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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]<sup>1</sup> 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.

<sup>1</sup> 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,  $\sigma$ , 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  $\nu_i$  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  $\nu_2$ , 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  $\nu_i$  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  $\nu_i$  is defined as the difference between the term values  $G(v_i = 1, \text{ all other } v_j = 0)$  and  $G(v_i = 0, \text{ and other } v_j = 0)$  expressed in  $\text{cm}^{-1}$ . Fundamental frequencies rather than harmonic frequencies ( $\omega_i$ ) 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  $1 \text{ cm}^{-1}$ .

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  $\text{cm}^{-1}$  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  $\nu_0$  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  $\zeta$  is the Coriolis coupling constant. This is in accord with the definition of  $\nu_0$  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  $\text{cm}^{-1}$ ) 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

- [1] Herzberg, G., *Spectra of Diatomic Molecules*, Second Edition (Van Nostrand, New York, 1950).
- [2] Herzberg, G., *Electronic Spectra of Polyatomic Molecules* (Van Nostrand, New York, 1966).
- [3] Wilson, E. Bright, Jr., Decius, J. C., Cross, Paul C., *Molecular Vibrations* (McGraw-Hill, New York, 1955).
- [4] Herzberg, G., *Infrared and Raman Spectra of Polyatomic Molecules* (Van Nostrand, New York, 1945).
- [5] Shimanouchi, T., *Molecular Force Field*, in *Physical Chemistry*, edited by Eyring, Henderson, and Jost. Vol. 4, chap. 6, New York, 1970 (Academic Press).
- [6] Starck, B., *Landolt-Börnstein Numerical Data and Functional Relationships in Science and Technology*, New Series, Group II, Vol. 4 (Springer-Verlag, Berlin, 1967).

## 4. Tables of Vibrational Frequencies

### C<sub>0</sub>-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, $\text{H}_2\text{O}$ .....	10
			5	Water-d <sub>1</sub> , $\text{HDO}$ .....	10

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

### C<sub>0</sub>-four-atomic molecules

14 Ammonia, NH <sub>3</sub>	15
15 Ammonia-d <sub>3</sub> , ND <sub>3</sub>	15
16 Nitrogen trifluoride, NF <sub>3</sub>	16
17 Phosphine, PH <sub>3</sub>	16
18 Phosphine-d <sub>3</sub> , PD <sub>3</sub>	17
19 Phosphorus trifluoride, PF <sub>3</sub>	17
20 Phosphorus trichloride, PCl <sub>3</sub>	18
21 Arsine, AsH <sub>3</sub>	18
22 Arsine-d <sub>3</sub> , AsD <sub>3</sub>	19
23 Stibine, SbH <sub>3</sub>	19
24 Stibine-d <sub>3</sub> , SbD <sub>3</sub>	20

### C<sub>0</sub>-five-atomic molecules

25 Silane, SiH <sub>4</sub>	20
26 Silane-d <sub>2</sub> , SiH <sub>2</sub> D <sub>2</sub>	21
27 Silane-d <sub>3</sub> , SiHD <sub>3</sub>	21
28 Silane-d <sub>4</sub> , SiD <sub>4</sub>	22
29 Silicon tetrafluoride, SiF <sub>4</sub>	22
30 Silicon tetrachloride, SiCl <sub>4</sub>	23
31 Silicon tetrabromide, SiBr <sub>4</sub>	23
32 Silicon tetraiodide, SiI <sub>4</sub>	24
33 Germane, GeH <sub>4</sub>	24
34 Germane-d <sub>1</sub> , GeH <sub>3</sub> D	25
35 Germane-d <sub>2</sub> , GeH <sub>2</sub> D <sub>2</sub>	25
36 Germane-d <sub>3</sub> , GeHD <sub>3</sub>	26
37 Germane-d <sub>4</sub> , GeD <sub>4</sub>	26
38 Germanium tetrachloride, GeCl <sub>4</sub>	27
39 Germanium tetrabromide, GeBr <sub>4</sub>	27
40 Tin tetrachloride, SnCl <sub>4</sub>	28
41 Tin tetrabromide, SnBr <sub>4</sub>	28
42 Silyl fluoride, SiH <sub>3</sub> F	29
43 Silyl chloride, SiH <sub>3</sub> Cl	29
44 Silyl bromide, SiH <sub>3</sub> Br	30
45 Bromotrichlorosilane, SiBrCl <sub>3</sub>	30
46 Trichloriodosilane, SiCl <sub>3</sub> I	31
47 Tribromochlorosilane, SiBr <sub>3</sub> Cl	31
48 Chlorotriiodosilane, SiClI <sub>3</sub>	32
49 Dibromodichlorosilane, SiBr <sub>2</sub> Cl <sub>2</sub>	32

### C<sub>0</sub>-seven-atomic molecules

50 Sulfur hexafluoride, SF <sub>6</sub>	33
51 Selenium hexafluoride, SeF <sub>6</sub>	33
52 Molybdenum hexafluoride, MoF <sub>6</sub>	34
53 Tungsten hexafluoride, WF <sub>6</sub>	34
54 Uranium hexafluoride, UF <sub>6</sub>	35

### C<sub>0</sub>-eight-atomic molecules

	Page
55 Diborane, <sup>10</sup> B <sub>2</sub> H <sub>6</sub>	36
56 Diborane, <sup>11</sup> B <sub>2</sub> H <sub>6</sub>	37
57 Diborane-d <sub>6</sub> , <sup>10</sup> B <sub>2</sub> D <sub>6</sub>	38

### C<sub>1</sub>-triatomic molecules

58 Carbon dioxide, <sup>12</sup> C <sup>16</sup> O <sub>2</sub>	39
59 Carbon dioxide, <sup>13</sup> C <sup>16</sup> O <sub>2</sub>	39
60 Carbon disulfide, <sup>12</sup> C <sup>32</sup> S <sub>2</sub>	40
61 Carbonyl sulfide, <sup>12</sup> C <sup>16</sup> O <sup>32</sup> S	40
62 Hydrogen cyanide, HCN	41
63 Deuterium cyanide, DCN	41
64 Cyanogen chloride, <sup>35</sup> ClCN	42
65 Cyanogen chloride, <sup>37</sup> ClCN	42
66 Cyanogen bromide, <sup>79</sup> BrCN	43
67 Cyanogen bromide, <sup>81</sup> BrCN	43

### C<sub>1</sub>-four-atomic molecules

68 Formaldehyde, H <sub>2</sub> CO	44
69 Formaldehyde-d <sub>1</sub> , HDCO	44
70 Formaldehyde-d <sub>2</sub> , D <sub>2</sub> CO	45

### C<sub>1</sub>-five-atomic molecules

71 Methane, CH <sub>4</sub>	45
72 Methane-d <sub>1</sub> , CH <sub>3</sub> D	46
73 Methane-d <sub>2</sub> , CH <sub>2</sub> D <sub>2</sub>	46
74 Methane-d <sub>3</sub> , CHD <sub>3</sub>	47
75 Methane-d <sub>4</sub> , CD <sub>4</sub>	47
76 Carbon tetrafluoride, CF <sub>4</sub>	48
77 Carbon tetrachloride, CCl <sub>4</sub>	48
78 Carbon tetrabromide, CBr <sub>4</sub>	49
79 Carbon tetraiodide, CI <sub>4</sub>	49
80 Methyl fluoride, CH <sub>3</sub> F	50
81 Methyl fluoride-d <sub>3</sub> , CD <sub>3</sub> F	50
82 Methyl chloride, CH <sub>3</sub> Cl	51
83 Methyl chloride-d <sub>3</sub> , CD <sub>3</sub> Cl	51
84 Methyl bromide, CH <sub>3</sub> Br	52
85 Methyl bromide-d <sub>3</sub> , CD <sub>3</sub> Br	52
86 Methyl iodide, CHI <sub>3</sub>	53
87 Methyl iodide-d <sub>3</sub> , CD <sub>3</sub> I	53
88 Trifluoromethane, CHF <sub>3</sub>	54
89 Trichloromethane, CHCl <sub>3</sub>	54
90 Trichloromethane-d <sub>1</sub> , CDCl <sub>3</sub>	55
91 Tribromomethane, CHBr <sub>3</sub>	55
92 Tribromomethane-d <sub>1</sub> , CDBr <sub>3</sub>	56
93 Bromotrichloromethane, CBrCl <sub>3</sub>	56
94 Tribromochloromethane, CBr <sub>3</sub> Cl	57
95 Dichloromethane, CH <sub>2</sub> Cl <sub>2</sub>	57
96 Dichloromethane-d <sub>1</sub> , CHDCl <sub>2</sub>	58
97 Dichloromethane-d <sub>2</sub> , CD <sub>2</sub> Cl <sub>2</sub>	58
98 Dibromomethane, CH <sub>2</sub> Br <sub>2</sub>	59
99 Dibromomethane-d <sub>1</sub> , CHDBr <sub>2</sub>	59
100 Dibromomethane-d <sub>2</sub> , CD <sub>2</sub> Br <sub>2</sub>	60
101 Dibromodichloromethane, CBr <sub>2</sub> Cl <sub>2</sub>	60
102 Bromochloromethane, CH <sub>2</sub> BrCl	61
103 Bromochloromethane-d <sub>1</sub> , CHDBrCl	61
104 Bromochloromethane-d <sub>2</sub> , CD <sub>2</sub> BrCl	62



		Page
105	Formic acid, $\text{HCOOH}$ .....	62
106	Formic acid- $\text{d}_2$ , $\text{DCOOD}$ .....	63

### C<sub>1</sub>-six-atomic molecules

107	Methanol, $\text{CH}_3\text{OH}$ (Gas).....	63
108	Methanol, $\text{CH}_3\text{OH}$ (Liquid).....	64
109	Methanol- $\text{d}_1$ , $\text{CH}_3\text{OD}$ (Gas).....	64
110	Methanol- $\text{d}_1$ , $\text{CH}_3\text{OD}$ (liquid).....	65
111	Methanol- $\text{d}_3$ , $\text{CD}_3\text{OH}$ (gas).....	65
112	Methanol- $\text{d}_3$ , $\text{CD}_3\text{OH}$ (liquid).....	66
113	Methanol- $\text{d}_4$ , $\text{CD}_3\text{OD}$ (gas).....	66

### C<sub>1</sub>-seven-atomic molecules

114	Methylamine, $\text{CH}_3\text{NH}_2$ .....	67
115	Methylamine- $\text{d}_2$ , $\text{CH}_3\text{ND}_2$ .....	68
116	Methylamine- $\text{d}_3$ , $\text{CD}_3\text{NH}_2$ .....	69
117	Methylamine- $\text{d}_5$ , $\text{CD}_3\text{ND}_2$ .....	70

### C<sub>2</sub>-four-atomic molecules

118	Acetylene, $\text{CHCH}$ .....	71
119	Acetylene- $\text{d}_1$ , $\text{CHCD}$ .....	71
120	Acetylene- $\text{d}_2$ , $\text{CDCD}$ .....	72
121	Fluoroacetylene, $\text{CHCF}$ .....	72
122	Chloroacetylene, $\text{CHCCl}$ .....	73
123	Bromoacetylene, $\text{CHCBr}$ .....	73

### C<sub>2</sub>-six-atomic molecules

124	Ethylene, $\text{CH}_2\text{CH}_2$ .....	74
125	Ethylene- $\text{d}_4$ , $\text{C}_2\text{D}_4$ .....	75
126	Tetrafluoroethylene, $\text{CF}_2\text{CF}_2$ .....	75
127	Tetrachloroethylene, $\text{CCl}_2\text{CCl}_2$ .....	76
128	Tetrabromoethylene, $\text{CBr}_2\text{CBr}_2$ .....	76
129	cis-1,2-Difluoroethylene, $\text{CHFCHF}$ .....	77
130	cis-1,2-Difluoroethylene- $\text{d}_1$ , $\text{CHFCHF}$ .....	77
131	cis-1,2-Difluoroethylene- $\text{d}_2$ , $\text{CDFCDF}$ .....	78
132	trans-1,2-Dichloroethylene, $\text{CHClCHCl}$ .....	78
133	trans-1,2-Dichloroethylene- $\text{d}_1$ , $\text{CHClCHCl}$ .....	79
134	trans-1,2-Dichloroethylene- $\text{d}_2$ , $\text{CDClCDCl}$ .....	79
135	cis-1,2-Dichloroethylene, $\text{CHClCHCl}$ .....	80
136	cis-1,2-Dichloroethylene- $\text{d}_1$ , $\text{CHClCHCl}$ .....	80
137	cis-1,2-Dichloroethylene- $\text{d}_2$ , $\text{CDClCDCl}$ .....	81
138	trans-1,2-Dichloro-1,2-difluoroethylene, $\text{CFCICFCl}$ .....	81
139	1,1-Dichloroethylene, $\text{CH}_2\text{CCl}_2$ .....	82
140	1,1-Dichloroethylene- $\text{d}_1$ , $\text{CHDCCl}_2$ .....	82
141	1,1-Dichloroethylene- $\text{d}_2$ , $\text{CD}_2\text{CCl}_2$ .....	83
142	1,1-Dichloro-2,2-difluoroethylene, $\text{CF}_2\text{CCl}_2$ .....	83
143	Methyl cyanide, $\text{CH}_3\text{CN}$ .....	84
144	Methyl cyanide- $\text{d}_3$ , $\text{CD}_3\text{CN}$ .....	84
145	Methylisocyanide, $\text{CH}_3\text{NC}$ .....	85
146	Methylisocyanide- $\text{d}_3$ , $\text{CD}_3\text{NC}$ .....	85

### C<sub>2</sub>-seven-atomic molecules

147	1,2,5-Oxadiazole, $\text{C}_2\text{H}_2\text{N}_2\text{O}$ .....	86
148	Silylacetylene, $\text{SiH}_3\text{CCH}$ .....	86

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149	Ethylene oxide, $\text{C}_2\text{H}_4\text{O}$ .....	87
150	Ethylene oxide- $\text{d}_4$ , $\text{C}_2\text{D}_4\text{O}$ .....	88
151	Acetaldehyde, $\text{CH}_3\text{CHO}$ .....	89
152	Acetaldehyde- $\text{d}_1$ , $\text{CH}_3\text{CDO}$ .....	90
153	Acetaldehyde- $\text{d}_4$ , $\text{CD}_3\text{CDO}$ .....	91

### C<sub>2</sub>-eight-atomic molecules

154	Ethane, $\text{CH}_3\text{CH}_3$ .....	92
155	Ethane-1,1,1- $\text{d}_3$ , $\text{CH}_3\text{CD}_3$ .....	93
156	Ethane- $\text{d}_6$ , $\text{CD}_3\text{CD}_3$ .....	94
157	Hexafluoroethane, $\text{CF}_3\text{CF}_3$ .....	95
158	Hexachloroethane, $\text{CCl}_3\text{CCl}_3$ .....	95
159	Hexabromoethane, $\text{CBr}_3\text{CBr}_3$ .....	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, $\text{HCOOCH}_3$ .....	107
171	Methyl formate- $\text{d}_1$ , $\text{DCOOCH}_3$ .....	108
172	Methyl formate- $\text{d}_3$ , $\text{HCOOCD}_3$ .....	109
173	Methyl formate- $\text{d}_4$ , $\text{DCOOCD}_3$ .....	110
174	Acetic acid, $\text{CH}_3\text{COOH}$ .....	111
175	Acetic acid- $\text{d}_1$ , $\text{CH}_3\text{COOD}$ .....	112

### C<sub>2</sub>-nine-atomic molecules

176	Dimethylether, $\text{CH}_3\text{OCH}_3$ .....	113
177	Dimethylether- $\text{d}_3$ , $\text{CH}_3\text{OCD}_3$ .....	114

### C<sub>3</sub>-seven-atomic molecules

178	Allene, $\text{CH}_2\text{CCH}_2$ .....	115
179	Methylacetylene, $\text{CH}_3\text{CCH}$ .....	116
180	Methylacetylene- $\text{d}_1$ , $\text{CH}_3\text{CCD}$ .....	116
181	Methyl- $\text{d}_3$ -acetylene, $\text{CD}_3\text{CCH}$ .....	117
182	Methylacetylene- $\text{d}_4$ , $\text{CD}_3\text{CCD}$ .....	117
183	Malononitrile, $\text{NCCH}_2\text{CN}$ .....	118
184	Malononitrile- $\text{d}_2$ , $\text{NCCD}_2\text{CN}$ .....	118

### C<sub>3</sub>-eight-atomic molecules

185	Propenal, $\text{CH}_2\text{CHCHO}$ .....	119
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### C<sub>3</sub>-nine-atomic molecules

186	Cyclopropane, $\text{C}_3\text{H}_6$ .....	120
187	Cyclopropane- $\text{d}_6$ , $\text{C}_3\text{D}_6$ .....	121
188	Ethylcyanide, $\text{CH}_3\text{CH}_2\text{CN}$ .....	122

	Page		Page
<b>C<sub>3</sub>-ten-atomic molecules</b>		209	1,3-Butadiene-d <sub>6</sub> , CD <sub>2</sub> CD <sub>2</sub> CD <sub>2</sub> ..... 143
189	Acetone, CH <sub>3</sub> COCH <sub>3</sub> ..... 123	210	2-Butyne, CH <sub>3</sub> CCCH <sub>3</sub> ..... 144
190	Acetone-α,α,α-d <sub>3</sub> , CH <sub>3</sub> COCD <sub>3</sub> ..... 124	<b>C<sub>4</sub>-12-atomic molecules</b>	
191	Acetone-d <sub>6</sub> , CD <sub>3</sub> COCD <sub>3</sub> ..... 125	211	Cyclobutane, C <sub>4</sub> H <sub>8</sub> ..... 145
<b>C<sub>3</sub>-11-atomic molecules</b>		212	Cyclobutane-d <sub>8</sub> , C <sub>4</sub> D <sub>8</sub> ..... 146
192	Propane, CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub> ..... 126	213	2-Methylpropene, (CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> ..... 147
193	Propane-2,2-d <sub>2</sub> , CH <sub>3</sub> CD <sub>2</sub> CH <sub>3</sub> ..... 127	214	2-Methyl-d <sub>3</sub> -propene-3,3,3-d <sub>3</sub> , (CD <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> ... 148
194	Propane-1,1,1-d <sub>3</sub> , CH <sub>3</sub> CH <sub>2</sub> CD <sub>3</sub> ..... 128	<b>C<sub>4</sub>-13-atomic molecules</b>	
195	Propane-1,1,1,3,3,3-d <sub>6</sub> , CD <sub>3</sub> CH <sub>2</sub> CD <sub>3</sub> ..... 129	215	2-Butanone CH <sub>3</sub> COCH <sub>2</sub> CH <sub>3</sub> (trans form)..... 149
196	Propane-d <sub>8</sub> , CD <sub>3</sub> CD <sub>2</sub> CD <sub>3</sub> ..... 130	<b>C<sub>4</sub>-14-atomic molecules</b>	
197	Methyl acetate, CH <sub>3</sub> COOCH <sub>3</sub> ..... 131	216	n-Butane, CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> (trans form)..... 150
198	Methyl acetate-d <sub>3</sub> , CD <sub>3</sub> COOCH <sub>3</sub> ..... 132	217	n-Butane, CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> (gauche form).... 151
199	Methyl-d <sub>3</sub> -acetate, CH <sub>3</sub> COOCD <sub>3</sub> ..... 133	<b>C<sub>6</sub>-12-atomic molecules</b>	
200	Methyl acetate-d <sub>6</sub> , CD <sub>3</sub> COOCD <sub>3</sub> ..... 134	218	Benzene, C <sub>6</sub> H <sub>6</sub> ..... 152
<b>C<sub>4</sub>-six-atomic molecules</b>		219	Benzene-d <sub>6</sub> , C <sub>6</sub> D <sub>6</sub> ..... 153
201	Butadiyne, HCCCCH..... 135	<b>C<sub>6</sub>-18-atomic molecules</b>	
<b>C<sub>4</sub>-nine-atomic molecules</b>		220	Cyclohexane, C <sub>6</sub> H <sub>12</sub> ..... 154
202	Furan, C <sub>4</sub> H <sub>4</sub> O..... 136	221	Cyclohexane-d <sub>12</sub> , C <sub>6</sub> D <sub>12</sub> ..... 155
203	Thiophene, C <sub>4</sub> H <sub>4</sub> S..... 137	<b>Polymer</b>	
204	Thiophene-d <sub>4</sub> , C <sub>4</sub> D <sub>4</sub> S..... 138	222	Poly (methylene), (CH <sub>2</sub> ) <sub>n</sub> ..... 156
<b>C<sub>4</sub>-ten-atomic molecules</b>		223	Poly (methylene-d <sub>2</sub> ), (CD <sub>2</sub> ) <sub>n</sub> ..... 157
205	1,3-Butadiene, CH <sub>2</sub> CHCHCH <sub>2</sub> ..... 139		
206	1,3-Butadiene-1-d <sub>1</sub> (trans), CH <sub>2</sub> CHCHCHD... 140		
207	1,3-Butadiene-1,1,2-d <sub>3</sub> , CH <sub>2</sub> CHCD <sub>2</sub> CD <sub>2</sub> ..... 141		
208	1,3-Butadiene-1,1,4,4-d <sub>4</sub> , CD <sub>2</sub> CHCHCD <sub>2</sub> ... 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 <sub>2</sub>	A, B	D <sub>3h</sub>	A <sub>1</sub> ', A <sub>1</sub> '', A <sub>2</sub> ', A <sub>2</sub> '', E', E''
C <sub>s</sub>	A', A''	D <sub>5h</sub>	A <sub>1</sub> ', A <sub>1</sub> '', A <sub>2</sub> ', A <sub>2</sub> '', E <sub>1</sub> ', E <sub>1</sub> '', E <sub>2</sub> ', E <sub>2</sub> ''
C <sub>i</sub>	A <sub>g</sub> , A <sub>u</sub>	D <sub>4h</sub>	A <sub>1g</sub> , A <sub>1u</sub> , A <sub>2g</sub> , A <sub>2u</sub> , B <sub>1g</sub> , B <sub>1u</sub> , B <sub>2g</sub> , B <sub>2u</sub> , E <sub>g</sub> , E <sub>u</sub>
C <sub>2v</sub>	A <sub>1</sub> , A <sub>2</sub> , B <sub>1</sub> , B <sub>2</sub>	D <sub>6h</sub>	A <sub>1g</sub> , A <sub>1u</sub> , A <sub>2g</sub> , A <sub>2u</sub> , B <sub>1g</sub> , B <sub>1u</sub> , B <sub>2g</sub> , B <sub>2u</sub> , E <sub>1g</sub> , E <sub>1u</sub> , E <sub>2g</sub> , E <sub>2u</sub>
C <sub>2h</sub>	A <sub>g</sub> , A <sub>u</sub> , B <sub>g</sub> , B <sub>u</sub>	D <sub>∞h</sub>	Σ <sub>g</sub> <sup>+</sup> , Σ <sub>u</sub> <sup>+</sup> , Σ <sub>g</sub> <sup>-</sup> , Σ <sub>u</sub> <sup>-</sup> , π <sub>g</sub> , π <sub>u</sub> , Δ <sub>g</sub> , Δ <sub>u</sub> , Φ <sub>g</sub> , Φ <sub>u</sub> , ...
D <sub>2</sub>	A, B <sub>1</sub> , B <sub>2</sub> , B <sub>3</sub>	C <sub>3</sub>	A, E
D <sub>2h</sub>	A <sub>g</sub> , A <sub>u</sub> , B <sub>1g</sub> , B <sub>1u</sub> , B <sub>2g</sub> , B <sub>2u</sub> , B <sub>3g</sub> , B <sub>3u</sub>	C <sub>6</sub>	A, B, E <sub>1</sub> , E <sub>2</sub>
C <sub>3v</sub>	A <sub>1</sub> , A <sub>2</sub> , E	S <sub>6</sub>	A <sub>g</sub> , A <sub>u</sub> , E <sub>g</sub> , E <sub>u</sub>
D <sub>3</sub>	A <sub>1</sub> , A <sub>2</sub> , E	C <sub>3h</sub>	A', A'', E', E''
C <sub>5v</sub>	A <sub>1</sub> , A <sub>2</sub> , E <sub>1</sub> , E <sub>2</sub>	C <sub>4h</sub>	A <sub>g</sub> , A <sub>u</sub> , B <sub>g</sub> , B <sub>u</sub> , E <sub>g</sub> , E <sub>u</sub>
C <sub>∞v</sub>	Σ <sup>+</sup> , Σ <sup>-</sup> , π, Δ, Φ, ...	C <sub>6h</sub>	A <sub>g</sub> , A <sub>u</sub> , B <sub>g</sub> , B <sub>u</sub> , E <sub>1g</sub> , E <sub>1u</sub> , E <sub>2g</sub> , E <sub>2u</sub>
C <sub>4v</sub> , D <sub>4</sub> , D <sub>2d</sub>	A <sub>1</sub> , A <sub>2</sub> , B <sub>1</sub> , B <sub>2</sub> , E	T <sub>d</sub> , O	A <sub>1</sub> , A <sub>2</sub> , E, F <sub>1</sub> , F <sub>2</sub>
C <sub>6v</sub> , D <sub>6</sub>	A <sub>1</sub> , A <sub>2</sub> , B <sub>1</sub> , B <sub>2</sub> , E <sub>1</sub> , E <sub>2</sub>	O <sub>h</sub>	A <sub>1g</sub> , A <sub>1u</sub> , A <sub>2g</sub> , A <sub>2u</sub> , E <sub>g</sub> , E <sub>u</sub> , F <sub>1g</sub> , F <sub>1u</sub> , F <sub>2g</sub> , F <sub>2u</sub>
D <sub>3d</sub>	A <sub>1g</sub> , A <sub>1u</sub> , A <sub>2g</sub> , A <sub>2u</sub> , E <sub>g</sub> , E <sub>u</sub>	T	A, E, F
D <sub>4d</sub>	A <sub>1</sub> , A <sub>2</sub> , B <sub>1</sub> , B <sub>2</sub> , E <sub>1</sub> , E <sub>2</sub> , E <sub>3</sub>		

TABLE II. Definition of local symmetry coordinates

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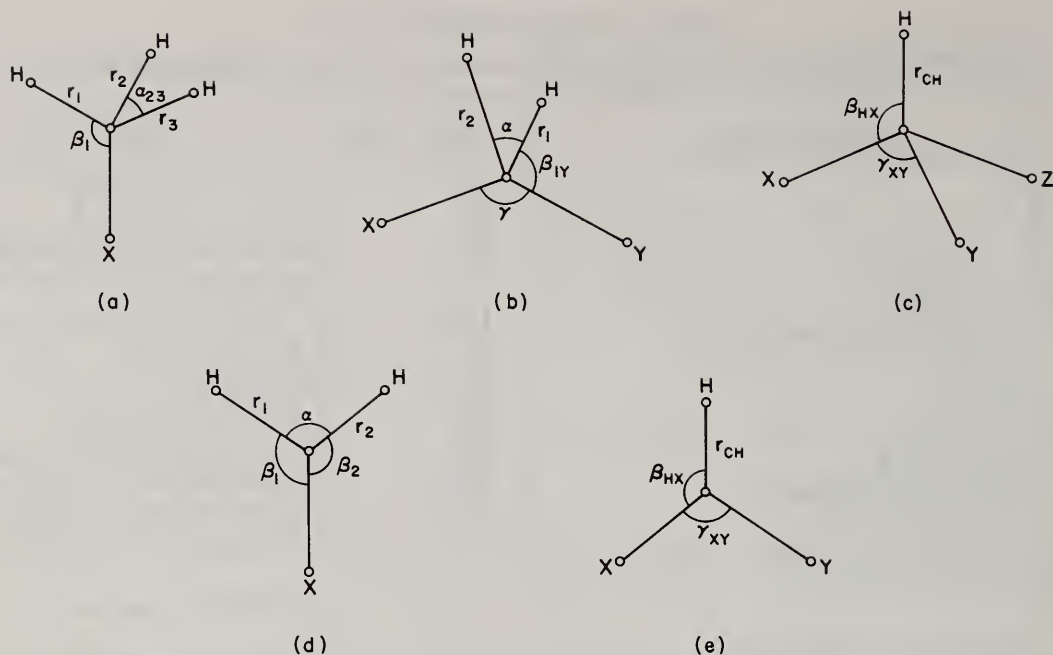


FIGURE 1. Parameters of methyl, methylene, and methin groups.

TABLE III. Uncertainty code for the selected values of frequencies

Notation	Uncertainty	Basis*
A	$\text{cm}^{-1}$ 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 $\text{cm}^{-1}$ for NaCl prism).
C	3 ~ 6	(i) Gas, prism spectrometer, low resolution (e.g., 1000 ~ 2000 $\text{cm}^{-1}$ for NaCl prism). (ii) Solid, liquid or solution, accurate measurement.
D	6 ~ 15	(i) Gas, prism spectrometer, very low resolution (e.g., >2000 $\text{cm}^{-1}$ 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
$\sigma^+$	$\nu_1$	NN stretch.....	2224 A	$\text{cm}^{-1}$ (Gas) 2223.7 VW	$\text{cm}^{-1}$ (Gas) 2224 W	
$\pi$	$\nu_2$	Bend.....	589 A	588.7 S	589 W	
$\sigma^+$	$\nu_3$	NO stretch.....	1285 A	1284.9 VS	1287 VS	

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- [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
$\sigma^+$	$\nu_1$	NN stretch.....	2202 A	$\text{cm}^{-1}$ (Gas) 2201.6	$\text{cm}^{-1}$	
$\pi$	$\nu_2$	Bend.....	585 A	585.3		
$\sigma^+$	$\nu_3$	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
$\sigma^+$	$\nu_1$	NN stretch.....	2155 A	$\text{cm}^{-1}$ (Gas) 2154.7	$\text{cm}^{-1}$	
$\pi$	$\nu_2$	Bend.....	572 A	571.9		
$\sigma^+$	$\nu_3$	NO stretch.....	1265 A	1265.3		

#### References

See No. 2.

Molecule: Water  $\text{H}_2\text{O}$   
 Symmetry  $\text{C}_{2v}$  Symmetry number  $\sigma = 2$

No. 4

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	3657 A	$\text{cm}^{-1}$ (Gas) 3656.65	$\text{cm}^{-1}$ (Gas) 3654	
	$\nu_2$	Bend.....	1595 A	1594.59		
$b_1$	$\nu_3$	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- $\text{d}_1$  HDO  
 Symmetry  $\text{C}_s$  Symmetry number  $\sigma = 1$

No. 5

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	OD stretch.....	2727 A	$\text{cm}^{-1}$ (Gas) 2726.73	$\text{cm}^{-1}$ (Gas) 2718	
	$\nu_2$	Bend.....	1402 A	1402.20		
	$\nu_3$	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-d<sub>2</sub> D<sub>2</sub>O  
 Symmetry C<sub>2v</sub> Symmetry number  $\sigma = 2$

No. 6

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	$\nu_1$	Sym. stretch.....	2671 A	<i>cm</i> <sup>-1</sup> (Gas) 2671.46	<i>cm</i> <sup>-1</sup> (Gas) 2666	
	$\nu_2$	Bend.....	1178 A	1178.33		
<i>b</i> <sub>1</sub>	$\nu_3$	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 F<sub>2</sub>O  
 Symmetry C<sub>2v</sub> Symmetry number  $\sigma = 2$

No. 7

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	$\nu_1$	Sym. stretch.....	928 B	<i>cm</i> <sup>-1</sup> (Gas) 928 S	<i>cm</i> <sup>-1</sup>	
	$\nu_2$	Bend.....	461 B	461 S		
<i>b</i> <sub>1</sub>	$\nu_3$	Antisym. stretch.....	831 B	831 VS		

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 [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  $\text{C}_{2v}$  Symmetry number  $\sigma = 2$

No. 8

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	639 D	$\text{cm}^{-1}$ (Gas) 638.6 VS (Ar matrix)	$\text{cm}^{-1}$	
	$\nu_2$	Bend.....	296 C	296.4 W (solid)		
$b_1$	$\nu_3$	Antisym. stretch.....	686 C	685.9 S		

#### References

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[2] IR.Th. K. Hedberg, J. Chem. Phys. 19, 509 (1951).  
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Molecule: Hydrogen sulfide  $\text{H}_2\text{S}$   
Symmetry  $\text{C}_{2v}$  Symmetry number  $\sigma = 2$

No. 9

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	2615 A	$\text{cm}^{-1}$ (Gas) 2614.6	$\text{cm}^{-1}$	
	$\nu_2$	Bend.....	1183 A	1182.7		
$b_1$	$\nu_3$	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).  
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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
$a_1$	$\nu_1$	Sym. stretch.....	1896 A	$cm^{-1}$ (Gas) 1896.38	$cm^{-1}$ (Gas) 1891.6	
	$\nu_2$	Bend.....	855 A	855.45		
$b_1$	$\nu_3$	Antisym. stretch.....	1999 E	1999		

#### References

- [1] IR. A. H. Nielsen and H. H. Nielsen, J. Chem. Phys. 5, 277 (1937).  
[2] R. G. M. Murphy and J. E. Vance, J. Chem. Phys. 6, 426 (1938).  
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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
$a_1$	$\nu_1$	Sym. stretch.....	1151 B	$cm^{-1}$ (Gas) 1151.4 S	$cm^{-1}$ (Gas) 1150.5 S, p	
	$\nu_2$	Bend.....	518 B	517.7 S	524.5 W, p (liquid)	
$b_1$	$\nu_3$	Antisym. stretch.....	1362 B	1361.8 S	1336.0 W, dp (liquid)	

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- [1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.  
[2] IR. R. 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  $\text{H}_2\text{Se}$   
 Symmetry  $\text{C}_{2v}$  Symmetry number  $\sigma = 2$

No. 12

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	2345 B	$\text{cm}^{-1}$ (Gas) 2344.5 S	$\text{cm}^{-1}$	
	$\nu_2$	Bend.....	1034 A	1034.2 S		
$b_1$	$\nu_3$	Antisym. stretch.....	2358 B	2357.8 S		

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- [1] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945), and references cited there.  
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Molecule: Hydrogen deuterium selenide  $\text{HDSe}$   
 Symmetry  $\text{C}_s$  Symmetry number  $\sigma = 1$

No. 13

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	SeD stretch.....	1691 C	$\text{cm}^{-1}$ (Gas) 1691	$\text{cm}^{-1}$	
	$\nu_2$	Bend.....	912 C	912		
	$\nu_3$	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 <sup>a</sup>	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	3337 A	$\text{cm}^{-1}$ 3336.2s 3337.2a	$\text{cm}^{-1}$	
	$\nu_2$	Sym. deform.....	950 C	932.5s 968.3a		
$e$	$\nu_3$	Deg. stretch.....	3444 A	3443.6s 3443.9a		
	$\nu_4$	Deg. deform.....	1627 A	1626.1s 1627.4a		

<sup>a</sup> "s" and "a" refer to symmetric and antisymmetric levels [2].

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- [2] IR. W. S. Benedict and E. K. Plyler, *Can. J. Phys.* 35, 1235 (1957).
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- [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 <sup>a</sup>	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	2420 C	$\text{cm}^{-1}$ (Gas) 2420.1s 2420.6a	$\text{cm}^{-1}$	
	$\nu_2$	Sym. deform.....	748 B	745.7s 749.4a		
$e$	$\nu_3$	Deg. stretch.....	2564 A	2564.0		
	$\nu_4$	Deg. deform.....	1191 B	1191		

<sup>a</sup> "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.
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- [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
$a_1$	$\nu_1$	Sym. stretch.....	1032 B	$\text{cm}^{-1}$ (Gas) 1032 S	$\text{cm}^{-1}$ (Liquid) 1050	
	$\nu_2$	Sym. deform.....	647 B	647 W	667	
$e$	$\nu_3$	Deg. stretch.....	907 C	907 S	905	
	$\nu_4$	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
$a_1$	$\nu_1$	Sym. stretch.....	2323 A	$\text{cm}^{-1}$ (Gas) 2322.9	$\text{cm}^{-1}$ (Liquid) 2306	
	$\nu_2$	Sym. deform.....	992 B	992.1	979	
$e$	$\nu_3$	Deg. stretch.....	2328 B	2327.7		
	$\nu_4$	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-d<sub>3</sub> PD<sub>3</sub>  
 Symmetry C<sub>3v</sub> Symmetry number  $\sigma = 3$

No. 18

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	1694 B	$cm^{-1}$ (Gas) 1694	$cm^{-1}$	CF [2].
	$\nu_2$	Sym. deform.....	730 B	730		
$e$	$\nu_3$	Deg. stretch.....	1687 D	.....	.....	
	$\nu_4$	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 PF<sub>3</sub>  
 Symmetry C<sub>3v</sub> Symmetry number  $\sigma = 3$

No. 19

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	892 B	$cm^{-1}$ (Gas) 892 S	$cm^{-1}$ (Liquid) 890 (10)	
	$\nu_2$	Sym. deform.....	487 B	487 M	486 (3)	
$e$	$\nu_3$	Deg. stretch.....	860 C	860 S	840 (10)	
	$\nu_4$	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).  
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 [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
$a_1$	$\nu_1$	Sym. stretch.....	504 C	$\text{cm}^{-1}$ (Gas) 504	$\text{cm}^{-1}$ (Liquid) 510 (10) p	
	$\nu_2$	Sym. deform.....	252 C	252	257 (6) p	
$e$	$\nu_3$	Deg. stretch.....	482 C	482	480 (3) dp	
	$\nu_4$	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
$a_1$	$\nu_1$	Sym. stretch.....	2116 A	$\text{cm}^{-1}$ (Gas) 2116.1	$\text{cm}^{-1}$	
	$\nu_2$	Sym. deform.....	906 B	906.0		
$e$	$\nu_3$	Deg. stretch.....	2123 B	2123.0		
	$\nu_4$	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-d<sub>3</sub>    AsD<sub>3</sub>  
 Symmetry    C<sub>3v</sub>                      Symmetry number  $\sigma = 3$

No. 22

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	1523 B	$cm^{-1}$ (Gas) 1523.1	$cm^{-1}$	
	$\nu_2$	Sym. deform.....	660 C	660.0		
$e$	$\nu_3$	Deg. stretch.....	1529 C	1529.3		
	$\nu_4$	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    SbH<sub>3</sub>  
 Symmetry    C<sub>3v</sub>                      Symmetry number  $\sigma = 3$

No. 23

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	1891 B	$cm^{-1}$ (Gas) 1890.9	$cm^{-1}$	
	$\nu_2$	Sym. deform.....	782 C	781.5		
$e$	$\nu_3$	Deg. stretch.....	1894 C	1894.2		
	$\nu_4$	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
$a_1$	$\nu_1$	Sym. stretch.....	1359 B	$cm^{-1}$ (Gas) 1358.8	$cm^{-1}$	
	$\nu_2$	Sym. deform.....	561 C	561.1		
$e$	$\nu_3$	Deg. stretch.....	1362 C	1362.0		
	$\nu_4$	Deg. deform.....	593 C	592.5		

## References

- [1] IR. W. H. Haynie and H. H. Nielsen, J. Chem. Phys. **21**, 1839 (1953).  
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	2187 B	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Gas) 2187.0 S	
$e$	$\nu_2$	Deg. deform.....	975 C	ia, <sup>a</sup> 974.6	978 W	
$f_2$	$\nu_3$	Deg. stretch.....	2191 A	2190.6		
	$\nu_4$	Deg. deform.....	914 B	914.2		

<sup>a</sup> Observed in the infrared through Coriolis interaction with  $\nu_4$ .

## References

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



Molecule: Silane-d<sub>2</sub> SiH<sub>2</sub>D<sub>2</sub>  
Symmetry C<sub>2v</sub> Symmetry number δ = 2

No. 26

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	SiH <sub>2</sub> s-stretch.....	2189 C	2189 S		
	<i>ν</i> <sub>2</sub>	SiD <sub>2</sub> s-stretch.....	1587 C	1587 S		
	<i>ν</i> <sub>3</sub>	SiH <sub>2</sub> scis.....	944 B	944 W		
	<i>ν</i> <sub>4</sub>	SiD <sub>2</sub> scis.....	683 B	682.5 M		
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>5</sub>	SiH <sub>2</sub> twist.....	844 E	ia	.....	CF [1].
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>6</sub>	SiH <sub>2</sub> a-stretch.....	2183 C	2183 S		
	<i>ν</i> <sub>7</sub>	SiH <sub>2</sub> rock.....	743 B	743 S		
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>8</sub>	SiD <sub>2</sub> a-stretch.....	1601 C	1601 S		
	<i>ν</i> <sub>9</sub>	SiH <sub>2</sub> wag.....	862 B	862 M		

### Reference

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

Molecule: Silane-d<sub>3</sub> SiHD<sub>3</sub>  
Symmetry C<sub>3v</sub> Symmetry number δ = 3

No. 27

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	SiH stretch.....	2182 C	2182 M		
	<i>ν</i> <sub>2</sub>	SiD <sub>3</sub> s-stretch.....	1573 C	1573 S		
	<i>ν</i> <sub>3</sub>	SiD <sub>3</sub> s-deform.....	683 C	683 S	.....	SF ( <i>ν</i> <sub>6</sub> ) [1].
<i>e</i>	<i>ν</i> <sub>4</sub>	SiD <sub>3</sub> d-stretch.....	1598 C	1598 S		
	<i>ν</i> <sub>5</sub>	SiH bend.....	851 B	851 S		
	<i>ν</i> <sub>6</sub>	SiD <sub>3</sub> d-deform.....	683 C	683 S	.....	SF ( <i>ν</i> <sub>3</sub> ) [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
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	Sym. stretch.....	1558 E	.....	.....	CF [4].
$e$	$\nu_2$	Deg. deform.....	700 E	.....	.....	CF [4].
$f_2$	$\nu_3$	Deg. stretch.....	1597 B	1597 S		
	$\nu_4$	Deg. deform.....	681 C	681 S		

#### References

- [1] IR. J. H. Meal and M. K. Wilson, J. Chem. Phys. 24, 385 (1956).
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	Sym. stretch.....	800 C	ia	800 S	
$e$	$\nu_2$	Deg. deform.....	268 C	ia	268 W	
$f_2$	$\nu_3$	Deg. stretch.....	1032 B	1031.8 S	1010 W	
	$\nu_4$	Deg. deform.....	389 B	389.35 S	390 W	

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- [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).
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Molecule: Silicon tetrachloride  $\text{SiCl}_4$   
Symmetry  $T_d$  Symmetry number  $\sigma = 12$

No. 30

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	424 C	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Liquid) 424 (5) p	
$e$	$\nu_2$	Deg. deform.....	150 C	ia	150 (4)	
$f_2$	$\nu_3$	Deg. stretch.....	621 C	621 VS	610 (2b)	
	$\nu_4$	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  $\text{SiBr}_4$   
Symmetry  $T_d$  Symmetry number  $\sigma = 12$

No. 31

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	249 C	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Liquid) 249 (4) p	
$e$	$\nu_2$	Deg. deform.....	90 C	ia	90 (3)	
$f_2$	$\nu_3$	Deg. stretch.....	487 C	.....	487 (1)	
	$\nu_4$	Deg. deform.....	137 C	.....	137 (3)	

#### References

- [1] R. B. Trumpy, Z. Phys. 68, 675 (1931).
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- [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
				$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	Sym. stretch.....	168 C	ia	168 S, p	
$e$	$\nu_2$	Deg. deform.....	63 C	ia	63 M, dp	
$f_2$	$\nu_3$	Deg. stretch.....	405 C	.....	405 W, dp	
	$\nu_4$	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
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	Sym. stretch.....	2106 B	ia	2106 S, p	
$e$	$\nu_2$	Deg. deform.....	931 D	ia, <sup>a</sup> 930.9	920 W	
$f_2$	$\nu_3$	Deg. stretch.....	2114 B	2113.6	2106 W (liquid)	
	$\nu_4$	Deg. deform.....	819 B	819.3	816 W (liquid)	

<sup>a</sup> Observed in the infrared through Coriolis interaction with  $\nu_4$ .

### References

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



Molecule: Germane-d<sub>1</sub> GeH<sub>3</sub>D  
 Symmetry C<sub>3v</sub> Symmetry number δ = 3

No. 34

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	GeH <sub>3</sub> s-stretch.....	2106 C	<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Gas)	
	<i>ν</i> <sub>2</sub>	GeD stretch.....	1520 B	1520.4 M	2106	
	<i>ν</i> <sub>3</sub>	GeH <sub>3</sub> s-deform.....	820 C	820 S		
<i>e</i>	<i>ν</i> <sub>4</sub>	GeH <sub>3</sub> d-stretch.....	2112 B	2112 S		
	<i>ν</i> <sub>5</sub>	GeH <sub>3</sub> d-deform.....	901 C	901 W		
	<i>ν</i> <sub>6</sub>	GeH <sub>3</sub> rock.....	706 C	706 S		

## References

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

Molecule: Germane-d<sub>2</sub> GeH<sub>2</sub>D<sub>2</sub>  
 Symmetry C<sub>2v</sub> Symmetry number δ = 2

No. 35

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

## Reference

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

Molecule: Germane-d<sub>3</sub> GeHD<sub>3</sub>  
 Symmetry C<sub>3v</sub> Symmetry number σ = 3

No. 36

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	GeH stretch.....	2112 B	<i>cm</i> <sup>-1</sup> (Gas) 2112.4	<i>cm</i> <sup>-1</sup> (Gas) 1504	
	<i>ν</i> <sub>2</sub>	GeD <sub>3</sub> s-stretch.....	1504 B	.....		
	<i>ν</i> <sub>3</sub>	GeD <sub>3</sub> s-deform.....	595 C	595		
<i>e</i>	<i>ν</i> <sub>4</sub>	GeD <sub>3</sub> d-stretch.....	1522 C	1522		
	<i>ν</i> <sub>5</sub>	GeH bend.....	792 B	792.3		
	<i>ν</i> <sub>6</sub>	GeD <sub>3</sub> d-deform.....	625 C	625		

### References

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

Molecule: Germane-d<sub>4</sub> GeD<sub>4</sub>  
 Symmetry T<sub>d</sub> Symmetry number σ = 12

No. 37

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

<sup>a</sup> Observed in the infrared through Coriolis interaction with *ν*<sub>4</sub>.

### Reference

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

Molecule: Germanium tetrachloride      GeCl<sub>4</sub>  
Symmetry    T<sub>d</sub>                      Symmetry number σ = 12

No. 38

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup>	cm <sup>-1</sup> (Liquid)	
a <sub>1</sub>	ν <sub>1</sub>	Sym. stretch.....	396 C	.....	396 (10)	
e	ν <sub>2</sub>	Deg. deform.....	134 C	.....	134 (6)	
f <sub>2</sub>	ν <sub>3</sub>	Deg. stretch.....	453 C	.....	453 (1)	
	ν <sub>4</sub>	Deg. deform.....	172 C	.....	172 (6)	

References

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

Molecule: Germanium tetrabromide      GeBr<sub>4</sub>  
Symmetry    T<sub>d</sub>                      Symmetry number σ = 12

No. 39

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup>	cm <sup>-1</sup> (Liquid)	
a <sub>1</sub>	ν <sub>1</sub>	Sym. stretch.....	235 C	.....	235	
e	ν <sub>2</sub>	Deg. deform.....	79 C	.....	79	
f <sub>2</sub>	ν <sub>3</sub>	Deg. stretch.....	327 C	.....	327	
	ν <sub>4</sub>	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  $\text{SnCl}_4$   
Symmetry  $T_d$  Symmetry number  $\sigma = 12$

No. 40

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	366 C	$\text{cm}^{-1}$ ia	$\text{cm}^{-1}$ (Liquid) 366 (10)	
$e$	$\nu_2$	Deg. deform.....	104 C	ia	104 (5)	
$f_2$	$\nu_3$	Deg. stretch.....	403 C	.....	403 (6)	
	$\nu_4$	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  $\text{SnBr}_4$   
Symmetry  $T_d$  Symmetry number  $\sigma = 12$

No. 41

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	220 C	$\text{cm}^{-1}$ ia	$\text{cm}^{-1}$ (Liquid) 220 (4)	
$e$	$\nu_2$	Deg. deform.....	64 C	ia	64 (2)	
$f_2$	$\nu_3$	Deg. stretch.....	279 C	.....	279 (3)	
	$\nu_4$	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  $\text{SiH}_3\text{F}$   
Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 42

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{SiH}_3$ s-stretch.....	2206 D	2206	.....	OV ( $\nu_4$ ).
	$\nu_2$	$\text{SiH}_3$ s-deform.....	990 C	990 S		
	$\nu_3$	$\text{SiF}$ stretch.....	872 B	872 M		
$e$	$\nu_4$	$\text{SiH}_3$ d-stretch.....	2196 C	2196 M		
	$\nu_5$	$\text{SiH}_3$ d-deform.....	956 C	<sup>a</sup> 956 M		
	$\nu_6$	$\text{SiH}_3$ rock.....	728 B	728.1 M		

<sup>a</sup> 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  $\text{SiH}_3\text{Cl}$   
Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 43

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{SiH}_3$ s-stretch.....	2201 D	2201	.....	OV ( $\nu_4$ ).
	$\nu_2$	$\text{SiH}_3$ s-deform.....	949 D	949	.....	OV ( $\nu_5$ ).
	$\nu_3$	$\text{SiCl}$ stretch.....	551 C	551 S		
$e$	$\nu_4$	$\text{SiH}_3$ d-stretch.....	2195 B	2195 S		
	$\nu_5$	$\text{SiH}_3$ d-deform.....	954 B	954.4 S		
	$\nu_6$	$\text{SiH}_3$ 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**  $\text{SiH}_3\text{Br}$   
 Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 44

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{SiH}_3$ s-stretch . . . . .	2200 D	2200	.....	OV ( $\nu_4$ ).
	$\nu_2$	$\text{SiH}_3$ s-deform . . . . .	930 C	930 S		
	$\nu_3$	$\text{SiBr}$ stretch . . . . .	430 C	430 M		
$e$	$\nu_4$	$\text{SiH}_3$ d-stretch . . . . .	2196 C	2196 S		
	$\nu_5$	$\text{SiH}_3$ d-deform . . . . .	950 B	950.4 S		
	$\nu_6$	$\text{SiH}_3$ 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**  $\text{SiBrCl}_3$   
 Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 45

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{SiCl}_3$ s-stretch . . . . .	545 C	.....	545 W, p	
	$\nu_2$	$\text{SiBr}$ stretch . . . . .	368 C	.....	368 S, p	
	$\nu_3$	$\text{SiCl}_3$ s-deform . . . . .	191 C	.....	191 M, p	
$e$	$\nu_4$	$\text{SiCl}_3$ d-stretch . . . . .	610 C	.....	610 M, dp	
	$\nu_5$	$\text{SiCl}_3$ rock . . . . .	205 C	.....	205 M, dp	
	$\nu_6$	$\text{SiCl}_3$ 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  $\text{SiCl}_3\text{I}$   
 Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 46

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{SiCl}_3$ s-stretch.....	519 C	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
	$\nu_2$	$\text{SiI}$ stretch.....	333 C	.....	519 W, p	
	$\nu_3$	$\text{SiCl}_3$ s-deform.....	169 C	.....	333 S, p	
$e$	$\nu_4$	$\text{SiCl}_3$ d-stretch.....	600 C	.....	169 M, p	
	$\nu_5$	$\text{SiCl}_3$ rock.....	197 C	.....	600 W, dp	
	$\nu_6$	$\text{SiCl}_3$ d-deform.....	123 C	.....	197 W, dp	
					123 M, dp	

#### References

See No. 45.

Molecule: Tribromochlorosilane  $\text{SiBr}_3\text{Cl}$   
 Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 47

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{SiCl}$ stretch.....	579 C	$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
	$\nu_2$	$\text{SiBr}_3$ s-stretch.....	288 C	.....	579 W, p	
	$\nu_3$	$\text{SiBr}_3$ s-deform.....	159 C	.....	288 S, p	
$e$	$\nu_4$	$\text{SiBr}_3$ d-stretch.....	498 C	.....	159 M, p	
	$\nu_5$	$\text{SiBr}_3$ d-deform.....	173 C	.....	498 M, dp	
	$\nu_6$	$\text{SiCl}$ bend.....	101 C	.....	173 W, dp	
					101 M, dp	

#### References

See No. 45.

Molecule: Chlorotriiodosilane  $\text{SiClI}_3$   
 Symmetry  $C_{3v}$  Symmetry number  $\sigma = 3$

No. 48

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	SiCl stretch.....	557 C	.....	557 W, p	
	$\nu_2$	SiI <sub>3</sub> s-stretch.....	220 C	.....	220 S, p	
	$\nu_3$	SiI <sub>3</sub> s-deform.....	114 C	.....	114 S, p	
$e$	$\nu_4$	SiI <sub>3</sub> d-stretch.....	411 C	.....	411 W, dp	
	$\nu_5$	SiI <sub>3</sub> d-deform.....	134 C	.....	134 W, dp	
	$\nu_6$	SiCl bend.....	73 C	.....	73 S, dp	

## References

See No. 45.

Molecule: Dibromodichlorosilane  $\text{SiBr}_2\text{Cl}_2$   
 Symmetry  $C_{2v}$  Symmetry number  $\sigma = 2$

No. 49

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	SiCl <sub>2</sub> s-stretch.....	563 C	.....	563 M, p	
	$\nu_2$	SiBr <sub>2</sub> s-stretch.....	326 C	.....	326 S, p	
	$\nu_3$	SiCl <sub>2</sub> scis.....	182 C	.....	182 S, p	
	$\nu_4$	SiBr <sub>2</sub> scis.....	111 C	.....	111 M, p	
$a_2$	$\nu_5$	SiCl <sub>2</sub> twist.....	122 C	.....	122 M, p	
$b_1$	$\nu_6$	SiCl <sub>2</sub> a-stretch.....	605 C	.....	605 W, dp	
	$\nu_7$	SiCl <sub>2</sub> rock.....	191 E	.....	191 VW	
$b_2$	$\nu_8$	SiBr <sub>2</sub> a-stretch.....	508 C	.....	508 W, dp	
	$\nu_9$	SiBr <sub>2</sub> rock.....	174 C	.....	174 W, dp	

## References

See No. 45.



Molecule: Sulfur hexafluoride SF<sub>6</sub>  
 Symmetry O<sub>h</sub> Symmetry number  $\sigma$  = 24

No. 50

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1g</sub>	$\nu_1$	Sym. stretch.....	774 B	<i>cm</i> <sup>-1</sup> (Gas) ia	<i>cm</i> <sup>-1</sup> (Gas) 773.5 VS	OC (2 $\nu_6$ ) [3].
<i>e</i> <sub>g</sub>	$\nu_2$	Deg. stretch.....	642 B	ia	641.7 W	
<i>f</i> <sub>1u</sub>	$\nu_3$	Deg. stretch.....	948 C	947.5	ia	
	$\nu_4$	Deg. deform.....	616 C	615.5	ia	
<i>f</i> <sub>2g</sub>	$\nu_5$	Deg. deform.....	525 C	ia	525 W	
<i>f</i> <sub>2u</sub>	$\nu_6$	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).

Molecule: Selenium hexafluoride SeF<sub>6</sub>  
 Symmetry O<sub>h</sub> Symmetry number  $\sigma$  = 24

No. 51

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1g</sub>	$\nu_1$	Sym. stretch.....	707 B	<i>cm</i> <sup>-1</sup> (Gas) ia	<i>cm</i> <sup>-1</sup> (Gas) 706.9 VS	OC (2 $\nu_6$ ) [3].
<i>e</i> <sub>g</sub>	$\nu_2$	Deg. stretch.....	659 B	ia	658.7 W	
<i>f</i> <sub>1u</sub>	$\nu_3$	Deg. stretch.....	780 C	780	ia	
	$\nu_4$	Deg. deform.....	437 C	437	ia	
<i>f</i> <sub>2g</sub>	$\nu_5$	Deg. deform.....	405 C	ia	405 W	
<i>f</i> <sub>2u</sub>	$\nu_6$	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
$a_{1g}$	$\nu_1$	Sym. stretch.....	742 B	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Gas) 741.5 VS, p	OC ( $2\nu_6$ ) [3].
$e_g$	$\nu_2$	Deg. stretch.....	652 B	ia	651.6 W, dp	
$f_{1u}$	$\nu_3$	Deg. stretch.....	741 C	741 VS	ia	
	$\nu_4$	Deg. deform.....	264 C	264 S	ia	
$f_{2g}$	$\nu_5$	Deg. deform.....	318 C	ia	318 W, dp	
$f_{2u}$	$\nu_6$	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
$a_{1g}$	$\nu_1$	Sym. stretch.....	771 B	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Gas) 771.0 VS, p	OC ( $2\nu_6$ ) [3].
$e_g$	$\nu_2$	Deg. stretch.....	677 B	ia	677.2 W, dp	
$f_{1u}$	$\nu_3$	Deg. stretch.....	712 C	712 VS	ia	
	$\nu_4$	Deg. deform.....	258 C	258 S	ia	
$f_{2g}$	$\nu_5$	Deg. deform.....	320 C	ia	320 W, dp	
$f_{2u}$	$\nu_6$	Deg. deform.....	127 E	ia	ia	

### References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_{1g}$	$\nu_1$	Sym. stretch.....	667 B	ia	667.1 VS	OC ( $2\nu_6$ ) [3].
$e_g$	$\nu_2$	Deg. stretch.....	533 B	ia	532.5 W	
$f_{1u}$	$\nu_3$	Deg. stretch.....	626 C	626	ia	
	$\nu_4$	Deg. deform.....	186 C	186.2	ia	
$f_{2g}$	$\nu_5$	Deg. deform.....	202 C	ia	202 W	
$f_{2u}$	$\nu_6$	Deg. deform.....	142 E	ia	ia	

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- [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
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_g$	$\nu_1$	$\text{BH}_2$ s-stretch.....	2537 C	ia	2537 VS	
	$\nu_2$	Ring stretch.....	2110 C	ia	2110 S	
	$\nu_3$	$\text{BH}_2$ scis.....	1186 C	ia	1186 M	
	$\nu_4$	Ring deform.....	816 C	ia	816 S	
$a_u$	$\nu_5$	$\text{BH}_2$ twist.....	833 C	ia, $^a 833.1$ VW	ia	
$b_{1g}$	$\nu_6$	Ring stretch.....	1768 C	ia	1768 W	
	$\nu_7$	$\text{BH}_2$ wag.....	850 E	ia		OC ( $\nu_7 + \nu_{10}$ ).
$b_{1u}$	$\nu_8$	$\text{BH}_2$ a-stretch.....	2625 C	2625 VS	ia	
	$\nu_9$	$\text{BH}_2$ rock.....	955 E		ia	CF [9].
	$\nu_{10}$	Ring puckering.....	368 C	368 S	ia	
$b_{2g}$	$\nu_{11}$	$\text{BH}_2$ a-stretch.....	2640 E	ia	2640 W, b	
	$\nu_{12}$	$\text{BH}_2$ rock.....	930 E	ia		OC ( $\nu_{10} + \nu_{12}$ ) [6].
$b_{2u}$	$\nu_{13}$	Ring stretch.....	1920 E	{ 1882 M (1992 W) }	ia	FR ( $\nu_9 + \nu_{15}$ ).
$b_{3g}$	$\nu_{14}$	$\text{BH}_2$ wag.....	977 C	977 S	ia	
	$\nu_{15}$	$\text{BH}_2$ twist.....	1012 E	ia		CF. <sup>b</sup>
$b_{3u}$	$\nu_{16}$	$\text{BH}_2$ s-stretch.....	2528 C	2528 VS	ia	
	$\nu_{17}$	Ring deform.....	1606 C	1606 VS	ia	
	$\nu_{18}$	$\text{BH}_2$ scis.....	1181 C	1181 VS	ia	

<sup>a</sup> Observed very weakly and also confirmed by combination bands.

<sup>b</sup> Estimated from  $\nu_{15}$  of  $^{11}\text{B}_2\text{H}_6$ .

## References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_g$	$\nu_1$	$\text{BH}_2$ s-stretch.....	2524 C	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Liquid) 2524 (10) p	
	$\nu_2$	Ring stretch.....	2104 C	ia	2104 (10) p	
	$\nu_3$	$\text{BH}_2$ scis.....	1180 C	ia	1180 (7)	
	$\nu_4$	Ring deform.....	794 C	ia	794 (10) p	
$a_u$	$\nu_5$	$\text{BH}_2$ twist.....	833 C	ia, $^{a}833.1$	ia	
$b_{1g}$	$\nu_6$	Ring stretch.....	1768 E	VW ia	{ 1788 (1) dp 1747 (1) dp }	FR ( $\nu_5 + \nu_9$ ).
	$\nu_7$	$\text{BH}_2$ wag.....	850 E	ia	.....	OC ( $\nu_7 + \nu_{10}$ ).
$b_{1u}$	$\nu_8$	$\text{BH}_2$ a-stretch.....	2612 C	2612 VS	ia	
	$\nu_9$	$\text{BH}_2$ rock.....	950 E	.....	ia	{ OC ( $\nu_5 + \nu_9$ ). OC ( $\nu_9 + \nu_{10}$ ). }
	$\nu_{10}$	Ring puckering.....	368 C	368 S	ia	
$b_{2g}$	$\nu_{11}$	$\text{BH}_2$ a-stretch.....	2591 C	ia	2591 (9) dp	
	$\nu_{12}$	$\text{BH}_2$ rock.....	915 E	ia	.....	OC ( $\nu_{10} + \nu_{12}$ ).
$b_{2u}$	$\nu_{13}$	Ring stretch.....	1915 E	{ 1887 M (1999 W) }	ia	
	$\nu_{14}$	$\text{BH}_2$ wag.....	973 C	973 S	ia	
$b_{3g}$	$\nu_{15}$	$\text{BH}_2$ twist.....	1012 C	ia	1012 (5) dp	
$b_{3u}$	$\nu_{16}$	$\text{BH}_2$ s-stretch.....	2525 C	2525 VS	ia	
	$\nu_{17}$	Ring deform.....	1602 C	1602 VS	ia	
	$\nu_{18}$	$\text{BH}_2$ scis.....	1177 C	1177 VS	ia	

<sup>a</sup> 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<sub>g</sub></i>	<i>ν</i> <sub>1</sub>	BD <sub>2</sub> s-stretch . . . . .	1860 E	<i>cm</i> <sup>-1</sup> (Gas) ia	<i>cm</i> <sup>-1</sup> (Liquid) { 1880 VS, p 1833 S, p	} FR (2 <i>ν</i> <sub>3</sub> ).
	<i>ν</i> <sub>2</sub>	Ring stretch . . . . .	1511 C	ia	1511 VS, p	
	<i>ν</i> <sub>3</sub>	BD <sub>2</sub> scis . . . . .	929 C	ia	929 p	
	<i>ν</i> <sub>4</sub>	Ring deform . . . . .	726 C	ia	726 VS, p	
<i>a<sub>u</sub></i>	<i>ν</i> <sub>5</sub>	BD <sub>2</sub> twist . . . . .	592 D	<sup>a</sup> 592 VW	ia	
<i>b<sub>1g</sub></i>	<i>ν</i> <sub>6</sub>	Ring stretch . . . . .	1273 C	ia	1273 (2) dp	OC ( <i>ν</i> <sub>5</sub> + <i>ν</i> <sub>7</sub> ).
	<i>ν</i> <sub>7</sub>	BD <sub>2</sub> wag . . . . .	870 E	ia		
<i>b<sub>1u</sub></i>	<i>ν</i> <sub>8</sub>	BD <sub>2</sub> a-stretch . . . . .	1999 C	1999 VS	ia	OC ( <i>ν</i> <sub>9</sub> + <i>ν</i> <sub>10</sub> ).
	<i>ν</i> <sub>9</sub>	BD <sub>2</sub> rock . . . . .	705 E		ia	
	<i>ν</i> <sub>10</sub>	Ring puckering . . . . .	262 C	262 M	ia	{ 1975 (9) dp (2000 (5))dp
<i>b<sub>2g</sub></i>	<i>ν</i> <sub>11</sub>	BD <sub>2</sub> a-stretch . . . . .	1980 E	ia		
	<i>ν</i> <sub>12</sub>	BD <sub>2</sub> rock . . . . .	740 E	ia		OC ( <i>ν</i> <sub>10</sub> + <i>ν</i> <sub>12</sub> ). FR ( <i>ν</i> <sub>5</sub> + <i>ν</i> <sub>7</sub> ).
<i>b<sub>2u</sub></i>	<i>ν</i> <sub>13</sub>	Ring stretch . . . . .	1465 E	{ 1491 M 1459 MS	ia	
	<i>ν</i> <sub>14</sub>	BD <sub>2</sub> wag . . . . .	728 C	728 S	ia	730 (4) dp
<i>b<sub>3g</sub></i>	<i>ν</i> <sub>15</sub>	BD <sub>2</sub> twist . . . . .	730 C	ia		
<i>b<sub>3u</sub></i>	<i>ν</i> <sub>16</sub>	BD <sub>2</sub> s-stretch . . . . .	1845 C	{ 1857 VS (1799 S)	ia	FR ( <i>ν</i> <sub>3</sub> + <i>ν</i> <sub>18</sub> ).
	<i>ν</i> <sub>17</sub>	Ring deform . . . . .	1205 C	1205 VS	ia	
	<i>ν</i> <sub>18</sub>	BD <sub>2</sub> scis . . . . .	881 C	881 VS	ia	

<sup>a</sup> 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
$\sigma_g^+$	$\nu_1$	Sym. stretch.....	1333 C	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Gas) { 1388.15 1285.40 ia ia	} FR ( $2\nu_2$ ).
$\pi_u$	$\nu_2$	Bend.....	667 A	667.38 S		
$\sigma_u^+$	$\nu_3$	Antisym. stretch.....	2349 A	2349.16 VS		

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- [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).
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- [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
$\sigma_g^+$	$\nu_1$	Sym. stretch.....	1334 C	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Gas) { 1369.90 1266.03 ia ia	} FR ( $2\nu_2$ ).
$\pi_u$	$\nu_2$	Bend.....	649 A	648.91 S		
$\sigma_u^+$	$\nu_3$	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
$\sigma_g^+$	$\nu_1$	Sym. stretch.....	658 A	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Gas) 657.98 ia	
$\pi_u$	$\nu_2$	Bend.....	397 B	396.8	ia	
$\sigma_u^+$	$\nu_3$	Antisym. stretch.....	1535 B	1535.35	ia	

#### References

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

Molecule: Carbonyl sulfide  $^{12}\text{C}^{16}\text{O}^{32}\text{S}$   
 Symmetry  $C_{\infty v}$  Symmetry number  $\sigma = 1$

No. 61

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$\sigma^+$	$\nu_1$	CO stretch.....	2062 A	$\text{cm}^{-1}$ (Gas) 2062.22	$\text{cm}^{-1}$ (Liquid) 2050 W	
$\pi$	$\nu_2$	Bend.....	520 A	520.41	521 W dp	
$\sigma^+$	$\nu_3$	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
$\sigma^+$	$\nu_1$	CH stretch.....	3311 A	$cm^{-1}$ (Gas) 3311.47 S	$cm^{-1}$ (Liquid) 3313 W	
$\pi$	$\nu_2$	Bend.....	712 A	711.98 VS	712 W	
$\sigma^+$	$\nu_3$	CN stretch.....	2097 A	2096.85 W	2089 S	

## References

- [1] R. Landolt-Börnstein, "Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik," 6. Auflage, I. Band, Atom-und Molekularphysik, 2. Teil, Molekeln I. (Springer-Verlag, Berlin, Göttingen, Heidelberg, 1951).  
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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
$\sigma^+$	$\nu_1$	CD stretch.....	2630 A	$cm^{-1}$ (Gas) 2630.30 S	$cm^{-1}$ (Liquid) 2630	
$\pi$	$\nu_2$	Bend.....	569 A	569.04 VS	569	
$\sigma^+$	$\nu_3$	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 <sup>35</sup>ClCN  
Symmetry C<sub>∞v</sub> Symmetry number σ = 1

No. 64

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ <sup>+</sup>	ν <sub>1</sub>	CN stretch.....	2216 A	cm <sup>-1</sup> (Gas) 2215.6 VS	cm <sup>-1</sup> (Liquid) 2206 (10)	RP [2]. FR (2ν <sub>2</sub> ) [2].
π	ν <sub>2</sub>	Bend.....	378 A	380 S	394 (3)	
σ <sup>+</sup>	ν <sub>3</sub>	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 <sup>37</sup>ClCN  
Symmetry C<sub>∞v</sub> Symmetry number σ = 1

No. 65

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
σ <sup>+</sup>	ν <sub>1</sub>	CN stretch.....	2215 A	cm <sup>-1</sup> (Gas) 2215.3 VS	cm <sup>-1</sup> (Liquid) 2206 (10)	RP [2]. FR (2ν <sub>2</sub> ) [2].
π	ν <sub>2</sub>	Bend.....	378 A	380 S	394 (3)	
σ <sup>+</sup>	ν <sub>3</sub>	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
$\sigma^+$	$\nu_1$	CN stretch.....	2198 A	$\text{cm}^{-1}$ (Gas) 2198.3	$\text{cm}^{-1}$ (Liquid) 2191	RP [2].
$\pi$	$\nu_2$	Bend.....	342 A	341.5	357	
$\sigma^+$	$\nu_3$	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
$\sigma^+$	$\nu_1$	CN stretch.....	2198 A	$\text{cm}^{-1}$ (Gas) 2198.3	$\text{cm}^{-1}$ (Liquid) 2191	RP [2].
$\pi$	$\nu_2$	Bend.....	342 A	341.5	357	
$\sigma^+$	$\nu_3$	CBr stretch.....	575 C	575	568	

#### References

See No. 66.

Molecule: Formaldehyde  $\text{H}_2\text{CO}$   
Symmetry  $\text{C}_{2v}$  Symmetry number  $\sigma = 2$

No. 68

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{CH}_2$ s-stretch.....	2783 A	2782.5 S	2781.6 S	
	$\nu_2$	CO stretch.....	1746 A	1746.1 VS	1742.3 W	
	$\nu_3$	$\text{CH}_2$ scis.....	1500 A	1500.1 S	1499.7 M	
$b_1$	$\nu_4$	$\text{CH}_2$ a-stretch.....	2843 A	2843.1 VS	2866 W	
$b_2$	$\nu_5$	$\text{CH}_2$ rock.....	1249 A	1249.1 S		
	$\nu_6$	$\text{CH}_2$ 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).
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- [4] IR.Th. T. Nakagawa, H. Kashiwagi, H. Kurihara, and Y. Morino, J. Mol. Spectrosc., **31**, 436 (1969).

Molecule: Formaldehyde- $\text{d}_1$   $\text{HDCO}$   
Symmetry  $\text{C}_s$  Symmetry number  $\sigma = 1$

No. 69

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a'$	$\nu_1$	CH stretch.....	2844 D	2844.1 S	2846.2 S	FR ( $\nu_3 + \nu_5$ ). FR ( $2\nu_6, 2\nu_5$ ).
	$\nu_2$	CD stretch.....	2121 D	2120.7 S	2120.3 S	
	$\nu_3$	CO stretch.....	1723 A	1723.4 VS	1723.2 VS	
	$\nu_4$	CHD scis.....	1400 B	1400.0 S	1397.4 M	
	$\nu_5$	CHD rock.....	1041 D	1041 S		
$a''$	$\nu_6$	CHD wag.....	1074 C	1074 S		

### Reference

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



Molecule: Formaldehyde-d<sub>2</sub> D<sub>2</sub>CO  
Symmetry C<sub>2v</sub> Symmetry number  $\sigma = 2$

No. 70

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	$\nu_1$	CD <sub>2</sub> s-stretch.....	2056 D	<i>cm</i> <sup>-1</sup> (Gas) 2056.4 S	<i>cm</i> <sup>-1</sup> .....	FR (2 $\nu_3$ ).
	$\nu_2$	CO stretch.....	1700 B	1700 VS		
	$\nu_3$	CD <sub>2</sub> scis.....	1106 C	1106.0 S		
<i>b</i> <sub>1</sub>	$\nu_4$	CD <sub>2</sub> a-stretch.....	2160 C	2160.3 VS		
	$\nu_5$	CD <sub>2</sub> rock.....	990 C	990.2 S		
<i>b</i> <sub>2</sub>	$\nu_6$	CD <sub>2</sub> wag.....	938 E	938 S		

### Reference

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

Molecule: Methane CH<sub>4</sub>  
Symmetry T<sub>d</sub> Symmetry number  $\sigma = 12$

No. 71

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	$\nu_1$	Sym. stretch.....	2917 A	<i>cm</i> <sup>-1</sup> (Gas) ia	<i>cm</i> <sup>-1</sup> (Gas) 2917.0	
<i>e</i>	$\nu_2$	Deg. deform.....	1534 A	ia, <sup>a</sup> 1533	1533.6	
<i>f</i> <sub>2</sub>	$\nu_3$	Deg. stretch.....	3019 A	3018.9	3019.5	
	$\nu_4$	Deg. deform.....	1306 C	1306.2		

<sup>a</sup> Observed in the infrared through Coriolis interaction with  $\nu_4$  [5].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	CH <sub>3</sub> s-stretch.....	2945 E	$\begin{matrix} cm^{-1} \\ (Gas) \\ \{2973 \text{ M} \\ 2914 \text{ M} \} \end{matrix}$	$\begin{matrix} cm^{-1} \\ (Gas) \\ \{ \dots \dots \dots \} \end{matrix}$	FR (2 $\nu_5$ ).
	$\nu_2$	CD stretch.....	2200 A	2200.0 M		
	$\nu_3$	CH <sub>3</sub> s-deform.....	1300 C	1300 M	1306	
$e$	$\nu_4$	CH <sub>3</sub> d-stretch.....	3017 B	3016.9 S		
	$\nu_5$	CH <sub>3</sub> d-deform.....	1471 C	1471 W		
	$\nu_6$	CH <sub>3</sub> rock.....	1155 C	1155 M	1156	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	CH <sub>2</sub> s-stretch.....	2974 C	$\begin{matrix} cm^{-1} \\ (Gas) \\ 2976 \text{ M} \end{matrix}$	$\begin{matrix} cm^{-1} \\ (Gas) \\ 2974 \end{matrix}$	
	$\nu_2$	CD <sub>2</sub> s-stretch.....	2202 C	2202 W		
	$\nu_3$	CH <sub>2</sub> scis.....	1436 C	1436 W		
	$\nu_4$	CD <sub>2</sub> scis.....	1033 C	1033 S	1034	
$a_2$	$\nu_5$	CH <sub>2</sub> twist.....	1333 C	ia, <sup>a</sup> 1329 W	1333	
$b_1$	$\nu_6$	CH <sub>2</sub> a-stretch.....	3013 C	3013 S		
	$\nu_7$	CH <sub>2</sub> rock.....	1090 C	1090 S	1090	
$b_2$	$\nu_8$	CD <sub>2</sub> a-stretch.....	2234 C	2234 M		
	$\nu_9$	CH <sub>2</sub> wag.....	1234 C	1234 M		

<sup>a</sup> Observed in the infrared through Coriolis interaction with  $\nu_9$ .

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Molecule: Methane-d<sub>3</sub> CHD<sub>3</sub>  
Symmetry C<sub>3v</sub> Symmetry number σ = 3

No. 74

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

## References

See No. 73.

Molecule: Methane-d<sub>4</sub> CD<sub>4</sub>  
Symmetry T<sub>d</sub> Symmetry number σ = 12

No. 75

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

<sup>a</sup> Observed in the infrared through Coriolis interaction with *ν*<sub>4</sub> [5].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	909 B	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Gas) 908.5 S	FR ( $2\nu_4$ ).
$e$	$\nu_2$	Deg. deform.....	435 B	ia	435.0 S	
$f_2$	$\nu_3$	Deg. stretch.....	1281 D	1282.6 VS 1260.9 VW	1283.0 W 1263 VW	
	$\nu_4$	Deg. deform.....	632 B	631.73 VS	631.2 S	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	Sym. stretch.....	459 C	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Liquid) 458.7 (10) p	FR ( $\nu_1 + \nu_4$ ).
$e$	$\nu_2$	Deg. deform.....	217 C	ia	217.0 (7) dp	
$f_2$	$\nu_3$	Deg. stretch.....	776 E	{ 789 VS 768 VS	{ 790.4 (4) dp 761.7 (4) dp	
	$\nu_4$	Deg. deform.....	314 C	309.9 W (liquid)	313.5 (9) dp	

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Molecule: Carbon tetrabromide  $\text{CBr}_4$   
 Symmetry  $T_d$  Symmetry number  $\sigma = 12$

No. 78

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Liquid)	$\text{cm}^{-1}$ (Benzene soln.)	
$a_1$	$\nu_1$	Sym. stretch.....	267 C	ia	267 (7) p	
$e$	$\nu_2$	Deg. deform.....	122 C	ia	122 (10) dp	
$f_2$	$\nu_3$	Deg. stretch.....	672 C	672 VS	671 (1) dp	
	$\nu_4$	Deg. deform.....	182 C	.....	182 (4) dp	

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Molecule: Carbon tetraiodide  $\text{CI}_4$   
 Symmetry  $T_d$  Symmetry number  $\sigma = 12$

No. 79

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Solid)	$\text{cm}^{-1}$ (Solid)	
$a_1$	$\nu_1$	Sym. stretch.....	178 D	ia	178 (10)	
$e$	$\nu_2$	Deg. deform.....	90 D	ia	90 (4)	
$f_2$	$\nu_3$	Deg. stretch.....	555 D	555 VS	123 (5)	
	$\nu_4$	Deg. deform.....	125 E	<sup>a</sup> $\left\{ \begin{array}{l} 123 \text{ W} \\ 127 \text{ W} \end{array} \right.$		

<sup>a</sup> Crystal field splitting.

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch . . . . .	2930 E	$\text{cm}^{-1}$ (Gas) 2964 VS 2863 S	$\text{cm}^{-1}$ }	FR ( $2\nu_5$ ).
	$\nu_2$	$\text{CH}_3$ s-deform . . . . .	1464 A	1464 S		
	$\nu_3$	CF stretch . . . . .	1049 A	1048.6 S		
$e$	$\nu_4$	$\text{CH}_3$ d-stretch . . . . .	3006 A	3005.8 S		
	$\nu_5$	$\text{CH}_3$ d-deform . . . . .	1467 A	1466.5 M		
	$\nu_6$	$\text{CH}_3$ rock . . . . .	1182 A	1182.4 M		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CD}_3$ s-stretch . . . . .	2110 E	$\text{cm}^{-1}$ (Gas) 2090 2150	$\text{cm}^{-1}$ }	FR ( $2\nu_5$ ).
	$\nu_2$	$\text{CD}_3$ s-deform . . . . .	1136 A	1136		
	$\nu_3$	CF stretch . . . . .	991 A	991		
$e$	$\nu_4$	$\text{CD}_3$ d-stretch . . . . .	2258 A	2258		
	$\nu_5$	$\text{CD}_3$ d-deform . . . . .	1072 A	1072		
	$\nu_6$	$\text{CD}_3$ rock . . . . .	903 A	903		

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Molecule: Methylchloride  $\text{CH}_3\text{Cl}$   
Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 82

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch . . . . .	2937 E	$\text{cm}^{-1}$ (Gas) 2967.78 M 2879.28 M	$\text{cm}^{-1}$ (Liquid) 2955 VS, p 2861 M	} FR ( $2\nu_5$ ).
	$\nu_2$	$\text{CH}_3$ s-deform . . . . .	1355 A	1354.9 S	1370 VW, p	
$e$	$\nu_3$	$\text{CCl}$ stretch . . . . .	732 A	732.1 S	709 VS, p	} FR ( $3\nu_6$ ) [6, 8].
	$\nu_4$	$\text{CH}_3$ d-stretch . . . . .	3039 B	3039.31 S 3042.75 S	3036 M, dp	
	$\nu_5$	$\text{CH}_3$ d-deform . . . . .	1452 A	1452.1 M	1446 W, dp	
	$\nu_6$	$\text{CH}_3$ rock . . . . .	1017 A	1017.3 M	1016 W, dp	

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Molecule: Methylchloride- $\text{d}_3$   $\text{CD}_3\text{Cl}$   
Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 83

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CD}_3$ s-stretch . . . . .	2160 A	$\text{cm}^{-1}$ (Gas) 2160.28 S	$\text{cm}^{-1}$	
	$\nu_2$	$\text{CD}_3$ s-deform . . . . .	1029 A	1028.7 S		
$e$	$\nu_3$	$\text{CCl}$ stretch . . . . .	701 A	701.4 S		
	$\nu_4$	$\text{CD}_3$ d-stretch . . . . .	2283 A	2283.3 S		
	$\nu_5$	$\text{CD}_3$ d-deform . . . . .	1060 A	1059.9 M		
	$\nu_6$	$\text{CD}_3$ rock . . . . .	768 A	767.6 M		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch . . . . .	2935 E	$\text{cm}^{-1}$ (Gas) { 2972 M 2862.1 M	$\text{cm}^{-1}$ (Liquid) 2972 VS 2862 W	} FR ( $2\nu_5$ ).
	$\nu_2$	$\text{CH}_3$ s-deform . . . . .	1306 A	1305.9 S	1309 W	
	$\nu_3$	CBr stretch . . . . .	611 A	611.1 S	609 S	
$e$	$\nu_4$	$\text{CH}_3$ d-stretch . . . . .	3056 A	3056.35 S	3068 VS	
	$\nu_5$	$\text{CH}_3$ d-deform . . . . .	1443 A	1442.7 M	1456 M	
	$\nu_6$	$\text{CH}_3$ rock . . . . .	955 A	954.7 M	956 VW	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CD}_3$ s-stretch . . . . .	2160 A	$\text{cm}^{-1}$ (Gas) 2159.8 VS	$\text{cm}^{-1}$	
	$\nu_2$	$\text{CD}_3$ s-deform . . . . .	992 A	992.0 VS		
	$\nu_3$	CBr stretch . . . . .	577 A	576.7 S		
$e$	$\nu_4$	$\text{CD}_3$ d-stretch . . . . .	2297 A	2297.3 M		
	$\nu_5$	$\text{CD}_3$ d-deform . . . . .	1056 A	1055.6 S		
	$\nu_6$	$\text{CD}_3$ rock . . . . .	713 A	713.0 M		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch.....	2933 E	$\text{cm}^{-1}$ (Gas) { 2969.8 M 2861.0 M }	$\text{cm}^{-1}$ .....	FR ( $2\nu_5$ ).
$e$	$\nu_2$	$\text{CH}_3$ s-deform.....	1252 A	1251.5 S		
	$\nu_3$	CI stretch.....	533 A	532.8 S		
	$\nu_4$	$\text{CH}_3$ d-stretch.....	3060 A	3060.06 S		
	$\nu_5$	$\text{CH}_3$ d-deform.....	1436 C	1435.5 M	.....	FR ( $\nu_3 + \nu_6$ ).
	$\nu_6$	$\text{CH}_3$ rock.....	882 A	882.4 M		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CD}_3$ s-stretch.....	2130 E	$\text{cm}^{-1}$ (Gas) { 2155.1 2081.0 }	$\text{cm}^{-1}$ .....	FR ( $2\nu_5$ ).
$e$	$\nu_2$	$\text{CD}_3$ s-deform.....	951 A	950.7		
	$\nu_3$	CI stretch.....	501 A	501.4		
	$\nu_4$	$\text{CD}_3$ d-stretch.....	2298 A	2298		
	$\nu_5$	$\text{CD}_3$ d-deform.....	1049 A	1049.3		
	$\nu_6$	$\text{CD}_3$ rock.....	656 A	655.9		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	CH stretch . . . . .	3036 C	$\text{cm}^{-1}$ (Gas) 3036 S	$\text{cm}^{-1}$ (Liquid) 3062 S, p	
	$\nu_2$	$\text{CF}_3$ s-stretch . . . . .	1117 C	1117 C	1117 VS, p	
	$\nu_3$	$\text{CF}_3$ s-deform . . . . .	700 C	700 M	697 S, p	
$e$	$\nu_4$	CH bend . . . . .	1372 C	1372 M	1376 S, dp	
	$\nu_5$	$\text{CF}_3$ d-stretch . . . . .	1152 C	1152 VS	1160 W, dp	
	$\nu_6$	$\text{CF}_3$ d-deform . . . . .	507 C	507 M	508 VS, dp	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	CH stretch . . . . .	3034 B	$\text{cm}^{-1}$ (Gas) 3034.1 M	$\text{cm}^{-1}$ (Gas) 3030 W	
	$\nu_2$	$\text{CCl}_3$ s-stretch . . . . .	680 B	680 S	672 S	
	$\nu_3$	$\text{CCl}_3$ s-deform . . . . .	363 C	366 (liquid)	363 M	
$e$	$\nu_4$	CH bend . . . . .	1220 B	1219.7 VS	1217 W	
	$\nu_5$	$\text{CCl}_3$ d-stretch . . . . .	774 B	774.0 VS	760 W	
	$\nu_6$	$\text{CCl}_3$ d-deform . . . . .	261 B	260 (liquid)	261 W	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a<sub>1</sub></i>	$\nu_1$	CD stretch . . . . .	2266 C	$cm^{-1}$ (Gas) 2266 W	$cm^{-1}$ (Liquid) 2255 (2) p	
	$\nu_2$	CCl <sub>3</sub> s-stretch . . . . .	659 B	658.5 S	649 (7) p	
	$\nu_3$	CCl <sub>3</sub> s-deform . . . . .	369 C	366 W (liquid)	369 (9) p	
<i>e</i>	$\nu_4$	CD bend . . . . .	914 B	913.9 VS	908 (1) dp	
	$\nu_5$	CCl <sub>3</sub> d-stretch . . . . .	749 B	748.5 VS	735 (2) dp	
	$\nu_6$	CCl <sub>3</sub> d-deform . . . . .	262 C	262 W (liquid)	262 (10) dp	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a<sub>1</sub></i>	$\nu_1$	CH stretch . . . . .	3042 B	$cm^{-1}$ (Gas) 3042 M	$cm^{-1}$ (Liquid) 3017 (6) p	
	$\nu_2$	CBr <sub>3</sub> s-stretch . . . . .	541 B	541 M	540 (4) p	
	$\nu_3$	CBr <sub>3</sub> s-deform . . . . .	222 C	.....	222 (10) p	
<i>e</i>	$\nu_4$	CH bend . . . . .	1149 B	1149 VS	1143 (2) dp	
	$\nu_5$	CBr <sub>3</sub> d-stretch . . . . .	669 B	669 VS	655 (2) dp	
	$\nu_6$	CBr d-deform . . . . .	155 C	.....	155 (5) dp	

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- [2] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS 47, 202 (1951).
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	CD stretch . . . . .	2251 C	$cm^{-1}$ (Liquid) 2251 M	$cm^{-1}$ (Liquid) 2247 (4)	
	$\nu_2$	CBr <sub>3</sub> s-stretch . . . . .	521 C	521 M	519.3 (7)	
	$\nu_3$	CBr <sub>3</sub> s-deform . . . . .	222 C	. . . . .	221.6 (10)	
$e$	$\nu_4$	CD bend . . . . .	850 D	{ 858 VS	856.5 (3)	} FR ( $\nu_3 + \nu_5$ ).
				{ 844 VS	840 (3)	
	$\nu_5$	CBr <sub>3</sub> d-stretch . . . . .	632 C	632 VS	628.5 (5)	
	$\nu_6$	CBr <sub>3</sub> d-deform . . . . .	153 C	. . . . .	153.4 (8)	

### References

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[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
$a_1$	$\nu_1$	CCl <sub>3</sub> s-stretch . . . . .	716 C	$cm^{-1}$ (Liquid) 719 VS	$cm^{-1}$ (Liquid) 716.3 (2) p	
	$\nu_2$	CBr stretch . . . . .	422 C	420 W	422.3 (10) p	
	$\nu_3$	CCl <sub>3</sub> s-deform . . . . .	247 C	. . . . .	247.3 (5) p	
$e$	$\nu_4$	CCl <sub>3</sub> d-stretch . . . . .	775 C	773 VS	775.3 (1) dp	
	$\nu_5$	CBr bend . . . . .	295 C	294 W	295.0 (3) dp	
	$\nu_6$	CCl <sub>3</sub> 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).  
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CCl stretch}$ .....	747 C	$\text{cm}^{-1}$ ( $\text{CS}_2$ , $\text{C}_7\text{H}_{14}$ soln.) 747 S	$\text{cm}^{-1}$ ( $\text{C}_6\text{H}_6$ , $\text{CCl}_4$ soln.) 748 (1)	CF [1].
	$\nu_2$	$\text{CBr}_3 \text{ s-stretch}$ .....	329 C	( $\text{CS}_2$ soln.) 329 W ( $\text{C}_7\text{H}_{14}$ soln.)	326 (10) p	
$e$	$\nu_3$	$\text{CBr}_3 \text{ s-deform}$ .....	210 C	.....	210 (10) p	
	$\nu_4$	$\text{CBr}_3 \text{ d-stretch}$ .....	675 C	675 S ( $\text{CS}_2$ soln.)	677 (4) dp	
	$\nu_5$	$\text{CCl bend}$ .....	211 E	.....	.....	
	$\nu_6$	$\text{CBr}_3 \text{ d-deform}$ .....	141 C	.....	141 (7) dp	

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- [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.
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$\text{CH}_2 \text{ s-stretch}$ .....	2999 B	$\text{cm}^{-1}$ (Gas) 2999 M	$\text{cm}^{-1}$ (Gas) 2996 S, p	
	$\nu_2$	$\text{CH}_2 \text{ scis}$ .....	1467 C	1467 W	1430.1 W, p	
	$\nu_3$	$\text{CCl}_2 \text{ s-stretch}$ .....	717 B	717 M	713 S, p	
	$\nu_4$	$\text{CCl}_2 \text{ scis}$ .....	282 B	284 (liquid)	281.5 M, p	
$a_2$	$\nu_5$	$\text{CH}_2 \text{ twist}$ .....	1153 B	$\text{cm}^{-1}$ 1153 <sup>a</sup> ia	1153 VW	
$b_1$	$\nu_6$	$\text{CH}_2 \text{ a-stretch}$ .....	3040 B	3045 (liquid)	3040 S, dp	
$b_2$	$\nu_7$	$\text{CH}_2 \text{ rock}$ .....	898 B	897.7 M	893 VW	
	$\nu_8$	$\text{CH}_2 \text{ wag}$ .....	1268 B	1268 S	1265 (liquid)	
	$\nu_9$	$\text{CCl}_2 \text{ a-stretch}$ .....	758 B	758 VS		

<sup>a</sup> In the spectrum of liquid  $\text{CH}_2\text{Cl}_2$ , a weak band is found at  $1156 \text{ cm}^{-1}$ , which may be assigned to  $\nu_5$ .

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- [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>	ν <sub>1</sub>	CH stretch.....	3024 B	cm <sup>-1</sup> (Gas) 3024	cm <sup>-1</sup> (Liquid) 3019 M, p	
	ν <sub>2</sub>	CD stretch.....	2249 B	2249	2246 M, p	
	ν <sub>3</sub>	CH bend.....	1282 B	1282	1276 VW	
	ν <sub>4</sub>	CD bend.....	778 C	778 (liquid)	779 W, p	
<i>a''</i>	ν <sub>5</sub>	CCl <sub>2</sub> s-stretch.....	692 B	692	682 S, p	
	ν <sub>6</sub>	CCl <sub>2</sub> scis.....	283 B	.....	283 M, p	
	ν <sub>7</sub>	CH bend.....	1223 A	1222.9	1221 VW	
	ν <sub>8</sub>	CD bend.....	890 A	889.8	886 VW	
	ν <sub>9</sub>	CCl <sub>2</sub> 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> <sub>1</sub>	ν <sub>1</sub>	CD <sub>2</sub> s-stretch.....	2205 B	cm <sup>-1</sup> (Gas) 2205 W	cm <sup>-1</sup> (Liquid) 2198 M, p	
	ν <sub>2</sub>	CD <sub>2</sub> scis.....	1052 D	.....	1052 VW, p	
	ν <sub>3</sub>	CCl <sub>2</sub> s-stretch.....	687 B	687 M	677 VS, p	
	ν <sub>4</sub>	CCl <sub>2</sub> scis.....	282 C	.....	282 S, p	
<i>a</i> <sub>2</sub>	ν <sub>5</sub>	CD <sub>2</sub> twist.....	826 C	ia	826 VW	
<i>b</i> <sub>1</sub>	ν <sub>6</sub>	CD <sub>2</sub> a-stretch.....	2304 C	2304 (liquid)	2304 VW	
<i>b</i> <sub>2</sub>	ν <sub>7</sub>	CD <sub>2</sub> rock.....	<sup>a</sup> 712 D	.....	.....	OV (ν <sub>9</sub> ).
	ν <sub>8</sub>	CD <sub>2</sub> wag.....	957 B	957 VS	.....	
	ν <sub>9</sub>	CCl <sub>2</sub> a-stretch.....	727 B	727 VS	716 W	

<sup>a</sup> 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
$a_1$	$\nu_1$	$\text{CH}_2$ s-stretch.....	3009 C	$\text{cm}^{-1}$ (Gas) 3009 W	$\text{cm}^{-1}$ (Gas) 3008 (1)	
	$\nu_2$	$\text{CH}_2$ scis.....	1382 C	1382 VW	1402 (0)	
	$\nu_3$	$\text{CBr}_2$ s-stretch.....	588 C	588 M	584 (10)	
	$\nu_4$	$\text{CBr}_2$ scis.....	169 C	.....	169 (10)	
$a_2$	$\nu_5$	$\text{CH}_2$ twist.....	1095 D	ia	<sup>a</sup> 1095	
$b_1$	$\nu_6$	$\text{CH}_2$ a-stretch.....	3073 B	3073 VW	<sup>a</sup> 3064	
	$\nu_7$	$\text{CH}_2$ rock.....	812 B	812 M	<sup>a</sup> 813	
$b_2$	$\nu_8$	$\text{CH}_2$ wag.....	1195 B	1195 VS	<sup>a</sup> 1194	
	$\nu_9$	$\text{CBr}$ a-stretch.....	653 B	653 VS	640 (0)	

<sup>a</sup> Liquid.

## References

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- [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
$a'$	$\nu_1$	CH stretch.....	3040 C	$\text{cm}^{-1}$ (Gas) 3040 W	$\text{cm}^{-1}$ (Liquid) 3028 VW, p	
	$\nu_2$	CD stretch.....	2249 D	2249 W (liquid)	2245 W, p	
	$\nu_3$	CH bend.....	1220 C	701 W	1239 W, p	
	$\nu_4$	CD bend.....	701 C	1220 W	702 M, p	
	$\nu_5$	$\text{CBr}_2$ s-stretch.....	565 C	565 VW	561 S, p	
	$\nu_6$	$\text{CBr}_2$ scis.....	172 D	.....	172 VS, p	
$a''$	$\nu_7$	CH bend.....	1154 B	1154 VS		
	$\nu_8$	CD bend.....	838 B	838 VS	835 VW, dp	
	$\nu_9$	$\text{CBr}_2$ 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> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CD <sub>2</sub> s-stretch.....	2214 C	<i>cm</i> <sup>-1</sup> (Gas) 2214 W	<i>cm</i> <sup>-1</sup> (Liquid) 2195 M, p	
	<i>ν</i> <sub>2</sub>	CD <sub>2</sub> scis.....	1026 D	1026 (liquid)	1028 W, p	
	<i>ν</i> <sub>3</sub>	CBr <sub>2</sub> s-stretch.....	559 C	559 M	551 S, p	
	<i>ν</i> <sub>4</sub>	CBr <sub>2</sub> scis.....	172 D	.....	172 VS, p	
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>5</sub>	CD <sub>2</sub> twist.....	782 D	ia	782 W, p	
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>6</sub>	CD <sub>2</sub> a-stretch.....	2324 C	2324 W	2313 VW, dp	
	<i>ν</i> <sub>7</sub>	CD <sub>2</sub> rock.....	625 B	625 VS	636 VW	
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>8</sub>	CD <sub>2</sub> wag.....	907 B	907 VS	902 W, dp	
	<i>ν</i> <sub>9</sub>	CBr <sub>2</sub> a-stretch.....	608 C	608 (liquid)	612 M, dp	

### References

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[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> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CCl <sub>2</sub> s-stretch.....	733 C	<i>cm</i> <sup>-1</sup> (Liquid) 733 VS	<i>cm</i> <sup>-1</sup> (Liquid) 734 (1) p	
	<i>ν</i> <sub>2</sub>	CBr <sub>2</sub> s-stretch.....	380 C	377 W	380 (10) p	
	<i>ν</i> <sub>3</sub>	CCl <sub>2</sub> scis.....	242 C	.....	242 (6) p	
	<i>ν</i> <sub>4</sub>	CBr <sub>2</sub> scis.....	154 C	.....	154 (4) p	
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>5</sub>	CCl <sub>2</sub> twist.....	175 C	ia	175 (2) dp	
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>6</sub>	CBr <sub>2</sub> a-stretch.....	683 C	683 VS	684 (3) dp	
	<i>ν</i> <sub>7</sub>	CCl <sub>2</sub> wag.....	229 C	.....	229 (2) dp	
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>8</sub>	CCl <sub>2</sub> a-stretch.....	768 C	768 VS	771 (0) dp	
	<i>ν</i> <sub>9</sub>	CCl <sub>2</sub> rock.....	262 C	.....	262 (1) dp	

### References

- [1] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS 47, 202 (1951), RP 2245.  
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	CH <sub>2</sub> s-stretch.....	3003 A	$cm^{-1}$ (Gas) 3003 S	$cm^{-1}$ (Liquid) 2986 M, p	
	$\nu_2$	CH <sub>2</sub> scis.....	1482 E	<sup>a</sup> 1482 M	1410 M, p	
	$\nu_3$	CH <sub>2</sub> wag.....	1231 B	1231 S	1229 W, p	
	$\nu_4$	CCl stretch.....	744 B	744 VS	731 M, p	
	$\nu_5$	CBr stretch.....	614 B	614 S	606 S, p	
<i>a''</i>	$\nu_6$	CBrCl scis.....	229 C	.....	229 S, p	
	$\nu_7$	CH <sub>2</sub> a-stretch.....	3066 B	3066 W	3055 M, dp	
	$\nu_8$	CH <sub>2</sub> twist.....	1128 C	1128 W (liquid)	1130 W	
	$\nu_9$	CH <sub>2</sub> rock.....	852 B	852 W	848 W	

<sup>a</sup> The corresponding frequency in the liquid state is found at 1407 cm<sup>-1</sup>. This band may be assigned to the overtone of the CCl stretching vibration.

#### References

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- [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>	$\nu_1$	CH stretch.....	3031 C	$cm^{-1}$ (Gas) 3031 S (liquid)	$cm^{-1}$ (Liquid) 3024 S, p	
	$\nu_2$	CD stretch.....	2252 C	2252 M (liquid)	2246 S, p	
	$\nu_3$	CH bend.....	1262 C	1262 S (liquid)	1264 W, p	
	$\nu_4$	CH bend.....	1188 B	1188 M	1179 W, p	
	$\nu_5$	CD bend.....	868 B	868 M	867 W	
	$\nu_6$	CD bend.....	746 B	746 W	743 VW	
	$\nu_7$	CCl stretch.....	711 B	711 S	707 M, p	
	$\nu_8$	CBr stretch.....	607 C	607 W	586 S, p	
	$\nu_9$	CBrCl scis.....	228 C	.....	228 S, p	

#### Reference

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

Molecule: Bromochloromethane-d<sub>2</sub> CD<sub>2</sub>BrCl  
Symmetry C<sub>s</sub> Symmetry number σ = 1

No. 104

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
a'	ν <sub>1</sub>	CD <sub>2</sub> s-stretch . . . . .	2208 B	2208 S	2196 M, p	
	ν <sub>2</sub>	CD <sub>2</sub> scis . . . . .	1050 B	1050 W	1042 M, p	
	ν <sub>3</sub>	CD <sub>2</sub> wag . . . . .	936 B	936 S	922 W, p	
	ν <sub>4</sub>	CCl stretch . . . . .	717 B	717 S	702 M, p	
	ν <sub>5</sub>	CBr stretch . . . . .	582 B	582 S	574 S, p	
a''	ν <sub>6</sub>	CBrCl scis . . . . .	226 C	.....	226 S, p	
	ν <sub>7</sub>	CD <sub>2</sub> a-stretch . . . . .	2305 C	2302 S (liquid)	2305 W, dp	
	ν <sub>8</sub>	CD <sub>2</sub> twist . . . . .	811 B	811 W	809 W, dp	
	ν <sub>9</sub>	CD <sub>2</sub> rock . . . . .	667 C	668 W (liquid)	667 W, dp	

### Reference

See No. 103.

Molecule: Formic acid HCOOH  
Symmetry C<sub>s</sub> Symmetry number σ = 1

No. 105

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a'	ν <sub>1</sub>	OH stretch . . . . .	3570 D	3570 M		
	ν <sub>2</sub>	CH stretch . . . . .	2943 C	2942.8 M		
	ν <sub>3</sub>	C=O stretch . . . . .	1770 C	1770 VS		
	ν <sub>4</sub>	CH bend . . . . .	1387 C	1387 VW		
	ν <sub>5</sub>	OH bend . . . . .	1229 C	1229 W		
	ν <sub>6</sub>	C—O stretch . . . . .	1105 C	1105.3 S		
a''	ν <sub>7</sub>	OCO deform . . . . .	625 C	625 M		
	ν <sub>8</sub>	CH bend . . . . .	1033 C	1033 W		
	ν <sub>9</sub>	Torsion . . . . .	638 C	638 S		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	OD stretch.....	2632 C	$cm^{-1}$ (Gas) 2632 W	$cm^{-1}$	
	$\nu_2$	CD stretch.....	2232 C	2231.8 M		
	$\nu_3$	C=O stretch.....	1742 C	1742 VS		
	$\nu_4$	CD bend.....	945 C	945 M		
	$\nu_5$	OD bend.....	1040 C	1040 W		
	$\nu_6$	C—O stretch.....	1171 C	1171.3 S		
<i>a''</i>	$\nu_7$	OCO deform.....	558 C	558 W		
	$\nu_8$	CD bend.....	873 C	873 W		
	$\nu_9$	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>	$\nu_1$	OH stretch.....	3681 A	$cm^{-1}$ (Gas) 3681 M	$cm^{-1}$ (Gas)	
	$\nu_2$	CH <sub>3</sub> d-stretch.....	3000 C	3000 M		
	$\nu_3$	CH <sub>3</sub> s-stretch.....	2844 A	2844 S		
	$\nu_4$	CH <sub>3</sub> d-deform.....	1477 B	1477 M	.....	OV ( $\nu_{10}$ )
	$\nu_5$	CH <sub>3</sub> s-deform.....	1455 A	1455 M		
	$\nu_6$	OH bend.....	1345 B	1345 S		
	$\nu_7$	CH <sub>3</sub> rock.....	1060 D	1060 W	.....	OV ( $\nu_8$ )
<i>a''</i>	$\nu_8$	CO stretch.....	1033 A	1033 VS	1032 (2)	
	$\nu_9$	CH <sub>3</sub> d-stretch.....	2960 C	2960 S	2955 (4)	
	$\nu_{10}$	CH <sub>3</sub> d-deform.....	1477 B	1477 M	.....	OV ( $\nu_4$ )
	$\nu_{11}$	CH <sub>3</sub> rock.....	1165 C	.....	1165 (1) (liquid)	
	$\nu_{12}$	Torsion.....	{ 295 (A) 200 (E) }	{ 80~300 }	.....	{ MW: <sup>a</sup> 295 (A) 200 (E) }

<sup>a</sup> The value of  $\nu_{12}$  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>	$\nu_1$	OH stretch . . . . .	3328 D	$cm^{-1}$ (Liquid) 3328 vb	$cm^{-1}$ (Liquid) 3270– 3480	OV ( $\nu_{10}$ ).
	$\nu_2$	CH <sub>3</sub> d-stretch . . . . .	2980 C	2980 M	2993 (3)	
	$\nu_3$	CH <sub>3</sub> s-stretch . . . . .	2834 C	2834 S	2834 (10)	
	$\nu_4$	CH <sub>3</sub> d-deform . . . . .	1480 C	1480 M	1464 (5b)	
	$\nu_5$	CH <sub>3</sub> s-deform . . . . .	1450 C	1450 M		
	$\nu_6$	OH bend . . . . .	1418 C	1418 M, b		
	$\nu_7$	CH <sub>3</sub> rock . . . . .	1115 C	1115 M	1107 (2)	
<i>a''</i>	$\nu_8$	CO stretch . . . . .	1030 C	1030 VS	1033 (6)	OV ( $\nu_4$ ).
	$\nu_9$	CH <sub>3</sub> d-stretch . . . . .	2946 C	2946 S	2940 (9)	
	$\nu_{10}$	CH <sub>3</sub> d-deform . . . . .	1480 C	1480 M	1464 (5b)	
	$\nu_{11}$	CH <sub>3</sub> rock . . . . .	1165 C		1165 (1)	
	$\nu_{12}$	Torsion . . . . .	655 D	655 vb		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	OD stretch . . . . .	2718 A	$cm^{-1}$ (Gas) 2718 M		SF ( $\nu_2$ of CH <sub>3</sub> OH).  OV ( $\nu_{10}$ ).
	$\nu_2$	CH <sub>3</sub> d-stretch . . . . .	3000 C	3000 M		
	$\nu_3$	CH <sub>3</sub> s-stretch . . . . .	2843 A	2843 S		
	$\nu_4$	CH <sub>3</sub> d-deform . . . . .	1473 B	1473 M		
	$\nu_5$	CH <sub>3</sub> s-deform . . . . .	1456 A	1456 M		
	$\nu_6$	OD bend . . . . .	864 A	864 S		
	$\nu_7$	CH <sub>3</sub> rock . . . . .	1230 B	1230 W		
<i>a''</i>	$\nu_8$	CO stretch . . . . .	1040 A	1040 VS		SF ( $\nu_9$ of CH <sub>3</sub> OH). OV ( $\nu_4$ ).  CF [5, 6].
	$\nu_9$	CH <sub>3</sub> d-stretch . . . . .	2960 C	2960 S		
	$\nu_{10}$	CH <sub>3</sub> d-deform . . . . .	1473 B	1473 M		
	$\nu_{11}$	CH <sub>3</sub> rock . . . . .	1160 C	1160 VW		
	$\nu_{12}$	Torsion . . . . .	213 E			

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



Molecule: Methanol-d<sub>1</sub> CH<sub>3</sub>OD (liquid)  
 Symmetry C<sub>s</sub> Symmetry number  $\sigma = 1$

No. 110

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	OD stretch . . . . .	2467 D	$cm^{-1}$ (Liquid) 2467 vb	$cm^{-1}$ (Liquid) 2420– 2560	OV ( $\nu_{10}$ ).
	$\nu_2$	CH <sub>3</sub> d-stretch . . . . .	2978 M	2978 M	2992 (3)	
	$\nu_3$	CH <sub>3</sub> s-stretch . . . . .	2838 C	2838 S	2834 (10)	
	$\nu_4$	CH <sub>3</sub> d-deform . . . . .	1469 C	1469 M	1463 (5b)	
	$\nu_5$	CH <sub>3</sub> s-deform . . . . .	1449 C	1449 M		
	$\nu_6$	OD bend . . . . .	940 C	940 M, b	955 (1)	
	$\nu_7$	CH <sub>3</sub> rock . . . . .	1231 C	1231 W	1226 (0)	
<i>a''</i>	$\nu_8$	CO stretch . . . . .	1038 C	1038 VS	1029 (6)	OV ( $\nu_4$ ).
	$\nu_9$	CH <sub>3</sub> d-stretch . . . . .	2951 C	2951 S	2943 (9)	
	$\nu_{10}$	CH <sub>3</sub> d-deform . . . . .	1469 C	1469 M	1463 (5b)	
	$\nu_{11}$	CH <sub>3</sub> rock . . . . .	1163 C	.....	1163 (1)	
	$\nu_{12}$	Torsion . . . . .	475 D	475 vb		

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

Molecule: Methanol-d<sub>3</sub> CD<sub>3</sub>OH (gas)  
 Symmetry C<sub>s</sub> Symmetry number  $\sigma = 1$

No. 111

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	OH stretch . . . . .	3690 D	$cm^{-1}$ (Gas) 3690 S	$cm^{-1}$	CF [1, 3].
	$\nu_2$	CD <sub>3</sub> d-stretch . . . . .	2260 E	2260 M, sh		
	$\nu_3$	CD <sub>3</sub> s-stretch . . . . .	2077 C	2077 S		
	$\nu_4$	CD <sub>3</sub> d-deform . . . . .	1047 D	1047 W		
	$\nu_5$	CD <sub>3</sub> s-deform . . . . .	1134 C	1134 VS		
	$\nu_6$	OH bend . . . . .	1297 C	1297 VS		
	$\nu_7$	CD <sub>3</sub> rock . . . . .	858 C	858 M		
<i>a''</i>	$\nu_8$	CO stretch . . . . .	988 C	988 VS		
	$\nu_9$	CD <sub>3</sub> d-stretch . . . . .	2235 D	2235 S		
	$\nu_{10}$	CD <sub>3</sub> d-deform . . . . .	1075 C	1075 W		
	$\nu_{11}$	CD <sub>3</sub> rock . . . . .	877 D	877 M		
	$\nu_{12}$	Torsion . . . . .	256 E			

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	OH stretch.....	3310 D	$cm^{-1}$ (Liquid) 3310 S, vb	$cm^{-1}$ (Liquid) 3350 W, vb	OV ( $\nu_{10}$ ).
	$\nu_2$	CD <sub>3</sub> d-stretch..	2235 D	<sup>a</sup> 2235 M	2230 M, dp	
	$\nu_3$	CD <sub>3</sub> s-stretch.....	2078 C	2078 S	2074 VS, p	
	$\nu_4$	CD <sub>3</sub> d-deform.....	1069 C	1069 W	1072 M, dp	
	$\nu_5$	CD <sub>3</sub> s-deform.....	1122 C	1122 VS	1127 M, p	
	$\nu_6$	OH bend.....	1391 C	1391 S, b	1360 VW, vb	
	$\nu_7$	CD <sub>3</sub> rock.....	882 C	882 M	894 M, dp	
<i>a''</i>	$\nu_8$	CO stretch.....	982 C	982 VS	986 VS, p	OV ( $\nu_{11}$ ).
	$\nu_9$	CD <sub>3</sub> d-stretch.....	2213 D	<sup>a</sup> 2213 M	2213 VW	
	$\nu_{10}$	CD <sub>3</sub> d-deform.....	1069 C	1069 W	1072 M, dp	
	$\nu_{11}$	CD <sub>3</sub> rock.....	882 D	882 M	894 M, dp	
	$\nu_{12}$	Torsion.....	665 D	665 S, vb		

<sup>a</sup> The value obtained in the vitreous solid (−180 °C).

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 [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>	$\nu_1$	OD stretch.....	2724 D	$cm^{-1}$ (Gas) 2724 S	$cm^{-1}$ .....	SF ( $\nu_2$ of CD <sub>3</sub> OH).
	$\nu_2$	CD <sub>3</sub> d-stretch.....	2260 E	2260		
	$\nu_3$	CD <sub>3</sub> s-stretch.....	2080 C	2080 S		
	$\nu_4$	CD <sub>3</sub> d-deform.....	1024 D	1024 W		
	$\nu_5$	CD <sub>3</sub> s-deform.....	1135 C	1135 VS		
	$\nu_6$	OD bend.....	1060 D	1060 W		
	$\nu_7$	CD <sub>3</sub> rock.....	776 C	776 S		
<i>a''</i>	$\nu_8$	CO stretch.....	983 C	983 VS		CF [1, 3].
	$\nu_9$	CD <sub>3</sub> d-stretch.....	2228 D	2228 S		
	$\nu_{10}$	CD <sub>3</sub> d-deform.....	1080 C	1080 W		
	$\nu_{11}$	CD <sub>3</sub> rock.....	892 C	892 W		
	$\nu_{12}$	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
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a'$	$\nu_1$	$\text{NH}_2$ s-stretch.....	3361 B	3361 W	3360 VS	
	$\nu_2$	$\text{CH}_3$ d-stretch.....	2961 B	2961 VS	2960 VS	
	$\nu_3$	$\text{CH}_3$ s-stretch.....	2820 B	2820 VS	2820 S	
	$\nu_4$	$\text{NH}_2$ scis.....	1623 B	1623 S		
	$\nu_5$	$\text{CH}_3$ d-deform.....	1473 B	1473 S	1460 M	
	$\nu_6$	$\text{CH}_3$ s-deform.....	1430 B	1430 M		
	$\nu_7$	$\text{CH}_3$ rock.....	1130 A	1130 M		
	$\nu_8$	CN stretch.....	1044 A	1044 S	1044 S	
$a''$	$\nu_9$	$\text{NH}_2$ wag.....	780 A	780 VS	781 W	
	$\nu_{10}$	$\text{NH}_2$ a-stretch.....	3427 C	3427 W	3470 W	
	$\nu_{11}$	$\text{CH}_3$ d-stretch.....	2985 C	2985 VS		
	$\nu_{12}$	$\text{CH}_3$ d-deform.....	1485 D	<sup>a</sup> 1485		
	$\nu_{13}$	$\text{NH}_2$ twist.....	1419 D	.....	.....	CF [5].
	$\nu_{14}$	$\text{CH}_3$ rock.....	1195 D	<sup>a</sup> 1195		
	$\nu_{15}$	Torsion.....	268 B	268	.....	MW: 272 (A). 265 (E).

<sup>a</sup> Estimated from  $\text{RQ}$  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> <sub>1</sub>	ND <sub>2</sub> s-stretch.....	2479 B	<i>cm</i> <sup>-1</sup> (Gas) 2479 W	<i>cm</i> <sup>-1</sup> (Gas) 2450 S	CF [5].
	<i>ν</i> <sub>2</sub>	CH <sub>3</sub> d-stretch.....	2961 B	2961 VS	2969 M	
	<i>ν</i> <sub>3</sub>	CH <sub>3</sub> s-stretch.....	2817 B	2817 S	2824 M	
	<i>ν</i> <sub>4</sub>	ND <sub>2</sub> scis.....	1234 B	1234 S	1214 M	
	<i>ν</i> <sub>5</sub>	CH <sub>3</sub> d-deform.....	1468 B	1468 S	1473 M	
	<i>ν</i> <sub>6</sub>	CH <sub>3</sub> s-deform.....	1430 B	1430 M		
	<i>ν</i> <sub>7</sub>	CH <sub>3</sub> rock.....	1117 A	1117 S		
	<i>ν</i> <sub>8</sub>	CN stretch.....	997 A	997 S	995 S	
<i>a''</i>	<i>ν</i> <sub>9</sub>	ND <sub>2</sub> wag.....	625 A	625 VS		
	<i>ν</i> <sub>10</sub>	ND <sub>2</sub> a-stretch.....	2556 B	2556 M	2527 M	
	<i>ν</i> <sub>11</sub>	CH <sub>3</sub> d-stretch.....	2985 C	2985 VS		
	<i>ν</i> <sub>12</sub>	CH <sub>3</sub> d-deform.....	1485 D	<sup>a</sup> 1485		
	<i>ν</i> <sub>13</sub>	ND <sub>2</sub> twist.....	1058 E	.....	.....	
	<i>ν</i> <sub>14</sub>	CH <sub>3</sub> rock.....	1187 C	1187 M		
	<i>ν</i> <sub>15</sub>	Torsion.....	228 C	228 S		

<sup>a</sup> Estimated from RQ branch frequency.

## References

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

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- [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> <sub>1</sub>	ND <sub>2</sub> s-stretch.....	2477 B	<i>cm</i> <sup>-1</sup> (Gas) 2477 W	<i>cm</i> <sup>-1</sup>	CF [2.]
	<i>ν</i> <sub>2</sub>	CD <sub>3</sub> d-stretch.....	2202 B	2202 VS		
	<i>ν</i> <sub>3</sub>	CD <sub>3</sub> s-stretch.....	2073 B	2073 VS		
	<i>ν</i> <sub>4</sub>	ND <sub>2</sub> scis.....	1227 B	1227 S		
	<i>ν</i> <sub>5</sub>	CD <sub>3</sub> d-deform.....	1065 D	.....		
	<i>ν</i> <sub>6</sub>	CD <sub>3</sub> s-deform.....	1123 B	1123 M		
	<i>ν</i> <sub>7</sub>	CD <sub>3</sub> rock.....	880 B	880 M		
	<i>ν</i> <sub>8</sub>	CN stretch.....	942 A	942 S		
	<i>ν</i> <sub>9</sub>	ND <sub>2</sub> wag.....	601 A	601 VS		
	<i>ν</i> <sub>10</sub>	ND <sub>2</sub> a-stretch.....	2556 C	2556 W		
	<i>ν</i> <sub>11</sub>	CD <sub>3</sub> d-stretch.....	2238 C	2238 VS		
	<i>ν</i> <sub>12</sub>	CD <sub>3</sub> d-deform.....	1077 C	1077 W		
	<i>ν</i> <sub>13</sub>	ND <sub>2</sub> twist.....	1072 D	.....		
	<i>ν</i> <sub>14</sub>	CD <sub>3</sub> rock.....	910 B	910 M		
	<i>ν</i> <sub>15</sub>	Torsion.....	201 C	.....		
<i>a''</i>						CF [2].
						CF [2].
						MW: 200 (A).
						203 (E).

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$\sigma_g^+$	$\nu_1$	CH stretch . . . . .	3374 C	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Gas) 3373.7 S	
	$\nu_2$	CC stretch . . . . .	1974 C	ia	1973.8 VS	
$\sigma_u^+$	$\nu_3$	CH stretch . . . . .	3289 B	$\left\{ \begin{array}{l} 3294.9 \text{ S} \\ 3281.9 \text{ VS} \end{array} \right\}$	ia	FR ( $\nu_2 + \nu_4 + \nu_5$ ).
$\pi_g$	$\nu_4$	CH bend . . . . .	612 C	ia	611.8 VW	
$\pi_u$	$\nu_5$	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
$\sigma^+$	$\nu_1$	CH stretch . . . . .	3336 A	$cm^{-1}$ (Gas) 3335.6 S	$cm^{-1}$ (Gas) 3335 S	
	$\nu_2$	CC stretch . . . . .	1854 A	1853.8 M	1851 S	
	$\nu_3$	CD stretch . . . . .	2584 A	2583.6 S		
$\pi$	$\nu_4$	CH bend . . . . .	518 A	518.38 S	.....	RP [4].
	$\nu_5$	CD bend . . . . .	678 A	677.8 S	.....	RP [4].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$\sigma_g^+$	$\nu_1$	CD stretch.....	2701 C	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Gas) 2700.5 S	OC ( $\nu_4 + \nu_5$ ) [1].
	$\nu_2$	CC stretch.....	1762 C	ia	1762.4 S	
$\sigma_u^+$	$\nu_3$	CD stretch.....	2439 A	2439.24 S	ia	
$\pi_g$	$\nu_4$	CD bend.....	505 C	ia	.....	
$\pi_u$	$\nu_5$	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
$\sigma^+$	$\nu_1$	CH stretch.....	3355 B	$cm^{-1}$ (Gas) 3355 VS	$cm^{-1}$	
	$\nu_2$	CC stretch.....	2255 B	2255 VS		
	$\nu_3$	CF stretch.....	1055 B	1055 VS		
$\pi$	$\nu_4$	CH bend.....	578 B	578 VS		
	$\nu_5$	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
$\sigma^+$	$\nu_1$	CH stretch.....	3340 B	$cm^{-1}$ (Gas) 3340 VS	$cm^{-1}$	
	$\nu_2$	CC stretch.....	2110 B	2110 VS		
	$\nu_3$	CCl stretch.....	756 B	756 VS		
$\pi$	$\nu_4$	CH bend.....	604 B	604 S		
	$\nu_5$	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
$\sigma^+$	$\nu_1$	CH stretch.....	3325 B	$cm^{-1}$ (Gas) 3325 VS	$cm^{-1}$	
	$\nu_2$	CC stretch.....	2085 B	2085 VS		
	$\nu_3$	CBr stretch.....	618 C	618 VS	.....	SF ( $\nu_4$ ).
$\pi$	$\nu_4$	CH bend.....	618 C	618 VS	.....	SF ( $\nu_3$ ).
	$\nu_5$	CCBr bend.....	295 B	295 W		

## References

See No. 121.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_g$	$\nu_1$	$\text{CH}_2$ s-stretch . . . . .	3026 B	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Gas) 3026.4 (10)p	FR ( $2\nu_{10}$ ).  OC ( $\nu_4 + \nu_6$ ) [7].
	$\nu_2$	CC stretch . . . . .	1623 D	ia	1622.6 (8)p	
	$\nu_3$	$\text{CH}_2$ scis . . . . .	1342 B	ia	1342.2 (10)p	
$a_u$	$\nu_4$	$\text{CH}_2$ twist . . . . .	1023 E	ia	ia	
$b_{1g}$	$\nu_5$	$\text{CH}_2$ a-stretch . . . . .	3103 B	ia	3102.5 (1)dp	
	$\nu_6$	$\text{CH}_2$ rock . . . . .	1236 C	ia	1236 (1)dp (liquid)	
$b_{1u}$	$\nu_7$	$\text{CH}_2$ wag . . . . .	949 A	949.3 M	ia	
$b_{2g}$	$\nu_8$	$\text{CH}_2$ wag . . . . .	943 C	ia	943 (1)dp (liquid)	
$b_{2u}$	$\nu_9$	$\text{CH}_2$ a-stretch . . . . .	3106 B	3105.5 S	ia	
	$\nu_{10}$	$\text{CH}_2$ rock . . . . .	826 A	826.0 W	ia	
$b_{3u}$	$\nu_{11}$	$\text{CH}_2$ s-stretch . . . . .	2989 A	2988.66 S	ia	
	$\nu_{12}$	$\text{CH}_2$ scis . . . . .	1444 B	1443.5 S	ia	

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Molecule: Ethylene-d<sub>4</sub> C<sub>2</sub>D<sub>4</sub>  
Symmetry D<sub>2h</sub> 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)	
$a_g$	$\nu_1$	CD <sub>2</sub> s-stretch.....	2251 C	ia	2251 VS	CF [4].
	$\nu_2$	CC stretch.....	1515 C	ia	1515 VS	
	$\nu_3$	CD <sub>2</sub> scis.....	981 C	ia	981 M	
$a_u$	$\nu_4$	CD <sub>2</sub> twist.....	728 E	ia	ia	
$b_{1g}$	$\nu_5$	CD <sub>2</sub> a-stretch.....	2304 C	ia	2304 W	
	$\nu_6$	CD <sub>2</sub> rock.....	1009 E	ia	.....	
$b_{1u}$	$\nu_7$	CD <sub>2</sub> wag.....	720 B	720.0 VS	ia	OC ( $\nu_6 + \nu_{10}$ ).
$b_{2g}$	$\nu_8$	CD <sub>2</sub> wag.....	780 C	ia	780 W	
$b_{2u}$	$\nu_9$	CD a-stretch.....	2345 C	2345 S	ia	CF. <sup>a</sup>
	$\nu_{10}$	CD <sub>2</sub> rock.....	586 E	.....	ia	
$b_{3u}$	$\nu_{11}$	CD <sub>2</sub> a-stretch.....	2200 C	2200.2 S	ia	
	$\nu_{12}$	CD <sub>2</sub> scis.....	1078 C	1077.9 S	ia	

<sup>a</sup> From product rule.

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Molecule: Tetrafluoroethylene CF<sub>2</sub>CF<sub>2</sub>  
Symmetry D<sub>2h</sub> 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)	
$a_g$	$\nu_1$	CC stretch.....	1872 C	ia	1872 M, p	CF [3].
	$\nu_2$	CF <sub>2</sub> s-stretch.....	778 C	ia	777.9 S, p	
	$\nu_3$	CF <sub>2</sub> scis.....	394 C	ia	394 W, p	
$a_u$	$\nu_4$	CF <sub>2</sub> twist.....	190 E	ia	ia	
$b_{1g}$	$\nu_5$	CF <sub>2</sub> a-stretch.....	1340 D	ia	1340 VW	
	$\nu_6$	CF <sub>2</sub> rock.....	551 D	ia	551 M (liquid)	
$b_{1u}$	$\nu_7$	CF <sub>2</sub> wag.....	406 C	406 S	ia	CF [3].
$b_{2g}$	$\nu_8$	CF <sub>2</sub> wag.....	508 D	ia	508 S (liquid)	
$b_{2u}$	$\nu_9$	CF <sub>2</sub> a-stretch.....	1337 C	1337 S	ia	CF [3].
	$\nu_{10}$	CF <sub>2</sub> rock.....	218 C	218 S	ia	
$b_{3u}$	$\nu_{11}$	CF <sub>2</sub> s-stretch.....	1186 C	1186 S	ia	
	$\nu_{12}$	CF <sub>2</sub> sciss.....	558 C	558 S	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_g$	$\nu_1$	CC stretch . . . . .	1571 D	$\text{cm}^{-1}$ (Liquid) ia	$\text{cm}^{-1}$ (Liquid) 1571 (7)p	OC ( $2\nu_4$ ) [2].
	$\nu_2$	$\text{CCl}_2$ s-stretch . . . . .	447 D	ia	447 (10)p	
	$\nu_3$	$\text{CCl}_2$ scis . . . . .	237 D	ia	237 (7)p	
$a_u$	$\nu_4$	$\text{CCl}_2$ twist . . . . .	110 E	ia	ia	
$b_{1g}$	$\nu_5$	$\text{CCl}_2$ a-stretch . . . . .	1000 D	ia	1000 (0)	
	$\nu_6$	$\text{CCl}_2$ rock . . . . .	347 D	ia	347 (4)dp	
$b_{1u}$	$\nu_7$	$\text{CCl}_2$ wag . . . . .	288 D	288 M	ia	
$b_{2g}$	$\nu_8$	$\text{CCl}_2$ wag . . . . .	512 D	ia	512 (4)dp	
$b_{2u}$	$\nu_9$	$\text{CCl}_2$ a-stretch . . . . .	908 C	908 S ( $\text{CS}_2$ soln.)	ia	
$b_{3u}$	$\nu_{10}$	$\text{CCl}_2$ rock . . . . .	176 C	176 S	ia	
	$\nu_{11}$	$\text{CCl}_2$ s-stretch . . . . .	777 C	777 S	ia	
	$\nu_{12}$	$\text{CCl}_2$ scis . . . . .	310 C	( $\text{CS}_2$ soln.) 310 W	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_g$	$\nu_1$	CC stretch . . . . .	1535 E	$\text{cm}^{-1}$ (Liquid) ia	$\text{cm}^{-1}$ (Liquid) {1547 (2)p 1515 (1)p}	FR ( $2\nu_9$ ) [1].  CF [2].
	$\nu_2$	$\text{CBr}_2$ s-stretch . . . . .	265 D	ia	265 (10)p	
	$\nu_3$	$\text{CBr}_2$ scis . . . . .	144 D	ia	144 (1)p	
$a_u$	$\nu_4$	$\text{CBr}_2$ twist . . . . .	66 E	ia	ia	
$b_{1g}$	$\nu_5$	$\text{CBr}_2$ a-stretch . . . . .	880 D	ia	880 (1)dp	
	$\nu_6$	$\text{CBr}_2$ rock . . . . .	208 D	ia	208 (2)dp	
$b_{1u}$	$\nu_7$	$\text{CBr}_2$ wag . . . . .	245 C	245 S	ia	
$b_{2g}$	$\nu_8$	$\text{CBr}_2$ wag . . . . .	464 D	ia	464 (1)dp	
$b_{2u}$	$\nu_9$	$\text{CBr}_2$ a-stretch . . . . .	766 C	766 S	ia	
$b_{3u}$	$\nu_{10}$	$\text{CBr}_2$ rock . . . . .	119 C	119 M	ia	
	$\nu_{11}$	$\text{CBr}_2$ s-stretch . . . . .	635 C	635 S	ia	
	$\nu_{12}$	$\text{CBr}_2$ scis . . . . .	188 C	188 M	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a</i> <sub>1</sub>	$\nu_1$	CH stretch.....	3135 D	3135 W	.....	SF ( $\nu_8$ ).
	$\nu_2$	CC stretch.....	1715 C	1715 S		
	$\nu_3$	CH bend.....	1266 C	1266 S		
	$\nu_4$	CF stretch.....	1014 C	1014 S		
	$\nu_5$	CCF deform.....	255 D	255 W		
<i>a</i> <sub>2</sub>	$\nu_6$	CH bend.....	866 E	ia	.....	CF. <sup>a</sup> CF. <sup>b</sup> SF ( $\nu_1$ ).
	$\nu_7$	Torsion.....	482 E	ia	.....	
<i>b</i> <sub>1</sub>	$\nu_8$	CH stretch.....	3135 D	3135 W	.....	
	$\nu_9$	CH bend.....	1376 C	1376 S		
	$\nu_{10}$	CF stretch.....	1127 C	1127 VS		
<i>b</i> <sub>2</sub>	$\nu_{11}$	CCF deform.....	768 B	768 S		
	$\nu_{12}$	CH bend.....	756 B	756 S		

<sup>a</sup> From product rule.

<sup>b</sup> 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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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a'</i>	$\nu_1$	CH stretch.....	3125 D	3125 W		
	$\nu_2$	CD stretch.....	2364 D	2364 W		
	$\nu_3$	CC stretch.....	1692 C	1692 S		
	$\nu_4$	CH bend.....	1330 C	1330 S		
	$\nu_5$	CF stretch.....	1167 C	1167 VS		
	$\nu_6$	CF stretch.....	1033 C	1033 VS		
	$\nu_7$	CD bend.....	889 B	889 M		
	$\nu_8$	CCF deform.....	757 B	757 S		
<i>a''</i>	$\nu_9$	CCF deform.....	255 D	255 W		
	$\nu_{10}$	CH bend.....	801 B	801 M		
	$\nu_{11}$	CD bend.....	633 B	633 M		
	$\nu_{12}$	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> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CD stretch.....	2320 D	2320 W	.....	SF ( <i>ν</i> <sub>8</sub> ).
	<i>ν</i> <sub>2</sub>	CC stretch.....	1675 C	1675 S		
	<i>ν</i> <sub>3</sub>	CF stretch.....	1054 C	1054 S		
	<i>ν</i> <sub>4</sub>	CD bend.....	847 B	847 M		
	<i>ν</i> <sub>5</sub>	CCF deform.....	255 D	255 W		
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>6</sub>	CD bend.....	656 E	ia	.....	CF. <sup>a</sup> CF. <sup>b</sup> SF ( <i>ν</i> <sub>1</sub> ).
	<i>ν</i> <sub>7</sub>	Torsion.....	459 E	ia	.....	
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>8</sub>	CD stretch.....	2320 D	2320 W	.....	
	<i>ν</i> <sub>9</sub>	CF stretch.....	1225 C	1225 VS		
	<i>ν</i> <sub>10</sub>	CD bend.....	937 B	937 M		
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>11</sub>	CCF deform.....	748 B	748 S		
	<i>ν</i> <sub>12</sub>	CD bend.....	597 B	597 M		

<sup>a</sup> From product rule.

<sup>b</sup> 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> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a</i> <sub>g</sub>	<i>ν</i> <sub>1</sub>	CH stretch.....	3073 C	ia	3073 S, p	
	<i>ν</i> <sub>2</sub>	CC stretch.....	1578 C	ia	1578 S, p	
	<i>ν</i> <sub>3</sub>	CH bend.....	1274 C	ia	1274 S, p	
	<i>ν</i> <sub>4</sub>	CCl stretch.....	846 C	ia	846 S, p	
	<i>ν</i> <sub>5</sub>	CCCl deform.....	350 C	ia	350 S, p	
<i>a</i> <sub>u</sub>	<i>ν</i> <sub>6</sub>	CH bend.....	900 B	899.8 VS	ia	
	<i>ν</i> <sub>7</sub>	Torsion.....	227 C	227 M	ia	
<i>b</i> <sub>g</sub>	<i>ν</i> <sub>8</sub>	CH bend.....	763 B	ia	763 M, dp	
<i>b</i> <sub>u</sub>	<i>ν</i> <sub>9</sub>	CH stretch.....	3090 C	3090 S	ia	
	<i>ν</i> <sub>10</sub>	CH bend.....	1200 B	1200 S	ia	
	<i>ν</i> <sub>11</sub>	CCl stretch.....	828 B	828 VS	ia	
	<i>ν</i> <sub>12</sub>	CCCl deform.....	250 D	250 W	ia	

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Molecule: **trans-1,2-Dichloroethylene-d<sub>1</sub>** **CHClCDCl**  
 Symmetry **C<sub>s</sub>** Symmetry number  **$\sigma = 1$**

No. 133

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	CH stretch.....	3087 C	<i>cm</i> <sup>-1</sup> (Gas) 3087 S	<i>cm</i> <sup>-1</sup> (Liquid) 3074 M	CF [6].
	$\nu_2$	CD stretch.....	2310 C	2310 S	2304 M	
	$\nu_3$	CC stretch.....	1574 D	1574 W (liquid)	1574 S	
	$\nu_4$	CH bend.....	1241 C	1241 S	1238 S	
	$\nu_5$	CD bend.....	963 C	963 VS	957 S	
	$\nu_6$	CCl stretch.....	823 C	825 VS (liquid)	823 W	
<i>a''</i>	$\nu_7$	CCl stretch.....	775 B	775 VS	775 M	
	$\nu_8$	CCCl deform.....	348 C	.....	348 VS	
	$\nu_9$	CCCl deform.....	245 E	.....	.....	
	$\nu_{10}$	CH bend.....	830 C	830 VS	834 W	
	$\nu_{11}$	CD bend.....	660 B	660 S	659 W	
	$\nu_{12}$	Torsion.....	224 E	.....	.....	CF [5, 6].

## References

See No. 132.

Molecule: **trans-1,2-Dichloroethylene-d<sub>2</sub>** **CDClCDCl**  
 Symmetry **C<sub>2h</sub>** Symmetry number  **$\sigma = 2$**

No. 134

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a<sub>g</sub></i>	$\nu_1$	CD stretch.....	2325 C	<i>cm</i> <sup>-1</sup> (Gas) ia	<i>cm</i> <sup>-1</sup> (Liquid) 2325 S	CF [5, 6].
	$\nu_2$	CC stretch.....	1570 C	ia	1570 S	
	$\nu_3$	CD bend.....	992 C	ia	992 S	
	$\nu_4$	CCl stretch.....	765 C	ia	765 M	
<i>a<sub>u</sub></i>	$\nu_5$	CCCl deform.....	346 C	ia	346 S	
	$\nu_6$	CD bend.....	660 B	660 S	ia	
	$\nu_7$	Torsion.....	221 E	.....	ia	
<i>b<sub>g</sub></i>	$\nu_8$	CD bend.....	657 C	ia	657 M	
<i>b<sub>u</sub></i>	$\nu_9$	CD stretch.....	2290 C	2290 S	ia	
	$\nu_{10}$	CD bend.....	916 C	916 VS	ia	
	$\nu_{11}$	CCl stretch.....	791 C	791 VS	ia	
	$\nu_{12}$	CCCl deform.....	240 E	.....	ia	CF [6].

## References

See No. 132.



Molecule: **cis-1,2-Dichloroethylene** **CHClCHCl**  
Symmetry **C<sub>2v</sub>** Symmetry number  **$\delta = 2$**

No. 135

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<b>a<sub>1</sub></b>	$\nu_1$	CH stretch.....	3077 C	$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
	$\nu_2$	CC stretch.....	1587 C	1590 S (liquid)	3077 1587 S, p	
	$\nu_3$	CH bend.....	1179 C	1183 W (liquid)	1179 S, p	
	$\nu_4$	CCl stretch.....	711 C	714 S (liquid)	711 S, p	
<b>a<sub>2</sub></b>	$\nu_5$	CCCl deform.....	173 C	.....	173 S, p	
	$\nu_6$	CH bend.....	876 C	ia	876 W, dp	
	$\nu_7$	Torsion.....	406 C	ia	406 S, dp	
<b>b<sub>1</sub></b>	$\nu_8$	CH stretch.....	3072 C	3072		
	$\nu_9$	CH bend.....	1303 C	1303		
	$\nu_{10}$	CCl stretch.....	857 B	857		
	$\nu_{11}$	CCCl deform.....	571 B	571	563 M, dp	
<b>b<sub>2</sub></b>	$\nu_{12}$	CH bend.....	697 B	697		

#### References

See No. 132.

Molecule: **cis-1,2-Dichloroethylene-d<sub>1</sub>** **CHClCDCl**  
Symmetry **C<sub>s</sub>** Symmetry number  **$\delta = 1$**

No. 136

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<b>a'</b>	$\nu_1$	CH stretch.....	3076 C	$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
	$\nu_2$	CD stretch.....	2306 C	3076 S (liquid)	3078 VS	
	$\nu_3$	CC stretch.....	1562 C	2306 S	2299 VS	
	$\nu_4$	CH bend.....	1253 C	1562 S	1553 S	
	$\nu_5$	CD bend.....	957 C	1253 VS	1245 M	
	$\nu_6$	CCl stretch.....	788 B	957 VS	950 M	
	$\nu_7$	CCl stretch.....	711 C	788 VS	781 W	
	$\nu_8$	CCl bend.....	558 C	711 VS	703 VS	
	$\nu_9$	CCl bend.....	175 D	558 S	561 S	
<b>a''</b>	$\nu_{10}$	CH bend.....	822 C	.....	175 VS	
	$\nu_{11}$	CD bend.....	589 C	822 VS	817 W	
	$\nu_{12}$	Torsion.....	387 C	589 VS	590 W	
				.....	387 S	

#### References

See No. 132.



Molecule: **cis-1,2-Dichloroethylene-d<sub>2</sub>** **CDCICDCI**  
Symmetry **C<sub>2v</sub>** Symmetry number  **$\sigma = 2$**

No. 137

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	$\nu_1$	CD stretch.....	2325 C	.....	2325 S	CF [6].
	$\nu_2$	CC stretch.....	1575 C	1575 S	1570 S	
	$\nu_3$	CD bend.....	850 C	.....	850 M	
	$\nu_4$	CCl stretch.....	700 C	700 S	689 S	
	$\nu_5$	CCCl deform.....	171 C	.....	171 S	
<i>a</i> <sub>2</sub>	$\nu_6$	CD bend.....	686 E	ia	.....	
	$\nu_7$	Torsion.....	368 C	ia	368 M	
<i>b</i> <sub>1</sub>	$\nu_8$	CD stretch.....	2280 B	2280	2280 S	
	$\nu_9$	CD bend.....	1051 B	1051	1040 VS	
	$\nu_{10}$	CCl stretch.....	766 B	766	761 VS	
	$\nu_{11}$	CCCl deform.....	558 C	.....	558 S	
<i>b</i> <sub>2</sub>	$\nu_{12}$	CD bend.....	540 C	.....	540 S	

## References

See No. 132.

Molecule: **trans-1,2-Dichloro-1,2-difluoroethylene** **CCIFCCIF**  
Symmetry **C<sub>2h</sub>** Symmetry number  **$\sigma = 2$**

No. 138

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a</i> <sub>g</sub>	$\nu_1$	CC stretch.....	1707 C	ia	1707 VS, p	CF [2].  FR ( $\nu_5 + \nu_{10}$ ).
	$\nu_2$	CF stretch.....	1186 C	ia	1186 W, p	
	$\nu_3$	CCl stretch.....	632 C	ia	632 M, p	
	$\nu_4$	CF bend.....	425 C	ia	425 M, p	
	$\nu_5$	CCl bend.....	288 C	ia	288 M, p	
<i>a</i> <sub>u</sub>	$\nu_6$	CFCl wag.....	333 C	333 M	ia	
	$\nu_7$	Torsion.....	140 D	.....	ia	
<i>b</i> <sub>g</sub>	$\nu_8$	CFCl wag.....	529 C	ia	529 M, dp	
<i>b</i> <sub>u</sub>	$\nu_9$	CF stretch.....	1190 E	{ 1214 VS 1167 VS }	ia	
	$\nu_{10}$	CCl stretch.....	892 B	892 VS	ia	
	$\nu_{11}$	CF bend.....	426 C	426 M	ia	
	$\nu_{12}$	CCl bend.....	175 C	175 M	ia	

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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
$a_1$	$\nu_1$	$\text{CH}_2$ s-stretch.....	3035 D	$\text{cm}^{-1}$ (Gas) $^a 3035$ W	$\text{cm}^{-1}$ (Liquid) 3035 VS, p	
	$\nu_2$	CC stretch.....	1627 C	1627 VS	1616 VS, p	
	$\nu_3$	$\text{CH}_2$ scis.....	1400 C	1400 M	1391 M, p	
	$\nu_4$	$\text{CCl}_2$ s-stretch.....	603 C	603 VS	601 VS, p	
	$\nu_5$	$\text{CCl}_2$ scis.....	299 C	299 W	299 S, p	
$a_2$	$\nu_6$	Torsion .....	686 D	ia	686 M, dp	
$b_1$	$\nu_7$	$\text{CH}_2$ a-stretch.....	3130 D	$^a 3130$ W	3130 S, dp	
	$\nu_8$	$\text{CH}_2$ rock.....	1095 C	1095 VS	1088 VW	
	$\nu_9$	$\text{CCl}_2$ a-stretch.....	800 B	800 VS	788 M, dp	
$b_2$	$\nu_{10}$	$\text{CCl}_2$ rock.....	372 C	372 M	375 S, dp	
	$\nu_{11}$	$\text{CH}_2$ wag.....	875 B	875 S	874 W	
	$\nu_{12}$	$\text{CCl}_2$ wag.....	460 B	460 S	458 M, dp	

<sup>a</sup>  $\text{CCl}_4$  solution.

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	CH stretch.....	3082 D	$cm^{-1}$ (Gas) <sup>a</sup> 3082 W	$cm^{-1}$	CF [1].
	$\nu_2$	CD stretch.....	2288 D	<sup>a</sup> 2288 W		
	$\nu_3$	CC stretch	1585 C	1585 S		
	$\nu_4$	CHD scis.....	1280 C	1280 M		
	$\nu_5$	CHD rock.....	999 C	999 VS		
	$\nu_6$	CCl <sub>2</sub> a-stretch.....	741 C	741 S		
	$\nu_7$	CCl <sub>2</sub> s-stretch.....	590 C	590 VS		
	$\nu_8$	CCl <sub>2</sub> rock.....	348 C	348 W		
$a''$	$\nu_9$	CCl <sub>2</sub> scis.....	306 E	.....	.....	
	$\nu_{10}$	CHD wag.....	819 B	819 S		
	$\nu_{11}$	Torsion.....	555 C	555 W		
	$\nu_{12}$	CCl <sub>2</sub> wag.....	444 B	444 M		

<sup>a</sup>  $\text{CCl}_4$  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> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CD <sub>2</sub> s-stretch.....	2262 D	<i>cm</i> <sup>-1</sup> (Gas) <sup>a</sup> 2262 W	<i>cm</i> <sup>-1</sup>	
	<i>ν</i> <sub>2</sub>	CC stretch.....	1565 C	1565 VS		
	<i>ν</i> <sub>3</sub>	CD <sub>2</sub> scis.....	1039 E			CF [1].
	<i>ν</i> <sub>4</sub>	CCl <sub>2</sub> s-stretch.....	580 C	580 VS		
	<i>ν</i> <sub>5</sub>	CCl <sub>2</sub> scis.....	305 E			CF [1].
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>6</sub>	Torsion.....	488 E	ia		CF [1].
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>7</sub>	CD <sub>2</sub> a-stretch.....	2380 D	<sup>a</sup> 2380 W		
	<i>ν</i> <sub>8</sub>	CD <sub>2</sub> rock.....	998 C	998 VS		
	<i>ν</i> <sub>9</sub>	CCl <sub>2</sub> a-stretch.....	697 C	697 S		SF ( <i>ν</i> <sub>11</sub> ).
	<i>ν</i> <sub>10</sub>	CCl <sub>2</sub> rock.....	327 C	327 M		
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>11</sub>	CD <sub>2</sub> wag.....	697 C	697 S		SF ( <i>ν</i> <sub>9</sub> ).
	<i>ν</i> <sub>12</sub>	CCl <sub>2</sub> wag.....	439 B	439 S		

<sup>a</sup> CCl<sub>4</sub> 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> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CC stretch	1749 B	<i>cm</i> <sup>-1</sup> (Gas) 1749 VS	<i>cm</i> <sup>-1</sup> (Liquid) 1738.8 S	
	<i>ν</i> <sub>2</sub>	CF stretch.....	1032 B	1032 VS	1027.6 M	
	<i>ν</i> <sub>3</sub>	CCl stretch.....	622 C	622 M	623.0 S	
	<i>ν</i> <sub>4</sub>	CF <sub>2</sub> scis.....	434 C	434	433.8 VS	
	<i>ν</i> <sub>5</sub>	CCl <sub>2</sub> scis.....	258 C	258 S	258 VS	
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>6</sub>	Torsion.....	167 D		167 VW	
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>7</sub>	CF stretch.....	1327 B	1327 VS	1313 VW	
	<i>ν</i> <sub>8</sub>	CCl stretch.....	989 B	989 VS	986 VW	
	<i>ν</i> <sub>9</sub>	CF <sub>2</sub> rock.....	459 C	459 VW	454 W	
	<i>ν</i> <sub>10</sub>	CCl <sub>2</sub> rock.....	192 C	192	187.8 W	
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>11</sub>	CF <sub>2</sub> wag.....	564 C	564 S	560.8 VS	
	<i>ν</i> <sub>12</sub>	CCl <sub>2</sub> wag.....	323 C	323 W		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch . . . . .	2954 A	2954.1 M	2942 VS	OC ( $\nu_3 + \nu_4$ ).
	$\nu_2$	CN stretch . . . . .	2267 A	2266.5 M	2249 S	
	$\nu_3$	$\text{CH}_3$ s-deform . . . . .	1385 C	.....	1376 M	
	$\nu_4$	CC stretch . . . . .	920 A	920.2 S	918 S	
$e$	$\nu_5$	$\text{CH}_3$ d-stretch . . . . .	3009 A	3009.2 S	2999 S	FR ( $\nu_7 + \nu_8$ ).
	$\nu_6$	$\text{CH}_3$ d-deform . . . . .	1448 D	1447.9 S	1440 M, b	
	$\nu_7$	$\text{CH}_3$ rock . . . . .	1041 A	1040.8 M		
	$\nu_8$	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
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CD}_3$ s-stretch . . . . .	2126 A	2125.6	2112 S	
	$\nu_2$	CN stretch . . . . .	2278 A	2277.6	2258 S	
	$\nu_3$	$\text{CD}_3$ s-deform . . . . .	1110 B	1110	1103 W	
	$\nu_4$	CC stretch . . . . .	831 A	831.3	834 W	
$e$	$\nu_5$	$\text{CD}_3$ d-stretch . . . . .	2257 A	2256.6	2258 S	
	$\nu_6$	$\text{CD}_3$ d-deform . . . . .	1046 A	1046.4	1041 W	
	$\nu_7$	$\text{CD}_3$ rock . . . . .	847 A	846.6		
	$\nu_8$	CCN bend . . . . .	331 B	331.2	348 M	

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Molecule: Methyl isocyanide  $\text{CH}_3\text{NC}$   
 Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 145

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch.....	2966 B	2965.8 M	2951 S	
	$\nu_2$	NC stretch.....	2166 B	2166.0 M	2161 S	
	$\nu_3$	$\text{CH}_3$ s-deform.....	1429 D	1429	1414 M	
	$\nu_4$	CN stretch.....	945 B	944.6 M	928 M	
$e$	$\nu_5$	$\text{CH}_3$ d-stretch.....	3014 B	3014.3 S	3002 W	
	$\nu_6$	$\text{CH}_3$ d-deform.....	1467 B	1466.9 S	1456 W	
	$\nu_7$	$\text{CH}_3$ rock.....	1129 B	1129.3 S		
	$\nu_8$	CNC bend.....	263 C	263 W	290 S	

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Molecule: Methyl isocyanide- $\text{d}_3$   $\text{CD}_3\text{NC}$   
 Symmetry  $\text{C}_{3v}$  Symmetry number  $\sigma = 3$

No. 146

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a_1$	$\nu_1$	$\text{CD}_3$ s-stretch.....	2251 B	2250.6 W		
	$\nu_2$	NC stretch.....	2165 B	2165.0 W		
	$\nu_3$	$\text{CD}_3$ s-deform.....	1117 B	1117.4 W		
	$\nu_4$	CN stretch.....	877 B	876.7 M		
$e$	$\nu_5$	$\text{CD}_3$ d-stretch.....	2263 B	2262.9 S		
	$\nu_6$	$\text{CD}_3$ d-deform.....	1058 B	1058.2 S		
	$\nu_7$	$\text{CD}_3$ rock.....	900 B	900.1 S		
	$\nu_8$	CNC bend.....	249 C	.....	.....	OC ( $\nu_2 + \nu_8$ )

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
$a_1$	$\nu_1$	CH stretch.....	3140 C	3140 VW	3144 VS, p	
	$\nu_2$	ip-Ring II.....	1418 B	1418 S	1422 VS, p	
	$\nu_3$	ip-Ring III.....	1316 B	1316 M	1315 VS, p	
	$\nu_4$	CH ip-bend.....	1038 D	1039 sh	1038 W, p	
	$\nu_5$	ip-Ring IV.....	1006 B	1006 S	998 M, p	
	$\nu_6$	ip-Ring VII.....	872 C	872 S	864 M, p	
$a_2$	$\nu_7$	CH op-bend.....	824 D	ia, 824 sh (liquid)	824 VW, dp	
	$\nu_8$	op-Ring I	635 E	ia	.....	OC ( $2\nu_8, \nu_4 + \nu_8, \nu_8 + \nu_{12}$ ).
$b_1$	$\nu_9$	CH stretch.....	3133 D	3133 sh (liquid)		
	$\nu_{10}$	ip-Ring I.....	1546 D	1546 VW (liquid)		
$b_2$	$\nu_{11}$	CH ip-bend.....	1177 B	1177 M	1172 VW, dp	
	$\nu_{12}$	ip-Ring V.....	952 B	952 S	951 W, dp	
	$\nu_{13}$	ip-Ring VI.....	889 B	889 S		
	$\nu_{14}$	CH op-bend.....	839 B	839 VS		
	$\nu_{15}$	op-Ring II.....	631 B	631 W	626 VW, dp	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$cm^{-1}$ (Gas)	$cm^{-1}$	
$a_1$	$\nu_1$	CH stretch.....	3311 B	3311.4 M		
	$\nu_2$	$SiH_3$ s-stretch.....	2192 B	2192.4 VS		
	$\nu_3$	CC stretch.....	2055 B	2054.9 S		
	$\nu_4$	$SiH_3$ s-deform.....	935 B	935.3 VS		
	$\nu_5$	SiC stretch.....	659 D	<sup>a</sup> 659 S		
$e$	$\nu_6$	$SiH_3$ d-stretch.....	2193 A	2192.9 VS		
	$\nu_7$	$SiH_3$ d-deform.....	946 D	<sup>a</sup> 946.4 VS		
	$\nu_8$	$SiH_3$ rock.....	685 D	<sup>a</sup> 685.4 VS		
	$\nu_9$	CH bend.....	668 D	<sup>a</sup> 668 VS		
	$\nu_{10}$	SiCC deform.....	220 E	220		

<sup>a</sup> These frequencies are taken from ref. 1. The band centers of  $\nu_5$ ,  $\nu_7$ ,  $\nu_8$ , and  $\nu_9$  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
$a_1$	$\nu_1$	$CH_2$ s-stretch.....	3006 C	$cm^{-1}$ (Gas) 3006 S	$cm^{-1}$ (Liquid) 3005 S, p	OV ( $\nu_{13}$ ).  OV ( $\nu_1$ ).
	$\nu_2$	$CH_2$ scis.....	1498 B	1498 W	1490 W, p	
	$\nu_3$	Ring stretch.....	1271 B	1271 S	1266 S, p	
	$\nu_4$	$CH_2$ wag.....	1120 D	1118 W ( $CS_2$ soln.)	1120 M, p	
$a_2$	$\nu_5$	Ring deform.....	877 B	877 VS	867 M, dp	
	$\nu_6$	$CH_2$ a-stretch.....	3063 D	ia	3063 W, dp	
	$\nu_7$	$CH_2$ twist.....	1300 E	ia		
	$\nu_8$	$CH_2$ rock.....	860 E	ia		
$b_1$	$\nu_9$	$CH_2$ s-stretch.....	3006 C	3006 S	3005 S, p	
	$\nu_{10}$	$CH_2$ scis.....	1472 B	1472 W		
	$\nu_{11}$	$CH_2$ wag.....	1151 D	1151 M	1150 W, dp	
	$\nu_{12}$	Ring deform.....	892 D	892 VS		
$b_2$	$\nu_{13}$	$CH_2$ a-stretch.....	3065 B	3065 S	3063 W, dp	
	$\nu_{14}$	$CH_2$ twist.....	1142 D	1142 M	1150 W, dp	
	$\nu_{15}$	$CH_2$ rock.....	822 B	822 M	807 M, dp	

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

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	$\text{CH}_3$ d-stretch.....	3005 C	3005 M	3001 W	
	$\nu_2$	$\text{CH}_3$ s-stretch.....	2917 D	.....	2917 S, p	
	$\nu_3$	CH stretch.....	2822 C	2822 M	2843 W, p	
	$\nu_4$	CO stretch.....	1743 C	1743 VS	1714 S, p	
	$\nu_5$	$\text{CH}_3$ d-deform.....	1441 C	1441 S	1426 S	
	$\nu_6$	CH bend.....	1400 C	1400 S	1391 S	
	$\nu_7$	$\text{CH}_3$ s-deform.....	1352 C	1352 S	1342 M	
	$\nu_8$	CC stretch.....	1113 C	1113 S	1109 M, p	
	$\nu_9$	$\text{CH}_3$ rock.....	919 C	919 M	911 M	
$a''$	$\nu_{10}$	CCO deform.....	509 C	509 S	512 S, p	
	$\nu_{11}$	$\text{CH}_3$ d-stretch.....	2967 C	2967 M	2964 W	
	$\nu_{12}$	$\text{CH}_3$ d-deform.....	1420 C	1420 S	1426 S, dp	
	$\nu_{13}$	$\text{CH}_3$ rock.....	867 C	867 M	885 M	
	$\nu_{14}$	CH bend.....	763 C	763 W	767 M, dp	
	$\nu_{15}$	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> <sub>1</sub>	CH <sub>3</sub> d-stretch.....	3028 C	<i>cm</i> <sup>-1</sup> (Gas) 3028 M	<i>cm</i> <sup>-1</sup> (Liquid) 2998 W	
	<i>ν</i> <sub>2</sub>	CH <sub>3</sub> s-stretch.....	2917 D	.....	2917 S, p	
	<i>ν</i> <sub>3</sub>	CD stretch.....	2071 C	2071 W	2097 W, p	
	<i>ν</i> <sub>4</sub>	CO stretch.....	1743 C	1743 VS	1702 S, p	
	<i>ν</i> <sub>5</sub>	CH <sub>3</sub> d-deform.....	1442 C	1442 S	1426 S	
	<i>ν</i> <sub>6</sub>	CD bend.....	1109 C	1109 S	1111 S, p	
	<i>ν</i> <sub>7</sub>	CD <sub>3</sub> s-deform.....	1353 C	1353 S	1343 M	
	<i>ν</i> <sub>8</sub>	CC stretch.....	1043 C	1043 W	1080 W	
	<i>ν</i> <sub>9</sub>	CH <sub>3</sub> rock.....	849 C	849 M	858 M	
	<i>ν</i> <sub>10</sub>	CCO deform.....	500 C	500 S	505 M, p	
<i>a''</i>	<i>ν</i> <sub>11</sub>	CH <sub>3</sub> d-stretch.....	2970 C	2970 M	2965 W	
	<i>ν</i> <sub>12</sub>	CH <sub>3</sub> d-deform.....	1420 C	1420 S	1426 S	
	<i>ν</i> <sub>13</sub>	CH <sub>3</sub> rock.....	802 C	802 W	820 W, sh	
	<i>ν</i> <sub>14</sub>	CD bend.....	668 C	668 W	674 W, dp	
	<i>ν</i> <sub>15</sub>	Torsion.....	145 D	145		

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

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_{1g}$	$\nu_1$	$\text{CH}_3$ s-stretch.....	2954 B	ia	2953.7	
	$\nu_2$	$\text{CH}_3$ s-deform.....	1388 B	ia	1388.4	
	$\nu_3$	CC stretch.....	995 A	ia	994.8	
$a_{1u}$	$\nu_4$	Torsion.....	289 B	289	ia	
$a_{2u}$	$\nu_5$	$\text{CH}_3$ s-stretch.....	2896 B	2895.8	ia	
	$\nu_6$	$\text{CH}_3$ s-deform.....	1379 A	1379.2	ia	
$e_g$	$\nu_7$	$\text{CH}_3$ d-stretch.....	2969 A	ia	2968.7	
	$\nu_8$	$\text{CH}_3$ d-deform.....	1468 A	ia	1468.1	
	$\nu_9$	$\text{CH}_3$ rock.....	1190 E	ia	.....	OC [2, 3].
$e_u$	$\nu_{10}$	$\text{CH}_3$ d-stretch.....	2985 A	2985.4	ia	
	$\nu_{11}$	$\text{CH}_3$ d-deform.....	1469 C	1469	ia	FR ( $\nu_4 + \nu_{12}$ ).
	$\nu_{12}$	$\text{CH}_3$ rock.....	822 A	821.6	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
a <sub>1</sub>	ν <sub>1</sub>	CH <sub>3</sub> s-stretch.....	2912 E	cm <sup>-1</sup> (Gas) { 2955.1 S 2897.4 S	cm <sup>-1</sup> (Gas) 2955.5 2898.2	} FR (2ν <sub>9</sub> ). } FR (2ν <sub>11</sub> ).
	ν <sub>2</sub>	CD <sub>3</sub> s-stretch.....	2098 E	{ 2139.6 S 2089.7 S	.....	
	ν <sub>3</sub>	CH <sub>3</sub> s-deform.....	1387 B	1386.6 W		
	ν <sub>4</sub>	CD <sub>3</sub> s-deform.....	1122 B	1122.0 W		
a <sub>2</sub> e	ν <sub>5</sub>	CC stretch.....	904 A	903.8 VW	904.7	
	ν <sub>6</sub>	Torsion.....	253 B	253 VW		
	ν <sub>7</sub>	CH <sub>3</sub> d-stretch.....	2977 D	2976.5 S	2976.6	
	ν <sub>8</sub>	CD <sub>3</sub> d-stretch.....	2240 E	2240 S		
	ν <sub>9</sub>	CH <sub>3</sub> d-deform.....	1471 A	1471.1 M		
	ν <sub>10</sub>	CH <sub>3</sub> rock.....	1115 B	1115.0 W		
	ν <sub>11</sub>	CD <sub>3</sub> d-deform.....	1066 B	1065.7 M	1062.6	
	ν <sub>12</sub>	CD <sub>3</sub> rock.....	678 A	678.4 M		

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I. Nakagawa and T. Shimanouchi, J. Mol. Spectrosc. 39, 255 (1971).

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

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

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_{1g}$	$\nu_1$	CC stretch . . . . .	1228 D	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Gas) 1228	OC. <sup>a</sup>  CF[2]
	$\nu_2$	$\text{CF}_3$ s-stretch . . . . .	807 C	ia	807 VS, p	
	$\nu_3$	$\text{CF}_3$ s-deform . . . . .	348 C	ia	348 W, p	
$a_{1u}$	$\nu_4$	Torsion . . . . .	68 D	ia	ia	
$a_{2u}$	$\nu_5$	$\text{CF}_3$ s-stretch . . . . .	1117 B	1117 VS	ia	
	$\nu_6$	$\text{CF}_3$ s-deform . . . . .	714 B	714 VS	ia	
$e_g$	$\nu_7$	$\text{CF}_3$ d-stretch . . . . .	1250 C	ia	1250 VW, dp	
	$\nu_8$	$\text{CF}_3$ d-deform . . . . .	619 C	ia	619 W, dp	
	$\nu_9$	$\text{CF}_3$ rock . . . . .	372 C	ia	372 W, dp	
$e_u$	$\nu_{10}$	$\text{CF}_3$ d-stretch . . . . .	1251 B	1251 VS	ia	
	$\nu_{11}$	$\text{CF}_3$ d-deform . . . . .	520 C	520 S	ia	
	$\nu_{12}$	$\text{CF}_3$ rock . . . . .	220 C	220 S	ia	

<sup>a</sup> Mean value of frequencies obtained from six combination bands [2].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_{1g}$	$\nu_1$	CC stretch . . . . .	975 C	$\text{cm}^{-1}$ (Solid) ia	$\text{cm}^{-1}$ (Solid) 975 VW, p	OC ( $\nu_4 + \nu_{10}$ , $\nu_4 + \nu_{11}$ ).
	$\nu_2$	$\text{CCl}_3$ s-stretch . . . . .	431 C	ia	431 VS, p	
	$\nu_3$	$\text{CCl}_3$ s-deform . . . . .	170 C	ia	170 W	
$a_{1u}$	$\nu_4$	Torsion . . . . .	61 D	ia	ia	
$a_{2u}$	$\nu_5$	$\text{CCl}_3$ s-stretch . . . . .	675 C	675 S	ia	
	$\nu_6$	$\text{CCl}_3$ s-deform . . . . .	372 C	372 S	ia	
$e_g$	$\nu_7$	$\text{CCl}_3$ d-stretch . . . . .	859 C	ia	859 W	
	$\nu_8$	$\text{CCl}_3$ d-deform . . . . .	340 C	ia	340 M	
	$\nu_9$	$\text{CCl}_3$ rock . . . . .	223 C	ia	223 S	
$e_u$	$\nu_{10}$	$\text{CCl}_3$ d-stretch . . . . .	778 C	778 VS	ia	
	$\nu_{11}$	$\text{CCl}_3$ d-deform . . . . .	271 C	271 S	ia	
	$\nu_{12}$	$\text{CCl}_3$ 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
				$\text{cm}^{-1}$ (Solid)	$\text{cm}^{-1}$ (Solid)	
$a_g$	$\nu_1$	CC stretch . . . . .	940 C	ia	940 M	OC ( $\nu_4 + \nu_{10}$ , $\nu_4 + \nu_{11}$ ).
	$\nu_2$	$\text{CBr}_3$ s-stretch . . . . .	255 C	ia	255 VS, p	
	$\nu_3$	$\text{CBr}_3$ s-deform . . . . .	120 C	ia	120 W	
$a_{1u}$	$\nu_4$	Torsion . . . . .	51 D	ia	ia	
$a_{2u}$	$\nu_5$	$\text{CBr}_3$ s-stretch . . . . .	559 C	559 S	ia	
	$\nu_6$	$\text{CBr}_3$ s-deform . . . . .	254 C	254 S	ia	
$e_g$	$\nu_7$	$\text{CBr}_3$ d-stretch . . . . .	768 C	ia	768 M, dp	
	$\nu_8$	$\text{CBr}_3$ d-deform . . . . .	204 C	ia	204 S, dp	
	$\nu_9$	$\text{CBr}_3$ rock . . . . .	139 C	ia	139 M	
$e_u$	$\nu_{10}$	$\text{CBr}_3$ d-stretch . . . . .	656 C	656 VS	ia	
	$\nu_{11}$	$\text{CBr}_3$ d-deform . . . . .	168 C	168 S	ia	
	$\nu_{12}$	$\text{CBr}_3$ 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> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a<sub>g</sub></i>	<i>ν</i> <sub>1</sub>	CH <sub>2</sub> s-stretch . . . . .	2957 D	ia	2957 (10) p	SF (gauche <i>ν</i> <sub>1</sub> , gauche <i>ν</i> <sub>11</sub> ).
	<i>ν</i> <sub>2</sub>	CH <sub>2</sub> scis . . . . .	1445 C	ia	1445 (4b) dp	
	<i>ν</i> <sub>3</sub>	CH <sub>2</sub> wag . . . . .	1304 C	ia	1304 (6) p	
	<i>ν</i> <sub>4</sub>	CC stretch . . . . .	1052 C	ia	1052 (4) p	
	<i>ν</i> <sub>5</sub>	CCl stretch . . . . .	754 C	ia	754 (10b) p	
	<i>ν</i> <sub>6</sub>	CCCl deform . . . . .	300 C	ia	300 (8) p	
<i>a<sub>u</sub></i>	<i>ν</i> <sub>7</sub>	CH <sub>2</sub> a-stretch . . . . .	3005 D	3005 W (liquid)	ia	
	<i>ν</i> <sub>8</sub>	CH <sub>2</sub> twist . . . . .	1123 B	1122.5 W	ia	
	<i>ν</i> <sub>9</sub>	CH <sub>2</sub> rock . . . . .	773 B	772.5 M	ia	
<i>b<sub>g</sub></i>	<i>ν</i> <sub>10</sub>	Torsion . . . . .	123 C	123 M	ia	
	<i>ν</i> <sub>11</sub>	CH <sub>2</sub> a-stretch . . . . .	3005 D	ia	3005 (8b) dp	
	<i>ν</i> <sub>12</sub>	CH <sub>2</sub> twist . . . . .	1264 C	ia	1264 (3) dp	
	<i>ν</i> <sub>13</sub>	CH <sub>2</sub> rock . . . . .	989 C	ia	989 (2) p	
<i>b<sub>u</sub></i>	<i>ν</i> <sub>14</sub>	CH <sub>2</sub> s-stretch . . . . .	2983 C	2983.3 M	ia	
	<i>ν</i> <sub>15</sub>	CH <sub>2</sub> scis . . . . .	1461 A	1460.6 S	ia	
	<i>ν</i> <sub>16</sub>	CH <sub>2</sub> wag . . . . .	1232 B	1232.3 S	ia	
	<i>ν</i> <sub>17</sub>	CCl stretch . . . . .	728 C	728.3 VS	ia	
	<i>ν</i> <sub>18</sub>	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>	$\nu_1$	$\text{CH}_2$ a-stretch . . . . .	3005 D	$\text{cm}^{-1}$ (Gas) 3005 W (liquid)	$\text{cm}^{-1}$ (Liquid) 3005 (8b) dp	SF ( $\nu_{11}$ , trans $\nu_7$ ).
	$\nu_2$	$\text{CH}_2$ s-stretch . . . . .	2957 D	2957 M (liquid)	2957 (10) p	SF (trans $\nu_1$ , trans $\nu_{14}$ ).
	$\nu_3$	$\text{CH}_2$ scis. . . . .	1433 C	1433 M (liquid)	1429 (6) dp	OV ( $\nu_{13}$ ).
	$\nu_4$	$\text{CH}_2$ wag. . . . .	1315 C	1315 W	1304 (6)	
	$\nu_5$	$\text{CH}_2$ twist . . . . .	1207 C	.....	1207 (5) p	
	$\nu_6$	CC stretch . . . . .	1027 D	1027 W	1031 (2) dp	
	$\nu_7$	$\text{CH}_2$ rock . . . . .	948 B	947.7 M	943 (5) p	
	$\nu_8$	CCl stretch . . . . .	669 C	669 M	654 (8) p	
	$\nu_9$	CCCl deform . . . . .	272 D	272 VW (liquid)	265 (5) p	
<i>b</i>	$\nu_{10}$	Torsion . . . . .	.....	.....	125 (5b)	
	$\nu_{11}$	$\text{CH}_2$ a-stretch . . . . .	3005 D	3005 W	3005 (8b) dp	SF ( $\nu_1$ , trans $\nu_7$ ).
	$\nu_{12}$	$\text{CH}_2$ s-stretch . . . . .	2957 C	2957.2 W		
	$\nu_{13}$	$\text{CH}_2$ scis. . . . .	1436 B	1436.3 W		
	$\nu_{14}$	$\text{CH}_2$ wag. . . . .	1292 B	1292.1 S		
	$\nu_{15}$	$\text{CH}_2$ twist . . . . .	1146 D	1146 VW	1145 (3) dp	
	$\nu_{16}$	$\text{CH}_2$ rock . . . . .	890 B	890.3 M	881 (4) dp	
	$\nu_{17}$	CCl stretch . . . . .	693 B	692.5 W	677 (6b) dp	
	$\nu_{18}$	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<sub>g</sub></i>	<i>ν</i> <sub>1</sub>	CH <sub>2</sub> s-stretch . . . . .	2972 D	<i>cm</i> <sup>-1</sup> (Liquid) ia	<i>cm</i> <sup>-1</sup> (Liquid) 2972 (10) p	SF ( <i>ν</i> <sub>12</sub> ).
	<i>ν</i> <sub>2</sub>	CH <sub>2</sub> scis . . . . .	1440 C	ia	1440 (5) dp	
	<i>ν</i> <sub>3</sub>	CH <sub>2</sub> wag . . . . .	1255 C	ia	1255 (10b) p	
	<i>ν</i> <sub>4</sub>	CC stretch . . . . .	1053 C	ia	1053 (9) dp	
	<i>ν</i> <sub>5</sub>	CBr stretch . . . . .	660 C	ia	660 (10b) p	
	<i>ν</i> <sub>6</sub>	CCBr deform . . . . .	190 C	ia	190 (10) p	
<i>a<sub>u</sub></i>	<i>ν</i> <sub>7</sub>	CH <sub>2</sub> a-stretch . . . . .	3037 D	3037 S	ia	SF ( <i>ν</i> <sub>3</sub> ).
	<i>ν</i> <sub>8</sub>	CH <sub>2</sub> twist . . . . .	1087 C	1087 M	ia	
	<i>ν</i> <sub>9</sub>	CH <sub>2</sub> rock . . . . .	753 C	753 S	ia	
	<i>ν</i> <sub>10</sub>	Torsion . . . . .	118 D	118 (gas)	132 (0)	
<i>b<sub>g</sub></i>	<i>ν</i> <sub>11</sub>	CH <sub>2</sub> a-stretch . . . . .	3013 D	ia	3013 (4b) dp	
	<i>ν</i> <sub>12</sub>	CH <sub>2</sub> twist . . . . .	1255 C	ia	1255 (10b) p	
<i>b<sub>u</sub></i>	<i>ν</i> <sub>13</sub>	CH <sub>2</sub> rock . . . . .	933 C	ia	933 (2) p	
	<i>ν</i> <sub>14</sub>	CH <sub>2</sub> s-stretch . . . . .	2974 D	2974 S	ia	
	<i>ν</i> <sub>15</sub>	CH <sub>2</sub> scis . . . . .	1441 D	1441 M	ia	
	<i>ν</i> <sub>16</sub>	CH <sub>2</sub> wag . . . . .	1186 C	1186 VS	1186 (0)	
	<i>ν</i> <sub>17</sub>	CBr stretch . . . . .	589 C	589 S	ia	
	<i>ν</i> <sub>18</sub>	CCBr deform . . . . .	193 D	193	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i>	$\nu_1$	$\text{CH}_2$ a-stretch.....	3005 D	$\text{cm}^{-1}$ (Liquid)	$\text{cm}^{-1}$ (Liquid)	SF ( $\nu_{11}$ ).
	$\nu_2$	$\text{CH}_2$ s-stretch.....	2953 D	2953 VS	2953 (8) p	SF ( $\nu_{12}$ ).
	$\nu_3$	$\text{CH}_2$ scis.....	1420 C	1420 M	1419 (3) dp	SF ( $\nu_{13}$ ).
	$\nu_4$	$\text{CH}_2$ wag.....	1278 C	1278 M	1276 (3)	
	$\nu_5$	$\text{CH}_2$ twist.....	1104 C	1104 M	1104 (1) dp	SF ( $\nu_{15}$ ).
	$\nu_6$	CC stretch.....	1019 C	1019 M	1019 (1)	
	$\nu_7$	$\text{CH}_2$ rock.....	898 C	898 M	899 (3) p	
	$\nu_8$	CBr stretch.....	550 C	550 M	551 (8)	
	$\nu_9$	CCBr deform.....	231 C		231 (3) p	
	$\nu_{10}$	Torsion.....	91 D		91 (2b) dp	
<i>b</i>	$\nu_{11}$	$\text{CH}_2$ a-stretch.....	3005 D		3005 (5)	SF ( $\nu_1$ ).
	$\nu_{12}$	$\text{CH}_2$ s-stretch.....	2953 D	2953 VS	2953 (8) p	SF ( $\nu_2$ ).
	$\nu_{13}$	$\text{CH}_2$ scis.....	1420 C	1420 M	1419 (3) dp	SF ( $\nu_3$ ).
	$\nu_{14}$	$\text{CH}_2$ wag.....	1245 C	1245 S	1243 (1)	
	$\nu_{15}$	$\text{CH}_2$ twist.....	1104 C	1104 W	1104 (1) dp	SF ( $\nu_5$ ).
	$\nu_{16}$	$\text{CH}_2$ rock.....	836 C	836 S	836 (2) dp	
	$\nu_{17}$	CBr stretch.....	589 C	589 S	583 (6b) dp	
	$\nu_{18}$	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 <sub>1</sub>	CH <sub>2</sub> s-stretch.....	2960 D	cm <sup>-1</sup> (Solid)	cm <sup>-1</sup> (Liquid)	SF (ν <sub>2</sub> , gauche ν <sub>3</sub> , gauche ν <sub>4</sub> ). SF (ν <sub>1</sub> , gauche ν <sub>3</sub> , gauche ν <sub>4</sub> ).  SF (gauche ν <sub>17</sub> ).
	ν <sub>2</sub>	CH <sub>2</sub> s-stretch.....	2960 D	.....	2960 (10vb)	
	ν <sub>3</sub>	CH <sub>2</sub> scis.....	1446 D	1446 S	.....	
	ν <sub>4</sub>	CH <sub>2</sub> scis.....	1444 C	.....	1444 (3b)	
	ν <sub>5</sub>	CH <sub>2</sub> wag.....	1284 C	1284 M	1284 (7) p	
	ν <sub>6</sub>	CH <sub>2</sub> wag.....	1203 C	1203 S	1203 (3)	
	ν <sub>7</sub>	CC stretch.....	1052 C	1056 M	1052 (4) dp	
	ν <sub>8</sub>	CCl stretch.....	726 C	722 S	726 (10b) p	
	ν <sub>9</sub>	CBr stretch.....	630 C	630 S	630 (9)	
	ν <sub>10</sub>	CCCl deform.....	251 C	.....	251 (10) p	
	ν <sub>11</sub>	CCBr deform.....	202 C	202.0 (CCl <sub>4</sub> soln.)	210 (2b)	
a''	ν <sub>12</sub>	CH <sub>2</sub> a-stretch.....	3010 D	.....	3010 (3vb)	SF (ν <sub>13</sub> , gauche ν <sub>1</sub> , gauche ν <sub>2</sub> ). SF (ν <sub>12</sub> , gauche ν <sub>1</sub> , gauche ν <sub>2</sub> ).  1259 (3) 961 (1b)
	ν <sub>13</sub>	CH <sub>2</sub> a-stretch.....	3010 D	.....	3010 (3vb)	
	ν <sub>14</sub>	CH <sub>2</sub> twist.....	1259 C	1258 VW	1259 (3)	
	ν <sub>15</sub>	CH <sub>2</sub> twist.....	1111 D	1111 M	.....	
	ν <sub>16</sub>	CH <sub>2</sub> rock.....	961 C	961 VW	961 (1b)	
	ν <sub>17</sub>	CH <sub>2</sub> rock.....	763 D	763 M	.....	
	ν <sub>18</sub>	Torsion.....	123 C	123 (CCl <sub>4</sub> soln.)	.....	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i>	$\nu_1$	$\text{CH}_2$ a-stretch . . . . .	3010 D	$\text{cm}^{-1}$ (Liquid)	$\text{cm}^{-1}$ (Liquid)	SF ( $\nu_2$ , trans $\nu_{12}$ , trans $\nu_{13}$ ).
	$\nu_2$	$\text{CH}_2$ a-stretch . . . . .	3010 D		3010 (3vb)	SF ( $\nu_1$ , trans $\nu_{12}$ , trans $\nu_{13}$ ).
	$\nu_3$	$\text{CH}_2$ s-stretch . . . . .	2960 D		2960 (10vb)	SF ( $\nu_4$ , trans $\nu_1$ , trans $\nu_2$ ).
	$\nu_4$	$\text{CH}_2$ s-stretch . . . . .	2960 D		2960 (10vb)	SF ( $\nu_3$ , trans $\nu_1$ , trans $\nu_2$ ).
	$\nu_5$	$\text{CH}_2$ scis . . . . .	1428 D	1428 S	1421 (3b)	OV ( $\nu_6$ ).
	$\nu_6$	$\text{CH}_2$ scis . . . . .	1428 D	1428 S	1421 (3b)	OV ( $\nu_5$ ).
	$\nu_7$	$\text{CH}_2$ wag . . . . .	1299 C	1299 S	1299 (1)	
	$\nu_8$	$\text{CH}_2$ wag . . . . .	1260 C	1260 S	1259 (3)	
	$\nu_9$	$\text{CH}_2$ twist . . . . .	1190 D	1190 M	1189 (2) p	
	$\nu_{10}$	$\text{CH}_2$ twist . . . . .	1127 C	1127 M	1128 (1) dp	
	$\nu_{11}$	CC stretch . . . . .	1025 C	1025 M	1023 (1)	
	$\nu_{12}$	$\text{CH}_2$ rock . . . . .	923 C	923 S	919 (3) p	
	$\nu_{13}$	$\text{CH}_2$ rock . . . . .	856 C	856 S	852 (2)	
	$\nu_{14}$	CCl stretch . . . . .	664 C	664 S	665 (6)	
	$\nu_{15}$	CBr stretch . . . . .	571 C	571 S	568 (9) p	
	$\nu_{16}$	CCCl deform . . . . .	385 C		385 (3) dp	
	$\nu_{17}$	CCBr deform . . . . .	251 D		251 (10)	SF (trans $\nu_{10}$ ).
	$\nu_{18}$	Torsion . . . . .	107 D		107 (2b)	

## References

See No. 164.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	$\text{CH}_3$ d-stretch.....	3003 D	$\text{cm}^{-1}$ (Gas) 3003 VS	$\text{cm}^{-1}$ (Liquid) 2986 VS, dp	OV ( $\nu_{12}, \nu_{13}$ ).
	$\nu_2$	$\text{CH}_2$ s-stretch.....	2941 D	2941	2941 VS, p	
	$\nu_3$	$\text{CH}_3$ s-stretch.....	2915 D	2915 S	2921 M	
	$\nu_4$	$\text{CH}_2$ scis.....	1479 C	1479 M	1480 W, b, dp	OV ( $\nu_{14}$ ).
	$\nu_5$	$\text{CH}_3$ d-deform.....	1449 D	1449 S	1458 M, b, dp	
	$\nu_6$	$\text{CH}_3$ s-deform.....	1395 C	1395 S	1393 W, p	
	$\nu_7$	$\text{CH}_2$ wag.....	1365 D	1365 M	1365 VW	
				(liquid)		
	$\nu_8$	$\text{CH}_3$ rock.....	1108 C	1108 VS	1103 S, p	OV ( $\nu_{16}$ ).
	$\nu_9$	CC stretch.....	1048 D	1048 VS	1041 M, b, dp	
$a''$	$\nu_{10}$	CF stretch.....	880 B	880 VS	873 VS, p	OV ( $\nu_1, \nu_{13}$ ).
	$\nu_{11}$	CCF deform.....	415 C	415	419 W, p	
	$\nu_{12}$	$\text{CH}_2$ a-stretch.....	3003 D	3003 VS	2986 VS, dp	
	$\nu_{13}$	$\text{CH}_3$ d-stretch.....	3003 D	3003 VS	2986 VS, dp	OV ( $\nu_1, \nu_{12}$ ).
	$\nu_{14}$	$\text{CH}_3$ d-deform.....	1449 D	1449 S	1458 M, b, dp	OV ( $\nu_5$ ).
	$\nu_{15}$	$\text{CH}_2$ twist.....	1277 C	1277	1276 W, b, dp	OV ( $\nu_9$ ).
	$\nu_{16}$	$\text{CH}_3$ rock.....	1048 D	1048 VS	1041 M, b, dp	
	$\nu_{17}$	$\text{CH}_2$ rock.....	810 C	810 W	815 WV	
	$\nu_{18}$	Torsion.....	243 B	243		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	$\text{CH}_2$ s-stretch.....	2967 D	$\text{cm}^{-1}$ (Gas) 2977 M (solid)	$\text{cm}^{-1}$ (Liquid) 2967 M, p	
	$\nu_2$	$\text{CH}_3$ d-stretch.....	2946 C	2946 S	2934 M, p	
	$\nu_3$	$\text{CH}_3$ s-stretch.....	2881 C	2881 S	2883 W, p	
	$\nu_4$	$\text{CH}_3$ d-deform.....	1463 D	1463 S (solid)		
	$\nu_5$	$\text{CH}_2$ scis.....	1448 D	1448 S	1453 M, dp	OV ( $\nu_{14}$ ).
	$\nu_6$	$\text{CH}_3$ s-deform.....	1385 C	1385 S	1383 W, dp	
	$\nu_7$	$\text{CH}_2$ wag.....	1289 C	1289 VS	1283 W, p	
	$\nu_8$	$\text{CH}_3$ rock.....	1081 D	1081 VW	1072 M, p	
	$\nu_9$	CC stretch.....	974 D	974 VS	969 W, dp	OV ( $\nu_{16}$ ).
	$\nu_{10}$	CCl stretch.....	677 C	677 VS	659 VS, p	
$a''$	$\nu_{11}$	CCCl deform.....	336 C	336 M	337 S, p	
	$\nu_{12}$	$\text{CH}_2$ a-stretch.....	3014 D	3014 VS	3013 W	
	$\nu_{13}$	$\text{CH}_3$ d-stretch.....	2986 D	2986 VS	2978 W	
	$\nu_{14}$	$\text{CH}_3$ d-deform.....	1448 D	1448 S	1453 M, dp	OV ( $\nu_5$ ).
	$\nu_{15}$	$\text{CH}_2$ twist.....	1251 D	1251 VW	1248 W, dp	
	$\nu_{16}$	$\text{CH}_3$ rock.....	974 D	974 VS	969 W, dp	OV ( $\nu_9$ ).
	$\nu_{17}$	$\text{CH}_2$ rock.....	786 B	786 M		
	$\nu_{18}$	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
$a'$	$\nu_1$	$\text{CH}_3$ d-stretch.....	2988 C	$\text{cm}^{-1}$ (Gas) 2988 S	$\text{cm}^{-1}$ (Liquid) 2971 (2b) p	OV ( $\nu_{13}$ ).
	$\nu_2$	$\text{CH}_2$ s-stretch.....	2937 B	2936.5 S	2924 (2) p	
	$\nu_3$	$\text{CH}_3$ s-stretch.....	2880 B	2879.8 S		
	$\nu_4$	$\text{CH}_2$ scis.....	1451 D	1451 M	1442 (2b) dp	OV ( $\nu_5, \nu_{14}$ ).
	$\nu_5$	$\text{CH}_3$ d-deform.....	1451 D	1451 M	1442 (2b) dp	OV ( $\nu_4, \nu_{14}$ ).
	$\nu_6$	$\text{CH}_3$ s-deform.....	1386 B	1386 M		
	$\nu_7$	$\text{CH}_2$ wag.....	1252 E	{ 1258 VS 1247 VS }	1248 (2b) p	FR ( $\nu_9 + \nu_{11}$ ).
	$\nu_8$	$\text{CH}_3$ rock.....	1061 D	1061 VW	1069 (1) p	
	$\nu_9$	CC stretch.....	964 B	964 S	960 (1b) dp	OV ( $\nu_{15}$ ).
	$\nu_{10}$	CBr stretch.....	583 B	583 VS	560 (10) p	
$a''$	$\nu_{11}$	CCBr deform.....	290 B	290 S	292 (3) p	
	$\nu_{12}$	$\text{CH}_2$ a-stretch.....	3018 B	3018 S		
	$\nu_{13}$	$\text{CH}_3$ d-stretch.....	2988 C	2988 S	2971 (2b) p	OV ( $\nu_1$ ).
	$\nu_{14}$	$\text{CH}_3$ d-deform.....	1451 D	1451 M	1442 (2b) dp	OV ( $\nu_4, \nu_5$ ).
	$\nu_{15}$	$\text{CH}_2$ twist.....	1248 E	.....	.....	CF [7].
	$\nu_{16}$	$\text{CH}_3$ rock.....	964 D	964 S	960 (1b) dp	OV ( $\nu_9$ ).
	$\nu_{17}$	$\text{CH}_2$ rock.....	770 B	770 M		
	$\nu_{18}$	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)	
$a'$	$\nu_1$	NH stretch.....	3338 C	3338 W	3302 M, p	OV ( $\nu_{11}$ ). OV ( $\nu_{12}$ ).
	$\nu_2$	CH <sub>2</sub> a-stretch.....	3079 D	3079 S	3059 M, dp	
	$\nu_3$	CH <sub>2</sub> s-stretch.....	3015 D	3015 S	2999 VS, p	
	$\nu_4$	CH <sub>2</sub> scis.....	1482 C	1482 W	1471 W, p	
	$\nu_5$	Ring stretch.....	1211 C	1211 S	1212 VS, p	
	$\nu_6$	CH <sub>2</sub> twist.....	1095 D	1095 S	1088 W, p	
	$\nu_7$	CH <sub>2</sub> wag.....	1090 D	1090 S	1088 W, p	
	$\nu_8$	NH bend.....	998 C	998 M	1028 W	
$a''$	$\nu_9$	Ring deform.....	856 C	856 VS	855 M, dp	OV ( $\nu_2$ ). OV ( $\nu_3$ ).
	$\nu_{10}$	CH <sub>2</sub> rock.....	773 C	773 S	787 W, dp	
	$\nu_{11}$	CH <sub>2</sub> a-stretch.....	3079 D	3079 S	3059 M, dp	
	$\nu_{12}$	CH <sub>2</sub> s-stretch.....	3015 D	3015 S	2999 VS, p	
	$\nu_{13}$	CH <sub>2</sub> scis.....	1463 C	1463 W	1452 W, dp	
	$\nu_{14}$	CH <sub>2</sub> twist.....	1268 C	1268 M	1276 VW	
	$\nu_{15}$	NH bend.....	1237 C	1237 M	1297 W, p	
	$\nu_{16}$	CH <sub>2</sub> wag.....	1131 C	1131 M	1130 VW	
	$\nu_{17}$	Ring deform.....	904 C	904 S		
	$\nu_{18}$	CH <sub>2</sub> rock.....	817 D	.....	817 M, dp	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	$CH_3$ d-stretch.....	3045 D	$cm^{-1}$ (Gas) 3045 M	$cm^{-1}$ (Liquid) 3030 (3b)	
	$\nu_2$	$CH_3$ s-stretch.....	2969 D	2969 S	2955 (10) p	
	$\nu_3$	CH stretch.....	2943 D	2943 S		
	$\nu_4$	C=O stretch.....	1754 C	1754 VS	1717 (5b) p	
	$\nu_5$	$CH_3$ d-deform.....	1454 D	1454 W ( $CCl_4$ soln.)		
	$\nu_6$	$CH_3$ s-deform.....	1445 D	1445 M		
	$\nu_7$	CH bend.....	1371 D	1371 W	1379 (4b) p	
	$\nu_8$	C-O stretch.....	1207 C	1207 VS	1207 (0.5b)	
	$\nu_9$	$CH_3$ rock.....	1166 D	1166 VS	1157 (1b)	
	$\nu_{10}$	O- $CH_3$ stretch.....	925 C	925 S	912 (10) p	
	$\nu_{11}$	OCO deform.....	767 C	767 M	765 (2)	
	$\nu_{12}$	COC deform.....	318 D	318 M		
	$\nu_{13}$	$CH_3$ d-stretch.....	3012 D	3012 M		
	$\nu_{14}$	$CH_3$ d-deform.....	1443 E	1443 W ( $CCl_4$ soln.)	1440 (3b)	
$a''$	$\nu_{15}$	$CH_3$ rock.....	1168 D	1168 M		
	$\nu_{16}$	CH bend.....	1032 C	1032 M	1030 (0.5)	
	$\nu_{17}$	C-O torsion.....	332 D	332 M	332 (3b) p	
	$\nu_{18}$	$CH_3$ 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>	$\nu_1$	CH <sub>3</sub> d-stretch.....	3041 C	<i>cm</i> <sup>-1</sup> (Gas) 3041 M	<i>cm</i> <sup>-1</sup> .....	FR (2 $\nu_{16}$ ).
	$\nu_2$	CH <sub>3</sub> s-stretch.....	2967 C	2967 S		
	$\nu_3$	CD stretch.....	2216 C	2216 S		
	$\nu_4$	C=O stretch.....	1739 E	{ 1755 VS 1716 VS		
	$\nu_5$	CH <sub>3</sub> d-deform.....	1448 E	1448 W (CCl <sub>4</sub> soln.)		
	$\nu_6$	CH <sub>3</sub> s-deform.....	1441 D	1441 M		
	$\nu_7$	CD bend.....	1048 D	1048 M		
	$\nu_8$	C-O stretch.....	1213 C	1213 VS		
	$\nu_9$	CH <sub>3</sub> rock.....	1157 D	1157 VS		
	$\nu_{10}$	O-CH <sub>3</sub> stretch.....	878 C	878 S		
	$\nu_{11}$	OCO deform.....	762 C	762 M		
	$\nu_{12}$	COC deform.....	315 E	315 M		
	$\nu_{13}$	CH <sub>3</sub> d-stretch.....	3007 D	3007 S		
	$\nu_{14}$	CH <sub>3</sub> d-deform.....	1440 E	1440 W (CCl <sub>4</sub> soln.)		
<i>a''</i>	$\nu_{15}$	CH <sub>3</sub> rock.....	1164 E	.....	.....	CF [2], OV ( $\nu_9$ ).
	$\nu_{16}$	CD bend.....	870 E	.....	.....	CF [2], OV ( $\nu_{10}$ ).
	$\nu_{17}$	C-O torsion.....	290 E	290 M	.....	.....
	$\nu_{18}$	CH <sub>3</sub> 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> <sub>1</sub>	CD <sub>3</sub> d-stretch.....	2284 D	<i>cm</i> <sup>-1</sup> (Gas) 2284 M	<i>cm</i> <sup>-1</sup>	
	<i>ν</i> <sub>2</sub>	CD <sub>3</sub> s-stretch.....	2087 D	2087 M		
	<i>ν</i> <sub>3</sub>	CH stretch.....	2931 D	2931 S		
	<i>ν</i> <sub>4</sub>	C=O stretch.....	1754 C	1754 VS		
	<i>ν</i> <sub>5</sub>	CD <sub>3</sub> d-deform.....	1060 E	1060 W	.....	OV ( <i>ν</i> <sub>14</sub> ).
	<i>ν</i> <sub>6</sub>	CD <sub>3</sub> s-deform.....	1102 E	1102 S		
	<i>ν</i> <sub>7</sub>	CH ip-bend.....	1368 D	1368 M		
	<i>ν</i> <sub>8</sub>	C-O stretch.....	1210 C	1210 VS		
	<i>ν</i> <sub>9</sub>	CD <sub>3</sub> rock.....	985 D	985 M		
	<i>ν</i> <sub>10</sub>	O-CD <sub>3</sub> stretch.....	877 C	877 M		
	<i>ν</i> <sub>11</sub>	OCO deform.....	714 C	714 M		
	<i>ν</i> <sub>12</sub>	COC deform.....	297 E	297 M		
<i>a''</i>	<i>ν</i> <sub>13</sub>	CD <sub>3</sub> d-stretch.....	2258 D	2258 M		
	<i>ν</i> <sub>14</sub>	CD <sub>3</sub> d-deform.....	1060 E	1060 W	.....	OV ( <i>ν</i> <sub>5</sub> ).
	<i>ν</i> <sub>15</sub>	CD <sub>3</sub> rock.....	905 D	905 W		
	<i>ν</i> <sub>16</sub>	CH op-bend.....	1040 E	1040 W		
	<i>ν</i> <sub>17</sub>	C-O torsion.....	312 E	312 M		
	<i>ν</i> <sub>18</sub>	CD <sub>3</sub> torsion.....	96 E	.....	.....	CF [2].

## References

See No. 171.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
<i>a'</i>	ν <sub>1</sub>	CD <sub>3</sub> d-stretch.....	2291 D	2291 M		
	ν <sub>2</sub>	CD <sub>3</sub> s-stretch.....	2100 D	2100 M		
	ν <sub>3</sub>	CD stretch.....	2210 D	2210 S		
	ν <sub>4</sub>	C=O stretch.....	1739 E	{ 1749 VS 1719 VS }	.....	FR (2ν <sub>16</sub> ).
	ν <sub>5</sub>	CD <sub>3</sub> d-deform.....	1060 E	1060 W	.....	OV (ν <sub>14</sub> ).
	ν <sub>6</sub>	CD <sub>3</sub> s-deform.....	1107 D	1107 S		
	ν <sub>7</sub>	CD bend.....	1041 E	1041 W		
	ν <sub>8</sub>	C-O stretch.....	1203 D	1203 VS		
	ν <sub>9</sub>	CD <sub>3</sub> rock.....	974 D	974 M		
	ν <sub>10</sub>	O-CD <sub>3</sub> stretch.....	840 D	840 M		
<i>a''</i>	ν <sub>11</sub>	OCO deform.....	708 D	708 M		
	ν <sub>12</sub>	COC deform.....	295 E	295 M		
	ν <sub>13</sub>	CD <sub>3</sub> d-stretch.....	2267 D	2267 M		
	ν <sub>14</sub>	CD <sub>3</sub> d-deform.....	1060 D	1060 W	.....	OV (ν <sub>4</sub> ).
	ν <sub>15</sub>	CD <sub>3</sub> rock.....	908 D	908 M		
	ν <sub>16</sub>	CD op-bend.....	870 D	870 W		
	ν <sub>17</sub>	C-O torsion.....	280 D	280 M		
	ν <sub>18</sub>	CD <sub>3</sub> torsion.....	96 E	.....	.....	CF [1].

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[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
$a'$	$\nu_1$	OH stretch.....	3583 B	$\text{cm}^{-1}$ (Gas) 3583 M	$\text{cm}^{-1}$	
	$\nu_2$	$\text{CH}_3$ d-stretch.....	3051 B	3051 VW		
	$\nu_3$	$\text{CH}_3$ s-stretch.....	2944 B	2944 VW		
	$\nu_4$	C=O stretch.....	1788 B	1788 VS		
	$\nu_5$	$\text{CH}_3$ d-deform.....	1430 C	1430 sh	.....	SF ( $\nu_{14}$ ).
	$\nu_6$	$\text{CH}_3$ s-deform.....	1382 B	1382 M		
	$\nu_7$	OH bend.....	1264 B	1264 M		
	$\nu_8$	C-O stretch.....	1182 B	1182 S		
	$\nu_9$	$\text{CH}_3$ rock.....	989 B	989 M		
	$\nu_{10}$	CC stretch.....	847 B	847 W		
	$\nu_{11}$	OCO deform.....	657 B	657 S		
$a''$	$\nu_{12}$	CCO deform.....	581 B	581 M		
	$\nu_{13}$	$\text{CH}_3$ d-stretch.....	2996 B	2996 VW		
	$\nu_{14}$	$\text{CH}_3$ d-deform.....	1430 C	1430 sh	.....	SF ( $\nu_5$ ).
	$\nu_{15}$	$\text{CH}_3$ rock.....	1048 B	1048 W		
	$\nu_{16}$	C=O op-bend.....	642 B	642 S		
	$\nu_{17}$	C-O torsion.....	534 B	534 M		
	$\nu_{18}$	$\text{CH}_3$ 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> <sub>1</sub>	CH <sub>3</sub> d-stretch.....	3039 B	<i>cm</i> <sup>-1</sup> (Gas) 3039 VW	<i>cm</i> <sup>-1</sup> .....	SF ( <i>ν</i> <sub>14</sub> ).
	<i>ν</i> <sub>2</sub>	CH <sub>3</sub> s-stretch.....	2952 B	2952 VW		
	<i>ν</i> <sub>3</sub>	OD stretch.....	2642 B	2642 M		
	<i>ν</i> <sub>4</sub>	C=O stretch.....	1775 B	1775 VS		
	<i>ν</i> <sub>5</sub>	CH <sub>3</sub> d-deform.....	1440 C	1440 sh		
	<i>ν</i> <sub>6</sub>	CH <sub>3</sub> s-deform.....	1383 B	1383 S		
	<i>ν</i> <sub>7</sub>	C-O stretch.....	1270 B	1270 S		
	<i>ν</i> <sub>8</sub>	CH <sub>3</sub> rock.....	990 D	990 sh		
	<i>ν</i> <sub>9</sub>	OD bend.....	955 B	955 S		
	<i>ν</i> <sub>10</sub>	CC stretch.....	840 B	840 W		
	<i>ν</i> <sub>11</sub>	OCO deform.....	609 B	609 M		
<i>a''</i>	<i>ν</i> <sub>12</sub>	CCO deform.....	543 B	543 M	.....	SF ( <i>ν</i> <sub>5</sub> ).
	<i>ν</i> <sub>13</sub>	CH <sub>3</sub> d-stretch.....	2997 D	2997 VW		
	<i>ν</i> <sub>14</sub>	CH <sub>3</sub> d-deform.....	1440 C	1440 sh		
	<i>ν</i> <sub>15</sub>	CH <sub>3</sub> rock.....	1052 B	1052 W		
	<i>ν</i> <sub>16</sub>	C=O ip-bend.....	603 B	603 M		
	<i>ν</i> <sub>17</sub>	C-O torsion.....	415 B	415 M		
	<i>ν</i> <sub>18</sub>	CH <sub>3</sub> torsion.....	93 E	.....		CF [3].

## References

See No. 174.



Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CH}_3$ d-stretch.....	2996 B	2996 S	2989 S	
	$\nu_2$	$\text{CH}_3$ s-stretch.....	2817 B	2817 S	2815 VS, p	
	$\nu_3$	$\text{CH}_3$ d-deform.....	1464 D	1464 M		
	$\nu_4$	$\text{CH}_3$ s-deform.....	1452 D	1452 M	1452 S, dp	
	$\nu_5$	$\text{CH}_3$ rock.....	1244 B	1244 W		
	$\nu_6$	CO s-stretch.....	928 B	928 S	922 S, p	
$a_2$	$\nu_7$	COC deform.....	418 C	418 M	428 M, p	
	$\nu_8$	$\text{CH}_3$ d-stretch.....	2952 C	ia	2952 S	
	$\nu_9$	$\text{CH}_3$ d-deform.....	1464 D	ia		SF ( $\nu_3$ ).
	$\nu_{10}$	$\text{CH}_3$ rock.....	1150 C	ia	1150 M, d	
$b_1$	$\nu_{11}$	Torsion.....	203 E	ia		CF [3].
	$\nu_{12}$	$\text{CH}_3$ d-stretch.....	2996 B	2996 S	2989 S	OV ( $\nu_1$ ).
	$\nu_{13}$	$\text{CH}_3$ s-stretch.....	2817 B	2817 S	2815 VS, p	OV ( $\nu_2$ ).
	$\nu_{14}$	$\text{CH}_3$ d-deform.....	1464 D	1464 M		OV ( $\nu_3$ ).
	$\nu_{15}$	$\text{CH}_3$ s-deform.....	1452 D	1452 M	1452 S, dp	OV ( $\nu_4$ ).
	$\nu_{16}$	$\text{CH}_3$ rock.....	1227 C		1227 W	
$b_2$	$\nu_{17}$	CO a-stretch.....	1102 B	1102 VS	1104 M, dp	
	$\nu_{18}$	$\text{CH}_3$ d-stretch.....	2925 B	2925 S		
	$\nu_{19}$	$\text{CH}_3$ d-deform.....	1464 D	1464 M		OV ( $\nu_3$ ).
	$\nu_{20}$	$\text{CH}_3$ rock.....	1179 B	1179 VS	1170 sh	
	$\nu_{21}$	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> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a'</i>	<i>ν</i> <sub>1</sub>	CH <sub>3</sub> d-stretch.....	2992 B	2992 S		
	<i>ν</i> <sub>2</sub>	CH <sub>3</sub> s-stretch.....	2819 B	2819 S		
	<i>ν</i> <sub>3</sub>	CD <sub>3</sub> d-stretch.....	2244 B	2244 S		
	<i>ν</i> <sub>4</sub>	CD <sub>3</sub> s-stretch.....	2058 B	2058 S		
	<i>ν</i> <sub>5</sub>	CH <sub>3</sub> d-deform.....	1465 C	1465 M		
	<i>ν</i> <sub>6</sub>	CH <sub>3</sub> s-deform.....	1453 C	1453 M		
	<i>ν</i> <sub>7</sub>	CH <sub>3</sub> rock.....	1212 B	1212 M		
	<i>ν</i> <sub>8</sub>	CO a-stretch.....	1156 C	1156 VS	.....	SF ( <i>ν</i> <sub>17</sub> ).
	<i>ν</i> <sub>9</sub>	CD <sub>3</sub> s-deform.....	1111 B	1111 S		
	<i>ν</i> <sub>10</sub>	CD <sub>3</sub> d-deform.....	1061 C	1061 M	.....	SF ( <i>ν</i> <sub>18</sub> ).
	<i>ν</i> <sub>11</sub>	CD <sub>3</sub> rock.....	947 C	947 W		
	<i>ν</i> <sub>12</sub>	CO s-stretch.....	860 C	860 M		
<i>a''</i>	<i>ν</i> <sub>13</sub>	COC deform.....	395 E	.....	.....	CF [2].
	<i>ν</i> <sub>14</sub>	CH <sub>3</sub> d-stretch.....	2932 B	2932 S		
	<i>ν</i> <sub>15</sub>	CD <sub>3</sub> d-stretch.....	2189 B	2189 S		
	<i>ν</i> <sub>16</sub>	CH <sub>3</sub> d-deform.....	1462 D	1462 M		
	<i>ν</i> <sub>17</sub>	CH <sub>3</sub> rock.....	1156 C	1156 VS	.....	SF ( <i>ν</i> <sub>8</sub> ).
	<i>ν</i> <sub>18</sub>	CD <sub>3</sub> d-deform.....	1061 C	1061 M	.....	SF ( <i>ν</i> <sub>10</sub> ).
	<i>ν</i> <sub>19</sub>	CD <sub>3</sub> rock.....	901 C	901 W		
	<i>ν</i> <sub>20</sub>	Torsion.....	227 E	.....	.....	CF [2].
	<i>ν</i> <sub>21</sub>	Torsion.....	164 E	.....	.....	CF [2].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Gas)	
$a_1$	$\nu_1$	$\text{CH}_2$ s-stretch.....	3015 A	.....	3015.0	
	$\nu_2$	$\text{CH}_2$ scis.....	1443 A	.....	1442.6	
	$\nu_3$	CC stretch.....	1073 A	.....	1072.6	
$b_1$	$\nu_4$	$\text{CH}_2$ twist.....	865 C	865	865 (liquid)	
$b_2$	$\nu_5$	$\text{CH}_2$ s-stretch.....	3007 A	3006.7		
	$\nu_6$	CC stretch.....	1957 C	1957	1960 (liquid)	
	$\nu_7$	$\text{CH}_2$ scis.....	1398 C	1398	1421 (liquid)	
$e$	$\nu_8$	$\text{CH}_2$ a-stretch.....	3086 A	3085.5		
	$\nu_9$	$\text{CH}_2$ rock.....	999 A	999.1		
	$\nu_{10}$	$\text{CH}_2$ wag.....	841 A	840.8		
	$\nu_{11}$	CCC deform.....	355 A	355.3		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	CH stretch . . . . .	3334 C	$\text{cm}^{-1}$ (Gas) 3334	$\text{cm}^{-1}$ (Liquid) 3305 M	FR ( $\nu_2 + 2\nu_7$ ) [2].
	$\nu_2$	$\text{CH}_3$ s-stretch . . . . .	2918 E	{ 2941 M 2881	{ 2941 VS, p	
	$\nu_3$	$\text{C}\equiv\text{C}$ stretch . . . . .	2142 A	2142.2 M	2142 VS, p	
	$\nu_4$	$\text{CH}_3$ s-deform . . . . .	1382 D		1382 S, dp	
	$\nu_5$	C-C stretch . . . . .	931 C	930.7 W	930 S, p (gas)	
$e$	$\nu_6$	$\text{CH}_3$ d-stretch . . . . .	3008 A	3008.3 M	2971 M	
	$\nu_7$	$\text{CH}_3$ d-deform . . . . .	1452 B	1452 M	1448 M	
	$\nu_8$	$\text{CH}_3$ rock . . . . .	1053 A	1052.5 W	1035 VW	
	$\nu_9$	CH bend . . . . .	633 C	633 S	643 S, dp	
	$\nu_{10}$	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
$a_1$	$\nu_1$	$\text{CH}_3$ s-stretch . . . . .	2920 E	$\text{cm}^{-1}$ (Gas) { 2941.0 M 2881.0 M	$\text{cm}^{-1}$ { . . . . .	FR ( $2\nu_7$ ) [1].
	$\nu_2$	CD stretch . . . . .	2617 B	2616.8 S		
	$\nu_3$	$\text{C}\equiv\text{C}$ stretch . . . . .	2060 C	2060.3 W		
	$\nu_4$	$\text{CH}_3$ s-deform . . . . .	1378 E	1378 W		
	$\nu_5$	C-C stretch . . . . .	886 E			
$e$	$\nu_6$	$\text{CH}_3$ d-stretch . . . . .	3009 B	3008.9 M		OV ( $\nu_7$ ). CF [1].
	$\nu_7$	$\text{CH}_3$ deform . . . . .	1454 B	1453.5 M		
	$\nu_8$	$\text{CH}_3$ rock . . . . .	1051 B	1051.0 W		
	$\nu_9$	CD bend . . . . .	498 B	497.5 S		
	$\nu_{10}$	CCC bend . . . . .	314 B	314 M		

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	CH stretch.....	3336 A	$cm^{-1}$ (Gas) 3335.8 S	$cm^{-1}$	
	$\nu_2$	CD <sub>3</sub> s-stretch.....	2110 E	{ 2121.0 M 2077.0 M }	.....	FR ( $\nu_2 + 2\nu_7$ ) [2].
	$\nu_3$	C $\equiv$ C stretch	2142 A	2142.0 M		
	$\nu_4$	CD <sub>3</sub> s-deform.....	1115 B	1115 M		
$e$	$\nu_5$	C-C stretch.....	830 B	830 W	.....	OV ( $\nu_8$ ).
	$\nu_6$	CD <sub>3</sub> d-stretch.....	2235 A	2234.9 M		
	$\nu_7$	CD <sub>3</sub> d-deform.....	1048 A	1048.2 M		
	$\nu_8$	CD <sub>3</sub> rock.....	835 A	835.4 W	.....	OV ( $\nu_5$ ).
	$\nu_9$	CH bend.....	633 B	633 S		
	$\nu_{10}$	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
$a_1$	$\nu_1$	CD stretch.....	2616 A	$cm^{-1}$ (Gas) 2616.3 VS	$cm^{-1}$	
	$\nu_2$	CD <sub>3</sub> s-stretch.....	2110 E	{ 2121 M 2077 M }	.....	FR ( $\nu_2 + 2\nu_7$ ) [2].
	$\nu_3$	C $\equiv$ C stretch.....	2008 A	2008.4 W		
	$\nu_4$	CD <sub>3</sub> s-deform.....	1110 A	1110.1 M		
$e$	$\nu_5$	C-C stretch.....	810 E	.....	.....	CF [1].
	$\nu_6$	CD <sub>3</sub> d-stretch.....	2235 A	2234.8 M		
	$\nu_7$	CD <sub>3</sub> d-deform.....	1048 A	1048.2 M		
	$\nu_8$	CD <sub>3</sub> rock.....	834 A	834.4 W		
	$\nu_9$	CD bend.....	492 B	492 VS		
	$\nu_{10}$	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)	
$a_1$	$\nu_1$	$CH_2$ s-stretch.....	2935 C	2935 VS	2929 (5)	SF ( $\nu_9$ ).
	$\nu_2$	CN s-stretch.....	2275 C	2275 M	2263 (7)	
	$\nu_3$	$CH_2$ scis.....	1395 C	1395 VS	1386 (4)	
	$\nu_4$	CC s-stretch.....	890 C	890 S	892 (5)	
	$\nu_5$	CCC deform.....	582 C	582 M	574 (3b)	
	$\nu_6$	CCN bend.....	167 C	.....	167 (10)	
$a_2$	$\nu_7$	$CH_2$ twist.....	1220 C	ia, 1220 VW	1214 (3)	SF ( $\nu_{12}$ ).
	$\nu_8$	CCN bend.....	367 C	ia, 371 M	367 (10)	
$b_1$	$\nu_9$	CN a-stretch.....	2275 C	2275 M	2263 (7)	SF ( $\nu_2$ ).
	$\nu_{10}$	$CH_2$ wag.....	1318 C	1318 W	1310 (2)	
	$\nu_{11}$	CC a-stretch.....	982 C	982 S	975 (1)	
	$\nu_{12}$	CCN bend.....	366 C	366 S	367 (10)	
$b_2$	$\nu_{13}$	$CH_2$ a-stretch.....	2968 C	2968 VS	2960 (1)	SF ( $\nu_8$ ).
	$\nu_{14}$	$CH_2$ rock.....	933 C	933 M		
	$\nu_{15}$	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.)	
$a_1$	$\nu_1$	$CD_2$ s-stretch.....	2146 C	2146 S	2146 (4)	SF ( $\nu_9$ ).
	$\nu_2$	CN s-stretch.....	2272 C	2272 M	2273 (8)	
	$\nu_3$	$CD_2$ scis.....	1037 C	1037 S	1033 (3)	
	$\nu_4$	CC s-stretch.....	858 C	858 M	854 (5)	
	$\nu_5$	CCC deform.....	577 C	577 M	581 (2)	
	$\nu_6$	CCN bend.....	163 C	.....	163 (4)	
$a_2$	$\nu_7$	$CD_2$ twist.....	892 C	ia, 892 VW	892 (1)	SF ( $\nu_{12}$ ).
	$\nu_8$	CCN bend.....	356 C	ia	356 (4)	
$b_1$	$\nu_9$	CN a-stretch.....	2272 C	2272 M	2273 (8)	SF ( $\nu_2$ ).
	$\nu_{10}$	$CD_2$ wag.....	1153 C	{ 1165 M 1142 M }	{ 1162 (0.5) 1130 (0.5) }	
$b_2$	$\nu_{11}$	CC a-stretch.....	829 C	829 M	828 (1)	SF ( $\nu_8$ ).
	$\nu_{12}$	CCN bend.....	356 C	356 S	356 (4)	
	$\nu_{13}$	$CD_2$ a-stretch.....	2230 C	2230 S	2228 (2)	
	$\nu_{14}$	$CD_2$ rock.....	795 C	795 W		
	$\nu_{15}$	CCN bend.....	302 C	.....	302 (1)	

#### Reference

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$	
$a'$	$\nu_1$	$\text{CH}_2$ a-stretch.....	3103 C	3103 M		
	$\nu_2$	$\text{CH}(\beta)$ stretch.....	3028 D	3028 M		
				(solid)		
	$\nu_3$	$\text{CH}_2$ s-stretch.....	3000 D	3000 M		
	$\nu_4$	$\text{CH}(\alpha)$ stretch.....	2800 C	2800 S		
	$\nu_5$	$\text{CO}$ stretch.....	1724 C	1724 VS		
	$\nu_6$	$\text{C}=\text{C}$ stretch.....	1625 C	1625 M		
	$\nu_7$	$\text{CH}_2$ scis.....	1420 C	1420 S		
	$\nu_8$	$\text{CH}(\alpha)$ ip-bend.....	1360 C	1360 M		
	$\nu_9$	$\text{CH}(\beta)$ ip-bend.....	1275 C	1275 W		
$a''$	$\nu_{10}$	$\text{C}-\text{C}$ stretch.....	1158 C	1158 S		
	$\nu_{11}$	$\text{CH}_2$ rock.....	912 C	912 S		
	$\nu_{12}$	$\text{CCO}$ deform.....	564 C	564 M		
	$\nu_{13}$	$\text{CCC}$ bend.....	327 C	327 M		
	$\nu_{14}$	$\text{CH}(\beta)$ op-bend.....	993 B	993 S		
	$\nu_{15}$	$\text{CH}(\alpha)$ op-bend.....	980 E	.....	.....	CF [1, 2].
	$\nu_{16}$	$\text{CH}_2$ wag.....	959 B	959 S		
	$\nu_{17}$	$\text{CH}_2$ twist.....	593 C	593 S		
	$\nu_{18}$	$\text{CC}$ torsion.....	157 C	157 M		

<sup>a</sup> 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
$a_1'$	$\nu_1$	$CH_2$ s-stretch . . . . .	3038 C	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Gas) 3038 S, p	} FR ( $2\nu_{14}$ ).
	$\nu_2$	$CH_2$ scis . . . . .	1479 D	ia	{ 1504 W, p 1453 W, p	
	$\nu_3$	Ring stretch . . . . .	1188 C	ia	1188 S, p	
$a_1''$	$\nu_4$	$CH_2$ twist . . . . .	1126 D	ia, 1126 VW	ia, 1133	
$a_2'$	$\nu_5$	$CH_2$ wag . . . . .	1070 D	ia, 1075 (solid)	ia	OC ( $\nu_5 + \nu_{10}$ ).
$a_2''$	$\nu_6$	$CH_2$ a-stretch . . . . .	3103 C	3103 S	ia	
	$\nu_7$	$CH_2$ rock . . . . .	854 C	854 S	ia	
$e'$	$\nu_8$	$CH_2$ s-stretch . . . . .	3025 C	3025 VS	3020 VS, p	
	$\nu_9$	$CH_2$ scis . . . . .	1438 C	1438 M	1442 M, dp	
	$\nu_{10}$	$CH_2$ wag . . . . .	1029 C	1029 S	1023 VW (liquid)	
	$\nu_{11}$	Ring deform . . . . .	866 C	866 VS	866 S, dp	
$e''$	$\nu_{12}$	$CH_2$ a-stretch . . . . .	3082 C	ia	3082 S, dp	
	$\nu_{13}$	$CH_2$ twist . . . . .	1188 C	ia	1188 M	
	$\nu_{14}$	$CH_2$ 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
$a_1'$	$\nu_1$	CD <sub>2</sub> s-stretch.....	2236 C	cm <sup>-1</sup> (Gas) ia	cm <sup>-1</sup> (Liquid) 2236 VS, p	CF [2].
	$\nu_2$	CD <sub>2</sub> scis.....	1274 D	ia	1274 S, p	
	$\nu_3$	Ring stretch.....	956 C	ia	956 S, p	
$a_1''$	$\nu_4$	CD <sub>2</sub> twist.....	800 D	ia, 800 VW	ia	
$a_2'$	$\nu_5$	CD <sub>2</sub> wag.....	870 D	ia, 875 (solid)	ia	CF [2], OC ( $\nu_5 + \nu_{11}$ ).
$a_2''$	$\nu_6$	CD <sub>2</sub> a-stretch.....	2336 C	2336 VS	ia	
	$\nu_7$	CD <sub>2</sub> rock.....	614 C	614 W	ia	
$e'$	$\nu_8$	CD <sub>2</sub> s-stretch.....	2211 C	2211 VS	2204 W, dp	
	$\nu_9$	CD <sub>2</sub> scis.....	1072 C	1072 S	1068 W, dp	CF [2], OC ( $2\nu_{13}$ ).
	$\nu_{10}$	CD <sub>2</sub> wag.....	885 C	885 M	884 M, dp	
	$\nu_{11}$	Ring deform.....	717 C	717 VS	721 M, dp	
$e''$	$\nu_{12}$	CD <sub>2</sub> a-stretch.....	2329 C	ia	2329 S, p	
	$\nu_{13}$	CD <sub>2</sub> twist.....	940 E	ia	.....	
	$\nu_{14}$	CD <sub>2</sub> rock.....	528 C	ia	528 W, dp	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Liquid)	$\text{cm}^{-1}$ (Liquid)	
$a'$	$\nu_1$	$\text{CH}_3$ d-stretch.....	3001 C	3001 VS	2999 S	OV ( $\nu_{14}$ ).
	$\nu_2$	$\text{CH}_2$ s-stretch.....	2955 C	2955 VS	2949 VS, p	
	$\nu_3$	$\text{CH}_3$ s-stretch.....	2900 C	2900 S	2898 S, p	SF ( $\nu_{16}$ ).
	$\nu_4$	CN stretch.....	2254 C	2254 VS	2251 VS, p	
	$\nu_5$	$\text{CH}_3$ d-deform.....	1465 C	1465 S	1466 VS, p	
	$\nu_6$	$\text{CH}_2$ scis.....	1433 C	1433 S	1436 M, p	
	$\nu_7$	$\text{CH}_3$ s-deform.....	1387 C	1387 M	1374 VW, p	
	$\nu_8$	$\text{CH}_2$ wag.....	1319 C	1319 M	1322 W, p	
	$\nu_9$	C-CN stretch.....	1077 C	1077 S	1078 M, p	
	$\nu_{10}$	CC stretch.....	1005 C	1005 M	1010 S, p	
	$\nu_{11}$	$\text{CH}_3$ rock.....	836 C	836 W	838 S, p	
	$\nu_{12}$	CCC deform.....	545 C	545 M	548 M, p	
$a''$	$\nu_{13}$	CCN bend.....	226 C	226 M	226 M, p	OV ( $\nu_1$ ).
	$\nu_{14}$	$\text{CH}_3$ d-stretch.....	3001 C	3001 VS	2999 S	
	$\nu_{15}$	$\text{CH}_2$ a-stretch.....	2849 C	2849 S	2850 M	SF ( $\nu_5$ ).
	$\nu_{16}$	$\text{CH}_3$ d-deform.....	1465 C	1465 S	1466 VS, dp	
	$\nu_{17}$	$\text{CH}_2$ twist.....	1256 C	1256 VW	1270 VW, dp	CF [2].
	$\nu_{18}$	$\text{CH}_3$ rock.....	1022 E	.....	.....	
	$\nu_{19}$	$\text{CH}_2$ rock.....	786 C	786 M	784 VW, dp	MW [2].
	$\nu_{20}$	CCN bend.....	378 C	378 M	378 M, dp	
	$\nu_{21}$	Torsion.....	222 C	.....	.....	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CH}_3$ d-stretch.....	3019 C	3018.5 S	3005.5 S	SF ( $\nu_{13}$ ).
	$\nu_2$	$\text{CH}_3$ s-stretch.....	2937 D	2937 S	2922 VS, p	SF ( $\nu_{14}$ ).
	$\nu_3$	CO stretch.....	1731 C	1731 VS	1710.5 S, p	
	$\nu_4$	$\text{CH}_3$ d-deform.....	1435 C	1435 S	1430 S	
	$\nu_5$	$\text{CH}_3$ s-deform.....	1364 C	1363.5 VS	1356 W	SF ( $\nu_{16}$ ).
	$\nu_6$	$\text{CH}_3$ rock.....	1066 C	.....	1066 M, p	
	$\nu_7$	CC stretch.....	777 C	777 W	787 VS, p	
	$\nu_8$	CCC deform.....	385 C	385 W	393 W, dp	
$a_2$	$\nu_9$	$\text{CH}_3$ d-stretch.....	2963 E	ia	.....	CF [4].
	$\nu_{10}$	$\text{CH}_3$ d-deform.....	1426 E	ia	.....	CF [4].
	$\nu_{11}$	$\text{CH}_3$ rock.....	877 E	ia	.....	CF [4].
	$\nu_{12}$	Torsion.....	105 D	ia	.....	CF [4]; MW: 102 [1].
$b_1$	$\nu_{13}$	$\text{CH}_3$ d-stretch.....	3019 C	3018.5 S	3005.5 S, dp	SF ( $\nu_1$ ).
	$\nu_{14}$	$\text{CH}_3$ s-stretch.....	2937 D	2937 S	2922 VS	SF ( $\nu_2$ ).
	$\nu_{15}$	$\text{CH}_3$ d-deform.....	1410 C	1410 S	.....	
	$\nu_{16}$	$\text{CH}_3$ s-deform.....	1364 C	1363.5 VS	.....	SF ( $\nu_5$ ).
	$\nu_{17}$	CC stretch.....	1216 C	1215.5 VS	1221 M, dp	
	$\nu_{18}$	$\text{CH}_3$ rock.....	891 C	891 M	902.5 W, dp	
$b_2$	$\nu_{19}$	CO ip-bend.....	530 C	530 S	531 M, dp	
	$\nu_{20}$	$\text{CH}_3$ d-stretch.....	2972 C	2972 S	2967 S	
	$\nu_{21}$	$\text{CH}_3$ d-deform.....	1454 C	1454 S	.....	
	$\nu_{22}$	$\text{CH}_3$ rock.....	1091 C	1090.5 M	.....	
	$\nu_{23}$	CO op-bend.....	484 C	484 W	493 W, dp	
	$\nu_{24}$	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
$a'$	$\nu_1$	CH <sub>3</sub> d-stretch.....	3018 C	$cm^{-1}$ (Gas) 3017.5 S	$cm^{-1}$ (Liquid) 3004.5 S	FR (2 $\nu_9$ ).
	$\nu_2$	CH <sub>3</sub> s-stretch.....	2922 C	.....	2921.5 VS, p	
	$\nu_3$	CD <sub>3</sub> d-stretch.....	2265 C	2265 M	2256 S	
	$\nu_4$	CD <sub>3</sub> s-stretch.....	2115 E	{ 2150 VVW 2095 VW	{ 2141.5 VS, p 2095.5 S, p	
	$\nu_5$	CO stretch.....	1734 C	1734 VS	1706 S	
	$\nu_6$	CH <sub>3</sub> d-deform.....	1430 C	1430 S	1427.5 M	
	$\nu_7$	CH <sub>3</sub> s-deform.....	1360 C	1360 VS	1361.5 VW	
	$\nu_8$	CC stretch.....	1225 C	1224.5 VS	1227.5 W	
	$\nu_9$	CD <sub>3</sub> s-deform.....	1058 C	.....	1057.5 W	
	$\nu_{10}$	CH <sub>3</sub> rock.....	1021 C	1021 S	1029.5 W	
	$\nu_{11}$	CD <sub>3</sub> d-deform.....	1003 C	.....	1003 M, p	
	$\nu_{12}$	CD <sub>3</sub> rock.....	781 C	781 W	780.5 VW	
	$\nu_{13}$	CC stretch.....	740 C	735 W	740 VS, p	
	$\nu_{14}$	CO ip-bend.....	502 C	501.5 S		
	$\nu_{15}$	CCC deform.....	352 C	352 W	356.5 W	
$a''$	$\nu_{16}$	CH <sub>3</sub> d-stretch.....	2968 C	2968 S	2965 S	
	$\nu_{17}$	CD <sub>3</sub> d-stretch.....	2222 C	2222 M	2217.5 S	
	$\nu_{18}$	CH <sub>3</sub> d-deform.....	1447 C	1447 S		
	$\nu_{19}$	CH <sub>3</sub> rock.....	1035 C	1035 S		
	$\nu_{20}$	CD <sub>3</sub> d-deform.....	999 C	999 S		
	$\nu_{21}$	CD <sub>3</sub> rock.....	764 D	764 M (solid)		
	$\nu_{22}$	CO op-bend.....	438 C	438	444 W	
	$\nu_{23}$	CH <sub>3</sub> torsion.....	106 E	.....	.....	CF [2].
	$\nu_{24}$	CD <sub>3</sub> torsion.....	78 E	.....	.....	CF [2].

## References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CD <sub>3</sub> d-stretch.....	2264 C	2263.5 S	.....	SF ( <i>ν</i> <sub>13</sub> ).
	<i>ν</i> <sub>2</sub>	CD <sub>3</sub> s-stretch.....	2123 C	2123 W	2108.5 VS, p	SF ( <i>ν</i> <sub>14</sub> ).
	<i>ν</i> <sub>3</sub>	CO stretch.....	1732 C	1732 VS	1700.5 S	
	<i>ν</i> <sub>4</sub>	CD <sub>3</sub> s-deform.....	1080 C	1080 M	1088 M, p	
	<i>ν</i> <sub>5</sub>	CD <sub>3</sub> d-deform.....	1035 D	1035 M	1036 M	
	<i>ν</i> <sub>6</sub>	CD <sub>3</sub> rock.....	887 C	887 W	889 M, p	
	<i>ν</i> <sub>7</sub>	CC stretch.....	689 C	689 W	695.5 VS, p	
	<i>ν</i> <sub>8</sub>	CCC deform.....	321 C	321 W	330 VW, dp	
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>9</sub>	CD <sub>3</sub> d-stretch.....	2219 E	ia	.....	CF [3].
	<i>ν</i> <sub>10</sub>	CD <sub>3</sub> d-deform.....	1021 E	ia	.....	CF [3].
	<i>ν</i> <sub>11</sub>	CD <sub>3</sub> rock.....	669 E	ia	.....	CF [3].
	<i>ν</i> <sub>12</sub>	Torsion.....	75 E	ia	.....	CF [3].
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>13</sub>	CD <sub>3</sub> d-stretch.....	2264 C	2263.5 S	2256.5 S	SF ( <i>ν</i> <sub>1</sub> ).
	<i>ν</i> <sub>14</sub>	CD <sub>3</sub> s-stretch.....	2123 C	2123 W	.....	SF ( <i>ν</i> <sub>2</sub> ).
	<i>ν</i> <sub>15</sub>	CC stretch.....	1242 C	1241.7 VS	1248.5 VW	
	<i>ν</i> <sub>16</sub>	CD <sub>3</sub> s-deform.....	1035 D	1035 M	1036 M	
	<i>ν</i> <sub>17</sub>	CD <sub>3</sub> d-deform.....	1004 C	1004 M	1006 sh	
	<i>ν</i> <sub>18</sub>	CD <sub>3</sub> rock.....	724 D	724 W		
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>19</sub>	CO ip-bend.....	475 C	475 S	478 W, dp	
	<i>ν</i> <sub>20</sub>	CD <sub>3</sub> d-stretch.....	2227 C	2226.5 S	2222 S	
	<i>ν</i> <sub>21</sub>	CD <sub>3</sub> d-deform.....	1050 C	1050 S		
	<i>ν</i> <sub>22</sub>	CD <sub>3</sub> rock.....	960 C	960 M		
	<i>ν</i> <sub>23</sub>	CO op-bend.....	405 C	405 W	410 VW, dp	
	<i>ν</i> <sub>24</sub>	Torsion.....	79 E	.....	.....	CF [3].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Liquid)	
$a_1$	$\nu_1$	$\text{CH}_3$ d-stretch.....	2977 C	2977		
	$\nu_2$	$\text{CH}_3$ s-stretch.....	2962 D	2962		
	$\nu_3$	$\text{CH}_2$ s-stretch.....	2887 C	2887		
	$\nu_4$	$\text{CH}_3$ d-deform.....	1476 C	1476		
	$\nu_5$	$\text{CH}_2$ scis.....	1462 C	1462		
	$\nu_6$	$\text{CH}_3$ s-deform.....	1392 C	1392		
	$\nu_7$	$\text{CH}_3$ rock.....	1158 C	1158	1152 W	
	$\nu_8$	CC stretch.....	869 C	869	867 S	
	$\nu_9$	CCC deform.....	369 C	369	375 W	
$a_2$	$\nu_{10}$	$\text{CH}_3$ d-stretch.....	2967 C	ia	2967 M	
	$\nu_{11}$	$\text{CH}_3$ d-deform.....	1451 C	ia	1451 S	
	$\nu_{12}$	$\text{CH}_2$ twist.....	1278 C	ia	1278 W	
	$\nu_{13}$	$\text{CH}_3$ rock.....	940 D	ia	940 VW	
	$\nu_{14}$	Torsion.....	<sup>a</sup> 216 C	ia	.....	MW [10,11].
$b_1$	$\nu_{15}$	$\text{CH}_3$ d-stretch.....	2968 C	2968		
	$\nu_{16}$	$\text{CH}_3$ s-stretch.....	2887 C	2887		OV ( $\nu_3$ ).
	$\nu_{17}$	$\text{CH}_3$ d-deform.....	1464 C	1464		
	$\nu_{18}$	$\text{CH}_3$ s-deform.....	1378 C	1378		
	$\nu_{19}$	$\text{CH}_2$ wag.....	1338 C	1338	1338 M	
	$\nu_{20}$	CC stretch.....	1054 C	1054	1054 M	
$b_2$	$\nu_{21}$	$\text{CH}_3$ rock.....	922 C	922		
	$\nu_{22}$	$\text{CH}_3$ d-stretch.....	2973 C	2973		
	$\nu_{23}$	$\text{CH}_2$ a-stretch.....	2968 C	2968		
	$\nu_{24}$	$\text{CH}_3$ d-deform.....	1472 C	1472		
	$\nu_{25}$	$\text{CH}_3$ rock.....	1192 C	1192		
	$\nu_{26}$	$\text{CH}_2$ rock.....	748 C	748		
	$\nu_{27}$	Torsion.....	<sup>a</sup> 268 C	.....	.....	MW [10,11].

<sup>a</sup> 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 <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a <sub>1</sub>	ν <sub>1</sub>	CH <sub>3</sub> d-stretch.....	2974 C	2974		
	ν <sub>2</sub>	CH <sub>3</sub> s-stretch.....	2883 C	2883		
	ν <sub>3</sub>	CD <sub>2</sub> s-stretch.....	2141 C	2141		
	ν <sub>4</sub>	CH <sub>3</sub> d-deform.....	1459 C	1459		
	ν <sub>5</sub>	CH <sub>3</sub> s-deform.....	1392 C	1392		
	ν <sub>6</sub>	CH <sub>3</sub> rock.....	1207 D	1207		
	ν <sub>7</sub>	CD <sub>2</sub> scis.....	1064 C	1064		
	ν <sub>8</sub>	CC stretch.....	843 C	843		
	ν <sub>9</sub>	CCC deform.....	362 E	.....	.....	CF [5].
a <sub>2</sub>	ν <sub>10</sub>	CH <sub>3</sub> d-stretch.....	2956 E	ia	.....	OC (ν <sub>10</sub> + ν <sub>18</sub> ) [4].
	ν <sub>11</sub>	CH <sub>3</sub> d-deform.....	1453 E	ia	.....	CF [5].
	ν <sub>12</sub>	CH <sub>3</sub> rock.....	1083 E	ia	.....	OC (ν <sub>12</sub> + ν <sub>16</sub> ) [4].
	ν <sub>13</sub>	CD <sub>2</sub> twist.....	777 E	ia	.....	CF [5].
	ν <sub>14</sub>	Torsion . . . . .	<sup>a</sup> 208 E	ia	.....	OC (ν <sub>18</sub> - ν <sub>14</sub> ) [4].
b <sub>1</sub>	ν <sub>15</sub>	CH <sub>3</sub> d-stretch . . . . .	2974 C	2974	.....	SF (ν <sub>1</sub> ).
	ν <sub>16</sub>	CH <sub>3</sub> s-stretch.....	2883 C	2883	.....	SF (ν <sub>2</sub> ).
	ν <sub>17</sub>	CH <sub>3</sub> d-deform.....	1461 C	1461		
	ν <sub>18</sub>	CH <sub>3</sub> s-deform.....	1374 C	1374		
	ν <sub>19</sub>	CC stretch.....	1203 C	1203		
	ν <sub>20</sub>	CH <sub>3</sub> rock.....	964 C	964		
	ν <sub>21</sub>	CD <sub>2</sub> wag.....	829 C	829		
	ν <sub>22</sub>	CH <sub>3</sub> d-stretch.....	2963 C	2963		
b <sub>2</sub>	ν <sub>23</sub>	CD <sub>2</sub> a-stretch.....	2182 C	2182		
	ν <sub>24</sub>	CH <sub>3</sub> d-deform.....	1476 C	1476		
	ν <sub>25</sub>	CH <sub>3</sub> rock.....	1146 C	1146		
	ν <sub>26</sub>	CD <sub>2</sub> rock.....	622 C	622		
	ν <sub>27</sub>	Torsion . . . . .	<sup>a</sup> 217 E	.....	.....	CF [4].

<sup>a</sup> Assigning frequencies higher than these by 10-20 percent may be more reasonable in view of the results for CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>.

## References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a'	ν <sub>1</sub>	CH <sub>3</sub> d-stretch.....	2966 C	2966		
	ν <sub>2</sub>	CH <sub>3</sub> s-stretch.....	2934 D	2934		
	ν <sub>3</sub>	CH <sub>2</sub> s-stretch.....	2882 C	2882		
	ν <sub>4</sub>	CD <sub>3</sub> d-stretch.....	2225 C	2225		
	ν <sub>5</sub>	CD <sub>3</sub> s-stretch.....	2075 C	2075		
	ν <sub>6</sub>	CH <sub>2</sub> scis.....	1461 D	1461		
	ν <sub>7</sub>	CH <sub>3</sub> d-deform.....	1460 D	1460		
	ν <sub>8</sub>	CH <sub>3</sub> s-deform.....	1383 C	1383		
	ν <sub>9</sub>	CH <sub>2</sub> wag.....	1332 C	1332		
	ν <sub>10</sub>	CC stretch.....	1132 C	1132		
	ν <sub>11</sub>	CH <sub>3</sub> rock.....	1101 C	1101		
	ν <sub>12</sub>	CD <sub>3</sub> d-deform.....	1062 C	1062		
	ν <sub>13</sub>	CD <sub>3</sub> s-deform.....	999 D	999		
	ν <sub>14</sub>	CC stretch.....	846 C	846		
	ν <sub>15</sub>	CD <sub>3</sub> rock.....	750 C	750		
a''	ν <sub>16</sub>	CCC deform.....	339 E	.....	.....	CF [2].
	ν <sub>17</sub>	CH <sub>3</sub> d-stretch.....	2966 C	2966	.....	SF (ν <sub>1</sub> ).
	ν <sub>18</sub>	CD <sub>2</sub> a-stretch.....	2935 C	2935		
	ν <sub>19</sub>	CD <sub>3</sub> d-stretch.....	2214 C	2214		
	ν <sub>20</sub>	CH <sub>3</sub> d-deform.....	1461 D	1461	.....	SF (ν <sub>6</sub> ).
	ν <sub>21</sub>	CH <sub>2</sub> twist.....	1285 D	1285		
	ν <sub>22</sub>	CH <sub>3</sub> rock.....	1129 C	1129		
	ν <sub>23</sub>	CD <sub>3</sub> d-deform.....	1063 C	1063		
	ν <sub>24</sub>	CH <sub>2</sub> rock.....	831 C	831		
	ν <sub>25</sub>	CD <sub>3</sub> rock.....	660 C	660		
	ν <sub>26</sub>	CH <sub>3</sub> torsion.....	<sup>a</sup> 216 E	.....	.....	CF [2].
	ν <sub>27</sub>	CD <sub>3</sub> torsion.....	<sup>a</sup> 161 E	.....	.....	CF [2].

<sup>a</sup> Assigning frequencies higher than these by 10–20 percent may be more reasonable in view of the results for CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>.

## References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a <sub>1</sub>	ν <sub>1</sub>	CH <sub>2</sub> s-stretch.....	2883 C	2883		
	ν <sub>2</sub>	CD <sub>3</sub> d-stretch.....	2225 C	2225	.....	SF (ν <sub>23</sub> ).
	ν <sub>3</sub>	CD <sub>3</sub> s-stretch.....	2091 C	2091	.....	SF (ν <sub>16</sub> ).
	ν <sub>4</sub>	CH <sub>2</sub> scis.....	1467 C	1467		
	ν <sub>5</sub>	CD <sub>3</sub> s-deform.....	1098 E	.....	.....	CF [4].
	ν <sub>6</sub>	CD <sub>3</sub> d-deform.....	1066 C	1066	.....	SF (ν <sub>19</sub> ).
	ν <sub>7</sub>	CD <sub>3</sub> rock.....	962 E	962		
	ν <sub>8</sub>	CC stretch.....	711 D	711		
	ν <sub>9</sub>	CCC deform.....	315 E	.....	.....	CF [4].
a <sub>2</sub>	ν <sub>10</sub>	CD <sub>3</sub> d-stretch.....	2222 E	ia	.....	CF [4].
	ν <sub>11</sub>	CH <sub>2</sub> twist.....	1257 E	ia	.....	CF [4].
	ν <sub>12</sub>	CD <sub>3</sub> d-deform.....	1052 E	ia	.....	CF [4].
	ν <sub>13</sub>	CD <sub>3</sub> rock.....	700 E	ia	.....	CF [4].
	ν <sub>14</sub>	Torsion.....	<sup>a</sup> 142 E	ia	.....	OC (ν <sub>14</sub> + ν <sub>21</sub> , ν <sub>21</sub> - 2ν <sub>14</sub> ) [3].
b <sub>1</sub>	ν <sub>15</sub>	CD <sub>3</sub> d-stretch.....	2227 C	2227		
	ν <sub>16</sub>	CD <sub>3</sub> s-stretch.....	2091 C	2091	.....	SF (ν <sub>3</sub> ).
	ν <sub>17</sub>	CH <sub>2</sub> wag.....	1331 C	1331		
	ν <sub>18</sub>	CC stretch.....	1131 C	1131		
	ν <sub>19</sub>	CD <sub>3</sub> d-deform.....	1066 C	1066	.....	SF (ν <sub>6</sub> ).
	ν <sub>20</sub>	CD <sub>3</sub> s-deform.....	920 E	920		
b <sub>2</sub>	ν <sub>21</sub>	CD <sub>3</sub> rock.....	725 C	725		
	ν <sub>22</sub>	CH <sub>2</sub> a-stretch.....	2929 C	2929		
	ν <sub>23</sub>	CD <sub>3</sub> d-stretch.....	2225 C	2225	.....	SF (ν <sub>2</sub> ).
	ν <sub>24</sub>	CD <sub>3</sub> d-deform.....	1087 C	1087		
	ν <sub>25</sub>	CH <sub>2</sub> rock.....	1066 D	1066		
	ν <sub>26</sub>	CD <sub>3</sub> rock.....	640 C	640		
	ν <sub>27</sub>	Torsion.....	<sup>a</sup> 173 E	.....	.....	OC (ν <sub>21</sub> + ν <sub>27</sub> - ν <sub>14</sub> ) [3].

<sup>a</sup> Assigning frequencies higher than these by 10-20 percent may be more reasonable in view of the results for CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>.

## References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm <sup>-1</sup> (Gas)	cm <sup>-1</sup>	
a <sub>1</sub>	ν <sub>1</sub>	CD <sub>3</sub> d-stretch.....	2225 C	2225		
	ν <sub>2</sub>	CD <sub>3</sub> s-stretch.....	2122 C	2122		
	ν <sub>3</sub>	CD <sub>2</sub> s-stretch.....	2081 C	2081		
	ν <sub>4</sub>	CD <sub>3</sub> s-deform.....	1086 D	1086		
	ν <sub>5</sub>	CD <sub>2</sub> scis.....	1064 D	1064		
	ν <sub>6</sub>	CD <sub>3</sub> d-deform.....	1064 D	1064		SF (ν <sub>5</sub> ).
	ν <sub>7</sub>	CD <sub>3</sub> rock.....	959 C	959		
	ν <sub>8</sub>	CC stretch.....	712 C	712		
	ν <sub>9</sub>	CCC deform.....	332 E			CF [3].
a <sub>2</sub>	ν <sub>10</sub>	CD <sub>3</sub> d-stretch.....	2221 E	ia		CF [4].
	ν <sub>11</sub>	CD <sub>3</sub> d-deform.....	1064 E	ia		CF [4].
	ν <sub>12</sub>	CD <sub>2</sub> twist.....	945 E	ia		CF [4].
	ν <sub>13</sub>	CD <sub>3</sub> rock.....	659 E	ia		CF [4].
	ν <sub>14</sub>	Torsion.....	<sup>a</sup> 143 E	ia		OC (ν <sub>14</sub> + ν <sub>22</sub> , ν <sub>14</sub> + ν <sub>24</sub> ) [3].
b <sub>1</sub>	ν <sub>15</sub>	CD <sub>3</sub> d-stretch.....	2224 C	2224		
	ν <sub>16</sub>	CD <sub>3</sub> s-stretch.....	2081 C	2081		SF (ν <sub>3</sub> ).
	ν <sub>17</sub>	CC stretch.....	1203 C	1203		
	ν <sub>18</sub>	CD <sub>3</sub> d-deform.....	1086 D	1086		SF (ν <sub>4</sub> ).
	ν <sub>19</sub>	CD <sub>3</sub> s-deform.....	1068 D	1068		
	ν <sub>20</sub>	CD <sub>2</sub> wag.....	862 D	862		
b <sub>2</sub>	ν <sub>21</sub>	CD <sub>3</sub> rock.....	688 C	688		
	ν <sub>22</sub>	CD <sub>3</sub> d-stretch.....	2224 C	2224		SF (ν <sub>15</sub> ).
	ν <sub>23</sub>	CD <sub>2</sub> a-stretch.....	2149 D	2149		
	ν <sub>24</sub>	CD <sub>3</sub> d-deform.....	1064 D	1064		SF (ν <sub>5</sub> , ν <sub>6</sub> ).
	ν <sub>25</sub>	CD <sub>3</sub> rock.....	949 D	949		
	ν <sub>26</sub>	CD <sub>2</sub> rock.....	544 D	544		
	ν <sub>27</sub>	Torsion.....	<sup>a</sup> 172 E			OC (ν <sub>25</sub> + ν <sub>27</sub> - ν <sub>21</sub> ) [3.]

<sup>a</sup> Assigning frequencies higher than 10-20 percent may be more reasonable in view of the results for CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>.

## References

- [1] IR. H. L. McMurphy and V. Thornton, J. Chem. Phys. 19, 1014 (1951).
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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	$\text{CH}_3(\text{O})$ d-stretch.....	3035 D	$\text{cm}^{-1}$ (Gas) 3035 M	$\text{cm}^{-1}$ (Liquid) 3028 (3b)	SF ( $\nu_2$ of $\text{CH}_3\text{COOCD}_3$ ).
	$\nu_2$	$\text{CH}_3(\text{C})$ d-stretch.....	3031 E	.....	.....	
	$\nu_3$	$\text{CH}_3(\text{O})$ s-stretch.....	2966 D	2966 S	2954 (3) p	SF ( $\nu_4$ of $\text{CH}_3\text{COOCD}_3$ ).
	$\nu_4$	$\text{CH}_3(\text{C})$ s-stretch.....	2964 E	.....	2942 (7b) p	
	$\nu_5$	$\text{C}=\text{O}$ stretch.....	1771 C	1771 VS	1738 (3b) p	OV ( $\nu_{20}$ ).
	$\nu_6$	$\text{CH}_3(\text{O})$ d-deform.....	1460 E	1460 W, sh ( $\text{CCl}_4$ soln.)	.....	
	$\nu_7$	$\text{CH}_3(\text{O})$ s-deform.....	1440 D	1440 M	.....	SF ( $\nu_3$ of $\text{CH}_3\text{COOCD}_3$ ).
	$\nu_8$	$\text{CH}_3(\text{C})$ d-deform.....	1430 E	.....	.....	
	$\nu_9$	$\text{CH}_3(\text{C})$ s-deform.....	1375 D	1375 S	1372 (0.5) p	OV ( $\nu_6$ ).
	$\nu_{10}$	$\text{C}-\text{O}$ stretch.....	1248 C	1248 VS	1254 (0)	
	$\nu_{11}$	$\text{CH}_3(\text{O})$ rock.....	1159 E	1159 VW (liquid)	.....	
$a''$	$\nu_{12}$	$\text{O}-\text{CH}_3$ stretch.....	1060 C	1060 S	1044 (2b)	
	$\nu_{13}$	$\text{CH}_3(\text{C})$ rock.....	980 C	980 W	980 (1b) p	
	$\nu_{14}$	$\text{CC}$ stretch.....	844 C	844 M	844 (8) p	
	$\nu_{15}$	$\text{C}=\text{O}$ ip-bend.....	639 C	639 M	640 (7) p	
	$\nu_{16}$	$\text{CCO}$ deform.....	429 C	429 M	433 (3) p	
	$\nu_{17}$	$\text{COC}$ deform.....	303 D	303 M	303 (1b) p	
	$\nu_{18}$	$\text{CH}_3(\text{O})$ d-stretch.....	3005 D	3005 M	3002 (3b)	
	$\nu_{19}$	$\text{CH}_3(\text{C})$ d-stretch.....	2994 D	2994 W	.....	
	$\nu_{20}$	$\text{CH}_3(\text{O})$ d-deform.....	1460 E	1460 W, sh ( $\text{CCl}_4$ soln.)	1449 (4b) dp	
	$\nu_{21}$	$\text{CH}_3(\text{C})$ d-deform.....	1430 E	1430 W	.....	
	$\nu_{22}$	$\text{CH}_3(\text{O})$ rock.....	1187 D	1187 W	1187 (0.5b)	
	$\nu_{23}$	$\text{CH}_3(\text{C})$ rock.....	1036 E	1036 W (solid)	.....	
	$\nu_{24}$	$\text{C}=\text{O}$ op-bend.....	607 D	607 M	610 (0) dp	
	$\nu_{25}$	$\text{C}-\text{O}$ torsion.....	187 D	187 W	.....	
	$\nu_{26}$	$\text{C}-\text{C}$ torsion.....	136 E	136 VW (liquid)	.....	
	$\nu_{27}$	$\text{O}-\text{CH}_3$ torsion.....	110 E	110 VW (liquid)	.....	

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- [4] IR.Th. S. Ichikawa, Y. Udagawa, and T. Shimanouchi, unpublished.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	CH <sub>3</sub> d-stretch.....	3032 D	$cm^{-1}$ (Gas) 3032 M	$cm^{-1}$ .....	OV ( $\nu_{20}$ ).
	$\nu_2$	CD <sub>3</sub> d-stretch.....	2275 E	2275 W		
	$\nu_3$	CH <sub>3</sub> s-stretch.....	2967 D	2967 S		
	$\nu_4$	CD <sub>3</sub> s-stretch.....	2087 E	2087 W		
	$\nu_5$	C=O stretch.....	1768 C	1768 VS		
	$\nu_6$	CH <sub>3</sub> d-deform.....	1455 E	1455 W, sh (CCl <sub>4</sub> soln.)		
	$\nu_7$	CH <sub>3</sub> s-deform.....	1439 D	1439 M		
	$\nu_8$	CD <sub>3</sub> d-deform.....	1007 D	1007 M		
	$\nu_9$	CD <sub>3</sub> s-deform.....	1086 C	1086 S		
	$\nu_{10}$	C-O stretch.....	1268 C	1268 VS		
	$\nu_{11}$	CH <sub>3</sub> rock.....	1160 D	1160 W		
	$\nu_{12}$	O-CH <sub>3</sub> stretch.....	1049 D	1049 W		
	$\nu_{13}$	CD <sub>3</sub> rock.....	780 C	780 M		
	$\nu_{14}$	CC stretch.....	860 C	860 M		
	$\nu_{15}$	C=O ip-bend.....	599 C	599 M		
	$\nu_{16}$	CCO deform.....	390 C	390 M		
<i>a''</i>	$\nu_{17}$	COC deform.....	298 D	298 M		
	$\nu_{18}$	CH <sub>3</sub> d-stretch.....	3004 D	3004 M		
	$\nu_{19}$	CD <sub>3</sub> d-stretch.....	2253 D	2253 W		OV ( $\nu_6$ ).
	$\nu_{20}$	CH <sub>3</sub> d-deform.....	1455 E	1455 W, sh (CCl <sub>4</sub> soln.)		
	$\nu_{21}$	CD <sub>3</sub> d-deform.....	1033 D	1033 W		
	$\nu_{22}$	CH <sub>3</sub> rock.....	1181 E	1181 W		
	$\nu_{23}$	CD <sub>3</sub> rock.....	918 C	918 M		
	$\nu_{24}$	C=O op-bend.....	525 D	525 M		
	$\nu_{25}$	C-O torsion.....	178 D	178 M		
	$\nu_{26}$	C-C torsion.....	98 E	.....		CF [2].
	$\nu_{27}$	O-CH <sub>3</sub> torsion.....	110 E	.....		CF [2].

## References

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



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

# References

See No. 198.

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

## References

See No. 198.

Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$\sigma_g^+$	$\nu_1$	CH stretch.....	3293 D	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Gas) 3293 VW (liquid)	
	$\nu_2$	$C\equiv C$ stretch.....	2184 C	ia	2184 VS	
	$\nu_3$	C-C stretch.....	874 C	ia	874 W	
$\sigma_u^+$	$\nu_4$	CH stretch.....	3329 C	3329 VS	ia	
	$\nu_5$	$C\equiv C$ stretch.....	2020 C	2020 M	ia	
$\pi_g$	$\nu_6$	CH bend.....	627 C	ia	627 M	
	$\nu_7$	CCC bend.....	482 C	ia	482 S	
$\pi_u$	$\nu_8$	CH bend.....	630 B	630 VS	ia	
	$\nu_9$	CCC bend.....	231 E	ia	231 VW (liquid)	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	$\nu_1$	CH stretch.....	3154 D	<i>cm</i> <sup>-1</sup> (Gas).....	<i>cm</i> <sup>-1</sup> (Liquid) 3154 VS, p	OC ( $\nu_9 + \nu_{16}$ , $\nu_9 + \nu_{17}$ , $\nu_9 + \nu_{19}$ , $\nu_9 + \nu_2$ ).
	$\nu_2$	CH stretch.....	3140 D	3140 sh		
	$\nu_3$	ip-Ring II.....	1491 C	1491 VS	1483 VS, p	
	$\nu_4$	ip-Ring III.....	1384 C	1384 M	1380 S, p	
	$\nu_5$	ip-Ring IV.....	1140 D	1140 sh (liquid)	1137 VS, p	
	$\nu_6$	CH ip-bend.....	1066 C	1066 S	1061 M, p	
	$\nu_7$	CH ip-bend.....	995 C	995 VS	986 M, p	
	$\nu_8$	ip-Ring VII.....	871 C	871 S		
<i>a</i> <sub>2</sub>	$\nu_9$	CH op-bend.....	863 C	ia	.....	
	$\nu_{10}$	CH op-bend.....	728 D	ia	728 W, dp	
<i>b</i> <sub>1</sub>	$\nu_{11}$	op-Ring I.....	613 D	ia	613 VW, dp	
	$\nu_{12}$	CH stretch.....	3161 C	3161 M		
	$\nu_{13}$	CH stretch.....	3129 C	3129 M	3121 S, dp	
	$\nu_{14}$	ip-Ring I.....	1556 C	1556 W		
	$\nu_{15}$	CH ip-bend.....	1267 C	1267 VW	1270 VW, dp	
	$\nu_{16}$	CH ip-bend.....	1180 C	1180 VS	1171 W, dp	
	$\nu_{17}$	ip-Ring V.....	1040 D	1040 sh (liquid)	1034 M, dp	
<i>b</i> <sub>2</sub>	$\nu_{18}$	ip-Ring VI.....	873 D	.....	873 W, dp	
	$\nu_{19}$	CH op-bend.....	838 C	838 VW	839 W, dp	
	$\nu_{20}$	CH op-bend.....	745 C	745 VS		
	$\nu_{21}$	op-Ring II.....	603 C	603 S	601 W, dp	

## References

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- [5] IR.R. M. Rico, M. Barrachina, and J. M. Orza, J. Mol. Spectrosc. 24, 133 (1967).



Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
$a_1$	$\nu_1$	CH stretch.....	3126 C	3126 M	3107 (10) p	
	$\nu_2$	CH stretch.....	3098 C	3098 S	3084 (5sh)	
	$\nu_3$	ip-Ring II.....	1409 C	1409 S	1407 (7) p	
	$\nu_4$	ip-Ring III.....	1360 C	1360 VW	1358 (5) p	
	$\nu_5$	CH ip-bend.....	1083 C	1083 S	1081 (5) p	
	$\nu_6$	CH ip-bend.....	1036 C	1036 S	1035	
	$\nu_7$	ip-Ring IV.....	839 C	839 VS	832 (5) p	
	$\nu_8$	ip-Ring VII.....	608 C	608 W	606 (2) p	
$a_2$	$\nu_9$	CH op-bend.....	903 D	ia, 900 VW (solid)	903 (0) dp	
	$\nu_{10}$	CH op-bend.....	688 D	ia	688 (0) dp	
	$\nu_{11}$	op-Ring I.....	567 D	ia, 565 VW (liquid)	567 (0) dp	
$b_1$	$\nu_{12}$	CH stretch.....	<sup>a</sup> 3125 E			
	$\nu_{13}$	CH stretch.....	3086 C	3086 S	3076 (sh)	
	$\nu_{14}$	ip-Ring I.....	1504 D	1504 VW (liquid)	1502 (0) dp	
	$\nu_{15}$	CH ip-bend.....	1256 C	1256 S	1257 (0)	
	$\nu_{16}$	CH ip-bend.....	<sup>a</sup> 1085 E			OV ( $\nu_5$ ).
$b_2$	$\nu_{17}$	ip-Ring V.....	872 C	872 M	869 (4) dp	
	$\nu_{18}$	ip-Ring VI.....	751 D	763 VW	751 (1) dp	
	$\nu_{19}$	CH op-bend.....	867 E			OC ( $\nu_9 + \nu_{19}, 2\nu_{19}$ ).
	$\nu_{20}$	CH op-bend.....	712 C	712 VS		
	$\nu_{21}$	op-Ring II.....	452 C	452 W	453 (0) dp	

<sup>a</sup> These frequencies were estimated from isotopic rule [3].

## References

- [1] IR. H. W. Thompson and R. B. Temple, Trans. Faraday Soc. 41, 27 (1945).
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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> <sub>1</sub>	$\nu_1$	CD stretch . . . . .	2343 C	<i>cm</i> <sup>-1</sup> (Gas) 2343 M	<i>cm</i> <sup>-1</sup> (Liquid) 2326 (6)	SF ( $\nu_{17}$ ).
	$\nu_2$	CD stretch . . . . .	2290 C	2290 M		
	$\nu_3$	ip-Ring II . . . . .	1376 C	1376 S	1372 (10) p	
	$\nu_4$	ip-Ring III . . . . .	1248 C	1248 W	1240 (5)	
	$\nu_5$	CD ip-bend . . . . .	896 C	896 M	891 (10) p	
	$\nu_6$	CD ip-bend . . . . .	785 C	785 M	780 (3) dp	
	$\nu_7$	ip-Ring IV . . . . .	731 C	731 VS	723 (3)	
	$\nu_8$	ip-Ring VII . . . . .	585 D	585 VW	582 (2) p	
<i>a</i> <sub>2</sub>	$\nu_9$	CD op-bend . . . . .	752 E	ia, 756 (solid)	752 (3) dp	
	$\nu_{10}$	CD op-bend . . . . .	532 D	ia	532 (2) dp	
<i>b</i> <sub>1</sub>	$\nu_{11}$	op-Ring I . . . . .	488 D	ia	488	
	$\nu_{12}$	CD stretch . . . . .	<sup>a</sup> 2340 E			
	$\nu_{13}$	CD stretch . . . . .	2305 C	2305 M	2286 (4) dp	
	$\nu_{14}$	ip-Ring I . . . . .	1459 C	1459 M		
	$\nu_{15}$	CD ip-bend . . . . .	1034 C	1034 S		
	$\nu_{16}$	CD ip-bend . . . . .	846 C	846 S	847 (2)	
	$\nu_{17}$	ip-Ring V . . . . .	752 D	756 (solid)	752 (3) dp	
<i>b</i> <sub>2</sub>	$\nu_{18}$	ip-Ring VI . . . . .	712 C	712 W		
	$\nu_{19}$	CD op-bend . . . . .	684 C	684 VW	682 (1)	
	$\nu_{20}$	CD op-bend . . . . .	531 C	531 VS		
	$\nu_{21}$	op-Ring II . . . . .	414 C	414 VW	411	

<sup>a</sup> 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
				$\text{cm}^{-1}$ (Gas)	$\text{cm}^{-1}$ (Solid)	
$a_g$	$\nu_1$	$\text{CH}_2$ a-stretch.....	3087 D	ia	3087 M	
	$\nu_2$	CH stretch.....	3003 D	ia	3003 M	
	$\nu_3$	$\text{CH}_2$ s-stretch.....	2992 D	ia	2992 S	
	$\nu_4$	C=C stretch.....	1630 D	ia	1630 VS	
	$\nu_5$	$\text{CH}_2$ scis.....	1438 D	ia	1438 S	
	$\nu_6$	CH bend.....	1280 D	ia	1280 S	
	$\nu_7$	C-C stretch.....	1196 D	ia	1196 S	
	$\nu_8$	$\text{CH}_2$ rock.....	894 D	ia	894 W	
	$\nu_9$	CCC deform.....	512 D	ia	512 S	
$a_u$	$\nu_{10}$	CH bend.....	1013 B	1013.4 VS	ia	
	$\nu_{11}$	$\text{CH}_2$ wag.....	908 B	907.8 VS	ia	
	$\nu_{12}$	$\text{CH}_2$ twist.....	522 B	522.2 M	ia	
	$\nu_{13}$	C-C torsion.....	162 B	162.3 VW	ia	
$b_g$	$\nu_{14}$	CH bend.....	976 D	ia	976 W	
	$\nu_{15}$	$\text{CH}_2$ wag.....	912 D	ia	912 S	
	$\nu_{16}$	$\text{CH}_2$ twist.....	770 D	ia	770 VW	
$b_u$	$\nu_{17}$	$\text{CH}_2$ a-stretch.....	3101 B	3100.6 S	ia	
	$\nu_{18}$	CH stretch.....	3055 B	3054.9 S	ia	
	$\nu_{19}$	$\text{CH}_2$ s-stretch.....	2984 B	2984.3 S	ia	
	$\nu_{20}$	C=C stretch.....	1596 B	1596.0 S	ia	
	$\nu_{21}$	$\text{CH}_2$ scis.....	1381 B	1380.7 W	ia	
	$\nu_{22}$	CH bend.....	1294 B	1294.3 W	ia	
	$\nu_{23}$	$\text{CH}_2$ rock.....	990 B	989.7 M	ia	
	$\nu_{24}$	CCC deform.....	301 B	300.6 VW	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a'</i>	$\nu_1$	CH <sub>2</sub> a-stretch.....	3100 C	<i>cm</i> <sup>-1</sup> (Gas) 3100.4 S	<i>cm</i> <sup>-1</sup> (Solid) 3090 M	CF [1].
	$\nu_2$	CH stretch.....	3075 D	.....	3075 W	
	$\nu_3$	CH stretch.....	3048 C	3047.9 S		
	$\nu_4$	CH stretch.....	3021 C	3020.5 S		
	$\nu_5$	CH <sub>2</sub> s-stretch.....	3003 D	.....	3003 M	
	$\nu_6$	CD stretch.....	2286 C	2285.9 M	2276 M	
	$\nu_7$	C=C stretch.....	1631 D	.....	1631 VS	
	$\nu_8$	C=C stretch.....	1580 B	1579.7 S	1572 M	
	$\nu_9$	CH <sub>2</sub> scis.....	1409 D	.....	1409 VW	
	$\nu_{10}$	CH ip-bend.....	1304 E	.....	.....	
	$\nu_{11}$	CH ip-bend.....	1288 D	.....	1288 S	
	$\nu_{12}$	CH ip-bend.....	1270 C	1270 M	1272 VW	
	$\nu_{13}$	C-C stretch.....	1183 D	1185 W	1183 S	
	$\nu_{14}$	CH <sub>2</sub> rock.....	964 D	964 W (solid)		
<i>a''</i>	$\nu_{15}$	CD ip-bend.....	793 D	.....	793 W	CF [1].
	$\nu_{16}$	CCC deform.....	511 D	.....	511 M	
	$\nu_{17}$	CCC deform.....	288 C	288 VW		
	$\nu_{18}$	CH op-bend.....	1008 B	1008.0 VS		
	$\nu_{19}$	CH op-bend.....	960 B	959.9 S		
	$\nu_{20}$	CH <sub>2</sub> wag.....	909 B	908.6 VS	921 M	
	$\nu_{21}$	CH op-bend.....	849 B	849.2 S	862 M	
	$\nu_{22}$	CD op-bend.....	674 C	673.9 VW		
	$\nu_{23}$	CH <sub>2</sub> twist.....	464 C	464.0 W		
	$\nu_{24}$	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)	$cm^{-1}$	
$\alpha'$	$\nu_1$	CH <sub>2</sub> a-stretch.....	3099 C	3099.1 S		
	$\nu_2$	CH stretch.....	3016 C	3016.4 S		
	$\nu_3$	CH <sub>2</sub> s-stretch.....	2995 C	2995.4 S		
	$\nu_4$	CD <sub>2</sub> a-stretch.....	2342 C	2341.9 S		
	$\nu_5$	CD stretch.....	2268 C	2267.9 S		
	$\nu_6$	CD <sub>2</sub> s-stretch.....	2217 C	2217.1 S		
	$\nu_7$	C=C stretch.....	1630 C	1630.4 M		
	$\nu_8$	C=C stretch.....	1549 B	1548.5 S		
	$\nu_9$	CH <sub>2</sub> scis.....	1425 C	1425 M		
	$\nu_{10}$	CH ip-bend.....	1298 C	1298 W		
	$\nu_{11}$	C-C stretch.....	1185 C	1185 W		
	$\nu_{12}$	CD <sub>2</sub> scis.....	1080 C	1080 W		
	$\nu_{13}$	CD ip-bend.....	992 D	991.8 W		
				(solid)		
$\alpha''$	$\nu_{14}$	CH <sub>2</sub> rock.....	880 D	879.9 M		
				(solid)		
	$\nu_{15}$	CD <sub>2</sub> rock.....	757 E	.....	.....	CF [1].
	$\nu_{16}$	CCC deform.....	476 E	.....	.....	CF [1].
	$\nu_{17}$	CCC deform.....	280 D	280 W		
	$\nu_{18}$	CH op-bend.....	991 B	990.6 VS		
	$\nu_{19}$	CH <sub>2</sub> wag.....	909 B	909.2 VS		
	$\nu_{20}$	CD op-bend.....	791 B	791.3 W		
	$\nu_{21}$	CD <sub>2</sub> wag.....	715 E	{ 734.0 S 710.1 VS }	.....	FR ( $\nu_{17} + \nu_{23}$ ).
	$\nu_{22}$	CH <sub>2</sub> twist.....	674 B	673.8 S		
	$\nu_{23}$	CD <sub>2</sub> twist.....	439 C	439.0 M		
	$\nu_{24}$	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> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Solid)	
<i>a<sub>g</sub></i>	<i>ν</i> <sub>1</sub>	CH stretch . . . . .	3010 D	ia	3010 M	CF [1].
	<i>ν</i> <sub>2</sub>	CD <sub>2</sub> a-stretch . . . . .	2315 D	ia	2315 S	
	<i>ν</i> <sub>3</sub>	CD <sub>2</sub> s-stretch . . . . .	2212 D	ia	2212 S	
	<i>ν</i> <sub>4</sub>	C=C stretch . . . . .	1610 D	ia	1610 VS	
	<i>ν</i> <sub>5</sub>	CH ip-bend . . . . .	1296 D	ia	1296 S	
	<i>ν</i> <sub>6</sub>	C-C stretch . . . . .	1170 D	ia	1170 S	
	<i>ν</i> <sub>7</sub>	CD <sub>2</sub> scis . . . . .	1040 D	ia	1040 S	
	<i>ν</i> <sub>8</sub>	CD <sub>2</sub> rock . . . . .	740 D	ia	740 W	
	<i>ν</i> <sub>9</sub>	CCC deform . . . . .	457 D	ia	457 S	
<i>a<sub>u</sub></i>	<i>ν</i> <sub>10</sub>	CH op-bend . . . . .	955 B	955.1 S	ia	
	<i>ν</i> <sub>11</sub>	CD <sub>2</sub> wag . . . . .	728 B	728.0 VS	ia	
	<i>ν</i> <sub>12</sub>	CD <sub>2</sub> twist . . . . .	397 C	397 W	ia	
<i>b<sub>g</sub></i>	<i>ν</i> <sub>13</sub>	C-C torsion . . . . .	149 E	.....	ia	
	<i>ν</i> <sub>14</sub>	CH op-bend . . . . .	948 D	ia	948 M	
	<i>ν</i> <sub>15</sub>	CD <sub>2</sub> wag . . . . .	728 D	ia	728 S	
<i>b<sub>u</sub></i>	<i>ν</i> <sub>16</sub>	CD <sub>2</sub> twist . . . . .	610 D	ia	610 VW	
	<i>ν</i> <sub>17</sub>	CH stretch . . . . .	3041 C	3040.8 S	ia	
	<i>ν</i> <sub>18</sub>	CD <sub>2</sub> a-stretch . . . . .	2350 D	2350 S	ia	
	<i>ν</i> <sub>19</sub>	CD <sub>2</sub> s-stretch . . . . .	2228 C	2228 S	ia	
	<i>ν</i> <sub>20</sub>	C=C stretch . . . . .	1535 B	1535.0 S	ia	
	<i>ν</i> <sub>21</sub>	CH ip-bend . . . . .	1335 C	1335.2 M	ia	
	<i>ν</i> <sub>22</sub>	CD <sub>2</sub> scis . . . . .	1031 C	1031.3 S	ia	
	<i>ν</i> <sub>23</sub>	CD <sub>2</sub> rock . . . . .	817 C	816.5 M	ia	
	<i>ν</i> <sub>24</sub>	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> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Solid)	
<i>a<sub>g</sub></i>	ν <sub>1</sub>	CD <sub>2</sub> a-stretch.....	2320 D	ia	2320 M	
	ν <sub>2</sub>	CD stretch.....	2250 D	ia	2250 M	
	ν <sub>3</sub>	CD <sub>2</sub> s-stretch.....	2210 D	ia	2210 M	
	ν <sub>4</sub>	C=C stretch.....	1580 D	ia	1580 VS	
	ν <sub>5</sub>	C-C stretch.....	1196 D	ia	1196 M	
	ν <sub>6</sub>	CD <sub>2</sub> scis.....	1045 D	ia	1045 W	
	ν <sub>7</sub>	CD ip-bend.....	918 D	ia	918 S	
	ν <sub>8</sub>	CD <sub>2</sub> rock.....	746 D	ia	746 M	
	ν <sub>9</sub>	CCC deform.....	439 D	ia	439 S	
<i>a<sub>u</sub></i>	ν <sub>10</sub>	CD op-bend.....	741 B	741.4 W	ia	
	ν <sub>11</sub>	CD <sub>2</sub> wag.....	718 B	718.4 S	ia	
	ν <sub>12</sub>	CD <sub>2</sub> twist.....	381 C	381.1 W	ia	
<i>b<sub>g</sub></i>	ν <sub>13</sub>	C-C torsion.....	140 C	140 VW	ia	
	ν <sub>14</sub>	CD op-bend.....	799 D	ia	799 S	
	ν <sub>15</sub>	CD <sub>2</sub> wag.....	705 D	ia	705 S	
<i>b<sub>u</sub></i>	ν <sub>16</sub>	CD <sub>2</sub> twist.....	603 D	ia	603 VW	
	ν <sub>17</sub>	CD <sub>2</sub> a-stretch.....	2320 D	2320.3 M	ia	
	ν <sub>18</sub>	CD stretch.....	2266 C	2265.9 M	ia	
	ν <sub>19</sub>	CD <sub>2</sub> s-stretch.....	2218 C	2218.0 M	ia	
	ν <sub>20</sub>	C=C stretch.....	1520 B	1519.6 S	ia	
	ν <sub>21</sub>	CD <sub>2</sub> scis.....	1048 C	1048.0 W	ia	
	ν <sub>22</sub>	CD ip-bend.....	1005 C	1005.4 M	ia	
	ν <sub>23</sub>	CD <sub>2</sub> rock.....	769 D	768.9 W	ia	
	ν <sub>24</sub>	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
$a'_1$	$\nu_1$	$\text{CH}_3$ s-stretch . . . . .	2916 C	$\text{cm}^{-1}$ (Gas) ia	$\text{cm}^{-1}$ (Liquid) 2916 S p	} FR ( $2\nu_8$ ).
	$\nu_2$	$\text{C}\equiv\text{C}$ stretch . . . . .	2240 E	ia	{ 2310 S p	
	$\nu_3$	$\text{CH}_3$ s-deform . . . . .	1380 C	ia	{ 2233 S p	
	$\nu_4$	$\text{C}-\text{C}$ stretch . . . . .	725 E	ia	1380 S	
$a''_1$	$\nu_5$	$\text{CH}_3$ torsion <sup>a</sup> . . . . .		ia	{ 774 M p	} FR ( $2\nu_{16}$ ).
$a''_2$	$\nu_6$	$\text{CH}_3$ s-stretch . . . . .	2938 B	2938 S	ia	
	$\nu_7$	$\text{CH}_3$ s-deform . . . . .	1382 B	1382 M	ia	
	$\nu_8$	$\text{C}-\text{C}$ stretch . . . . .	1152 B	1152 W	ia	
$e'$	$\nu_9$	$\text{CH}_3$ d-stretch . . . . .	2973 B	2973 S		
	$\nu_{10}$	$\text{CH}_3$ d-deform . . . . .	1456 B	1456 S		
	$\nu_{11}$	$\text{CH}_3$ rock . . . . .	1054 B	1054 M		
$e''$	$\nu_{12}$	CCC deform . . . . .	213 C		213 VW	
	$\nu_{13}$	$\text{CH}_3$ d-stretch . . . . .	2966 D	ia	2966 W	
	$\nu_{14}$	$\text{CH}_3$ d-deform . . . . .	1448 C	ia	1448 M dp	
	$\nu_{15}$	$\text{CH}_3$ rock . . . . .	1029 C	ia	1029 M dp	
	$\nu_{16}$	CCC deform . . . . .	371 C	ia	371 S dp	

<sup>a</sup> Free rotation [5].

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a_1$	$\nu_1$	$CH_2$ s-stretch . . . . .	2895 D	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Liquid) 2916 p 2866 p	} FR ( $2\nu_2, 2\nu_{13}$ ).
	$\nu_2$	$CH_2$ scis . . . . .	1443 C	ia	1443 p	
	$\nu_3$	Ring stretch . . . . .	1001 C	ia	1001 p	SF ( $\nu_{13}$ ).
	$\nu_4$	$CH_2$ a-stretch . . . . .	2975 E	ia	.....	SF ( $\nu_{14}$ ).
	$\nu_5$	$CH_2$ rock . . . . .	741 C	ia	741 dp	CF [3].
	$\nu_6$	Ring puckering . . . . .	197 C	ia	197	CF [3].
$a_2$	$\nu_7$	$CH_2$ wag . . . . .	1260 E	ia	ia	CF [3].
	$\nu_8$	$CH_2$ twist . . . . .	1257 E	ia	ia	CF [3].
$b_1$	$\nu_9$	$CH_2$ wag . . . . .	1219 C	ia	1219 dp	
	$\nu_{10}$	Ring deform . . . . .	926 C	ia	926 dp	
	$\nu_{11}$	$CH_2$ twist . . . . .	1222 E	ia	.....	CF [3].
$b_2$	$\nu_{12}$	$CH_2$ s-stretch . . . . .	2893 E	.....	.....	CF [3].
	$\nu_{13}$	$CH_2$ scis . . . . .	1443 C	.....	1443 dp	SF ( $\nu_2$ ).
	$\nu_{14}$	Ring deform . . . . .	1001 D	.....	1001 p	SF ( $\nu_3$ ).
	$\nu_{15}$	$CH_2$ a-stretch . . . . .	2987 C	2987 S		
	$\nu_{16}$	$CH_2$ rock . . . . .	627 C	627 S		
$e$	$\nu_{17}$	$CH_2$ a-stretch . . . . .	2952 C	.....	2952	
	$\nu_{18}$	$CH_2$ twist . . . . .	1223 C	1223 W		
	$\nu_{19}$	$CH_2$ rock . . . . .	749 C	749 W		
	$\nu_{20}$	$CH_2$ s-stretch . . . . .	2887 D	{ 2897 S 2878 S }		
	$\nu_{21}$	$CH_2$ scis . . . . .	1447 C	1447 S		
	$\nu_{22}$	$CH_2$ wag . . . . .	1257 C	1257 S		
	$\nu_{23}$	Ring deform . . . . .	898 C	898 S		

## References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				<i>cm</i> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup> (Liquid)	
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CD <sub>2</sub> s-stretch.....	2124 E	ia	.....	CF [2].
	<i>ν</i> <sub>2</sub>	CD <sub>2</sub> scis.....	1160 C	ia	1160 p	
	<i>ν</i> <sub>3</sub>	Ring stretch.....	882 C	ia	882 p	
	<i>ν</i> <sub>4</sub>	CD <sub>2</sub> a-stretch.....	2224 E	ia	.....	CF [2].
	<i>ν</i> <sub>5</sub>	CD <sub>2</sub> rock.....	632 E	ia	.....	CF [2].
	<i>ν</i> <sub>6</sub>	Ring puckering.....	158 D	ia	.....	RP [3].
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>7</sub>	CD <sub>2</sub> wag.....	1010 E	ia	ia	CF [2].
	<i>ν</i> <sub>8</sub>	CD <sub>2</sub> twist.....	889 E	ia	ia	CF [2].
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>9</sub>	CD <sub>2</sub> wag.....	1078 C	ia	1078 dp	
	<i>ν</i> <sub>10</sub>	Ring deform.....	746 C	ia	746 dp	
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>11</sub>	CD <sub>2</sub> twist.....	864 E	ia	.....	CF [2].
	<i>ν</i> <sub>12</sub>	CD <sub>2</sub> s-stretch.....	2115 E	.....	.....	CF [2].
	<i>ν</i> <sub>13</sub>	CD <sub>2</sub> scis.....	1040 D	.....	1040 dp	
	<i>ν</i> <sub>14</sub>	Ring deform.....	938 D	.....	938 dp	SF ( <i>ν</i> <sub>18</sub> ).
	<i>ν</i> <sub>15</sub>	CD <sub>2</sub> a-stretch.....	2242 C	2242 S	.....	
	<i>ν</i> <sub>16</sub>	CD rock.....	483 C	483 S	.....	
<i>e</i>	<i>ν</i> <sub>17</sub>	CD <sub>2</sub> a-stretch.....	2230 C	.....	2230 dp	
	<i>ν</i> <sub>18</sub>	CD <sub>2</sub> twist.....	938 D	.....	938 dp	SF ( <i>ν</i> <sub>14</sub> ).
	<i>ν</i> <sub>19</sub>	CD <sub>2</sub> rock.....	556 C	556 W	.....	
	<i>ν</i> <sub>20</sub>	CD <sub>2</sub> s-stretch.....	2103 E	.....	.....	CF [2].
	<i>ν</i> <sub>21</sub>	CD <sub>2</sub> scis.....	1078 C	1078 S	.....	
	<i>ν</i> <sub>22</sub>	CD <sub>2</sub> wag.....	1048 C	1048 S	.....	
	<i>ν</i> <sub>23</sub>	Ring deform.....	734 C	734 S	.....	

## References

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
<i>a</i> <sub>1</sub>	ν <sub>1</sub>	CH <sub>2</sub> s-stretch.....	2989 D	cm <sup>-1</sup> (Gas) 2991 M (solid)	cm <sup>-1</sup> (Liquid) 2989 S, p	
	ν <sub>2</sub>	CH <sub>3</sub> d-stretch.....	2941 C	2940.8	2930 W, p	
	ν <sub>3</sub>	CH <sub>3</sub> s-stretch.....	2911 D	2919 W	2911 S, p	
	ν <sub>4</sub>	C=C stretch.....	1661 C	1661.1 S	1655 S, p	
	ν <sub>5</sub>	CH <sub>3</sub> d-deform.....	1470 C	1469.6 S	1462 VW	
	ν <sub>6</sub>	CH <sub>2</sub> scis.....	1416 D	1419 W (solid)	1416 S, p	
	ν <sub>7</sub>	CH <sub>3</sub> s-deform.....	1366 D	.....	1366 VW, p	
	ν <sub>8</sub>	CH <sub>3</sub> rock.....	1064 C	1063.9 S	1058 W, p	
	ν <sub>9</sub>	C-C stretch.....	801 C	801 W	803 VS, p	
	ν <sub>10</sub>	C=CC <sub>2</sub> ip-deform.....	383 D	384 W (solid)	383 W	
<i>a</i> <sub>2</sub>	ν <sub>11</sub>	CH <sub>3</sub> d-stretch.....	2970 D	ia	2970 W, p	OV (ν <sub>17</sub> ).
	ν <sub>12</sub>	CH <sub>3</sub> d-deform.....	1459 D	ia	1459 VW	
	ν <sub>13</sub>	CH <sub>3</sub> rock.....	1076 E	ia	.....	CF [4].
	ν <sub>14</sub>	CH <sub>2</sub> twist.....	981 E	ia	.....	CF [4].
	ν <sub>15</sub>	CH <sub>3</sub> torsion.....	193 E	ia	.....	CF [3].
<i>b</i> <sub>1</sub>	ν <sub>16</sub>	CH <sub>2</sub> a-stretch.....	3086 C	3086.0 S	3079 W, dp	
	ν <sub>17</sub>	CH <sub>3</sub> d-stretch.....	2980 C	2980.4	2970 W, dp	OV (ν <sub>11</sub> ).
	ν <sub>18</sub>	CH <sub>3</sub> s-stretch.....	2893 C	2892.9 W	2892 W, dp	
	ν <sub>19</sub>	CH <sub>3</sub> d-deform.....	1458 C	1458.4 S		
	ν <sub>20</sub>	CH <sub>3</sub> s-deform.....	1381 C	1381.2 S	1386 W	
	ν <sub>21</sub>	C-C stretch.....	1282 C	1281.9 S	1281 W	
	ν <sub>22</sub>	CH <sub>3</sub> rock.....	1043 E	.....	.....	CF [4].
	ν <sub>23</sub>	CH <sub>2</sub> rock.....	974 C	973.7 W	972 VW	
	ν <sub>24</sub>	C=CC <sub>2</sub> ip-deform.....	430 D	430 sh (solid)		
	ν <sub>25</sub>	CH <sub>3</sub> d-stretch.....	2945 C	2944.9 S		
<i>b</i> <sub>2</sub>	ν <sub>26</sub>	CH <sub>3</sub> d-deform.....	1444 C	1443.7 S	1439 VW	
	ν <sub>27</sub>	CH <sub>3</sub> rock.....	1079 C	1079.0 S		
	ν <sub>28</sub>	CH <sub>2</sub> wag.....	890 C	889.7 VS	883 W, dp	
	ν <sub>29</sub>	C=CC <sub>2</sub> op-deform.....	429 C	429.1 S	431 W, dp	
	ν <sub>30</sub>	CH <sub>3</sub> 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> <sup>-1</sup> (Gas)	<i>cm</i> <sup>-1</sup>	
<i>a</i> <sub>1</sub>	<i>ν</i> <sub>1</sub>	CH <sub>2</sub> s-stretch . . . . .	2996 C	2996 M		
	<i>ν</i> <sub>2</sub>	CD <sub>3</sub> d-stretch . . . . .	2166 D	2166 W		
				(solid)		
	<i>ν</i> <sub>3</sub>	CD <sub>3</sub> s-stretch . . . . .	2111 C	2111 W		
	<i>ν</i> <sub>4</sub>	C = C stretch . . . . .	1650 C	1650 S		
	<i>ν</i> <sub>5</sub>	CH <sub>2</sub> scis . . . . .	1410 C	1410 W		
	<i>ν</i> <sub>6</sub>	CD <sub>3</sub> s-deform . . . . .	1092 D	1092 W		
				(solid)		
	<i>ν</i> <sub>7</sub>	CD <sub>3</sub> d-deform . . . . .	1056 D	1056 M		
				(solid)		
	<i>ν</i> <sub>8</sub>	CD <sub>3</sub> rock . . . . .	850 E	.....	.....	CF [1].
	<i>ν</i> <sub>9</sub>	C-C stretch . . . . .	718 D	718 W		
				(solid)		
<i>a</i> <sub>2</sub>	<i>ν</i> <sub>10</sub>	C = CC <sub>2</sub> ip-deform . . . . .	319 C	319 W		
	<i>ν</i> <sub>11</sub>	CD <sub>3</sub> d-stretch . . . . .	2208 E	ia	.....	CF [1].
	<i>ν</i> <sub>12</sub>	CD <sub>3</sub> d-deform . . . . .	1054 E	ia	.....	CF [1].
	<i>ν</i> <sub>13</sub>	CD <sub>3</sub> rock . . . . .	731 E	ia	.....	CF [1].
	<i>ν</i> <sub>14</sub>	CH <sub>2</sub> twist . . . . .	664 E	ia	.....	CF [1].
<i>b</i> <sub>1</sub>	<i>ν</i> <sub>15</sub>	CD <sub>3</sub> torsion . . . . .	138 E	ia	.....	CF [1].
	<i>ν</i> <sub>16</sub>	CH <sub>2</sub> a-stretch . . . . .	3085 C	3085 S		
	<i>ν</i> <sub>17</sub>	CD <sub>3</sub> d-stretch . . . . .	2236 C	2236 S		
	<i>ν</i> <sub>18</sub>	CD <sub>3</sub> s-stretch . . . . .	2072 C	2072 M		
	<i>ν</i> <sub>19</sub>	C-C stretch . . . . .	1294 C	1294 M		
	<i>ν</i> <sub>20</sub>	CD <sub>3</sub> d-deform . . . . .	1074 C	1074 W		
	<i>ν</i> <sub>21</sub>	CD <sub>3</sub> s-deform . . . . .	1052 D	1052 M		
				(solid)		
	<i>ν</i> <sub>22</sub>	CH <sub>2</sub> rock . . . . .	880 E	.....	.....	CF [1].
<i>b</i> <sub>2</sub>	<i>ν</i> <sub>23</sub>	CD <sub>3</sub> rock . . . . .	745 C	745 W		
	<i>ν</i> <sub>24</sub>	C = CC <sub>2</sub> ip-deform . . . . .	400 C	400 M		
	<i>ν</i> <sub>25</sub>	CD <sub>3</sub> d-stretch . . . . .	2204 C	2204 S		
	<i>ν</i> <sub>26</sub>	CD <sub>3</sub> d-deform . . . . .	1055 C	1055 S		
	<i>ν</i> <sub>27</sub>	CD <sub>3</sub> rock . . . . .	923 C	923 M		
	<i>ν</i> <sub>28</sub>	CH <sub>2</sub> wag . . . . .	884 C	884 VS		
	<i>ν</i> <sub>29</sub>	C = CC <sub>2</sub> op-deform . . . . .	369 C	369 S		
	<i>ν</i> <sub>30</sub>	CD <sub>3</sub> torsion . . . . .	143 E	.....	.....	CF [1].

## Reference

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
$a'$	$\nu_1$	$\text{CH}_3(1)$ d-stretch . . . . .	2983 D	$\text{cm}^{-1}$ (Solid) 2983 S (liquid)	$\text{cm}^{-1}$ (Liquid) 2983 M	OV ( $\nu_2, \nu_{21}, \nu_{22}$ ).
	$\nu_2$	$\text{CH}_3(4)$ d-stretch . . . . .	2983 D	2983 S (liquid)	2983 M	OV ( $\nu_1, \nu_{21}, \nu_{22}$ ).
	$\nu_3$	$\text{CH}_3(1)$ s-stretch . . . . .	2910 D	2910 S (liquid)	2924 S, p	OV ( $\nu_4$ ).
	$\nu_4$	$\text{CH}_3(4)$ s-stretch . . . . .	2910 D	2910 S (liquid)	2924 S, p	OV ( $\nu_3$ ).
	$\nu_5$	$\text{CH}_2$ s-stretch . . . . .	2884 D	2884 S (liquid)		
	$\nu_6$	CO stretch . . . . .	1716 C	1716 S	1715 M, p	
	$\nu_7$	$\text{CH}_3(4)$ d-deform . . . . .	1460 D	1460 M	1450 M	OV ( $\nu_{24}$ ).
	$\nu_8$	$\text{CH}_2$ scis . . . . .	1422 C	1422 S	1419 M	
	$\nu_9$	$\text{CH}_3(1)$ d-deform . . . . .	1413 D	1413 S	.....	OV ( $\nu_{25}$ ).
	$\nu_{10}$	$\text{CH}_3(4)$ s-deform . . . . .	1373 C	1373 S		
	$\nu_{11}$	$\text{CH}_3(1)$ s-deform . . . . .	1346 C	1346 S	1345 W	
	$\nu_{12}$	$\text{CH}_2$ wag . . . . .	1263 D	1263 W	1258 W	OV ( $\nu_{26}$ ).
	$\nu_{13}$	CC(12) stretch . . . . .	1182 C	1182 S	1169 W	
	$\nu_{14}$	$\text{CH}_3(4)$ rock . . . . .	1089 C	1089 M	1087 M, p	
	$\nu_{15}$	CC(34) stretch . . . . .	997 C	997	999 W	
	$\nu_{16}$	$\text{CH}_3(1)$ rock . . . . .	939 C	939	951 W	
	$\nu_{17}$	CC(23) stretch . . . . .	760 D	760 S (liquid)	760 M, p	
$a''$	$\nu_{18}$	CO ip-bend . . . . .	590 C	590 S	591 W	
	$\nu_{19}$	CCC(123) deform . . . . .	413 C	413 S	410 W	
	$\nu_{20}$	CCC(234) deform . . . . .	260 C	260 S	264 W	
	$\nu_{21}$	$\text{CH}_3(1)$ d-stretch . . . . .	2983 D	2983 S (liquid)	2983	OV ( $\nu_1, \nu_2, \nu_{22}$ ).
	$\nu_{22}$	$\text{CH}_3(4)$ d-stretch . . . . .	2983 D	2983 S (liquid)	2983	OV ( $\nu_1, \nu_2, \nu_{21}$ ).
	$\nu_{23}$	$\text{CH}_2$ d-stretch . . . . .	2941 D	2941 S (liquid)		
	$\nu_{24}$	$\text{CH}_3(4)$ d-deform . . . . .	1460 D	1460 M	1450 M	OV ( $\nu_7$ ).
	$\nu_{25}$	$\text{CH}_3(1)$ d-deform . . . . .	1413 D	1413 S	.....	OV ( $\nu_9$ ).
	$\nu_{26}$	$\text{CH}_2$ twist . . . . .	1263 D	1263 W	1258 W	OV ( $\nu_{12}$ ).
	$\nu_{27}$	$\text{CH}_3(4)$ rock . . . . .	1108 C	1108 W		
	$\nu_{28}$	$\text{CH}_3(1)$ rock . . . . .	952 C	952 sh	951 W	
	$\nu_{29}$	$\text{CH}_2$ rock . . . . .	768 D	768 S (liquid)		
	$\nu_{30}$	CO op-bend . . . . .	460 C	460 VW		
	$\nu_{31}$	CC(34) torsion . . . . .	201 E	.....	.....	CF [4].
	$\nu_{32}$	CC(12) torsion . . . . .	106 E	.....	.....	CF [4].
	$\nu_{33}$	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 <sup>-1</sup> (Matrix isolation)	cm <sup>-1</sup> (Solid)	
<i>a<sub>g</sub></i>	$\nu_1$	CH <sub>3</sub> d-stretch.....	2965 C	ia	2965 (9)	SF ( $\nu_{20}$ ).
	$\nu_2$	CH <sub>3</sub> s-stretch.....	2872 C	ia	2872 (8)	
	$\nu_3$	CH <sub>2</sub> s-stretch.....	2853 D	ia	2853 (8)	
	$\nu_4$	CH <sub>3</sub> d-deform.....	1460 C	ia	1460 (2)	SF ( $\nu_{22}$ ).
	$\nu_5$	CH <sub>2</sub> scis.....	1442 D	ia	1442 (3)	
	$\nu_6$	CH <sub>3</sub> s-deform.....	1382 C	ia	.....	CF [9].
	$\nu_7$	CH <sub>2</sub> wag.....	1361 D	ia	.....	CF [9].
	$\nu_8$	CH <sub>3</sub> rock.....	1151 C	ia	1151 (4)	
	$\nu_9$	CC stretch.....	1059 C	ia	1059 (5)	
	$\nu_{10}$	CC stretch.....	837 C	ia	837 (6)	
	$\nu_{11}$	CCC deform.....	425 C	ia	425 (4)	
<i>a<sub>u</sub></i>	$\nu_{12}$	CH <sub>3</sub> d-stretch.....	2968 C	2968 S	ia	SF ( $\nu_{27}$ ).
	$\nu_{13}$	CH <sub>2</sub> a-stretch.....	2930 C	2930 S	ia	
	$\nu_{14}$	CH <sub>3</sub> d-deform.....	1461 C	1461 S	ia	SF ( $\nu_{30}$ ), OV ( $\nu_{30}$ , $\nu_{31}$ )
	$\nu_{15}$	CH <sub>2</sub> twist.....	1257 C	1257 W (solid)	ia	
	$\nu_{16}$	CH <sub>3</sub> rock.....	948 B	948 M	ia	
	$\nu_{17}$	CH <sub>2</sub> rock.....	731 B	731 S	ia	
	$\nu_{18}$	CH <sub>3</sub> -CH <sub>2</sub> torsion.....	194 E	.....	ia	CF [9].
	$\nu_{19}$	CH <sub>2</sub> -CH <sub>2</sub> torsion.....	102 E	.....	ia	CF [9].
	$\nu_{20}$	CH <sub>3</sub> d-stretch.....	2965 C	ia	2965 (9)	SF ( $\nu_1$ ).
	$\nu_{21}$	CH <sub>2</sub> a-stretch.....	2912 C	ia	2912 (4)	
	$\nu_{22}$	CH <sub>3</sub> d-deform.....	1460 C	ia	1460 (2)	SF ( $\nu_4$ ).
<i>b<sub>g</sub></i>	$\nu_{23}$	CH <sub>2</sub> twist.....	1300 C	ia	1300 (4)	
	$\nu_{24}$	CH <sub>3</sub> rock.....	1180 D	ia	.....	CF [9].
	$\nu_{25}$	CH <sub>2</sub> rock.....	803 D	ia	.....	CF [9].
	$\nu_{26}$	CH <sub>3</sub> -CH <sub>2</sub> torsion.....	225 E	ia	.....	CF [9].
	$\nu_{27}$	CH <sub>3</sub> d-stretch.....	2968 C	2968 S	ia	SF ( $\nu_{12}$ ).
	$\nu_{28}$	CH <sub>3</sub> s-stretch.....	2870 C	2870 S	ia	
	$\nu_{29}$	CH <sub>2</sub> s-stretch.....	2853 E	.....	ia	SF ( $\nu_3$ ).
	$\nu_{30}$	CH <sub>3</sub> d-deform.....	1461 C	1461 S	ia	SF ( $\nu_{14}$ ), OV ( $\nu_{14}$ , $\nu_{31}$ ).
	$\nu_{31}$	CH <sub>2</sub> scis.....	1461 C	1461 S	ia	OV ( $\nu_{14}$ , $\nu_{30}$ ).
	$\nu_{32}$	CH <sub>3</sub> s-deform.....	1379 B	1379 M	ia	
	$\nu_{33}$	CH <sub>2</sub> wag.....	1290 B	1290 W	ia	
	$\nu_{34}$	CC stretch.....	1009 C	1009 W (solid)	ia	
<i>b<sub>u</sub></i>	$\nu_{35}$	CH <sub>3</sub> rock.....	964 B	964 M	ia	
	$\nu_{36}$	CCC deform.....	271 E		ia	CF [9].

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<sup>a</sup> 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
$a_{1g}$	$\nu_1$	CH stretch.....	3062 C	$cm^{-1}$ (Gas) ia	$cm^{-1}$ (Liquid) 3061.9 VS, p	
	$\nu_2$	Ring stretch.....	992 C	ia	991.6 VS, p	
$a_{2g}$	$\nu_3$	CH bend.....	1326 E	ia	1326 VW	
$a_{2u}$	$\nu_4$	CH bend.....	673 B	673 S	ia	
$b_{1u}$	$\nu_5$	CH stretch.....	3068 C	3067.57 VW (solid)	ia	
	$\nu_6$	Ring deform.....	1010 C	1010 W (solid)	ia	
$b_{2g}$	$\nu_7$	CH bend.....	995 E	ia	ia	OC ( $\nu_{19} + \nu_7, \nu_{20} + \nu_7$ ).
	$\nu_8$	Ring deform.....	703 E	ia	ia	OC ( $\nu_{19} + \nu_8, \nu_{20} + \nu_8$ ).
$b_{2u}$	$\nu_9$	Ring stretch.....	1310 C	1310 W (liquid)	ia	
	$\nu_{10}$	CH bend.....	1150 C	1150 W (liquid)	ia	
$e_{1g}$	$\nu_{11}$	CH bend.....	849 C	ia	848.9 M, dp	
$e_{1u}$	$\nu_{12}$	CH stretch.....	3063 E	{ 3080 S 3030 S (liquid)	ia	FR ( $\nu_{13} + \nu_{16}$ ).
	$\nu_{13}$	Ring stretch + deform.....	1486 B	1486 S	ia	
	$\nu_{14}$	CH bend.....	1038 B	1038 S	ia	
$e_{2g}$	$\nu_{15}$	CH stretch.....	3047 C	ia	3046.8 S, dp	
	$\nu_{16}$	Ring stretch.....	1596 E	ia	{ 1606.4 S, dp 1584.6 S, dp	FR ( $\nu_2 + \nu_{18}$ ).
	$\nu_{17}$	CH bend.....	1178 C	ia	1178.0 S, dp	
	$\nu_{18}$	Ring deform.....	606 C	ia	605.6 S, dp	
$e_{2u}$	$\nu_{19}$	CH bend.....	975 C	975 W (liquid)	ia	
	$\nu_{20}$	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> <sub>1g</sub>	<i>ν</i> <sub>1</sub>	CD stretch.....	2293 C	<i>cm</i> <sup>-1</sup> (Gas) ia	<i>cm</i> <sup>-1</sup> (Liquid) 2292.6 VS, p	OC ( <i>ν</i> <sub>3</sub> + <i>ν</i> <sub>14</sub> , <i>ν</i> <sub>3</sub> + <i>ν</i> <sub>16</sub> ).
	<i>ν</i> <sub>2</sub>	Ring stretch.....	943 C	ia	943.2 VS, p	
<i>a</i> <sub>2g</sub>	<i>ν</i> <sub>3</sub>	CD bend.....	1037 E	ia	ia	
<i>a</i> <sub>2u</sub>	<i>ν</i> <sub>4</sub>	CD bend.....	497 C	496.5 S (liquid)	ia	
<i>b</i> <sub>1u</sub>	<i>ν</i> <sub>5</sub>	CD stretch.....	2292 E	2292 VW (solid)	ia	OC ( <i>ν</i> <sub>7</sub> + <i>ν</i> <sub>19</sub> ). OC ( <i>ν</i> <sub>8</sub> + <i>ν</i> <sub>19</sub> ).
	<i>ν</i> <sub>6</sub>	Ring deform.....	969 C	{ 970.48 969.77 966.76 (solid)	ia	
<i>b</i> <sub>2g</sub>	<i>ν</i> <sub>7</sub>	CD bend.....	827 E	ia	ia	
	<i>ν</i> <sub>8</sub>	Ring deform.....	601 E	ia	ia	
<i>b</i> <sub>2u</sub>	<i>ν</i> <sub>9</sub>	Ring stretch.....	1286 C	{ 1287.51 1286.41 1285.14 (solid)	ia	OC ( <i>ν</i> <sub>7</sub> + <i>ν</i> <sub>19</sub> ). OC ( <i>ν</i> <sub>8</sub> + <i>ν</i> <sub>19</sub> ).
	<i>ν</i> <sub>10</sub>	CD bend.....	824 C	{ 825.2 822.57 (solid)	ia	
<i>e</i> <sub>1g</sub>	<i>ν</i> <sub>11</sub>	CD bend.....	662 C	ia	661.7 M, dp	
<i>e</i> <sub>1u</sub>	<i>ν</i> <sub>12</sub>	CD stretch.....	2287 C	2287 S	ia	
	<i>ν</i> <sub>13</sub>	Ring stretch + deform.....	1335 B	1335 M	ia	OC ( <i>ν</i> <sub>4</sub> + <i>ν</i> <sub>20</sub> , <i>ν</i> <sub>14</sub> + <i>ν</i> <sub>20</sub> ).
	<i>ν</i> <sub>14</sub>	CD bend.....	814 B	814 S	ia	
<i>e</i> <sub>2g</sub>	<i>ν</i> <sub>15</sub>	CD stretch.....	2265 C	ia	2264.9 S, dp	
	<i>ν</i> <sub>16</sub>	Ring stretch.....	1552 C	ia	1551.5 S, dp	
	<i>ν</i> <sub>17</sub>	CD bend.....	867 C	ia	867.3 S, dp	OC ( <i>ν</i> <sub>4</sub> + <i>ν</i> <sub>20</sub> , <i>ν</i> <sub>14</sub> + <i>ν</i> <sub>20</sub> ).
	<i>ν</i> <sub>18</sub>	Ring deform.....	577 C	ia	577.4 M, dp	
<i>e</i> <sub>2u</sub>	<i>ν</i> <sub>19</sub>	CD bend.....	795 C	{ 799.91 797.37 794.64 790.9 790.3 (solid)	ia	
	<i>ν</i> <sub>20</sub>	Ring deform.....	352 E	ia	ia	

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Sym. species	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				$cm^{-1}$ (Gas)	$cm^{-1}$ (Liquid)	
$a_{1g}$	$\nu_1$	CH <sub>2</sub> a-stretch.....	2930 E	ia	{ 2938 VS, p 2923 VS, p }	FR ( $2\nu_3$ ).
	$\nu_2$	CH <sub>2</sub> s-stretch.....	2852 C	ia	2852 VS, p	
	$\nu_3$	CH <sub>2</sub> scis.....	1465 C	ia	1465 M, p	
	$\nu_4$	CH <sub>2</sub> rock.....	1157 C	ia	1157 S, p	
	$\nu_5$	CC stretch.....	802 C	ia	802 VS, p	
	$\nu_6$	CCC deform + CC torsion.....	383 C	ia	383 M, p	
$a_{1u}$	$\nu_7$	CH <sub>2</sub> twist.....	1383 C	<sup>a</sup> 1383	ia	SF ( $\nu_2, \nu_{13}, \nu_{26}$ ).  FR ( $\nu_{23} + \nu_{32}$ ).  SF ( $\nu_1, \nu_{12}, \nu_{25}$ ).
	$\nu_8$	CH <sub>2</sub> wag.....	1157 C	<sup>a</sup> 1157	ia	
	$\nu_9$	CC stretch + CC torsion.....	1057 C	<sup>a</sup> 1057	ia	
$a_{2g}$	$\nu_{10}$	CH <sub>2</sub> wag.....	1437 C	<sup>a</sup> 1437	ia	
	$\nu_{11}$	CH <sub>2</sub> twist.....	1090 C	<sup>a</sup> 1090	ia	
$a_{2u}$	$\nu_{12}$	CH <sub>2</sub> a-stretch.....	2915 E	2915 M	ia	
	$\nu_{13}$	CH <sub>2</sub> s-stretch.....	2860 E	.....	ia	
	$\nu_{14}$	CH <sub>2</sub> scis.....	1437 C	1437 M	ia	
	$\nu_{15}$	CH <sub>2</sub> rock.....	1030 D	{ 1040 M 1016 M }	ia	
	$\nu_{16}$	CCC deform.....	523 A	523 W	ia	
$e_g$	$\nu_{17}$	CH <sub>2</sub> a-stretch.....	2930 E	ia	.....	SF ( $\nu_1, \nu_{12}, \nu_{25}$ ).
	$\nu_{18}$	CH <sub>2</sub> s-stretch.....	2897 E	ia	2897 M, vb	
	$\nu_{19}$	CH <sub>2</sub> scis.....	1443 C	ia	1443 S, dp	
	$\nu_{20}$	CH <sub>2</sub> wag.....	1347 C	ia	1347 S, dp	
	$\nu_{21}$	CH <sub>2</sub> twist.....	1266 C	ia	1266 VS, dp	
	$\nu_{22}$	CC stretch.....	1027 C	ia	1027 VS, dp	
	$\nu_{23}$	CH <sub>2</sub> rock.....	785 C	<sup>a</sup> 785	785 VW, dp	
	$\nu_{24}$	CCC deform + CC torsion.....	426 C	ia	426 S, dp	
	$\nu_{25}$	CH <sub>2</sub> a-stretch.....	2933 A	2933 VS	ia	
$e_u$	$\nu_{26}$	CH <sub>2</sub> s-stretch.....	2863 A	2863 VS	ia	
	$\nu_{27}$	CH <sub>2</sub> scis.....	1457 A	1457 VS	ia	
	$\nu_{28}$	CH <sub>2</sub> wag.....	1355 B	1355 W	ia	
	$\nu_{29}$	CH <sub>2</sub> twist.....	1261 A	1261 S	ia	
	$\nu_{30}$	CH <sub>2</sub> rock.....	907 B	907 S	ia	
	$\nu_{31}$	CC stretch.....	863 A	863 S	ia	
	$\nu_{32}$	CCC deform. + CC torsion.....	248 C	248 VW (liquid)	ia	

<sup>a</sup> 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 <sup>-1</sup> (Gas)	cm <sup>-1</sup> (Liquid)	
<i>a<sub>1g</sub></i>	<i>ν</i> <sub>1</sub>	CD <sub>2</sub> a-stretch.....	2152 C	ia	2152 VS, p	
	<i>ν</i> <sub>2</sub>	CD <sub>2</sub> s-stretch.....	2082 C	ia	2082 VS, p	
	<i>ν</i> <sub>3</sub>	CD <sub>2</sub> scis.....	1117 C	ia	1117 M, p	
	<i>ν</i> <sub>4</sub>	CD <sub>2</sub> rock.....	1012 C	ia	1012 W, p	
	<i>ν</i> <sub>5</sub>	CC stretch.....	723 C	ia	723 VS, p	
	<i>ν</i> <sub>6</sub>	CCC deform. + CC torsion.....	298 C	ia	298 W, p	
<i>a<sub>1u</sub></i>	<i>ν</i> <sub>7</sub>	CD <sub>2</sub> twist.....	864 E	ia	ia	CF [4].
	<i>ν</i> <sub>8</sub>	CD <sub>2</sub> wag.....	842 E	ia	ia	CF [4].
	<i>ν</i> <sub>9</sub>	CC stretch. + CC torsion.....	1187 E	ia	ia	CF [4].
<i>a<sub>2g</sub></i>	<i>ν</i> <sub>10</sub>	CD <sub>2</sub> wag.....	1126 E	ia	ia	CF [4].
	<i>ν</i> <sub>11</sub>	CD <sub>2</sub> twist.....	778 E	ia	ia	CF [4].
<i>a<sub>2u</sub></i>	<i>ν</i> <sub>12</sub>	CD <sub>2</sub> a-stretch.....	2206 C	2206 VS	ia	OV ( <i>ν</i> <sub>25</sub> ).
	<i>ν</i> <sub>13</sub>	CD <sub>2</sub> s-stretch.....	2108 C	2108 VS	ia	OV ( <i>ν</i> <sub>26</sub> ).
	<i>ν</i> <sub>14</sub>	CD <sub>2</sub> scis.....	1091 B	1091 VS	ia	
	<i>ν</i> <sub>15</sub>	CD <sub>2</sub> rock.....	917 A	917 VS	ia	
	<i>ν</i> <sub>16</sub>	CCC deform.....	395 B	395 S	ia	
	<i>ν</i> <sub>17</sub>	CD <sub>2</sub> a-stretch.....	2199 C	ia	2199 VS, dp	
<i>e<sub>g</sub></i>	<i>ν</i> <sub>18</sub>	CD s-stretch.....	2104 C	ia	2104 VS, dp	
	<i>ν</i> <sub>19</sub>	CD <sub>2</sub> scis.....	1071 C	ia	1071 M, dp	
	<i>ν</i> <sub>20</sub>	CD <sub>2</sub> wag.....	1212 C	ia	1212 M, dp	
	<i>ν</i> <sub>21</sub>	CD <sub>2</sub> twist.....	937 C	ia	937 S, dp	
	<i>ν</i> <sub>22</sub>	CC stretch.....	795 C	ia	795 S, dp	
	<i>ν</i> <sub>23</sub>	CD <sub>2</sub> rock.....	637 C	ia	637 W, dp	
	<i>ν</i> <sub>24</sub>	CCC deform. + CC torsion.....	373 C	ia	373 M, dp	
	<i>ν</i> <sub>25</sub>	CD <sub>2</sub> a-stretch.....	2206 C	2206 VS	ia	OV ( <i>ν</i> <sub>12</sub> ).
<i>e<sub>u</sub></i>	<i>ν</i> <sub>26</sub>	CD <sub>2</sub> s-stretch.....	2108 C	2108 VS	ia	OV ( <i>ν</i> <sub>13</sub> ).
	<i>ν</i> <sub>27</sub>	CD <sub>2</sub> scis.....	1069 C	1069 M (liquid)	ia	
	<i>ν</i> <sub>28</sub>	CD <sub>2</sub> wag.....	1165 A	1165 VS	ia	
	<i>ν</i> <sub>29</sub>	CD <sub>2</sub> twist.....	991 A	991 VS	ia	
	<i>ν</i> <sub>30</sub>	CD <sub>2</sub> rock.....	687 B	687 S	ia	
	<i>ν</i> <sub>31</sub>	CC stretch.....	720 A	720 S	ia	
	<i>ν</i> <sub>32</sub>	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> <sup>-1</sup> (Solid)	<i>cm</i> <sup>-1</sup> (Solid)	
<i>a<sub>g</sub></i>	<i>ν</i> <sub>1</sub>	CH <sub>2</sub> s-stretch.....	2848 C	ia	2848 S	
	<i>ν</i> <sub>2</sub>	CH <sub>2</sub> scis.....	1440 C	ia	1440 M	
	<i>ν</i> <sub>3</sub>	CC stretch.....	1131 C	ia	1131 M	
<i>a<sub>u</sub></i>	<i>ν</i> <sub>4</sub>	CH <sub>2</sub> twist.....	<sup>a</sup> 1050 D	ia, 1050 VW	ia	
<i>b<sub>1g</sub></i>	<i>ν</i> <sub>5</sub>	CH <sub>2</sub> wag.....	1370 D	ia	1370 VW	
	<i>ν</i> <sub>6</sub>	CC stretch.....	1061 C	ia	1061 M	
<i>b<sub>1u</sub></i>	<i>ν</i> <sub>7</sub>	CH <sub>2</sub> a-stretch.....	2919 C	2919 S	ia	
	<i>ν</i> <sub>8</sub>	CH <sub>2</sub> rock.....	725 C	<sup>b</sup> { 731 S 720 S }	ia	
<i>b<sub>2g</sub></i>	<i>ν</i> <sub>9</sub>	CH <sub>2</sub> twist.....	1295 C	ia	1295 M	
<i>b<sub>2u</sub></i>	<i>ν</i> <sub>10</sub>	CH <sub>2</sub> s-stretch.....	2851 C	2851 S	ia	
	<i>ν</i> <sub>11</sub>	CH <sub>2</sub> scis.....	1468 C	<sup>b</sup> { 1473 S 1463 S }	ia	
<i>b<sub>3g</sub></i>	<i>ν</i> <sub>12</sub>	CH <sub>2</sub> a-stretch.....	2883 C	ia	2883 S	
	<i>ν</i> <sub>13</sub>	CH <sub>2</sub> rock.....	1168 C	ia	1168 W	
<i>b<sub>3u</sub></i>	<i>ν</i> <sub>14</sub>	CH <sub>2</sub> wag.....	1176 C	1176 VW	ia	

<sup>a</sup> 1063 *cm*<sup>-1</sup> is given to this mode in ref. 6.

<sup>b</sup> 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> <sup>-1</sup> (Solid)	<i>cm</i> <sup>-1</sup> (Solid)	
<i>a<sub>g</sub></i>	<i>ν</i> <sub>1</sub>	CD <sub>2</sub> s-stretch . . . . .	2102 C	ia	2102 S	CF [5].
	<i>ν</i> <sub>2</sub>	CD <sub>2</sub> scis . . . . .	1146 C	ia	1146 M	
	<i>ν</i> <sub>3</sub>	CC stretch . . . . .	966 E	ia	966 VW	
<i>a<sub>u</sub></i>	<i>ν</i> <sub>4</sub>	CD <sub>2</sub> twist . . . . .	743 E	ia	ia	
<i>b<sub>1g</sub></i>	<i>ν</i> <sub>5</sub>	CD <sub>2</sub> wag . . . . .	1249 C	ia	1249 W	
	<i>ν</i> <sub>6</sub>	CC stretch . . . . .	820 E	ia	.....	CF [5].
<i>b<sub>1u</sub></i>	<i>ν</i> <sub>7</sub>	CD <sub>2</sub> a-stretch . . . . .	2192 C	2192 S	ia	
	<i>ν</i> <sub>8</sub>	CD <sub>2</sub> rock . . . . .	526 C	<sup>a</sup> { 528 M 522 M }	ia	
<i>b<sub>2g</sub></i>	<i>ν</i> <sub>9</sub>	CD <sub>2</sub> twist . . . . .	916 C	ia	916 M	
<i>b<sub>2u</sub></i>	<i>ν</i> <sub>10</sub>	CD <sub>2</sub> s-stretch . . . . .	2088 C	2088 S	ia	
	<i>ν</i> <sub>11</sub>	CD <sub>2</sub> scis . . . . .	1090 C	<sup>a</sup> { 1092 S 1087 S }	ia	
<i>b<sub>3g</sub></i>	<i>ν</i> <sub>12</sub>	CD <sub>2</sub> a-stretch . . . . .	2197 C	ia	2197 M	CF [5].
	<i>ν</i> <sub>13</sub>	CD <sub>2</sub> rock . . . . .	991 C	ia	991 M	
<i>b<sub>3u</sub></i>	<i>ν</i> <sub>14</sub>	CD <sub>2</sub> wag . . . . .	889 E	.....	ia	

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

### Compounds Containing Carbon

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

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