasshi 82, 1304 (1961).
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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	$\text{C}=\text{O}$ 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_3 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}	$\text{C}-\text{O}$ stretch.....	1248 C	1248 VS	1254 (0)	
	ν_{11}	$\text{CH}_3(\text{O})$ rock.....	1159 E	1159 VW (liquid)		
a''	ν_{12}	$\text{O}-\text{CH}_3$ stretch.....	1060 C	1060 S	1044 (2b)	
	ν_{13}	$\text{CH}_3(\text{C})$ rock.....	980 C	980 W	980 (1b) p	
	ν_{14}	CC stretch.....	844 C	844 M	844 (8) p	
	ν_{15}	$\text{C}=\text{O}$ 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	
	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}	$\text{C}=\text{O}$ op-bend.....	607 D	607 M	610 (0) dp	
	ν_{25}	$\text{C}-\text{O}$ torsion.....	187 D	187 W		
	ν_{26}	$\text{C}-\text{C}$ torsion.....	136 E	136 VW (liquid)		
	ν_{27}	$\text{O}-\text{CH}_3$ torsion.....	110 E	110 VW (liquid)		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	ν_1	CH ₃ d-stretch.....	3032 D	cm^{-1} (Gas) 3032 M	cm^{-1}	OV (ν_{20}).
	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.)		
	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		OV (ν_6).
	ν_{19}	CD ₃ d-stretch.....	2253 D	2253 W		
	ν_{20}	CH ₃ d-deform.....	1455 E	1455 W, sh (CCl ₄ soln.)		
	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

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

References

See No. 198.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm ⁻¹ (Gas)	cm ⁻¹	
a'	ν ₁	CD ₃ (O) d-stretch	2285 D	2285 M		
	ν ₂	CD ₃ (C) d-stretch	2275 E			SF (ν ₂ of CD ₃ COOCH ₃).
	ν ₃	CD ₃ (O) s-stretch	2099 D	2099 M		
	ν ₄	CD ₃ (C) s-stretch	2087 E			SF (ν ₄ of CD ₃ COOCH ₃).
	ν ₅	C=O stretch	1767 C	1767 VS		
	ν ₆	CD ₃ (O) d-deform	1059 E	1059 W		OV (ν ₂₀).
	ν ₇	CD ₃ (O) s-deform	1106 C	1106 S		
	ν ₈	CD ₃ (C) d-deform	1003 E	1003 W		
	ν ₉	CD ₃ (C) s-deform	1086 E			SF (ν ₉ of CD ₃ COOCH ₃).
	ν ₁₀	C-O stretch	1282 C	1282 VS		
	ν ₁₁	CD ₃ (O) rock	975 D	975 M		
	ν ₁₂	O-CH ₃ stretch	1045 E	1045 W		
	ν ₁₃	CD ₃ (C) rock	828 E	828 W		
	ν ₁₄	CC stretch	747 C	747 M		
	ν ₁₅	C=O ip-bend	585 C	585 M		
	ν ₁₆	CCO deform	334 C	334 M		
	ν ₁₇	COC deform	266 D	266 M		
	ν ₁₈	CD ₃ (O) d-stretch	2264 D	2264 M		
	ν ₁₉	CD ₃ (C) d-stretch	2253 E			SF (ν ₁₉ of CD ₃ COOCH ₃).
a''	ν ₂₀	CD ₃ (O) d-deform	1059 D	1059 W		OV (ν ₆).
	ν ₂₁	CD ₃ (C) d-deform	1038 E	1038 W		
	ν ₂₂	CD ₃ (O) rock	908 E			SF (ν ₂₂ of CH ₃ COOCD ₃).
	ν ₂₃	CD ₃ (C) rock	925 D	925 M		
	ν ₂₄	C=O op-bend	522 D	522 M		
	ν ₂₅	C-O torsion	160 D	160 W		
	ν ₂₆	C-C torsion	100 E			CF [2].
	ν ₂₇	O-CH ₃ torsion	80 E			CF [2].

References

See No. 198.

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	
	ν_3	C-C stretch.....	874 C	ia	874 W	
σ_u^+	ν_4	CH stretch.....	3329 C	3329 VS	ia	
	ν_5	$C\equiv C$ stretch.....	2020 C	2020 M	ia	
π_g	ν_6	CH bend.....	627 C	ia	627 M	
	ν_7	CCC bend.....	482 C	ia	482 S	
π_u	ν_8	CH bend.....	630 B	630 VS	ia	
	ν_9	CCC bend.....	231 E	ia	231 VW (liquid)	

Reference

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

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) 3154 VS, p	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		
	ν_3	ip-Ring II.....	1491 C	1491 VS	1483 VS, p	
	ν_4	ip-Ring III.....	1384 C	1384 M	1380 S, p	
	ν_5	ip-Ring IV.....	1140 D	1140 sh (liquid)	1137 VS, p	
	ν_6	CH ip-bend.....	1066 C	1066 S	1061 M, p	
	ν_7	CH ip-bend.....	995 C	995 VS	986 M, p	
	ν_8	ip-Ring VII.....	871 C	871 S		
a_2	ν_9	CH op-bend.....	863 C	ia		
	ν_{10}	CH op-bend.....	728 D	ia	728 W, dp	
b_1	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	
	ν_{17}	ip-Ring V.....	1040 D	1040 sh (liquid)	1034 M, dp	
b_2	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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH stretch.....	3126 C	3126 M	3107 (10) p	
	ν_2	CH stretch.....	3098 C	3098 S	3084 (5sh)	
	ν_3	ip-Ring II.....	1409 C	1409 S	1407 (7) p	
	ν_4	ip-Ring III.....	1360 C	1360 VW	1358 (5) p	
	ν_5	CH ip-bend.....	1083 C	1083 S	1081 (5) p	
	ν_6	CH ip-bend.....	1036 C	1036 S	1035	
	ν_7	ip-Ring IV.....	839 C	839 VS	832 (5) p	
	ν_8	ip-Ring VII.....	608 C	608 W	606 (2) p	
a_2	ν_9	CH op-bend.....	903 D	ia, 900 VW (solid)	903 (0) dp	
	ν_{10}	CH op-bend.....	688 D	ia	688 (0) dp	
	ν_{11}	op-Ring I.....	567 D	ia, 565 VW (liquid)	567 (0) dp	
b_1	ν_{12}	CH stretch.....	^a 3125 E			
	ν_{13}	CH stretch.....	3086 C	3086 S	3076 (sh)	
	ν_{14}	ip-Ring I.....	1504 D	1504 VW (liquid)	1502 (0) dp	
	ν_{15}	CH ip-bend.....	1256 C	1256 S	1257 (0)	
b_2	ν_{16}	CH ip-bend.....	^a 1085 E			OV (ν_5).
	ν_{17}	ip-Ring V.....	872 C	872 M	869 (4) dp	
	ν_{18}	ip-Ring VI.....	751 D	763 VW	751 (1) dp	
	ν_{19}	CH op-bend.....	867 E			OC ($\nu_9 + \nu_{19}, 2\nu_{19}$).
	ν_{20}	CH op-bend.....	712 C	712 VS		
	ν_{21}	op-Ring II.....	452 C	452 W	453 (0) dp	

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

References

- [1] IR. H. W. Thompson and R. B. Temple, Trans. Faraday Soc. 41, 27 (1945).
- [2] R. K. W. Kohlrausch and H. Schreiner, Acta Phys. Austriaca 1, 373 (1948).
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- [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
<i>a</i> ₁	ν_1	CD stretch	2343 C	<i>cm</i> ⁻¹ (Gas) 2343 M	<i>cm</i> ⁻¹ (Liquid) 2326 (6)	SF (ν_{17}).
	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	
<i>a</i> ₂	ν_9	CD op-bend	752 E	ia, 756 (solid)	752 (3) dp	
	ν_{10}	CD op-bend	532 D	ia	532 (2) dp	
<i>b</i> 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	
<i>b</i> 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
				cm^{-1} (Gas)	cm^{-1} (Solid)	
a_g	ν_1	CH_2 a-stretch.....	3087 D	ia	3087 M	
	ν_2	CH stretch.....	3003 D	ia	3003 M	
	ν_3	CH_2 s-stretch.....	2992 D	ia	2992 S	
	ν_4	C=C stretch.....	1630 D	ia	1630 VS	
	ν_5	CH_2 scis.....	1438 D	ia	1438 S	
	ν_6	CH bend.....	1280 D	ia	1280 S	
	ν_7	C-C stretch.....	1196 D	ia	1196 S	
	ν_8	CH_2 rock.....	894 D	ia	894 W	
	ν_9	CCC deform.....	512 D	ia	512 S	
a_u	ν_{10}	CH bend.....	1013 B	1013.4 VS	ia	
	ν_{11}	CH_2 wag.....	908 B	907.8 VS	ia	
	ν_{12}	CH_2 twist.....	522 B	522.2 M	ia	
	ν_{13}	C-C torsion.....	162 B	162.3 VW	ia	
b_g	ν_{14}	CH bend.....	976 D	ia	976 W	
	ν_{15}	CH_2 wag.....	912 D	ia	912 S	
	ν_{16}	CH_2 twist.....	770 D	ia	770 VW	
b_u	ν_{17}	CH_2 a-stretch.....	3101 B	3100.6 S	ia	
	ν_{18}	CH stretch.....	3055 B	3054.9 S	ia	
	ν_{19}	CH_2 s-stretch.....	2984 B	2984.3 S	ia	
	ν_{20}	C=C stretch.....	1596 B	1596.0 S	ia	
	ν_{21}	CH_2 scis.....	1381 B	1380.7 W	ia	
	ν_{22}	CH bend.....	1294 B	1294.3 W	ia	
	ν_{23}	CH_2 rock.....	990 B	989.7 M	ia	
	ν_{24}	CCC deform.....	301 B	300.6 VW	ia	

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

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	<i>cm</i> ⁻¹ (Gas) 3100.4 S	<i>cm</i> ⁻¹ (Solid) 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			

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
				cm^{-1} (Gas)	cm^{-1}	
α'	ν_1	CH ₂ a-stretch.....	3099 C	3099.1 S		
	ν_2	CH stretch.....	3016 C	3016.4 S		
	ν_3	CH ₂ s-stretch.....	2995 C	2995.4 S		
	ν_4	CD ₂ a-stretch.....	2342 C	2341.9 S		
	ν_5	CD stretch.....	2268 C	2267.9 S		
	ν_6	CD ₂ s-stretch.....	2217 C	2217.1 S		
	ν_7	C=C stretch.....	1630 C	1630.4 M		
	ν_8	C=C stretch.....	1549 B	1548.5 S		
	ν_9	CH ₂ scis.....	1425 C	1425 M		
	ν_{10}	CH ip-bend.....	1298 C	1298 W		
	ν_{11}	C-C stretch.....	1185 C	1185 W		
	ν_{12}	CD ₂ scis.....	1080 C	1080 W		
	ν_{13}	CD ip-bend.....	992 D	991.8 W		
				(solid)		
α''	ν_{14}	CH ₂ rock.....	880 D	879.9 M		
				(solid)		
	ν_{15}	CD ₂ rock.....	757 E			CF [1].
	ν_{16}	CCC deform.....	476 E			CF [1].
	ν_{17}	CCC deform.....	280 D	280 W		
	ν_{18}	CH op-bend.....	991 B	990.6 VS		
	ν_{19}	CH ₂ wag.....	909 B	909.2 VS		
	ν_{20}	CD op-bend.....	791 B	791.3 W		
	ν_{21}	CD ₂ wag.....	715 E	{ 734.0 S 710.1 VS }		FR ($\nu_{17} + \nu_{23}$).
	ν_{22}	CH ₂ twist.....	674 B	673.8 S		
	ν_{23}	CD ₂ twist.....	439 C	439.0 M		
	ν_{24}	C-C torsion.....	153 E			CF [1].

Reference

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Solid)	
<i>a_g</i>	<i>ν</i> ₁	CH stretch	3010 D	ia	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	ia	
	<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>cm</i> ⁻¹ (Gas)	<i>cm</i> ⁻¹ (Solid)	
<i>a_g</i>	ν ₁	CD ₂ a-stretch.....	2320 D	ia	2320 M	
	ν ₂	CD stretch.....	2250 D	ia	2250 M	
	ν ₃	CD ₂ s-stretch.....	2210 D	ia	2210 M	
	ν ₄	C=C stretch.....	1580 D	ia	1580 VS	
	ν ₅	C-C stretch.....	1196 D	ia	1196 M	
	ν ₆	CD ₂ scis.....	1045 D	ia	1045 W	
	ν ₇	CD ip-bend.....	918 D	ia	918 S	
	ν ₈	CD ₂ rock.....	746 D	ia	746 M	
	ν ₉	CCC deform.....	439 D	ia	439 S	
<i>a_u</i>	ν ₁₀	CD op-bend.....	741 B	741.4 W	ia	
	ν ₁₁	CD ₂ wag.....	718 B	718.4 S	ia	
	ν ₁₂	CD ₂ twist.....	381 C	381.1 W	ia	
<i>b_g</i>	ν ₁₃	C-C torsion.....	140 C	140 VW	ia	
	ν ₁₄	CD op-bend.....	799 D	ia	799 S	
	ν ₁₅	CD ₂ wag.....	705 D	ia	705 S	
<i>b_u</i>	ν ₁₆	CD ₂ twist.....	603 D	ia	603 VW	
	ν ₁₇	CD ₂ a-stretch.....	2320 D	2320.3 M	ia	
	ν ₁₈	CD stretch.....	2266 C	2265.9 M	ia	
	ν ₁₉	CD ₂ s-stretch.....	2218 C	2218.0 M	ia	
	ν ₂₀	C=C stretch.....	1520 B	1519.6 S	ia	
	ν ₂₁	CD ₂ scis.....	1048 C	1048.0 W	ia	
	ν ₂₂	CD ip-bend.....	1005 C	1005.4 M	ia	
	ν ₂₃	CD ₂ rock.....	769 D	768.9 W	ia	
	ν 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	$\text{C}-\text{C}$ stretch	725 E	ia	1380 S	
a''_1	ν_5	CH_3 torsion ^a		ia	{ 774 M p	} FR ($2\nu_{16}$).
a''_2	ν_6	CH_3 s-stretch	2938 B	2938 S	ia	
	ν_7	CH_3 s-deform	1382 B	1382 M	ia	
	ν_8	$\text{C}-\text{C}$ stretch	1152 B	1152 W	ia	
e'	ν_9	CH_3 d-stretch	2973 B	2973 S		
	ν_{10}	CH_3 d-deform	1456 B	1456 S		
	ν_{11}	CH_3 rock	1054 B	1054 M		
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].

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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 ($2\nu_2, 2\nu_{13}$).
	ν_2	CH_2 scis	1443 C	ia	1443 p	
	ν_3	Ring stretch	1001 C	ia	1001 p	SF (ν_{13}).
	ν_4	CH_2 a-stretch	2975 E	ia		SF (ν_{14}).
	ν_5	CH_2 rock	741 C	ia	741 dp	CF [3].
	ν_6	Ring puckering	197 C	ia	197	CF [3].
a_2	ν_7	CH_2 wag	1260 E	ia	ia	CF [3].
	ν_8	CH_2 twist	1257 E	ia	ia	CF [3].
b_1	ν_9	CH_2 wag	1219 C	ia	1219 dp	
	ν_{10}	Ring deform	926 C	ia	926 dp	
	ν_{11}	CH_2 twist	1222 E	ia		CF [3].
b_2	ν_{12}	CH_2 s-stretch	2893 E			CF [3].
	ν_{13}	CH_2 scis	1443 C		1443 dp	SF (ν_2).
	ν_{14}	Ring deform	1001 D		1001 p	SF (ν_3).
	ν_{15}	CH_2 a-stretch	2987 C	2987 S		
	ν_{16}	CH_2 rock	627 C	627 S		
e	ν_{17}	CH_2 a-stretch	2952 C		2952	
	ν_{18}	CH_2 twist	1223 C	1223 W		
	ν_{19}	CH_2 rock	749 C	749 W		
	ν_{20}	CH_2 s-stretch	2887 D	{ 2897 S 2878 S }		
	ν_{21}	CH_2 scis	1447 C	1447 S		
	ν_{22}	CH_2 wag	1257 C	1257 S		
	ν_{23}	Ring deform	898 C	898 S		

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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.....	2124 E	ia		CF [2].
	<i>ν</i> ₂	CD ₂ scis.....	1160 C	ia	1160 p	
	<i>ν</i> ₃	Ring stretch.....	882 C	ia	882 p	
	<i>ν</i> ₄	CD ₂ a-stretch.....	2224 E	ia		CF [2].
	<i>ν</i> ₅	CD ₂ rock.....	632 E	ia		CF [2].
	<i>ν</i> ₆	Ring puckering.....	158 D	ia		RP [3].
<i>a</i> ₂	<i>ν</i> ₇	CD ₂ wag.....	1010 E	ia	ia	CF [2].
	<i>ν</i> ₈	CD ₂ twist.....	889 E	ia	ia	CF [2].
<i>b</i> ₁	<i>ν</i> ₉	CD ₂ wag.....	1078 C	ia	1078 dp	
	<i>ν</i> ₁₀	Ring deform.....	746 C	ia	746 dp	
<i>b</i> ₂	<i>ν</i> ₁₁	CD ₂ twist.....	864 E	ia		CF [2].
	<i>ν</i> ₁₂	CD ₂ s-stretch.....	2115 E			CF [2].
	<i>ν</i> ₁₃	CD ₂ scis.....	1040 D		1040 dp	
	<i>ν</i> ₁₄	Ring deform.....	938 D		938 dp	SF (<i>ν</i> ₁₈).
	<i>ν</i> ₁₅	CD ₂ a-stretch.....	2242 C	2242 S		
	<i>ν</i> ₁₆	CD rock.....	483 C	483 S		
<i>e</i>	<i>ν</i> ₁₇	CD ₂ a-stretch.....	2230 C		2230 dp	
	<i>ν</i> ₁₈	CD ₂ twist.....	938 D		938 dp	SF (<i>ν</i> ₁₄).
	<i>ν</i> ₁₉	CD ₂ rock.....	556 C	556 W		
	<i>ν</i> ₂₀	CD ₂ s-stretch.....	2103 E			CF [2].
	<i>ν</i> ₂₁	CD ₂ scis.....	1078 C	1078 S		
	<i>ν</i> ₂₂	CD ₂ wag.....	1048 C	1048 S		
	<i>ν</i> 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	cm^{-1} (Gas) 2991 M (solid)	cm^{-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>b</i> ₂	<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>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 (liquid)	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	999 W	
	ν_{16}	$\text{CH}_3(1)$ rock	939 C	939	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
				cm ⁻¹ (Matrix isolation)	cm ⁻¹ (Solid)	
<i>a_g</i>	ν_1	CH ₃ d-stretch.....	2965 C	ia	2965 (9)	SF (ν_{20}).
	ν_2	CH ₃ s-stretch.....	2872 C	ia	2872 (8)	
	ν_3	CH ₂ s-stretch.....	2853 D	ia	2853 (8)	
	ν_4	CH ₃ d-deform.....	1460 C	ia	1460 (2)	SF (ν_{22}).
	ν_5	CH ₂ scis.....	1442 D	ia	1442 (3)	
	ν_6	CH ₃ s-deform.....	1382 C	ia		CF [9].
	ν_7	CH ₂ wag.....	1361 D	ia		CF [9].
	ν_8	CH ₃ rock.....	1151 C	ia	1151 (4)	
	ν_9	CC stretch.....	1059 C	ia	1059 (5)	
	ν_{10}	CC stretch.....	837 C	ia	837 (6)	
	ν_{11}	CCC deform.....	425 C	ia	425 (4)	
<i>a_u</i>	ν_{12}	CH ₃ d-stretch.....	2968 C	2968 S	ia	SF (ν_{27}).
	ν_{13}	CH ₂ a-stretch.....	2930 C	2930 S	ia	
	ν_{14}	CH ₃ d-deform.....	1461 C	1461 S	ia	SF (ν_{30}), OV (ν_{30} , ν_{31})
	ν_{15}	CH ₂ twist.....	1257 C	1257 W (solid)	ia	
	ν_{16}	CH ₃ rock.....	948 B	948 M	ia	
	ν_{17}	CH ₂ rock.....	731 B	731 S	ia	
	ν_{18}	CH ₃ -CH ₂ torsion.....	194 E		ia	CF [9].
	ν_{19}	CH ₂ -CH ₂ torsion.....	102 E		ia	CF [9].
	ν_{20}	CH ₃ d-stretch.....	2965 C	ia	2965 (9)	SF (ν_1).
	ν_{21}	CH ₂ a-stretch.....	2912 C	ia	2912 (4)	
	ν_{22}	CH ₃ d-deform.....	1460 C	ia	1460 (2)	SF (ν_4).
<i>b_g</i>	ν_{23}	CH ₂ twist.....	1300 C	ia	1300 (4)	
	ν_{24}	CH ₃ rock.....	1180 D	ia		CF [9].
	ν_{25}	CH ₂ rock.....	803 D	ia		CF [9].
	ν_{26}	CH ₃ -CH ₂ torsion.....	225 E	ia		CF [9].
	ν_{27}	CH ₃ d-stretch.....	2968 C	2968 S	ia	SF (ν_{12}).
	ν_{28}	CH ₃ s-stretch.....	2870 C	2870 S	ia	
	ν_{29}	CH ₂ s-stretch.....	2853 E		ia	SF (ν_3).
	ν_{30}	CH ₃ d-deform.....	1461 C	1461 S	ia	SF (ν_{14}), OV (ν_{14} , ν_{31}).
	ν_{31}	CH ₂ scis.....	1461 C	1461 S	ia	OV (ν_{14} , ν_{30}).
	ν_{32}	CH ₃ s-deform.....	1379 B	1379 M	ia	
	ν_{33}	CH ₂ wag.....	1290 B	1290 W	ia	
	ν_{34}	CC stretch.....	1009 C	1009 W (solid)	ia	
<i>b_u</i>	ν_{35}	CH ₃ rock.....	964 B	964 M	ia	
	ν_{36}	CCC deform.....	271 E		ia	CF [9].

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^a Deduced from the corresponding frequencies of the trans form.

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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	
b_{2g}	ν_7	CH bend.....	995 E	ia	ia	OC ($\nu_{19} + \nu_7, \nu_{20} + \nu_7$).
	ν_8	Ring deform.....	703 E	ia	ia	OC ($\nu_{19} + \nu_8, \nu_{20} + \nu_8$).
b_{2u}	ν_9	Ring stretch.....	1310 C	1310 W (liquid)	ia	
	ν_{10}	CH bend.....	1150 C	1150 W (liquid)	ia	
e_{1g}	ν_{11}	CH bend.....	849 C	ia	848.9 M, dp	
e_{1u}	ν_{12}	CH stretch.....	3063 E	{ 3080 S 3030 S (liquid)	ia	FR ($\nu_{13} + \nu_{16}$).
	ν_{13}	Ring stretch + deform.....	1486 B	1486 S	ia	
	ν_{14}	CH bend.....	1038 B	1038 S	ia	
e_{2g}	ν_{15}	CH stretch.....	3047 C	ia	3046.8 S, dp	
	ν_{16}	Ring stretch.....	1596 E	ia	{ 1606.4 S, dp 1584.6 S, dp	FR ($\nu_2 + \nu_{18}$).
	ν_{17}	CH bend.....	1178 C	ia	1178.0 S, dp	
	ν_{18}	Ring deform.....	606 C	ia	605.6 S, dp	
e_{2u}	ν_{19}	CH bend.....	975 C	975 W (liquid)	ia	
	ν_{20}	Ring deform.....	410 C	{ 417.7 403.0 (solid)	ia	

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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	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	943.2 VS, p	
<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	OC (<i>ν</i> ₇ + <i>ν</i> ₁₉). OC (<i>ν</i> ₈ + <i>ν</i> ₁₉).
	<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	
	<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	OC (<i>ν</i> ₇ + <i>ν</i> ₁₉). OC (<i>ν</i> ₈ + <i>ν</i> ₁₉).
	<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	OC (<i>ν</i> ₄ + <i>ν</i> ₂₀ , <i>ν</i> ₁₄ + <i>ν</i> ₂₀).
	<i>ν</i> ₁₄	CD bend.....	814 B	814 S	ia	
<i>e</i> _{2g}	<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	OC (<i>ν</i> ₄ + <i>ν</i> ₂₀ , <i>ν</i> ₁₄ + <i>ν</i> ₂₀).
	<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	

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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 ($2\nu_3$).
	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 ($\nu_2, \nu_{13}, \nu_{26}$).
	ν_{14}	CH_2 scis.....	1437 C	1437 M	ia	
	ν_{15}	CH_2 rock.....	1030 D	{ 1040 M 1016 M	ia	FR ($\nu_{23} + \nu_{32}$).
				523 W	ia	
e_g	ν_{16}	CCC deform.....	523 A			SF ($\nu_1, \nu_{12}, \nu_{25}$).
	ν_{17}	CH_2 a-stretch.....	2930 E	ia		
	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
				cm ⁻¹ (Gas)	cm ⁻¹ (Liquid)	
<i>a_{1g}</i>	<i>ν</i> ₁	CD ₂ a-stretch.....	2152 C	ia	2152 VS, p	
	<i>ν</i> ₂	CD ₂ s-stretch.....	2082 C	ia	2082 VS, p	
	<i>ν</i> ₃	CD ₂ scis.....	1117 C	ia	1117 M, p	
	<i>ν</i> ₄	CD ₂ rock.....	1012 C	ia	1012 W, p	
	<i>ν</i> ₅	CC stretch.....	723 C	ia	723 VS, p	
	<i>ν</i> ₆	CCC deform. + CC torsion.....	298 C	ia	298 W, p	
<i>a_{1u}</i>	<i>ν</i> ₇	CD ₂ twist.....	864 E	ia	ia	CF [4].
	<i>ν</i> ₈	CD ₂ wag.....	842 E	ia	ia	CF [4].
	<i>ν</i> ₉	CC stretch. + CC torsion.....	1187 E	ia	ia	CF [4].
<i>a_{2g}</i>	<i>ν</i> ₁₀	CD ₂ wag.....	1126 E	ia	ia	CF [4].
	<i>ν</i> ₁₁	CD ₂ twist.....	778 E	ia	ia	CF [4].
<i>a_{2u}</i>	<i>ν</i> ₁₂	CD ₂ a-stretch.....	2206 C	2206 VS	ia	OV (<i>ν</i> ₂₅).
	<i>ν</i> ₁₃	CD ₂ s-stretch.....	2108 C	2108 VS	ia	OV (<i>ν</i> ₂₆).
	<i>ν</i> ₁₄	CD ₂ scis.....	1091 B	1091 VS	ia	
	<i>ν</i> ₁₅	CD ₂ rock.....	917 A	917 VS	ia	
	<i>ν</i> ₁₆	CCC deform.....	395 B	395 S	ia	
	<i>ν</i> ₁₇	CD ₂ a-stretch.....	2199 C	ia	2199 VS, dp	
<i>e_g</i>	<i>ν</i> ₁₈	CD s-stretch.....	2104 C	ia	2104 VS, dp	
	<i>ν</i> ₁₉	CD ₂ scis.....	1071 C	ia	1071 M, dp	
	<i>ν</i> ₂₀	CD ₂ wag.....	1212 C	ia	1212 M, dp	
	<i>ν</i> ₂₁	CD ₂ twist.....	937 C	ia	937 S, dp	
	<i>ν</i> ₂₂	CC stretch.....	795 C	ia	795 S, dp	
	<i>ν</i> ₂₃	CD ₂ rock.....	637 C	ia	637 W, dp	
	<i>ν</i> ₂₄	CCC deform. + CC torsion.....	373 C	ia	373 M, dp	
	<i>ν</i> ₂₅	CD ₂ a-stretch.....	2206 C	2206 VS	ia	OV (<i>ν</i> ₁₂).
<i>e_u</i>	<i>ν</i> ₂₆	CD ₂ s-stretch.....	2108 C	2108 VS	ia	OV (<i>ν</i> ₁₃).
	<i>ν</i> ₂₇	CD ₂ scis.....	1069 C	1069 M (liquid)	ia	
	<i>ν</i> ₂₈	CD ₂ wag.....	1165 A	1165 VS	ia	
	<i>ν</i> ₂₉	CD ₂ twist.....	991 A	991 VS	ia	
	<i>ν</i> ₃₀	CD ₂ rock.....	687 B	687 S	ia	
	<i>ν</i> ₃₁	CC stretch.....	720 A	720 S	ia	
	<i>ν</i> 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>ν</i> ₁	CH ₂ s-stretch.....	2848 C	ia	2848 S	
	<i>ν</i> ₂	CH ₂ scis.....	1440 C	ia	1440 M	
	<i>ν</i> ₃	CC stretch.....	1131 C	ia	1131 M	
<i>a_u</i>	<i>ν</i> ₄	CH ₂ twist.....	^a 1050 D	ia, 1050 VW	ia	
<i>b_{1g}</i>	<i>ν</i> ₅	CH ₂ wag.....	1370 D	ia	1370 VW	
	<i>ν</i> ₆	CC stretch.....	1061 C	ia	1061 M	
<i>b_{1u}</i>	<i>ν</i> ₇	CH ₂ a-stretch.....	2919 C	2919 S	ia	
	<i>ν</i> ₈	CH ₂ rock.....	725 C	^b { 731 S 720 S }	ia	
<i>b_{2g}</i>	<i>ν</i> ₉	CH ₂ twist.....	1295 C	ia	1295 M	
<i>b_{2u}</i>	<i>ν</i> ₁₀	CH ₂ s-stretch.....	2851 C	2851 S	ia	
	<i>ν</i> ₁₁	CH ₂ scis.....	1468 C	^b { 1473 S 1463 S }	ia	
<i>b_{3g}</i>	<i>ν</i> ₁₂	CH ₂ a-stretch.....	2883 C	ia	2883 S	
	<i>ν</i> ₁₃	CH ₂ rock.....	1168 C	ia	1168 W	
<i>b_{3u}</i>	<i>ν</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>cm</i> ⁻¹ (Solid)	<i>cm</i> ⁻¹ (Solid)	
<i>a_g</i>	<i>ν</i> ₁	CD ₂ s-stretch	2102 C	ia	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</i> _{1<i>g</i>}	<i>ν</i> ₅	CD ₂ wag	1249 C	ia	1249 W	
	<i>ν</i> ₆	CC stretch	820 E	ia		CF [5].
<i>b</i> _{1<i>u</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</i> _{2<i>g</i>}	<i>ν</i> ₉	CD ₂ twist	916 C	ia	916 M	
<i>b</i> _{2<i>u</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</i> _{3<i>g</i>}	<i>ν</i> ₁₂	CD ₂ a-stretch	2197 C	ia	2197 M	CF [5].
	<i>ν</i> ₁₃	CD ₂ rock	991 C	ia	991 M	
<i>b</i> _{3<i>u</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
ClI 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 ¹⁶ 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 ₂ N ₂	Malononitrile	183
C ₂ Br ₄	Tetrabromoethylene	128	C ₃ H ₂ 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 ₃ H ₄	Methylacetylene-d ₁	180
C ₂ Cl ₂ F ₂	1,1-Dichloro-2,2-difluoroethylene	142	C ₃ H ₄	Methylacetylene-d ₃	181
C ₂ Cl ₄	Tetrachloroethylene	127	C ₃ H ₄	Methylacetylene-d ₄	182
C ₂ Cl ₆	Hexachloroethane	158	C ₃ H ₄ O	Propenal	185
C ₂ F ₄	Tetrafluoroethylene	126	C ₃ H ₅ N	Ethylecyanide	188
C ₂ F ₆	Hexafluoroethane	157	C ₃ H ₆	Cyclopropane	186
C ₂ HBr	Bromoacetylene	123	C ₃ H ₆	Cyclopropane-d ₆	187
C ₂ HCl	Chloroacetylene	122	C ₃ H ₆ O	Acetone	189
C ₂ HF	Fluoroacetylene	121	C ₃ H ₆ O	Acetone-d ₃	190
C ₂ H ₂	Acetylene	118	C ₃ H ₆ O	Acetone-d ₆	191
C ₂ H ₂	Acetylene-d ₁	119	C ₃ H ₆ O ₂	Methyl acetate	197
C ₂ H ₂	Acetylene-d ₂	120	C ₃ H ₆ O ₂	Methyl-d ₃ -acetate	198
C ₂ H ₂ Cl ₂	Trans-1,2-Dichloroethylene	132	C ₃ H ₆ O ₂	Methyl acetate-d ₃	199
C ₂ H ₂ Cl ₂	Trans-1,2-Dichloroethylene-d ₁	133	C ₃ H ₆ O ₂	Methyl acetate-d ₆	200
C ₂ H ₂ Cl ₂	Trans-1,2-Dichloroethylene-d ₂	134	C ₃ H ₈	Propane	192
C ₂ H ₂ Cl ₂	Cis-1,2-Dichloroethylene	135	C ₃ H ₈	Propane-d ₃	193
C ₂ H ₂ Cl ₂	Cis-1,2-Dichloroethylene-d ₁	136	C ₃ H ₈	Propane-d ₂	194
C ₂ H ₂ Cl ₂	Cis-1,2-Dichloroethylene-d ₂	137	C ₃ H ₈	Propane-d ₆	195
C ₂ H ₂ Cl ₂	1,1-Dichloroethylene	139	C ₃ H ₈	Propane-d ₃	196
C ₂ H ₂ Cl ₂	1,1-Dichloroethylene-d ₁	140	C ₄ H ₂	Butadiyne	201
C ₂ H ₂ Cl ₂	1,1-Dichloroethylene-d ₂	141	C ₄ H ₄ O	Furan	202
C ₂ H ₂ F ₂	Cis-1,2-Difluoroethylene	129	C ₄ H ₄ S	Thiophene	203
C ₂ H ₂ F ₂	Cis-1,2-Difluoroethylene-d ₁	130	C ₄ H ₄ S	Thiophene-d ₄	204
C ₂ H ₂ F ₂	Cis-1,2-Difluoroethylene-d ₂	131	C ₄ H ₆	1,3-Butadiene	205
C ₂ H ₂ N ₂ O	1,2,5-Oxadiazole	147	C ₄ H ₆	1,3-Butadiene-d ₁ , trans	206
C ₂ H ₃ N	Methyl cyanide	143	C ₄ H ₆	1,3-Butadiene-1,1,2-d ₃	207
C ₂ H ₃ N	Methyl cyanide-d ₃	144	C ₄ H ₆	1,3-Butadiene-1,1,4,4-d ₄	208
C ₂ H ₃ N	Methyl isocyanide	145	C ₄ H ₆	1,3-Butadiene-d ₆	209

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

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