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Tables of
Molecular Vibrational Frequencies
Part 1.

UNITED STATES DEPARTMENT OF COMMERCE
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Foreword

The National Standard Reference Data System is a government-wide effort to give to the technical community of the United States optimum access to the quantitative data of physical science, critically evaluated and compiled for convenience. This program was established in 1963 by the President's Office of Science and Technology, acting upon the recommendation of the Federal Council for Science and Technology. The National Bureau of Standards has been assigned responsibility for administering the effort. The general objective of the System is to coordinate and integrate existing data evaluation and compilation activities into a systematic, comprehensive program, supplementing and expanding technical coverage when necessary, establishing and maintaining standards for the output of the participating groups, and providing mechanisms for the dissemination of the output as required.

The NSRDS is conducted as a decentralized operation of nation-wide scope with central coordination by NBS. It comprises a complex of data centers and other activities, carried on in government agencies, academic institutions, and nongovernmental laboratories. The independent operational status of existing critical data projects is maintained and encouraged. Data centers that are components of the NSRDS produce compilations of critically evaluated data, critical reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data.

For operational purposes, NSRDS compilation activites are organized into seven categories as listed below. The data publications of the NSRDS, which may consist of monographs, looseleaf sheets, computer tapes, or any other useful product, will be classified as belonging to one or another of these categories. An additional "General" category of NSRDS publications will include reports on detailed classification schemes, lists of compilations considered to be Standard Reference Data, status reports, and similar material. Thus, NSRDS publications will appear in the following eight categories:

Category	*Title*
1	General
2	Nuclear Properties
3	Atomic and Molecular Properties
4	Solid State Properties
5	Thermodynamic and Transport Properties
6	Chemical Kinetics
7	Colloid and Surface Properties
8	Mechanical Properties of Materials

The present compilation is in category 3 of the above list. It constitutes the sixth publication in a new NBS series known as the National Standard Reference Data Series.

A. V. ASTIN, *Director.*

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Tables of Molecular Vibrational Frequencies

Part 1.

T. Shimanouchi

A compilation of vibrational frequency data for selected molecules is being conducted at the University of Tokyo in cooperation with the National Standard Reference Data Program of the National Bureau of Standards as a part of an international effort to compile and evaluate physical and chemical data. This report, first of a series of annual reports, contains fundamental vibrational frequencies of 59 molecules together with vibrational assignments, sources of data, brief comments, and citations of references. The fundamental frequencies are obtained mainly from the infrared and Raman spectra. When these are not available, other experimental data such as microwave results are taken into account. The selection of vibrational fundamentals from observed spectral data is based upon careful studies of the spectral data and comprehensive mathematical analyses. These tables were designed to provide a concise summary needed for the computation of ideal gas thermodynamic properties. They may also provide a convenient source of information to those who require vibrational energy levels and related properties in molecular spectroscopy, analytical chemistry, and other fields of physics and chemistry.

Key Words: Molecular, vibrational, frequencies, data, tables, force, constants, spectral.

I. Introduction

A compilation of vibrational frequency data for selected molecules is being conducted as a part of a broad program on the compilation and critical evaluation of physical and chemical data of many substances. Vibrational frequency data of molecules are not only useful in research on molecular structure, but are also essential to accurate computation of ideal gas thermodynamic properties. These tables will be a convenient source of information in any field of physics or chemistry in which the vibrational energy levels and related properties are needed. These data may also be useful to those who utilize infrared or Raman spectra as a technique in analytical chemistry.

This is the first of a series of annual reports being prepared in cooperation with the National Standard Reference Data Program of the National Bureau of Standards. It contains fundamental vibrational frequencies and assignments for 59 molecules, as well as sources of data, brief comments, and citations of references. The fundamental frequencies are obtained mainly from the infrared and Raman spectra. When this information is not available, other experimental data such as microwave results are taken into account.

In many cases there are several possible ways of assigning the observed frequencies of a molecule, and only tentative assignments have been given in the literature. In the present table the fundamental frequencies and assignments are adopted only when they are definitely supported by the calculation of normal vibrations based on a consistent set of force constants which correlate the frequencies of molecules having similar structures. These calculations also give reliable predictions for the frequencies of the optically inactive vibrations.

The approach adopted in selecting force constants and the techniques employed in calculating normal vibrations are described in some detail in other publications by this author. The reader is directed especially to references 1 to 5. Further development of this expository material is contained in several papers now being prepared for publication. A later report in this series of Tables of Molecular Vibration Frequencies will supply additional references. Specific details may be found in several of the references which follow the individual tables.

General comments concerning the format and convention adopted in this compilation are discussed below. The objective was to achieve a very concise presentation of the essential information in a form that would be useful in the computation of thermodynamic properties. The molecules included in this first report were selected from a list of molecules that have been analyzed by mathematical techniques. It is hoped that this compilation can be continued until all of the more important organic and inorganic molecules are included. Needless to say, there will be revisions of these tables from time to time as new information becomes available. The author of this report would appreciate such information as well as comments concerning the scope and format of the reports.

I express my sincere thanks to many members of the National Bureau of Standards, especially C. W. Beckett, D. R. Lide, Jr., and E. L. Brady who offered helpful suggestions in the planning of the tables.

I also acknowledge the assistance of my colleagues at the University of Tokyo: I. Nakagawa, C. Tanaka, S. Suzuki, M. Tasumi, T. Fujiyama, J. Hiraishi, I. Harada, Y. Abo, M. Oka, T. Ueda, M. Ishii, Y. Noto, and H. Yoshioka.

References

[1] T. Shimanouchi, Pure and Applied Chemistry **7**, 131 (1963).

[2] T. Shimanouchi, I. Nakagawa, J. Hiraishi and M. Ishii, J. Molecular Spectroscopy, in press.

[3] T. Shimanouchi and I. Suzuki, J. Chem. Phys. **42**, 296 (1965), **43**, 1854 (1965).

[4] H. Takahashi, T. Shimanouchi, K. Fukushima and T. Miyazawa, J. Mol. Spectr. **13**, 43 (1964).

[5] M. Tasumi, T. Shimanouchi and T. Miyazawa, J. Mol. Spectr. **9**, 261 (1962), **11**, 422 (1963).

II. Explanation of Tables

1. Observed fundamental vibrational frequencies in the gaseous state are tabulated unless otherwise noted.

2. When vibrational frequencies in the liquid or the solid state are significantly different from those in the gaseous state, they are tabulated on a separate sheet. (Examples: CH_3OH and $CH_3CONHCH_3$.)

3. The notation of Herzberg[1] for the symmetry classes and vibrational numbering is adopted unless otherwise mentioned. In the case of deuterium compounds the same numbering used for the analogous hydrogen compound is adopted.

4. "Approximate type of mode" is a descriptive name indicating the local symmetry coordinate which makes the maximum contribution in the corresponding normal coordinates. (See below for the definition of the local symmetry coordinates of CH_3, CH_2, and CH groups.) When there is a strong coupling among two or more symmetry coordinates (more than 30% in the potential energy distribution), the notation (ν_i) is used. (ν_i) means that the contribution of the coordinate given in the ν_i row is also considerable. The following abbreviations are used:

stretch.	stretching	twist.	twisting
deform.	deformation	wag.	wagging
rock.	rocking	bend.	bending
sym.	symmetric	deg.	degenerate
anti.	antisymmetric		

5. Observed infrared and Raman frequencies are tabulated, when available, for each normal mode. In addition a selected value for the fundamental vibrational frequency is listed. No corrections have been made for anharmonicity. As the selected value of frequency, that in the gaseous state is adopted when available. When this is not available, the value found in the liquid state, in the solid state, or in solution is adopted. When no observed frequency is available, the calculated frequency is adopted. Comments on the calculated frequencies are given in notes.

6. The uncertainties of the selected values are given by the symbol, A, B, C, D, or E. The range of uncertainty in cm^{-1} and the basis on which it is estimated is given in table I.

TABLE I. *Uncertainty of the selected value*

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

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

7. Abbreviations used with "Infrared" and "Raman" data are as follows:

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

The intensity of a Raman line may also be indicated by $(1) \sim (10)$, which gives a rough estimation of relative intensity.

8. Abbreviations used in "comments" are as follows:

FR	Fermi Resonance with an overtone or a combination tone indicated in the parentheses which follow
OC	Frequency estimated from an overtone or a combination tone indicated in the parentheses
CF	Calculated frequency

---

[1] G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).

SF	Calculation shows that the frequency approximately equals that of the vibration indicated in the parentheses
TA	Tentative assignment
OV	Overlapped by the band indicated in the parentheses
ρ	Depolarization degree.

9. "References" are not comprehensive. Only the papers from which the data are taken or which contain important information related to the given assignments are cited. The abbreviations, IR, R, and Th, denote infrared, Raman, and theoretical, respectively.

10. The vibrational contributions to the ideal gas thermodynamic properties can be calculated from the fundamental vibrational frequencies given in the tables. The statistical weight is one for the vibrations belonging to the species designated by "*a*" and "*b*", two for those designated by "*e*" and three for those designated by "*f*". The harmonic vibration approximation can be used for almost all the vibrations except the torsional motions, the inversions of NH_3-like molecules, and the ring puckering motions. For these motions more refined treatments are needed especially when the frequencies are low.

11. Definition of local symmetry coordinates:

(a) Local symmetry coordinates for the CH_3 group (see fig. 1a)

CH_3 symmetrical stretching: $(\Delta r_1+\Delta r_2+\Delta r_3)/\sqrt{3}$
CH_3 degenerate stretching: $(2\Delta r_1-\Delta r_2-\Delta r_3)/\sqrt{6}$
CH_3 symmetrical deformation: $(\Delta r_2-\Delta r_3)/\sqrt{2}$
$(\Delta\alpha_{23}+\Delta\alpha_{31}+\Delta\alpha_{12}-\Delta\beta_1-\Delta\beta_2-\Delta\beta_3)/\sqrt{6}$
CH_3 degenerate deformation: $(2\Delta\alpha_{23}-\Delta\alpha_{31}-\Delta\alpha_{12})/\sqrt{6}$
$(\Delta\alpha_{31}-\Delta\alpha_{12})/\sqrt{2}$
CH_3 rocking: $(2\Delta\beta_1-\Delta\beta_2-\Delta\beta_3)/\sqrt{6}$
$(\Delta\beta_2-\Delta\beta_3)/\sqrt{2}$.

(b) Local symmetry coordinates for the CH_2 group (see fig. 1b)

CH_2 symmetrical stretching: $(\Delta r_1+\Delta r_2)/\sqrt{2}$
CH_2 antisymmetrical stretching: $(\Delta r_1-\Delta r_2)/\sqrt{2}$
CH_2 scissors: $(4\Delta\alpha-\Delta\beta_{1X}-\Delta\beta_{2X}-\Delta\beta_{1Y}-\Delta\beta_{2Y})/\sqrt{20}$
CH_2 wagging: $(\Delta\beta_{1X}+\Delta\beta_{2X}-\Delta\beta_{1Y}-\Delta\beta_{2Y})/2$
CH_2 twisting: $(\Delta\beta_{1X}-\Delta\beta_{2X}-\Delta\beta_{1Y}+\Delta\beta_{2Y})/2$
CH_2 rocking: $(\Delta\beta_{1X}-\Delta\beta_{2X}+\Delta\beta_{1Y}-\Delta\beta_{2Y})/2$.

(c) Local symmetry coordinates for the CH group (see fig. 1c)

CH stretching: Δr_{CH}
CH bending: $(2\Delta\beta_{HX}-\Delta\beta_{HY}-\Delta\beta_{HZ})/\sqrt{6}$
$(\Delta\beta_{HY}-\Delta\beta_{HZ})/\sqrt{2}$

(d) Local symmetry coordinates for the planar CH_2 group (see fig. 1d)

CH_2 symmetrical stretching: $(\Delta r_1+\Delta r_2)/\sqrt{2}$
CH_2 antisymmetrical stretching: $(\Delta r_1-\Delta r_2)/\sqrt{2}$
CH_2 scissors: $(2\Delta\alpha-\Delta\beta_1-\Delta\beta_2)/\sqrt{6}$
CH_2 rocking: $(\Delta\beta_1-\Delta\beta_2)/\sqrt{2}$
CH_2 wagging: $\Delta\theta_X\cdot\sin\alpha$.

(e) Local symmetry coordinates for the planar CH group (see fig. 1e)

CH stretching: Δr_{CH}
in-plane CH bending: $(\Delta\beta_{HX}-\Delta\beta_{HY})/\sqrt{2}$
out-of-plane CH bending: $\Delta\theta_H\cdot\sin\gamma_{XY}$.

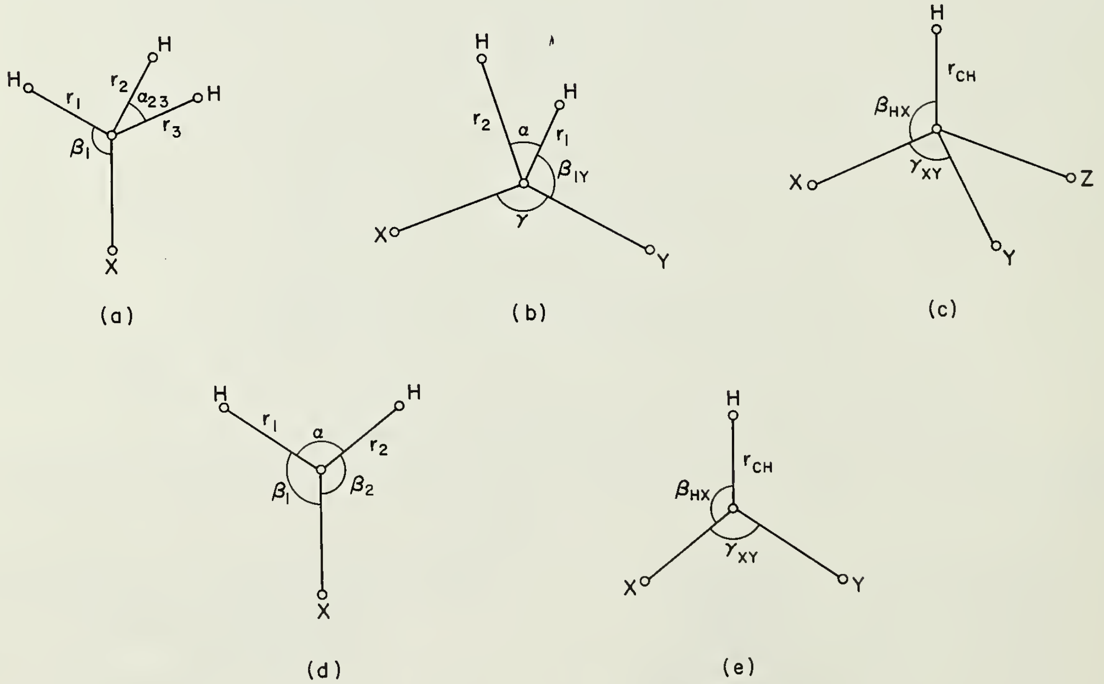

FIGURE 1. *Parameters of methyl, methylene, and methin groups.*

III. Tables of Vibrational Frequencies

Pages 7 to 54

No. 1

Molecule: Ammonia NH_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared[a]	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	NH_3 sym. stretch.	3337 A	3336.2 s 3337.2 a		
	ν_2	NH_3 sym. deform.	950 C	932.5 s 968.3 a		
e	ν_3	NH_3 deg. stretch.	3444 A	3443.6 s 3443.9 a		
	ν_4	NH_3 deg. deform.	1627 A	1626.1 s 1627.4 a		

[a] "a" refers to the antisymmetric levels and "s" to the symmetric levels. (See reference 2.)

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945) and references cited there.
[2] IR. W. S. Benedict and E. K. Plyer, Can. J. Phys. **35**, 1235 (1957).
[3] IR. J. S. Garing, H. H. Nielsen, and K. N. Rao, J. Mol. Spectr. **3**, 496 (1959).
[4] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20**, 523 (1964).

No. 2

Molecule: Ammonia-*d*3 ND_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared[a]	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	ND_3 sym. stretch.	2420 A	2420.1 s 2420.6 a		
	ν_2	ND_3 sym. deform.	748 B	745.7 s 749.4 a		
e	ν_3	ND_3 deg. stretch.	2564 A	2464.0		
	ν_4	ND_3 deg. deform.	1191 B	1191		

[a] "a" refers to the antisymmetric levels and "s" to the symmetric levels.

References

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

No. 3

Molecule: Phosphine PH_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	PH_3 sym. stretch.	2323 A	2322.9	2306	
	ν_2	PH_3 sym. deform.	992 B	992.1	979	
e	ν_3	PH_3 deg. stretch.	2328 B	2327.7		
	ν_4	PH_3 deg. deform.	1118 A	1118.3	1115	

References

[1] IR. R. Robertson and J. J. Fox, Proc. Roy. Soc. (London) **A120,** 161 (1928).
[2] IR. L. W. Fung and E. F. Barker, Phys. Rev. **45,** 238 (1934).
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[4] IR. H. H. Nielsen, J. Chem. Phys. **20,** 759 (1952).
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[7] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20,** 523 (1964).

No. 4

Molecule: Phosphine-d_3 PD_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	PD_3 sym. stretch.	1694 B	1694		
	ν_2	PD_3 sym. deform.	730 B	730		
e	ν_3	PD_3 deg. stretch.	1700 D			CF[3].
	ν_4	PD_3 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).

No. 5

Molecule: Arsine AsH_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared[a]	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	AsH_3 sym. stretch.	2116 A	2116.1		
	ν_2	AsH_3 sym. deform.	906 B	904.4 s 906.9 a		
e	ν_3	AsH_3 deg. stretch.	2123 B	2123.0		
	ν_4	AsH_3 deg. deform.	1003 B	1003		

[a] "a" refers to the antisymmetric level and "s" to the symmetric level. (See references 4 and 5.)

References

[1] IR. R. Robertson and J. J. Fox, Proc. Roy. Soc. (London) **A120,** 161 (1928).
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[3] IR. V. M. McConaghie and H. H. Nielsen, Phys. Rev. **75,** 633 (1949).
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[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).

No. 6

Molecule: Arsine-d_3 AsD_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	AsD_3 sym. stretch.	1523 A	1523.1		
	ν_2	AsD_3 sym. deform.	660 B	660.0		
e	ν_3	AsD_3 deg. stretch.	1529 B	1529.3		
	ν_4	AsD_3 deg. deform.	714 B	714		

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[1] IR. E. Lee and C. K. Wu, Trans. Faraday Soc. **35,** 1366 (1939).
[2] IR. V. M. McConaghie and H. H. Nielsen, Phys. Rev. **75,** 633 (1949).
[3] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20,** 523 (1964).

No. 7

Molecule: Stibine SbH_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$	
a_1	ν_1	SbH_3 sym. stretch.	1891 A	1890.9		
	ν_2	SbH_3 sym. deform.	782 B	781.5		
e	ν_3	SbH_3 deg. stretch.	1894 B	1894.2		
	ν_4	SbH_3 deg. deform.	831 B	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).

No. 8

Molecule: Stibine-*d*$_3$ SbD_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$	
a_1	ν_1	SbD_3 sym. stretch.	1359 A	1358.8		
	ν_2	SbD_3 sym. deform.	561 B	561.1		
e	ν_3	SbD_3 deg. stretch.	1362 B	1362.0		
	ν_4	SbD_3 deg. deform.	593 B	592.5		

References

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

No. 9

Molecule: Carbon tetrafluoride CF_4

Symmetry T_d **Symmetry number = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared cm^{-1}	Raman cm^{-1}	Comments
a_1	ν_1	CF_4 sym. stretch.	908 B	ia	908.5 S	
e	ν_2	CF_4 deg. deform.	435 B	ia	435.0 S	
f_2	ν_3	CF_4 deg. stretch.	1283 D	1283 VS	1283.0 W	FR($2\nu_4$).
	ν_4	CF_4 deg. deform.	632 B	631.73 VS	631.2 S	

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[1] R. D. M. Yost, E. N. Lassettre, and S. T. Gross, J. Chem. Phys. **4**, 325 (1936).
[2] IR. C. R. Baeley, J. B. Hale, and J. W. Thompson, Proc. Roy. Soc. (London) **167**, 555 (1938).
[3] IR. Th. E. K. Plyler and W. S. Benedict, J. Res. NBS **47**, 202 (1951) RP2245.
[4] IR. P. J. H. Woltz and A. H. Nielsen, J. Chem. Phys. **20**, 307 (1952).
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No. 10

Molecule: Carbon tetrachloride CCl_4

Symmetry T_d **Symmetry number = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	CCl_4 sym. stretch.	458 C	ia	458.7 (10)p (liquid)	
e	ν_2	CCl_4 deg. deform.	218 C	ia	217.0 (7)dp (liquid)	
f_2	ν_3	CCl_4 deg. stretch.	776 E	789 VS 768 VS	790.4 (4)dp 761.7 (4)dp (liquid)	FR($\nu_1 + \nu_4$).
	ν_4	CCl_4 deg. deform.	314 C	309.9 W (liquid)	313.5 (9)dp (liquid)	

References

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[2] R. J. P. Zietlow, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **18**, 1076 (1950).
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[5] IR. H. Yoshinaga, J. Chem. Phys. **23**, 2206 (1955).
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[7] R. M. Ito, Spectrochim. Acta **21**, 731 (1965).

No. 11

Molecule: Carbon tetrabromide CBr_4

Symmetry T_d **Symmetry number = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Benzene soln.)	
a_1	ν_1	CBr_4 sym. stretch.	267 C	ia	267 (7)p	
e	ν_2	CBr_4 deg. deform.	123 C	ia	122 (10)dp	
f_2	ν_3	CBr_4 deg. stretch.	672 C	672 VS	671 (1)dp	
	ν_4	CBr_4 deg. deform.	183 C		182 (4)dp	

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

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No. 12

Molecule: Carbon tetraiodide CI_4

Symmetry T_d **Symmetry number = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	CI_4 sym. stretch.	178 D	ia	178 (10) (solid)	
e	ν_2	CI_4 deg. deform.	90 D	ia	90 (4) (solid)	
f_2	ν_3	CI_4 deg. stretch.	555 D	555 VS (solid)		
	ν_4	CI_4 deg. deform.	123 E	[a] 123 W 127 W (solid)	123 (5) (solid)	

[a] Crystal field splitting.

Reference

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

Molecule: Dichloromethane CH_2Cl_2

Symmetry C_{2v} **Symmetry number = 2**

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

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

References

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

No. 14

Molecule: Dichloromethane-d_1 $CHDCl_2$

Symmetry C_s Symmetry number = 1

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a'	ν_1	CH stretch.	3024 B	3024	3019 M,p	
	ν_2	CD stretch.	2249 B	2249	2246 M,p	
	ν_3	CH bend.	1282 B	1282	1276 VW	
	ν_4	CD bend.	778 C	[a] 787 (R-branch) 778 (liquid)	779 W,p	
	ν_5	CCl_2 sym. stretch.	692 B	692	682 S,p	
	ν_6	CCl_2 scissors	283 B		283 M,p	
a''	ν_7	CH bend.	1223 A	1222.9	1221 VW	
	ν_8	CD bend.	890 A	889.8	886 VW	
	ν_9	CCl_2 anti. stretch.	738 B	738	725 W,dp	

[a] Due to the strong ν_9 band, the P-branch of this band is blurred out.

References

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

Molecule: Dichloromethane-d_2 CD_2Cl_2

Symmetry C_{2v} Symmetry number = 2

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_1	ν_1	CD_2 sym. stretch.	2205 B	2205 W	2198 M,p	
	ν_2	CD_2 scissors	1006 D	[a]1006 W	[a]1052 VW,p	
	ν_3	CCl_2 sym. stretch.	687 B	687 M	677 VS,p	
	ν_4	CCl_2 scissors	282 C		282 S,p	
a_2	ν_5	CD_2 twist.	826 C	ia	826 VW	
b_1	ν_6	CD_2 anti. stretch.	2304 C	2304 (liquid)	2304 VW	
	ν_7	CD_2 rock.	712 D			Calculated from product rule.
b_2	ν_8	CD_2 wag.	957 B	957 VS		
	ν_9	CCl_2 anti. stretch.	727 B	727 VS	716 W	

[a] Palma et al., assigned a Raman line at 1052 cm^{-1} to this vibrational mode, although the corresponding band does not appear in the infrared spectrum of CD_2Cl_2 in the gaseous and the liquid states.

References

[1] IR. T. Shimanouchi and I. Suzuki, J. Mol. Spectry. **8,** 222 (1962).
[2] IR.R. F. E. Palma, E. A. Piotrowski, S. Sundram, and F. F. Cleveland, J. Mol. Spectry. **13,** 118 (1964).

No. 16

Molecule: Methane CH_4

Symmetry T_d **Symmetry number = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_1	ν_1	CH_4 sym. stretch.	2917 A	ia	2917.0	
e	ν_2	CH_4 deg. deform.	1534 A	ia	1533.6	
f_2	ν_3	CH_4 deg. stretch.	3019 A	3018.9	3018.9	
	ν_4	CH_4 deg. deform.	1306 C	1306.2		

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR. H. C. Allen, Jr. and E. K. Plyler, J. Chem. Phys. **26**, 972 (1957).
[3] R. M. A. Thomas and H. L. Welsh, Can. J. Phys. **38**, 1291 (1960).

No. 17

Molecule: Methane-*d*$_1$ CH_3D

Symmetry C_{3v} **Symmetry number = 3**

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

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[2] IR. J. K. Wilmshurst and H. J. Bernstein, Can. J. Chem. **35**, 226 (1957).
[3] IR. H. C. Allen, Jr., and E. K. Plyler, J. Res. NBS **63**, 145 (1959).
[4] IR. L. H. Jones, J. Mol. Spec. **4**, 86 (1960).

No. 18

Molecule: Methane-d_2 CH_2D_2

Symmetry C_{2v} **Symmetry number = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$	
a_1	ν_1	CH_2 sym. stretch.	2976 D	2984 M 2969 M	2974	
	ν_2	CD_2 sym. stretch.	2202 C	2208 W 2196 W		
	ν_3	CH_2 scissors	1436 C	1442 W 1430 W		
	ν_4	CD_2 scissors	1033 C	1033 S	1034	
a_2	ν_5	CH_2 twist.	1329 C	1329 W		
b_1	ν_6	CH_2 anti. stretch.	3013 C	3013 S		
	ν_7	CH_2 rock.	1090 C	1090 S	1090	
b_2	ν_8	CD_2 anti. stretch.	2234 C	2234 M		
	ν_9	CH_2 wag.	1234 C	1234 M		

References

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

[2] IR. J. K. Wilmshurst and H. J. Bernstein, Can. J. Chem. **35**, 226 (1957).

No. 19

Molecule: Methane-d_3 CHD_3

Symmetry C_{3v} **Symmetry number = 3**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$	
a_1	ν_1	CH stretch.	2993 C	2993 M		
	ν_2	CD_3 sym. stretch.	2142 C	2142 M	2141	
	ν_3	CD_3 sym. deform.	1003 C	1003 M		
e	ν_4	CD_3 deg. stretch.	2263 C	2263 M	2269	
	ν_5	CH bend.	1291 C	1291 M	1299	
	ν_6	CD_3 deg. deform.	1036 C	1036 S	1046	

References

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

[2] IR. J. K. Wilmshurst and H. J. Bernstein, Can. J. Chem. **35**, 226 (1957).

Molecule: Methane-d_4 CD_4

Symmetry T_d **Symmetry number = 12**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$	
a_1	ν_1	CD_4 sym. stretch.	2109 B	ia	2108.9	
e	ν_2	CD_4 deg. deform.	1092 B	[a]1092	1091.9	
f_2	ν_3	CD_4 deg. stretch.	2259 A	2259.3	2259.3	
	ν_4	CD_4 deg. deform.	996 B	996.0		

[a] Coriolis interaction between ν_2 and ν_4.

References

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

[2] IR. H. M. Kaylor and A. H. Nielsen, J. Chem. Phys. **23**, 2139 (1955).

[3] R. G. C. Shepherd and H. L. Welsh, J. Mol. Spectry. **1**, 277 (1957).

[4] R. R. A. Olafson, M. A. Thomas, and H. L. Welsh, Can. J. Phys. **39**, 419 (1961).

No. 21

Molecule: **Methanol** **CH_3OH (gas)**

Symmetry C_s **Symmetry number = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a'	ν_1	OH stretch.	3681 A	3681 M		
	ν_2	CH_3 deg. stretch.	[a]3005 C	3000 M		
	ν_3	CH_3 sym. stretch.	2844 A	2844 S		
	ν_4	CH_3 deg. deform.	1477 B	1477 M		OV(ν_{10}).
	ν_5	CH_3 sym. deform.	1455 A	1455 M		
	ν_6	OH bend. (ν_7)	1345 B	1345 S		
	ν_7	CH_3 rock. (ν_6)	[b]1060 D	1060 W		
	ν_8	CO stretch.	1033 A	1033 VS	1032 (2)	
a''	ν_9	CH_3 deg. stretch.	[a]2965 C	2960 S	2955 (4)	
	ν_{10}	CH_3 deg. deform.	1477 B	1477 M		OV(ν_4).
	ν_{11}	CH_3 rock.	[c]1165 C			
	ν_{12}	C-O torsion	[d] 270 D	50 ~ 860		

[a] The value obtained by the matrix isolation method [4].

[b] Buried under the R-branch of very strong CO stretching band centered at 1033 cm^{-1} [3].

[c] Frequency in the liquid state (Raman). It is also possible to assign this vibration to a very weak infrared band at 1230 cm^{-1}. However, the latter assignment is not consistent with those of related compounds.

[d] See References [2] and [5].

References

[1] R. J. R. Nielsen and N. E. Ward, J. Chem. Phys. **10**, 81 (1942).
[2] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[3] IR. C. Tanaka, K. Kuratani, and S. Mizushima, Spectrochim. Acta **9**, 265 (1957).
[4] IR. M. Van Thiel, E. D. Becker, and G. C. Pimentel, J. Chem. Phys. **27**, 95 (1957).
[5] IR.Th. D. G. Burkhard and D. M. Dennison, J. Mol Spectr. **3**, 299 (1959).
[6] Th. M. Margottin-Maclou, J. Phys. Radium **21**, 634 (1960).
[7] IR. M. Falk and E. Whalley, J. Chem. Phys. **34**, 1554 (1961) and references cited there.
[8] Th. G. Zerbi, J. Overend, and B. Crawford, J. Chem. Phys. **38**, 122 (1963).
[9] IR.Th. C. Tanaka and T. Shimanouchi, unpublished.

No. 22

Molecule: **Methanol** **CH_3OH (liquid)**

Symmetry C_s **Symmetry number = 1**

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

References

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

Molecule: **Methanol-d_1** **CH_3OD (gas)**

Symmetry C_s **Symmetry number = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$	
a'	ν_1	OD stretch.	2718 A	2718 M		
	ν_2	CH_3 deg. stretch.	3005 C	3000 M		SF(ν_2 of CH_3OH).
	ν_3	CH_3 sym. stretch.	2843 A	2843 S		
	ν_4	CH_3 deg. deform.	1473 B	1473 M		OV(ν_{10}).
	ν_5	CH_3 sym. deform.	1456 A	1456 M		
	ν_6	OD bend.	864 A	864 S		
	ν_7	CH_3 rock.	1230 B	1230 W		
	ν_8	CO stretch.	1040 A	1040 VS		
a"	ν_9	CH_3 deg. stretch.	2965 C	2960 S		SF(ν_9 of CH_3OH).
	ν_{10}	CH_3 deg. deform.	1473 B	1473 M		OV(ν_4).
	ν_{11}	CH_3 rock.	1160 C	1160 VW		
	ν_{12}	C-O torsion	213 E			CF[2, 4]

References

[1] IR. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).

[2] IR. C. Tanaka, K. Kuratani, and S. Mizushima, Spectrochim. Acta **9**, 265 (1957).

[3] Th. M. Margottin-Maclou, J. Phys. Radium **21**, 634 (1960).

[4] IR. M. Falk and E. Whalley, J. Chem. Phys. **34**, 1554 (1961) and references cited there.

[5] Th. G. Zerbi, J. Overend, and B. Crawford, Jr., J. Chem. Phys. **38**, 122 (1963).

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

Molecule: **Methanol-d_1** **CH_3OD (liquid)**

Symmetry C_s **Symmetry number = 1**

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

References

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

[2] R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).

[3] IR.R. M. Falk and E. Whalley, J. Chem. Phys. **34,** 1554 (1961) and references cited there.

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

No. 25

Molecule: Methanol-d_3 CD_3OH (gas)

Symmetry C_s **Symmetry number = 1**

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

[a] The value used by Margottin-Maclou for her normal coordinate treatment.

References

[1] Th. M. Margottin-Maclou, J. Phys. Radium **21**, 634 (1960).
[2] IR. M. Falk and E. Whalley, J. Chem. Phys. **34**, 1554 (1961) and references cited there.
[3] Th. G. Zerbi, J. Overend, and B. Crawford, Jr., J. Chem. Phys. **38**, 122 (1963).
[4] Th. C. Tanaka and T. Shimanouchi, unpublished.

No. 26

Molecule: Methanol-d_3 CD_3OH (liquid)

Symmetry C_s **Symmetry number = 1**

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

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

References

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

No. 27

Molecule: **Methanol-d_4** **CD_3OD (gas)**

Symmetry C_s **Symmetry number = 1**

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

[a] The value used by Margottin-Maclou for her normal coordinate treatment.

References

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

No. 28

Molecule: **Tetrafluoroethylene** CF_2CF_2

Symmetry D_{2h} **Symmetry number = 4**

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

References

[1] IR.R. J. R. Nielsen, H. H. Claassen, and D. C. Smith, J. Chem. Phys. **18**, 812 (1950).
[2] R. A. Monfils and J. Duchesne, J. Chem. Phys. **18**, 1415 (1950).
[3] IR. D. E. Mann, N. Acquista, and E. K. Plyler, J. Res. NBS **52**, 67 (1954) RP2474.

No. 29

Molecule: Tetrachloroethylene CCl_2CCl_2

Symmetry D_{2h} Symmetry number = 4

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid)	cm^{-1} (Liquid)	
a_g	ν_1	CC stretch.	1571 D	ia	1571 (7)p	
	ν_2	CCl_2 sym. stretch.	447 D	ia	447 (10)p	
	ν_3	CCl_2 scissors	237 D	ia	237 (7)p	
a_u	ν_4	CCl_2 twist.	110 E	ia	ia	OC($2\nu_4 = 218$)[1].
b_{1g}	ν_5	CCl_2 anti. stretch.	1000 D	ia	1000 (0)	
	ν_6	CCl_2 rock.	347 D	ia	347 (4)dp	
b_{1u}	ν_7	CCl_2 wag.	288 D	288 M	ia	
b_{2g}	ν_8	CCl_2 wag.	512 D	ia	512 (4)dp	
b_{2u}	ν_9	CCl_2 anti. stretch.	908 C	908 S (CS_2 soln.)	ia	
	ν_{10}	CCl_2 rock.	176 C	176 S	ia	
b_{3u}	ν_{11}	CCl_2 sym. stretch.	777 C	777 S (CS_2 soln.)	ia	
	ν_{12}	CCl_2 scissors	310 C	310 W	ia	

References

[1] IR. D. E. Mann, N. Acquista, and E. K. Plyler, J. Res. NBS **52**, 67 (1954) RP2474.
[2] IR. D. E. Mann, J. H. Meal and E. K. Plyler, J. Chem. Phys. **24**, 1018 (1956).
[3] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945) and references cited there.

No. 30

Molecule: Tetrabromoethylene CBr_2CBr_2

Symmetry D_{2h} **Symmetry number = 4**

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

References

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

No. 31

Molecule: 1,1-Difluoro 2,2-dichloroethylene CF_2CCl_2

Symmetry C_{2v} **Symmetry number = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CC stretch.	1749 B	1749 VS	1738.8 S	
	ν_2	CF stretch.	1032 B	1032 VS	1027.6 M	
	ν_3	CCl stretch.	622 C	622 M	623.0 S	
	ν_4	CF_2 scissors	434 C	434	433.8 VS	
	ν_5	CCl_2 scissors	258 C	258 S	258 VS	
a_2	ν_6	Torsion	167 D		167 VVW	
b_1	ν_7	CF stretch.	1327 B	1328 VS	1313 VVW	
	ν_8	CCl stretch.	989 B	989 VS	986 VW	
	ν_9	CF_2 rock.	459 C	459 VW	454 W	
	ν_{10}	CCl_2 rock.	192 C	192	187.8 W	
b_2	ν_{11}	CF_2 wag.	564 C	564 S	560.8 VS	
	ν_{12}	CCl_2 wag.	323 C	323 W		

References

[1] IR.R. J. R. Nielsen and H. H. Claassen, J. Chem. Phys. **18**, 485 (1950).
[2] IR. D. E. Mann and E. K. Plyler, J. Chem. Phys. **23**, 1989 (1955).
[3] Th. D. E. Mann, L. Fano, J. H. Meal, and T. Shimanouchi, J. Chem. Phys. **27**, 51 (1957).

No. 32

Molecule: ***trans*-Difluorodichloroethylene** **CFClCFCl**

Symmetry C_{2h} **Symmetry number = 2**

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

References

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

No. 33

Molecule: **Hexafluoroethane** **CF_3CF_3**

Symmetry D_{3d} **Symmetry number = 6**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Gas)	
a_g	ν_1	CC stretch.	1228 D	ia	1228	OC.[a]
	ν_2	CF_3 sym. stretch.	807 C	ia	807 VS,p	
	ν_3	CF_3 sym. deform.	348 C	ia	348 W,p	
a_{1u}	ν_4	Torsion	67 D	ia	ia	(b)
a_{2u}	ν_5	CF_3 sym. stretch.	1117 B	1117 VS	ia	
	ν_6	CF_3 sym. deform.	714 B	714 VS	ia	
e_g	ν_7	CF_3 deg. stretch.	1243 C	ia	1250 VW,dp	
	ν_8	CF_3 deg. deform.	619 C	ia	619 W,dp	
	ν_9	CF_3 rock.	376 C	ia	372 W,dp	
e_u	ν_{10}	CF_3 deg. stretch.	1251 B	1251 VS	ia	
	ν_{11}	CF_3 deg. deform.	523 C	520 S	ia	
	ν_{12}	CF_3 rock.	220 C	220 S	ia	

[a] The mean value of frequencies obtained from six combination bands.

[b] Obtained from thermodynamic data [3].

References

[1] IR.R. R. A. Carney, E. A. Piotrowski, A. G. Meister, J. H. Broun, and F. F. Cleveland, J. Mol. Spectr. **7**, 209 (1961).
[2] Th. T. Fujiyama and T. Shimanouchi, unpublished.
[3] D. E. Mann and E. K. Plyler, J. Chem. Phys. **21**, 1116 (1953).

No. 34

Molecule: Hexachloroethane CCl_3CCl_3

Symmetry D_{3d} **Symmetry number = 6**

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

[a] Obtained from $\nu_7 + \nu_4$ and $\nu_8 + \nu_4$.

References

[1] IR.R.Th. T. Fujiyama and T. Shimanouchi, unpublished.

[2] IR.R. R. A. Carney, E. A. Piotrowski, A. G. Meister, J. H. Broun, and F. F. Cleveland, J. Mol. Spectr. **7**, 209 (1961).

No. 35

Molecule: **Hexabromoethane** **CBr_3CBr_3**

Symmetry D_{3d} **Symmetry number = 6**

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

[a] Obtained from $\nu_7 + \nu_4$ and $\nu_8 + \nu_4$.

References

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

No. 36

Molecule: Ethylene CH_2CH_2

Symmetry D_{2h} **Symmetry number = 4**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1}	
a_g	ν_1	CH_2 sym. stretch.	3026 B	ia	3026.4 (10)p	
	ν_2	CC stretch.	1623 D	ia	1622.6 (8)p	FR($2\nu_{10}$).
	ν_3	CH_2 scissors	1342 B	ia	1342.2 (10)p	
a_u	ν_4	CH_2 twist.	1023 E	ia	ia	OC($\nu_4 + \nu_6$)[4].
	ν_5	CH_2 anti. stretch.	3103 B	ia	3102.5 (1)dp	
	ν_6	CH_2 rock.	1236 C	ia	1236 (1)dp (liquid)	
b_{1u}	ν_7	CH_2 wag.	949 A	949.3 M	ia	
b_{2g}	ν_8	CH_2 wag.	943 C	ia	943 (1)dp (liquid)	
b_{2u}	ν_9	CH_2 anti. stretch.	3106 B	3105.5 S	ia	
	ν_{10}	CH_2 rock.	826 A	826.0 W	ia	
b_{3u}	ν_{11}	CH_2 sym. stretch.	2989 A	2988.66 S	ia	
	ν_{12}	CH_2 scissors	1444 B	1443.5 S	ia	

References

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

No. 37

Molecule: 1,2-Dichloroethane CH_2ClCH_2Cl
(trans form)

Symmetry C_{2h} **Symmetry number = 2**

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

[a] Torsional vibration appears at 134 cm^{-1} in the liquid state.

References

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

[2] IR.R. S. Mizushima, Y. Morino, I. Watanabe, T. Shimanouchi, and S. Yamaguchi, J. Chem. Phys. **17**, 591 (1949).

[3] IR.R. John T. Neu and Wm. D. Gwinn, J. Chem. Phys. **18**, 1642 (1950).

[4] IR.R. J. K. Brown and N. Sheppard, Trans. Faraday Soc. **48**, 128 (1952).

[5] Th. I. Nakagawa and S. Mizushima, J. Chem. Phys. **21**, 2195 (1953).

[6] IR. I. Ichishima, H. Kamiyama, T. Shimanouchi, and S. Mizushima, J. Chem. Phys. **29**, 1190 (1958).

[7] IR. S. Mizushima, T. Shimanouchi, I. Ichishima and H. Kamiyama, Revue Universelle des Mines **15**, 447 (1959).

No. 38

Molecule: 1,2-Dichloroethane CH_2ClCH_2Cl (gauche form)

Symmetry C_2 **Symmetry number = 2**

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

See references for the trans form.

No. 39

Molecule: **1,2-Dibromoethane** **CH_2BrCH_2Br**
(trans form)

Symmetry C_{2h} **Symmetry number = 2**

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

[a] Torsional frequency in the liquid state was observed at 127 cm^{-1}.

References

[1] IR.R. S. Mizushima, Y. Morino, I. Watanabe, T. Shimanouchi and S. Yamaguchi, J. Chem. Phys. **17**, 591 (1949).

[2] IR.R. John T. Neu and Wm. D. Gwinn, J. Chem. Phys. **18**, 1642 (1950).

[3] IR.R. J. K. Brown and N. Sheppard, Trans. Faraday Soc. **48**, 128 (1952).

[4] IR. I. Ichishima, H. Kamiyama, T. Shimanouchi and S. Mizushima, J. Chem. Phys. **29**, 1190 (1958).

No. 40

Molecule: 1,2-Dibromoethane CH_2BrCH_2Br (gauche form)

Symmetry C_2 **Symmetry number = 2**

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

See references for the trans form.

No. 41

Molecule: **1,2-Chlorobromoethane** **CH_2ClCH_2Br**
(trans form)

Symmetry C_s **Symmetry number = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Solid)	cm^{-1} (Liquid)	
a'	ν_1	CH_2 sym. stretch.	2960 D		2960 (10vb)	SF(ν_2,gauche ν_3, gauche ν_4).
	ν_2	CH_2 sym. stretch.	2960 D		2960 (10vb)	SF(ν_1, gauche ν_3, gauche ν_4).
	ν_3	CH_2 scissors	1446 D	1446 S		
	ν_4	CH_2 scissors	1444 C		1444 (3b)	
	ν_5	CH_2 wag.	1284 C	1284 M	1284 (7)p	
	ν_6	CH_2 wag.	1203 C	1203 S	1203 (3)	
	ν_7	CC stretch.	1052 C	1056 M	1052 (4)dp	
	ν_8	CCl stretch. (ν_9)	726 C	722 S	726 (10b)p	
	ν_9	CBr stretch. (ν_8)	630 C	630 S	630 (9)	
	ν_{10}	CCCl deform. (ν_{11})	251 C		251 (10)p	SF(gauche ν_{17}).
	ν_{11}	CCBr deform. (ν_{10})	202 C	202.0 (CCl_4 soln.)	210 (2b)	
a''	ν_{12}	CH_2 anti. stretch.	3010 D		3010 (3vb)	SF(ν_{13}, gauche ν_1, gauche ν_2).
	ν_{13}	CH_2 anti. stretch.	3010 D		3010 (3vb)	SF(ν_{12}, gauche ν_1, gauche ν_2).
	ν_{14}	CH_2 twist.	1259 C	1258 VW	1259 (3)	
	ν_{15}	CH_2 twist.	1111 D	1111 M		
	ν_{16}	CH_2 rock.	961 C	961 VW	961 (1b)	
	ν_{17}	CH_2 rock.	763 D	763 M		
	ν_{18}	Torsion	123 C	123.0 (CCl_4 soln.)		

References

[1] R. S. Mizushima, Y. Morino, Y. Miyahara, and M. Tomura, Sci. Pop. Inst. Physic. Chem. Res. Japan **39**, 387 (1942).
[2] IR.R. J. K. Brown and N. Sheppard, Trans. Faraday Soc. **48**, 128 (1952).
[3] IR. L. R. Blaine, J. Res. NBS **67C** (Engr. and Instr.) No. 3, 207 (1963).

No. 42

Molecule: 1,2-Chlorobromoethane CH_2ClCH_2Br
(gauche form)

Symmetry C_1 Symmetry number = 1

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

See references for the trans form.

Molecule: **Ethyl floride** CH_3CH_2F

Symmetry C_s **Symmetry number = 1**

Sym. class	No.	Approximate type of mode	Selected value of fre-quency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$ (Liquid)	
a'	ν_1	CH_3 deg. stretch.	3003 D	3003 VS	2986 VS,dp	OV(ν_{12},ν_{13}).
	ν_2	CH_2 sym. stretch.	2941 D	2941	2941 VS,p	
	ν_3	CH_3 sym. stretch.	2915 D	2915 S	2921 M	
	ν_4	CH_2 scissors	1479 C	1479 M	1480 W,b,dp	
	ν_5	CH_3 deg. deform.	1449 D	1449 S	1458 M,b,dp	OV(ν_{14}).
	ν_6	CH_3 sym. deform.	1395 C	1395 S	1393 W,p	
	ν_7	CH_2 wag.	1365 D	1365 M (liquid)	1365 VW	
	ν_8	CH_3 rock.	1108 C	1108 VS	1103 S,p	
	ν_9	CC stretch.	1048 D	1048 VS	1041 M,b,dp	
	ν_{10}	CF stretch.	880 B	880 VS	873 VS,p	
	ν_{11}	CCF deform.	415 C	415	419 W,p	
a"	ν_{12}	CH_2 anti. stretch.	3003 D	3003 VS	2986 VS,dp	OV(ν_1,ν_{13}).
	ν_{13}	CH_3 deg. stretch.	3003 D	3003 VS	2986 VS,dp	OV(ν_1,ν_{12}).
	ν_{14}	CH_3 deg. deform.	1449 D	1449 S	1458 M,b,dp	OV(ν_5).
	ν_{15}	CH_2 twist.	1277 C	1277	1276 W,b,dp	
	ν_{16}	CH_3 rock.	1048 D	1048 VS	1041 M,b,dp	OV(ν_9).
	ν_{17}	CH_2 rock.	810 C	810 W	815 VW	
	ν_{18}	Torsion	243 B	242.7		

References

[1] IR.R. D. C. Smith, R. A. Saunders, J. Rud Nielsen, and E. E. Ferguson, J. Chem. Phys. **20,** 847 (1952).

[2] IR. E. Catalano and K. S. Pitzer, J. Phys. Chem. **62,** 873 (1958).

[3] IR. G. Sage and W. Klemperer, J. Chem. Phys. **39,** 371 (1963).

Molecule: Ethyl chloride CH_3CH_2Cl

Symmetry C_s **Symmetry number = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$ (Liquid)	
a'	ν_1	CH_3 deg. stretch.	2983 D	2983 S	2966 (10)p	
	ν_2	CH_2 sym. stretch.	2946 B	2945.8 S	2933 (10)p	
	ν_3	CH_3 sym. stretch.	2890 D	2890 S	2880 (4)p	
	ν_4	CH_2 scissors	1452 D	1452 VS	1452 (2)p	OV(ν_5,ν_{14}).
	ν_5	CH_3 deg. deform.	1452 D	1452 VS	1452 (2)p	OV(ν_4,ν_{14}).
	ν_6	CH_3 sym. deform.	1383 C	1383 VS	1380	
	ν_7	CH_2 wag.	1287 C	1287 VS	1280	
	ν_8	CH_3 rock.	1080 D	1080 W	1072 (1)p	
	ν_9	CC stretch.	972 D	972 VS	970 (1b)p	
	ν_{10}	CCl stretch.	676 B	676 VS	658 (8)p	
	ν_{11}	CCCl deform.	336 B	336 VS	335 (2)p	
a''	ν_{12}	CH_2 anti. stretch.	3012 D	3012 S	3020 (7)dp	
	ν_{13}	CH_3 deg. stretch.	2983 D	2983 S	2983 (7)dp	
	ν_{14}	CH_3 deg. deform.	1452 D	1452 VS	1452 (2)p	OV(ν_4,ν_5).
	ν_{15}	CH_2 twist.	1244 E		1244	
	ν_{16}	CH_3 rock.	972 D	972 VS	970 (1)p	OV(ν_9).
	ν_{17}	CH_2 rock.	785 A	785.1 M		
	ν_{18}	Torsion	243 B	243 W		

References

[1] IR.R. L. W. Daasch, C. Y. Liang, and J. Rud Nielsen, J. Chem. Phys. **22**, 1293 (1954).
[2] R. G. Allen and H. J. Bernstein, Can. J. Chem. **32**, 1124 (1954).
[3] IR. R. N. Dixon, Spectrochim. Acta **9**, 59 (1957).
[4] IR. W. G. Fateley and F. A. Miller, Spectrochim. Acta **17**, 857 (1961).
[5] IR. N. T. McDevitt, A. L. Rozek, F. F. Bentley, and A. D. Davidson, J. Chem. Phys. **42**, 1173 (1965).

Molecule: Ethyl bromide CH_3CH_2Br

Symmetry C_s **Symmetry number = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a'	ν_1	CH_3 deg. stretch.	2988 C	2988 S	2971 (2b)p	OV(ν_{13}).
	ν_2	CH_2 sym. stretch.	2937 B	2936.5 S	2924 (2)p	
	ν_3	CH_3 sym. stretch.	2880 B	2879.8 S		
	ν_4	CH_2 scissors	1451 D	1451 M	1442 (2b)dp	OV(ν_5,ν_{14}).
	ν_5	CH_3 deg. deform.	1451 D	1451 M	1442 (2b)dp	OV(ν_4,ν_{14}).
	ν_6	CH_3 sym. deform.	1386 B	1386 M		
	ν_7	CH_2 wag.	1252 E	$\begin{cases}1258\ \text{VS}\\1247\ \text{VS}\end{cases}$	1248 (2b)p	FR($\nu_9+\nu_{11}$).
	ν_8	CH_3 rock.	1061 D	1061 VW	1069 (1)p	
	ν_9	CC stretch.	964 B	964 S	960 (1b)dp	
	ν_{10}	CBr stretch.	583 B	583 VS	560 (10)p	
	ν_{11}	CCBr deform.	290 B	290 S	293 (3)p	
a''	ν_{12}	CH_2 anti. stretch.	3018 B	3018 S		
	ν_{13}	CH_3 deg. stretch.	2988 C	2988 S	2971 (2b)p	OV(ν_1).
	ν_{14}	CH_3 deg. deform.	1451 D	1451 M	1442 (2b)dp	
	ν_{15}	CH_2 twist.	1248 E			CF.
	ν_{16}	CH_3 rock.	964 D	964 S	960 (1b)dp	OV(ν_9).
	ν_{17}	CH_2 rock.	770 B	770 M		
	ν_{18}	Torsion	247 B	247		

Note. The CH_2 twisting frequency, ν_{15}, was calculated from the modified Urey-Bradley force constants which were transferred from hydrocarbons and halogenoethanes [5].

References

[1] R. J. Wagner, Zeit. Phys. Chem. **B40**, 439 (1938).
[2] R. J. K. Brown and N. Sheppard, Trans. Faraday Soc. **50**, 535 (1954).
[3] IR. R. N. Dixon, Spectrochim. Acta **9**, 59 (1957).
[4] IR. N. T. McDevitt, A. L. Rozek, F. F. Bentley, and A. D. Davidson, J. Chem. Phys. **42**, 1173 (1965).
[5] IR.Th. T. Shimanouchi and S. Takayama, unpublished.
[6] IR. S. Kinumaki and Y. Musha, unpublished.

No. 46

Molecule: **Ethane** CH_3CH_3

Symmetry D_{3d} **Symmetry number = 6**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	*cm*$^{-1}$	
a_{1g}	ν_1	CH_3 sym. stretch.	2915 E	ia	2899.2 S,p 2955.1 S,p	FR($2\nu_{11}$).
	ν_2	CH_3 sym. deform.	1400 E	ia		OC [1, 2].
	ν_3	CC stretch.	993 A	ia	993.0 S,p	
a_{1u}	ν_4	Torsion.	275 D	ia	ia	CF.[a]
a_{2u}	ν_5	CH_3 sym. stretch.	2915 E	2954.0 S 2895.6 M	ia	FR($\nu_8+\nu_{11}$).
	ν_6	CH_3 sym. deform.	1379 A	1379.2 W	ia	
e_u	ν_7	CH_3 deg. stretch.	2995 A	2995.5 M	ia	
	ν_8	CH_3 deg. deform.	1472 A	1472.2 S	ia	
	ν_9	CH_3 rock.	822 A	821.52 S	ia	
e_g	ν_{10}	CH_3 deg. stretch.	2955 C	ia	2963 W (liquid)	
	ν_{11}	CH_3 deg. deform.	1460 C	ia	1460 M,dp (liquid)	
	ν_{12}	CH_3 rock.	1190 E	ia		OC [1, 2].

[a] Calculated from specific heat data.

References

[1] IR.R. G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945) and references cited there.
[2] IR. L. G. Smith, J. Chem. Phys. **17, 139** (1949).
[3] IR. G. E. Hansen and D. M. Dennison, J. Chem. Phys. **20,** 313 (1952).

No. 47

Molecule: **Ethane-d_6** CD_3CD_3

Symmetry D_{3d} **Symmetry number = 6**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_{1g}	ν_1	CD_3 sym. stretch.	2100 E	ia	2147 S 2083 S	FR($2\nu_{11}$).
	ν_2	CD_3 sym. deform.	1158 C	ia	1158 M	
	ν_3	CC stretch.	852 C	ia	852 S	
a_{1u}	ν_4	Torsion	200 D	ia	ia	CF.[a]
a_{2u}	ν_5	CD_3 sym. stretch.	2095 E	2087.3 S 2139.7	ia	FR($\nu_8+\nu_{11}$).
	ν_6	CD_3 sym. deform.	1077 A	1077 S	ia	
e_u	ν_7	CD_3 deg. stretch.	2236 A	2236 S	ia	
	ν_8	CD_3 deg. deform.	1082 A	1082 S	ia	
	ν_9	CD_3 rock.	594 A	593.7 S	ia	
e_g	ν_{10}	CD_3 deg. stretch.	2225 C	ia	2225 S,b	
	ν_{11}	CD_3 deg. deform.	1055 C	ia	1055 M,b	
	ν_{12}	CD_3 rock.	970 C	ia	970 W,b	

[a] Calculated from specific heat data.

References

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

[2] IR. G. E. Hansen and D. M. Dennison, J. Chem. Phys. **20**, 313 (1952).

No. 48

Molecule: Dimethylether CH_3OCH_3

Symmetry C_{2v} **Symmetry number = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Gas)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 deg. stretch.	2996 B	2996 S	2989 S	
	ν_2	CH_3 sym. stretch.	2817 B	2817 S	2815 VS,p	
	ν_3	CH_3 deg. deform.	1464 D	1464 M		
	ν_4	CH_3 sym. deform.	1452 D	1452 M	1452 S,dp	
	ν_5	CH_3 rock.	1244 B	1244 W		
	ν_6	CO sym. stretch.	928 B	928 S	922 S,p	
	ν_7	COC deform.	418 C	418 M	428 M,p	
a_2	ν_8	CH_3 deg. stretch.	2952 C	ia	2952 S	
	ν_9	CH_3 deg. deform.	1464 D	ia		SF(ν_3).
	ν_{10}	CH_3 rock.	1150 C	ia	1150 M,d	
	ν_{11}	C-O torsion	203 E	ia		CF [3].
b_1	ν_{12}	CH_3 deg. stretch.	2996 B	2996 S	2989 S	OV(ν_1).
	ν_{13}	CH_3 sym. stretch.	2817 B	2817 S	2815 VS,p	OV(ν_2).
	ν_{14}	CH_3 deg. deform.	1464 D	1464 M		OV(ν_3).
	ν_{15}	CH_3 sym. deform.	1452 D	1452 M	1452 S,dp	OV(ν_4).
	ν_{16}	CH_3 rock.	1227 C		1227 W	
	ν_{17}	CO anti. stretch.	1102 B	1102 VS	1104 M,dp	
b_2	ν_{18}	CH_3 deg. stretch.	2925 B	2925 S		
	ν_{19}	CH_3 deg. deform.	1464 D	1464 M		OV(ν_3).
	ν_{20}	CH_3 rock.	1179 B	1179 VS	1170 sh	
	ν_{21}	C-O torsion	242 C	242 W^2		

References

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

[2] R. R. C. Taylor and G. L. Vidale, J. Chem. Phys. **26**, 122 (1957).

[3] IR.R. Y. Kanazawa and K. Nukada, Bull. Chem. Soc. Japan **35**, 612 (1962).

[4] IR. W. G. Fateley and F. A. Miller, Spectrochim. Acta **18**, 977 (1962).

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

No. 49

Molecule: Dimethylether-d_3 CH_3OCD_3

Symmetry C_s Symmetry number = 1

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

References

[1] IR. J. P. Perchard, Théses faculté des sciences de L'université de Paris (1962).
[2] Th. T. Shimanouchi and M. Oka, unpublished.

No. 50

Molecule: Malononitrile $NCCH_2CN$

Symmetry C_{2v} Symmetry number = 2

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

[a] Activated only in solid phase.

References

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

[2] R. K. W. F. Kohlrausch and G. Prinz Ypsilanti, Zeits. Physik. Chemie B. **29**, 274 (1934).

No. 51

Molecule: Malononitrile-d_2 $NCCD_2CN$

Symmetry C_{2v} Symmetry number = 2

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

Reference

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

Molecule: Ethylcyanide CH_3CH_2CN

Symmetry C_s **Symmetry number = 1**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Liquid) [1]	cm^{-1} (Liquid) [1]	
a'	ν_1	CH_3 deg. stretch.	3001 C	3001 VS	2999 S	OV(ν_{14}).
	ν_2	CH_2 sym. stretch.	2955 C	2955 VS	2949 VS,p	
	ν_3	CH_3 sym. stretch.	2900 C	2900 S	2898 S,p	
	ν_4	$C \equiv N$ stretch.	2254 C	2254 VS	2251 VS,p	
	ν_5	CH_3 deg. deform.	1465 C	1465 S	1466 VS,p	SF(ν_{16}).
	ν_6	CH_2 scissors	1433 C	1433 S	1436 M,p	
	ν_7	CH_3 sym. deform.	1387 B	1387 M	1374 VW,p	
	ν_8	CH_2 wag.	1319 B	1319 M	1322 W,p	
	ν_9	C—CN stretch.	1077 B	1077 S	1078 M,p	
	ν_{10}	CC stretch.	1005 B	1005 M	1010 S,p	
	ν_{11}	CH_3 rock.	836 B	836 W	838 S,p	
	ν_{12}	CCC deform.	545 B	545 M	548 M,p	
	ν_{13}	CCN bend.	226 B	226 M	226 M,p	
a''	ν_{14}	CH_3 deg. stretch.	3001 C	3001 VS	2999 S	OV(ν_1)
	ν_{15}	CH_2 anti. stretch.	2849 C	2849 S	2850 M	
	ν_{16}	CH_3 deg. deform.	1465 C	1465 S	1466 VS,dp	
	ν_{17}	CH_2 twist.	1256 B	1256 VW	1270 VW,dp	
	ν_{18}	CH_3 rock.	1022 E			CF
	ν_{19}	CH_2 rock.	786 B	786 M	784 VW,dp	
	ν_{20}	CCN bend.	378 B	378 M	378 M,dp	
	ν_{21}	CH_3 torsion	274 C	274 W		

References

[1] IR.R. N. E. Duncan and G. J. Janz, J. Chem. Phys. **23**, 434 (1955).
[2] IR.R.Th. T. Fujiyama and T. Shimanouchi, unpublished.

Molecule: **Propane** $CH_3CH_2CH_3$

Symmetry C_{2v} **Symmetry number = 2**

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1} (Matrix isolation)	cm^{-1} (Liquid)	
a_1	ν_1	CH_3 deg. stretch.	2962 C	2962 S		SF(ν_{15},ν_{22}).
	ν_2	CH_3 sym. stretch.	2876 C	2876 S		OV(ν_3), SF(ν_{16}).
	ν_3	CH_2 sym. stretch.	2876 C	2876 S		OV(ν_2).
	ν_4	CH_3 deg. deform.	1470 C	1470 S		SF(ν_{17}, ν_{24}).
	ν_5	CH_2 scissors	1449 C	1449 W (solid)		
	ν_6	CH_3 sym. deform.	1388 B	1388 M		
	ν_7	CH_3 rock.	1154 B	1154 M	1152 W	
	ν_8	CC stretch.	870 B	870 S	867 S	
	ν_9	CCC deform.	371 B	370.6 (gas)	375 W	
a_2	ν_{10}	CH_3 deg. stretch.	2967 C	ia	2967 M	
	ν_{11}	CH_3 deg. deform.	1451 C	ia	1451 S	
	ν_{12}	CH_2 twist.	1278 C	ia	1278 W	
	ν_{13}	CH_3 rock.	940 D	ia	940 VW	
	ν_{14}	CH_3 torsion	200 E	ia		CF [7].
b_1	ν_{15}	CH_3 deg. stretch.	2962 C	2962 S		SF(ν_1,ν_{22}).
	ν_{16}	CH_3 sym. stretch.	2876 C	2876 S		SF(ν_2).
	ν_{17}	CH_3 deg. deform.	1470 C	1470 S		SF(ν_4, ν_{24}).
	ν_{18}	CH_3 sym. deform.	1375 B	1375 S		
	ν_{19}	CH_2 wag.	1336 B	1336 M	1338 M	
	ν_{20}	CC stretch.	1051 B	1051 M	1054 M	
	ν_{21}	CH_3 rock.	918 B	918 M		
b_2	ν_{22}	CH_3 deg. stretch.	2962 C	2962 S		SF(ν_1,ν_{15}).
	ν_{23}	CH_2 anti. stretch.	2910 C	2910 S		
	ν_{24}	CH_3 deg. deform.	1470 C	1470 S		SF(ν_4,ν_{17}).
	ν_{25}	CH_3 rock.	1186 B	1186 M		
	ν_{26}	CH_2 rock.	741 B	741 S		
	ν_{27}	CH_3 torsion	220			CF [7].

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Molecule: *n*-Butane $CH_3CH_2CH_2CH_3$ (trans form)
Symmetry C_{2h} Symmetry number = 2

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

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No. 55

Molecule: ***n*-Butane** **$CH_3CH_2CH_2CH_3$**
(gauche form)

Symmetry C_2 **Symmetry number = 2**

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

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

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No. 56

Molecule: Benzene C_6H_6

Symmetry D_{6h} Symmetry number = 12

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

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No. 57

Molecule: **Benzene-d_6** **C_6D_6**

Symmetry D_{6h} **Symmetry number = 12**

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

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Molecule: Cyclohexane C_3H_{12}

Symmetry D_{3h} Symmetry number = 6

Sym. class	No.	Approximate type of mode	Selected value of frequency	Infrared	Raman	Comments
				cm^{-1}	cm^{-1} (Liquid)	
a_{1g}	ν_1	CH_2 anti. stretch.	2930 E	ia	2938 VS,p 2923 VS,p	FR($2\nu_3$).
	ν_2	CH_2 sym. stretch.	2852 C	ia	2852 VS,p	
	ν_3	CH_2 scissors	1465 C	ia	1465 M,p	
	ν_4	CH_2 rock.	1157 C	ia	1157 S,p	
	ν_5	CC stretch.	802 C	ia	802 VS,p	
	ν_6	CCC deform. + CC torsion	383 C	ia	383 M,p	
a_{1u}	ν_7	CH_2 twist. (ν_8)	1383 C	ia, 1383*	ia	CF[3,5].
	ν_8	CH_2 wag. (ν_7)	1157 C	ia, 1157*	ia	CF[3,5].
	ν_9	CC stretch. + CC torsion	1057 C	ia, 1057*	ia	CF[3,5].
a_{2g}	ν_{10}	CH_2 wag.	1437 C	ia, 1437*	ia	CF[3,5].
	ν_{11}	CH_2 twist.	1090 C	ia, 1090*	ia	CF[3,5].
a_{2u}	ν_{12}	CH_2 anti. stretch.	2915 E	2915 M	ia	
	ν_{13}	CH_2 sym. stretch.	2860 E		ia	SF(ν_2,ν_{18},ν_{26}).
	ν_{14}	CH_2 scissors	1437 C	1437 M	ia	
	ν_{15}	CH_2 rock. (ν_{16})	1030 D	1040 M 1016 M	ia	FR($\nu_{23}+\nu_{32}$).
	ν_{16}	CCC deform. (ν_{15})	523 A	523 W	ia	
e_g	ν_{17}	CH_2 anti. stretch.	2930 E	ia		SF(ν_1, ν_{12}, ν_{25}).
	ν_{18}	CH_2 sym. stretch.	2897 E	ia	2897 M,vb	
	ν_{19}	CH_2 scissors	1443 C	ia	1443 S,dp	
	ν_{20}	CH_2 wag.	1347 C	ia	1347 S,dp	
	ν_{21}	CH_2 twist.	1266 C	ia	1266 VS,dp	
	ν_{22}	CC stretch.	1027 C	ia	1027 VS,dp	
	ν_{23}	CH_2 rock.	785 C	ia, 785*	785 VW,dp	
	ν_{24}	CCC deform. + CC torsion	426 C	ia	426 S,dp	
e_u	ν_{25}	CH_2 anti. stretch.	2933 A	2933 VS	ia	
	ν_{26}	CH_2 sym. stretch.	2863 A	2863 VS	ia	
	ν_{27}	CH_2 scissors	1457 A	1457 VS	ia	
	ν_{28}	CH_2 wag.	1355 B	1355 W	ia	
	ν_{29}	CH_2 twist.	1261 A	1261 S	ia	
	ν_{30}	CH_2 rock.	907 B	907 S	ia	
	ν_{31}	CC stretch.	863 A	863 S	ia	
	ν_{32}	CCC deform. + CC torsion	248 C	248 VW (liquid)	ia	

Note 1. Reference 3 gives the frequencies calculated from the modified Urey-Bradley force constants for hydrocarbons. Reference 5 gives those from the general internal force constants for hydrocarbons. These two sets of calculated frequencies are in agreement with each other within the deviation of 65 cm⁻¹ for the A_{1u} and A_{2g} vibrations.

Note 2. Reference 4 gives different assignments for the CH_2 rocking and skeletal deformation vibrations.

Note 3. The frequencies with asterisk are observed in the crystalline state at about 90 °K (ref. 9).

Note 4. An alternative assignment for ν_{15} is 910 cm^{-1} (see refs. 9 and 3).

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Molecule: Cyclohexane-d_{12} C_6D_{12}

Symmetry D_{3h} **Symmetry number = 6**

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

Note 1. As for the calculated frequencies, see C_6H_{12}.

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