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# Tables of Molecular Vibrational Frequencies Part 2.

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University of Tokyo

Tokyo, Japan




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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. The 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 activities are organized into seven categories as listed below. The data publications of the NSRDS, which may consist of monographs, loose-leaf 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 classifications 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 eleventh 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 2.

**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, as a continuation of Part I published as NSRDS–NBS–6, contains fundamental vibrational frequencies of 54 molecules together with vibrational assignments, sources of data, brief comments, and citations of references. The procedures used for the preparation of tables are the same as given in Part I. The fundamental frequencies are obtained mainly from the infrared and Raman spectra. When these are not avialable, other experimental data such as microwave results are taken into account. The selection of vibrational fundamentals from observed 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: Data, force constants, infrared spectra, modes of vibration, molecular vibrational frequencies, molecular spectra, Raman spectra.

## 1. 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 second of a series of annual reports being prepared in cooperation with the National Standard Reference Data Program of the National Bureau of Standards. The first report, which has been published as NSRDS-NBS 6, contains data for 59 molecules. This second report contains another 54 molecules with the serial numbers 60 113. These molecules have been selected from compounds for which experimental data are available and normal coordinate treatments have been made in detail. General comments on the procedures by which the tables are prepared and on the explanations of notation and abbreviations are given in Part 1 (NSRDS-NBS 6). Only the important notation and abbreviations are reproduced in the following tables.

The author expresses his sincere thanks to many members of the National Bureau of Standards, especially C. W. Beckett, D. R. Lide, Jr., E. L. Brady, and S. A. Rossmassler who helped me in the planning, the preparation, and the publication of the tables.

The author also acknowledges the assistance of his colleagues at the University of Tokyo: I. Nakagawa, A. Hirakawa, I. Suzuki, M. Tasumi, T. Fujiyama, I. Harada, M. Ishii, T. Ueda, H. Yoshioka, and K. Ishii.

TABLE 1. *Abbreviations for approximate type of mode*

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

TABLE 2. *Uncertainty for the selective values of frequencies*

| Notation | Uncertainty | Basis* |
|---|---|---|
| | $cm^{-1}$ | |
| A | $0 \sim 1$ | (i) Gas, grating spectrometer, rotational fine structure accurately analyzed.<br>(ii) Gas, grating spectrometer, a sharp $Q$ branch. |
| B | $1 \sim 3$ | (i) Gas, grating spectrometer, rotational fine structure partly analyzed.<br>(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).<br>(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.).<br>(ii) Solid, liquid or solution, inaccurate measurement. |
| E | $15 \sim 30$ | (i) Value estimated from Fermi resonance doublet.<br>(ii) Value estimated from overtone or combination tone.<br>(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.

TABLE 3. *Abbreviations used with "infrared" and "Raman"*

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

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

TABLE 4. *Abbreviations used in "Comments"*

| | |
|---|---|
| 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. |
| 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. |
| $\rho$ | Depolarization degree. |

## II. Tables of Vibrational Frequencies

**Pages 5 to 38**

**Molecule: Diborane $^{10}B_2H_6$**

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared [6] | Raman [8] | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Gas) | |
| $a_g$ | $\nu_1$ | $BH_2$ sym. stretch..... | 2537 C | ia | 2537 VS | |
| | $\nu_2$ | BH ring stretch..... | 2110 C | ia | 2110 S | |
| | $\nu_3$ | $BH_2$ scissors..... | 1186 C | ia | 1186 M | |
| | $\nu_4$ | Ring deform..... | 816 C | ia | 816 S<br>[b] 820 (2) (liquid) | |
| $a_u$ | $\nu_5$ | $BH_2$ twist..... | 829 D | [a] 829 VW | ia | |
| $b_{1g}$ | $\nu_6$ | BH ring stretch..... | 1768 C | ia | 1768 W | |
| | $\nu_7$ | $BH_2$ wag..... | 1044 E | ia | ..... | OC($\nu_5+\nu_7$) [6]. |
| $b_{1u}$ | $\nu_8$ | $BH_2$ anti. stretch..... | 2625 C | 2625 VS | ia | |
| | $\nu_9$ | $BH_2$ rock..... | 955 E | ..... | ia | CF [9]. |
| | $\nu_{10}$ | Ring puckering..... | 368 C | 368 S | ia | |
| $b_{2g}$ | $\nu_{11}$ | $BH_2$ anti. stretch..... | 2640 E | ia | 2640 W, b | |
| | $\nu_{12}$ | $BH_2$ rock..... | 930 E | ia | ..... | OC($\nu_{10}+\nu_{12}$)[6]. |
| $b_{2u}$ | $\nu_{13}$ | BH ring stretch..... | [b] 1920 E | 1882 M (1992 W) | ia | |
| $b_{2u}$ | $\nu_{14}$ | $BH_2$ wag..... | 977 C | 977 S | ia | |
| $b_{3g}$ | $\nu_{15}$ | $BH_2$ twist..... | 1012 E | ia | ..... | CF.[c] |
| $b_{3u}$ | $\nu_{16}$ | $BH_2$ sym. stretch..... | 2528 C | 2528 VS | ia | |
| | $\nu_{17}$ | BH ring stretch. and deform. | 1606 C | 1606 VVS | ia | |
| | $\nu_{18}$ | $BH_2$ scissors..... | 1181 C | 1181 VS | ia | |

[a] Forbidden by the selection rule, observed very weakly, and also confirmed by a combination band.
[b] Corrected for a presumed shift due to Fermi resonance.
[c] Expected frequency from $\nu_{15}$ of $^{11}B_2H_6$.

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[1] R. T. F. Anderson and A. B. Burg, J. Chem. Phys. **6,** 586 (1938).
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**Symmetry $D_{2h}$** **Symmetry number $\sigma = 4$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared [2] | Raman [2] | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_g$ | $\nu_1$ | $BD_2$ sym. stretch | [a] 1860 E | ia | 1880 VS, p<br>1833 S, p | FR($2\nu_3$). |
| | $\nu_2$ | BD ring stretch | 1511 C | ia | 1511 VS, p | |
| | $\nu_3$ | $BD_2$ scissors | 929 C | ia | 929 p | |
| | $\nu_4$ | Ring deform | 726 C | ia | 726 VS, p | |
| $a_u$ | $\nu_5$ | $BD_2$ twist | 592 D | [b] 592 VVW | ia | OC($\nu_5+\nu_7$).[b]<br>OC($\nu_5+\nu_{15}$). |
| $b_{1g}$ | $\nu_6$ | BD ring stretch | 1273 C | ia | 1273 (2) dp | |
| | $\nu_7$ | $BD_2$ wag | 870 E | ia | ..... | OC($\nu_5+\nu_7$). |
| $b_{1u}$ | $\nu_8$ | $BD_2$ anti. stretch | 1999 C | 1999 VS | ia | |
| | $\nu_9$ | $BD_2$ rock | 705 E | ..... | ia | OC($\nu_9+\nu_{10}$). |
| | $\nu_{10}$ | Ring puckering | 262 C | 262M | ia | |
| $b_{2g}$ | $\nu_{11}$ | $BD_2$ anti. stretch | [a] 1980 E | ia | 1975 (9) dp<br>(2000 (5)) dp | FR($\nu_6+\nu_{15}$). |
| | $\nu_{12}$ | $BD_2$ rock | 740 E | ia | ..... | OC($\nu_{10}+\nu_{12}$). |
| $b_{2u}$ | $\nu_{13}$ | BD ring stretch | [a] 1465 E | 1491 M<br>1459 MS | ia | FR($\nu_5+\nu_7$). |
| $b_{2u}$ | $\nu_{14}$ | $BD_2$ wag | 728 C | 728 S | ia | |
| $b_{3g}$ | $\nu_{15}$ | $BD_2$ twist | 730 C | ia | 730 (4) dp | |
| $b_{3u}$ | $\nu_{16}$ | $BD_2$ sym. stretch | 1845 C | 1857 VS<br>(1799 S) | ia | FR($\nu_3+\nu_{18}$). |
| | $\nu_{17}$ | BD ring stretch. and deform. | 1205 C | 1205 VVS | ia | |
| | $\nu_{18}$ | $BD_2$ scissors | 881 C | 881 VS | ia | |

[a] Corrected for a presumed shift due to Fermi resonance.
[b] Forbidden, by the selection rule, observed very weakly, and also confirmed by a combination band.

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[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. Emergy, Spectrochim. Acta **10**, 419 (1958).
[4] Th. T. Ogawa and T. Miyazawa, Spectrochim. Acta **20**, 557 (1964).

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared [6] | Raman [6], | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_g$ | $\nu_1$ | $BH_2$ sym. stretch..... | 2524 C | ia | 2524 (10) p | |
| | $\nu_2$ | BH ring stretch..... | 2104C | ia | 2104 (10) p | |
| | $\nu_3$ | $BH_2$ scissors..... | 1180 C | ia | 1180 (7) | |
| | $\nu_4$ | Ring deform..... | 794 C | ia | 794 (10) p | |
| $a_u$ | $\nu_5$ | $BH_2$ twist..... | 829 D | [a] 829 VW | ia | OC($\nu_5+\nu_7$).[a] OC($\nu_5+\nu_9$). |
| $b_{1g}$ | $\nu_6$ | BH ring stretch..... | [b] 1768 E | ia | 1788 (1) dp<br>1747 (1) dp | FR($\nu_5+\nu_9$). |
| | $\nu_7$ | $BH_2$ wag..... | 1035 E | ia | ..... | OC($\nu_5+\nu_7$). |
| $b_{1u}$ | $\nu_8$ | $BH_2$ anti. stretch..... | 2612 C | 2612 VS | ia | |
| | $\nu_9$ | $BH_2$ rock..... | 950 E | ..... | ia | OC($\nu_5+\nu_9$). OC($\nu_9+\nu_{10}$). |
| | $\nu_{10}$ | Ring puckering..... | 368 C | 368 S | ia | |
| $b_{2g}$ | $\nu_{11}$ | $BH_2$ anti. stretch..... | 2591 C | ia | 2591 (9) dp | |
| | $\nu_{12}$ | $BH_2$ rock..... | 920 E | ia | ..... | OC($\nu_{10}+\nu_{12}$). |
| $b_{2u}$ | $\nu_{13}$ | BH ring stretch..... | [b] 1915 E | 1887 M (1999 W) | ia | |
| | $\nu_{14}$ | $BH_2$ wag..... | 973 C | 973 S | ia | |
| $b_{3g}$ | $\nu_{15}$ | $BH_2$ twist..... | 1012 C | ia | 1012 (5) dp | |
| $b_{3u}$ | $\nu_{16}$ | $BH_2$ sym. stretch..... | 2525 C | 2525 VS | ia | |
| | $\nu_{17}$ | BH ring stretch. and deform. | 1602 C | 1602 VVS | ia | |
| | $\nu_{18}$ | $BH_2$ scissors..... | 1177 C | 1177 VS | ia | |

[a] Forbidden by the selection rule, observed very weakly, and also confirmed by a combination band.
[b] Corrected for a presumed shift due to Fermi resonance.

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[1] R. T. F. Anderson and A. B. Burg, J. Chem. Phys. **6**, 586 (1938).
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**Molecule: Silicon tetrabromide $SiBr_4$** No. 63

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $SiBr_4$ sym. stretch..... | 249 C | ia | 249 (4) p | |
| $e$ | $\nu_2$ | $SiBr_4$ deg. deform..... | 90 C | ia | 90 (3) | |
| $f_2$ | $\nu_3$ | $SiBr_4$ deg. stretch..... | 487 C | ..... | 487 (1) | |
| | $\nu_4$ | $SiBr_4$ deg. deform..... | 137 C | ..... | 137 (3) | |

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**Molecule: Silicon tetrachloride $SiCl_4$** No. 64

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $SiCl_4$ sym. stretch ..... | 424 C | ia | 424 (5) p | |
| $e$ | $\nu_2$ | $SiCl_4$ deg. deform..... | 150 C | ia | 150 (4) | |
| $f_2$ | $\nu_3$ | $SiCl_4$ deg. stretch..... | 621 C | 621 VS | 610 (2b) | |
| | $\nu_4$ | $SiCl_4$ deg. deform..... | 221 C | ..... | 221 (4) | |

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**Molecule: Silicon tetrafluoride $SiF_4$** No. 65

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $SiF_4$ sym. stretch | 801 C | ia | 800 S | |
| $e$ | $\nu_2$ | $SiF_4$ deg. deform | 264 C | ia | 268 W | |
| $f_2$ | $\nu_3$ | $SiF_4$ deg. stretch | 1032 B | [a] 1031.8 S | 1010 W | |
| | $\nu_4$ | $SiF_4$ deg. deform | 389 B | [a] 389.35 S | 390 W | |

[a] $^{28}Si^{23}F_4$.

## References


[1] R.IR. E. A. Jones, J. S. Kirby-Smith, P. J. H. Woltz, and A. H. Nielsen, J. Chem. Phys. **19,** 242 (1951).
[2] IR. J. Heicklen and V. Knight, Spectrochim. Acta **20,** 295 (1964).
[3] Th. J. L. Duncan and I. M. Mills, Spectrochim. Acta **20,** 1089 (1964).


**Molecule: Silane $SiH_4$** No. 66

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $SiH_4$ sym. stretch | 2187 B | ia | 2187.0 S | |
| $e$ | $\nu_2$ | $SiH_4$ deg. deform | 975 C | [a] 974.6 | 978 W | |
| $f_2$ | $\nu_3$ | $SiH_4$ deg. stretch | 2191 A | 2190.6 | | |
| | $\nu_4$ | $SiH_4$ deg. deform | 914 B | 914.2 | | |

[a] Coriolis interaction between $\nu_2$ and $\nu_4$.

## 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] G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules (Van Nostrand, New York, 1945).
[4] IR. D. F. Ball and D. C. McKean, Spectrochim. Acta **18,** 1019; 1029 (1962).
[5] IR. I. W. Levin and W. T. King, J. Chem. Phys. **37,** 1375 (1962).

**Molecule: Silane-$d_2$ $SiH_2D_2$** No. 67

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $SiH_2$ sym. stretch | 2189 C | 2189 S | | |
| | $\nu_2$ | $SiD_2$ sym. stretch | 1587 C | 1587 S | | |
| | $\nu_3$ | $SiH_2$ scissors | 944 B | 944 W | | |
| | $\nu_4$ | $SiD_2$ scissors | 683 B | 682.5 M | | |
| $a_2$ | $\nu_5$ | $SiH_2$ twist | 844 E | ia | ..... | CF [1]. |
| $b_1$ | $\nu_6$ | $SiH_2$ anti. stretch | 2183 C | 2183 S | | |
| | $\nu_7$ | $SiH_2$ rock | 743 B | 743 S | | |
| $b_2$ | $\nu_8$ | $SiD_2$ anti. stretch | 1601 C | 1601 S | | |
| | $\nu_9$ | $SiH_2$ wag | 862 B | 862 M | | |

## Reference

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

**Molecule: Silane-$d_3$ $SiHD_3$** No. 68

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | SiH stretch | 2182 C | 2182 M | | |
| | $\nu_2$ | $SiD_3$ sym. stretch | 1573 C | 1573 S | | |
| | $\nu_3$ | $SiD_3$ sym. deform | 683 C | 683 S | ..... | SF($\nu_6$). |
| $e$ | $\nu_4$ | $SiD_3$ deg. stretch | 1598 C | 1598 S | | |
| | $\nu_5$ | SiH bend | 851 B | 851 S | | |
| | $\nu_6$ | $SiD_3$ deg. deform | 683 C | 683 S | ..... | SF($\nu_3$). |

## References

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

**Molecule: Silane-$d_4$ $SiD_4$** No. 69

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $SiD_4$ sym. stretch..... | 1558 E | ..... | ..... | CF [4]. |
| $e$ | $\nu_2$ | $SiD_4$ deg. deform..... | 700 E | ..... | ..... | CF [4]. |
| $f_2$ | $\nu_3$ | $SiD_4$ deg. stretch..... | 1597 B | 1597 S | | |
| | $\nu_4$ | $SiD_4$ deg. deform..... | 681 C | 681 S | | |

## References


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


**Molecule: Silicon tetriodide $SiI_4$** No. 70

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $SiI_4$ sym. stretch..... | 168 C | ia | 168 S, p | |
| $e$ | $\nu_2$ | $SiI_4$ deg. deform..... | 63 C | ia | 63 M, dp | |
| $f_2$ | $\nu_3$ | $SiI_4$ deg. stretch..... | 405 C | ..... | 405 W, dp | |
| | $\nu_4$ | $SiI_4$ deg. deform..... | 94 C | ..... | 94 S, dp | |

## Reference


[1] R. M. L. Delwaulle, J. Phys. Chem. **56,** 355 (1952).

**Molecule: Germane $GeH_4$** No. 71

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $GeH_4$ sym. stretch..... | 2106 B | ia | 2106 S, p | |
| $e$ | $\nu_2$ | $GeH_4$ deg. deform..... | 931 D | [a] 930.9 | 920 W | |
| $f_2$ | $\nu_3$ | $GeH_4$ deg. stretch..... | 2114 B | 2113.6 | 2106 W (liquid) | |
| | $\nu_4$ | $GeH_4$ deg. deform..... | 819 B | 819.3 | 816 W (liquid) | |

[a] Coriolis interaction between $\nu_2$ and $\nu_4$.

## 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. Physik. Chem. **193,** 334 (1944).
[3] 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. Physik. Chem. (Frankfurt) **9,** 29 (1956).
[5] IR. A. A. Chalmers and D. C. McKean, Spectrochim. Acta **21,** 1941 (1965).


**Molecule: Germane-$d_1$ $GeH_3D$** No. 72

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $GeH_3$ sym. stretch ..... | 2106 C | ..... | 2106 | |
| | $\nu_2$ | GeD stretch..... | 1520 B | 1520.4 M | | |
| | $\nu_3$ | $GeH_3$ sym. deform..... | 820 C | 820 S | | |
| $e$ | $\nu_4$ | $GeH_3$ deg. stretch..... | 2112 B | 2112 S | | |
| | $\nu_5$ | $GeH_3$ deg. deform..... | 901 C | 901 W | | |
| | $\nu_6$ | $GeH_3$ rock..... | 706 C | 706 S | | |

## References


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

**Molecule: Germane-$d_2$ $GeH_2D_2$** No. 73

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $GeH_2$ sym. stretch..... | 2112 C | 2112 | | |
| | $\nu_2$ | $GeD_2$ sym. stretch..... | 1512 C | 1512 | | |
| | $\nu_3$ | $GeH_2$ scissors..... | 881 B | 881 | | |
| | $\nu_4$ | $GeD_2$ scissors..... | 620 C | 620 | | |
| $a_2$ | $\nu_5$ | $GeH_2$ twist..... | 807 E | 807 | | |
| $b_1$ | $\nu_6$ | $GeH_2$ anti. stretch..... | 2112 C | 2112 | | |
| | $\nu_7$ | $GeH_2$ rock..... | 657 C | 657 | | |
| $b_2$ | $\nu_8$ | $GeD_2$ anti. stretch..... | 1522 C | 1522 | | |
| | $\nu_9$ | $GeH_2$ wag..... | 770 C | 770 | | |

**Reference**

[1] IR. L. P. Lindeman and M. K. Wilson, Z. Physik. Chem. (Frankfurt) **9**, 29 (1956).

**Molecule: Germane-$d_3$ $GeHD_3$** No. 74

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | GeH stretch..... | 2112 B | 2112.4 | | |
| | $\nu_2$ | $GeD_3$ sym. stretch..... | 1504 B | ..... | 1504 | |
| | $\nu_3$ | $GeD_3$ sym. deform..... | 593 C | 595 | | |
| $e$ | $\nu_4$ | $GeD_3$ deg. stretch..... | 1522 C | 1522 | | |
| | $\nu_5$ | GeH bend..... | 792 B | 792.3 | | |
| | $\nu_6$ | $GeD_3$ deg. 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. Physik. Chem. (Frankfurt) **9**, 29 (1956).



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**Molecule: Germane-$d_4$ $GeD_4$** No. 75

**Symmetry $T_d$** **Symmetry number $\sigma = 12$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $GeD_4$ sym. stretch..... | 1504 C | ia | 1504 | |
| $e$ | $\nu_2$ | $GeD_4$ deg. deform..... | 665 D | [a] 665 W | | |
| $f_2$ | $\nu_3$ | $GeD_4$ deg. stretch..... | 1522 B | 1522.2 S | | |
| | $\nu_4$ | $GeD_4$ deg. deform..... | 596 C | 596 S | | |

[a] Coriolis interaction between $\nu_2$ and $\nu_4$.

## Reference


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


**Molecule: Nitrogen trifluoride $NF_3$** No. 76

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $NF_3$ sym. stretch..... | 1032 C | 1032 S | 1050 | |
| | $\nu_2$ | $NF_3$ sym. deform..... | 647 C | 647 W | 667 | |
| $e$ | $\nu_3$ | $NF_3$ deg. stretch..... | 905 C | 905 S | 905 | |
| | $\nu_4$ | $NF_3$ deg. deform..... | 493 C | 493 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).
[3] IR.R. E. L. Pace and L. Pierce, J. Chem. Phys. **23**, 1248 (1955).
[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).

**Molecule: Phosphorus trichloride $PCl_3$** No. 77

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $PCl_3$ sym. stretch..... | 504 C | 504 | 510 (10) p | |
| | $\nu_2$ | $PCl_3$ sym. deform..... | 252 C | 252 | 257 (6) p | |
| $e$ | $\nu_3$ | $PCl_3$ deg. stretch..... | 482 C | 482 | 480 (3) dp | |
| | $\nu_4$ | $PCl_3$ 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. Oetzen, J. Mol. Spectry. **2**, 253 (1958).
[3] IR. V. Lorenzelli, Compt. Rend. **252**, 3219 (1961).
[4] Th. A. M. Mirri, F. Scappini, and P. G. Favero, Spectrochim. Acta **21**, 965 (1965).


**Molecule: Phosphorus trifluoride $PF_3$** No. 78

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $PF_3$ sym. stretch..... | 892 C | 892 S | 890 (10) | |
| | $\nu_2$ | $PF_3$ sym. deform..... | 487 C | 487 M | 486 (3) | |
| $e$ | $\nu_3$ | $PF_3$ deg. stretch..... | 860 D | 860 S | 840 (10) | |
| | $\nu_4$ | $PF_3$ deg. deform..... | 344 C | 344 M | | |

**References**


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

**Molecule: Tribromochloromethane $CBr_3Cl$** No. 79

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ ($C_6H_6$ $CCl_4$ soln.) | |
| $a_1$ | $\nu_1$ | CCl stretch | 745 C | 747 S ($CS_2$ soln.) | 748 (1) | |
| | $\nu_2$ | $CBr_3$ sym. stretch | 327 C | 329 W ($C_7H_{14}$ soln.) | 326 (10) p | |
| | $\nu_3$ | $CBr_3$ sym. deform | 211 C | ..... | 210 (10) p | SF($\nu_5$). |
| $e$ | $\nu_4$ | $CBr_3$ deg. stretch | 677 C | 675 S ($CS_2$ soln.) | 677 (4) dp | |
| | $\nu_5$ | CCl bend. ($\nu_6$) | 211 E | ..... | ..... | SF($\nu_3$). |
| | $\nu_6$ | $CBr_3$ deg. deform. ($\nu_5$) | 140 C | ..... | 141 (7) dp | |

**References**


[1] R.IR. A. G. Meister, S. E. Rosser, and F. F. Cleveland, J. Chem. Phys. **18,** 346 (1950).
[2] IR. E. K. Plyler, W. H. Smith, and N. Acquista, J. Res. NBS **44,** 503 (1950), RP2097.
[3] R. M. L. Delwaulle, M. B. Buisset, and M. Delhaye, J. Am. Chem. Soc. **74,** 5768 (1952).
[4] R. R. H. Krupp, S. M. Ferogle, and A. Weber, J. Chem. Phys. **24,** 355 (1956).


**Molecule: Dibromodichloromethane $CBr_2Cl_2$** No. 80

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Liquid) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CCl_2$ sym. stretch | 733 C | 733 VS | 734 (1) p | |
| | $\nu_2$ | $CBr_2$ sym. stretch | 380 C | 377 W | 380 (10) p | |
| | $\nu_3$ | $CCl_2$ scissors ($\nu_4$) | 242 C | ..... | 242 (6) p | |
| | $\nu_4$ | $CBr_2$ scissors ($\nu_3$) | 154 C | ..... | 154 (4) p | |
| $a_2$ | $\nu_5$ | $CCl_2$ twist | 175 C | ..... | 175 (2) dp | |
| $b_1$ | $\nu_6$ | $CBr_2$ anti. stretch | 683 C | 683 VS | 684 (3) dp | |
| | $\nu_7$ | $CCl_2$ wag | 230 C | ..... | 229 (2) dp | |
| $b_2$ | $\nu_8$ | $CCl_2$ anti. stretch | 768 C | 768 VS | 771 (0) dp | |
| | $\nu_9$ | $CCl_2$ rock | 262 C | ..... | 262 (1) dp | |

**References**


[1] IR. E. K. Plyler and W. S. Benedict, J. Res. NBS **47,** 202 (1951), RP 2245.
[2] R. IR. A. Davis, F. F. Cleveland, and A. G. Meister, J. Chem. Phys. **20,** 454 (1952).

**Molecule: Bromotrichlromethane $CBrCl_3$** No. 81

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Liquid) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CCl_3$ sym. stretch | 716 C | 719 VS | 716.3 (2) p | |
| | $\nu_2$ | CBr stretch | 422 C | 420 W | 422.3 (10) p | |
| | $\nu_3$ | $CCl_3$ sym. deform | 247 C | ..... | 247.3 (5) p | |
| $e$ | $\nu_4$ | $CCl_3$ deg. stretch | 775 C | 773 VS | 775.3 (1) dp | |
| | $\nu_5$ | CBr bend. ($\nu_6$) | 295 C | 294 W | 295.0 (3) dp | |
| | $\nu_6$ | $CCl_3$ deg. deform. ($\nu_5$) | 193 C | ..... | 193.3 (4) dp | |

## References


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


**Molecule: Dibromomethane $CH_2Br_2$** No. 82

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Liquid) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CH_2$ sym. stretch | 2989 C | 2989 W | 2988 M, p | |
| | $\nu_2$ | $CH_2$ scissors | 1389 C | 1389 M | 1387 M, p | |
| | $\nu_3$ | $CBr_2$ sym. stretch | 579 C | 579 M | 577 S, p | |
| | $\nu_4$ | $CBr_2$ scissors | 174 C | ..... | 174 S, p | |
| $a_2$ | $\nu_5$ | $CH_2$ twist | 1096 C | [a] 1096 W | 1089 W, dp | |
| $b_1$ | $\nu_6$ | $CH_2$ anti. stretch | 3065 C | 3065 S | 3061 W, dp | |
| | $\nu_7$ | $CH_2$ rock | 813 C | 813 M | | |
| $b_2$ | $\nu_8$ | $CH_2$ wag | 1192 C | 1192 S | 1183 W, dp | |
| | $\nu_9$ | $CBr_2$ anti. stretch | 638 C | 638 S | 639 W, dp | |

[a] Apparently the $C_{2v}$ selection rule does not hold in the liquid state.

## References


[1] R. J. Wagner, Z. Physik. Chem. **B45,** 69 (1939).
[2] R. M. L. Delwaulle and F. Francois, J. Phys. Radium **7,** 15 (1946).
[3] IR. E. K. Plyler, W. A. Smith, and N. Acquista, J. Res. NBS **44,** 503 (1950) RP2097.
[4] IR. I. Suzuki, unpublished work.

**Molecule: Dibromomethane-$d_1$ $CHDBr_2$** No. 83

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Liquid) | $cm^{-1}$ (Liquid) | |
| $a'$ | $\nu_1$ | CH stretch | 3030 C | 3030 M | | |
| | $\nu_2$ | CD stretch | 2247 C | 2247 W | | |
| | $\nu_3$ | CH bend | 1245 C | 1245 W | | |
| | $\nu_4$ | CD bend | 702 C | 702 M | | |
| | $\nu_5$ | $CBr_2$ sym. stretch | 563 C | 563 M | | |
| | $\nu_6$ | $CBr_2$ scissors | [a] 174 D | ..... | | |
| $a''$ | $\nu_7$ | CH bend | 1151 C | 1151 S | | |
| | $\nu_8$ | CD bend | 836 C | 836 M | | |
| | $\nu_9$ | $CBr_2$ anti. stretch | 622 C | 622 W | | |

[a] Assumed to have the same value as the corresponding frequencies of $CH_2Br_2$ and $CD_2Br_2$.

## References


[1] IR. I. Suzuki, unpublished work.


**Molecule: Dibromomethane-$d_2$ $CD_2Br_2$** No. 84

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Liquid) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CD_2$ sym. stretch | 2192 C | 2192 M | 2195 | |
| | $\nu_2$ | $CD_2$ scissors | 1028 C | 1028 W | 1023 | |
| | $\nu_3$ | $CBr_2$ sym. stretch | 553 C | 553 W | 548 | |
| | $\nu_4$ | $CBr_2$ scissors | 174 C | ..... | 174 | |
| $a_2$ | $\nu_5$ | $CD_2$ twist | 779 C | [a] 779 W | | |
| $b_1$ | $\nu_6$ | $CD_2$ anti. stretch | 2313 C | 2313 S | 2235 | |
| | $\nu_7$ | $CD_2$ rock | 637 C | 637 M | | |
| $b_2$ | $\nu_8$ | $CD_2$ wag | 901 C | 901 S | | |
| | $\nu_9$ | $CBr_2$ anti. stretch | 779 C | 779 S | | |

[a] Apparently the $C_{2v}$ selection rule does not hold in the liquid state.

## References


[1] R. B. Trumpy, Z. Physik. **100,** 250 (1936).
[2] IR. I. Suzuki, unpublished work.

**Molecule: Chlorobromomethane $CH_2ClBr$** No. 85

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a'$ | $\nu_1$ | $CH_2$ sym. stretch | 3003 A | 3003 S | 2986 M, p | |
| | $\nu_2$ | $CH_2$ scissors | 1482 D | [a] 1482 M | 1410 M, p | |
| | $\nu_3$ | $CH_2$ 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 | |
| | $\nu_6$ | $CCl_2$ scissors | 229 C | ..... | 229 S, p | |
| $a''$ | $\nu_7$ | $CH_2$ anti. stretch | 3066 B | 3066 W | 3055 M, dp | |
| | $\nu_8$ | $CH_2$ twist | 1128 C | 1127 W (liquid) | 1130 W | |
| | $\nu_9$ | $CH_2$ rock | 852 B | 852 W | 848 W | |

[a] The corresponding frequency in the liquid state is found at 1407 $cm^{-1}$. This band may be assigned to the overtone of the CCl stretching vibration.

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[1] IR. E. K. Plyler, W. A. Smith, and W. Acquista, J. Res. NBS **44**, 503 (1950) RP2097.
[2] IR.R. A. Weber, A. G. Meister, and F. F. Cleveland, J. Chem. Phys. **21**, 930 (1953).
[3] IR.R. A. N. Tanaka, K. V. Narasimham, A. G. Meister, J. M. Dowling, F. F. Cleveland, S. Sundaram, E. A. Piotrowski, R. B. Bernstein, and S. I. Miller, J. Mol. Spectry. **15**, 319 (1965).
[4] IR. I. Suzuki, unpublished work.


**Molecule: Chlorobromomethane-$d_1$ CHDClBr** No. 86

**Symmetry $C_1$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a$ | $\nu_1$ | CH stretch | 3031 C | [a] 3031 S | 3024 S, p | |
| | $\nu_2$ | CD stretch | 2252 C | [a] 2252 M | 2245 S, p | |
| | $\nu_3$ | CH bend | 1262 C | [a] 1262 S | 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 scissors | 228 C | ..... | 228 S, p | |

[a] The value in the liquid state.

**References**


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

**Molecule: Chlorobromomethane-$d_2$ $CD_2ClBr$** No. 87

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a'$ | $\nu_1$ | $CD_2$ sym. stretch | 2208 B | 2208 S | 2196 M, p | |
| | $\nu_2$ | $CD_2$ scissors | 1050 B | 1050 W | 1042 M, p | |
| | $\nu_3$ | $CD_2$ wag | 936 B | 936 S | 922 W, p | |
| | $\nu_4$ | CCl stretch | 717 B | 717 S | 702 M, p | |
| | $\nu_5$ | CBr stretch | 582 B | 582 S | 574 S, p | |
| | $\nu_6$ | CBrCl scissors | 226 C | ..... | 226 S, p | |
| $a''$ | $\nu_7$ | $CD_2$ anti. stretch | 2305 C | [a] 2305 S | 2305 W, dp | |
| | $\nu_8$ | $CD_2$ twist | 811 B | 811 W | 809 W, dp | |
| | $\nu_9$ | $CD_2$ rock | 667 C | [a] 668 W | 667 W, dp | |

[a] The value in the liquid state.

## References


[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. Spectry. **15**, 319 (1965).


**Molecule: Formaldehyde $H_2CO$** No. 88

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CH_2$ sym. stretch | 2766 E | 2766.4 S | 2781.6 S | |
| | $\nu_2$ | CO stretch | 1746 A | 1746.1 VS | 1742.3 W | |
| | $\nu_3$ | $CH_2$ scissors | 1501 A | 1500.6 S | 1499.7 M | |
| $b_1$ | $\nu_4$ | $CH_2$ anti. stretch | [a] 2843 E | 2843.4 VS | 2866 W | |
| | $\nu_5$ | $CH_2$ rock | 1247 B | 1247.4 S | | |
| $b_2$ | $\nu_6$ | $CH_2$ wag | 1164 B | 1163.5 S | | |

[a] The frequency has uncertainty due to the Fermi resonance between $\nu_4$ and $\nu_2 + \nu_5$.

## 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. Spectry. **1**, 124 (1957).
[3] IR. K. B. Harvey and J. F. Ogilvie, Can. J. Chem. **40**, 85 (1962).

**Molecule: Formaldehyde-$d_1$ HDCO** No. 89

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a'$ | $\nu_1$ | CH stretch | [a] 2844 E | 2844.1 S | 2846.2 S | |
| | $\nu_2$ | CD stretch | [b] 2121 B | 2120.7 S | 2120.3 S | |
| | $\nu_3$ | CO stretch | 1723 A | 1723.4 VS | 1723.2 VS | |
| | $\nu_4$ | CHD scissors | 1400 A | 1400.0 S | 1397.4 M | |
| | $\nu_5$ | CHD rock | 1041 E | 1041 S | | |
| $a''$ | $\nu_6$ | CHD wag | 1074 E | 1074 S | | |

[a] The frequency has uncertainty due to the Fermi resonance between $\nu_1$ and $\nu_3+\nu_5$.
[b] The frequency has uncertainty due to the Fermi resonances among $\nu_2$, $2\nu_6$, and $2\nu_5$.

## References


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


**Molecule: Formaldehyde-$d_2$ $D_2CO$** No. 90

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CD_2$ sym. stretch | [a] 2056 E | 2056.4 S | | |
| | $\nu_2$ | CO stretch | 1700 C | 1700 VS | | |
| | $\nu_3$ | $CD_2$ scissors | 1106 C | 1106.0 S | | |
| $b_1$ | $\nu_4$ | $CD_2$ anti. stretch | 2160 E | 2160.3 VS | | |
| | $\nu_5$ | $CD_2$ rock | 990 E | 990.2 S | | |
| $b_2$ | $\nu_6$ | $CD_2$ wag | 938 E | 938 S | | |

[a] The frequency has uncertainty due to the Fermi resonance between $\nu_1$ and $2\nu_3$.

## References


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

**Molecule: Methylbromide $CH_3Br$** No. 91

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CH_3$ sym. stretch..... | 2935 E | 2972 M<br>2861 M | 2972 VS<br>2862 W | FR($2\nu_5$). |
| | $\nu_2$ | $CH_3$ sym. deform..... | 1305 A | 1305 S | 1309 W | |
| | $\nu_3$ | CBr stretch..... | 611 A | 611 S | 609 S | |
| $e$ | $\nu_4$ | $CH_3$ deg. stretch..... | 3057 A | 3056.7 S | 3068 VS | |
| | $\nu_5$ | $CH_3$ deg. deform..... | 1443 A | 1442.8 M | 1456 M | |
| | $\nu_6$ | $CH_3$ rock..... | 954 A | 954.3 M | 956 VW | |

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[1] R. H. L. Welsh, M. F. Crawford, T. R. Thomas, and G. R. Love, Can. J. Phys. **30,** 577 (1952).
[2] IR. H. B. Weissman, R. B. Bernstein, S. E. Rosser, A. G. Meister, and F. F. Cleveland, J. Chem. Phys. **23,** 544 (1955).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38,** 443 (1965).
[4] IR. Y. Morino, J. Nakamura, and S. Yamamoto, Bull. Chem. Soc. Japan **38,** 459 (1965).
[5] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22,** 647 (1966).


**Molecule: Methylbromide-$d_3$ $CD_3Br$** No. 92

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CD_3$ sym. stretch..... | 2157 E | 2157 VS | ..... | FR($2\nu_5$). |
| | $\nu_2$ | $CD_3$ sym. deform..... | 993 A | 993.4 VS | | |
| | $\nu_3$ | CBr stretch..... | 578 A | 577.9 S | | |
| $e$ | $\nu_4$ | $CD_3$ deg. stretch..... | 2296 A | 2296.3 M | | |
| | $\nu_5$ | $CD_3$ deg. deform..... | 1056 A | 1055.6 S | | |
| | $\nu_6$ | $CD_3$ rock..... | 713 A | 713.1 M | | |

**References**


[1] IR. H. B. Weissman, R. B. Bernstein, S. E. Roser, A. G. Meister, and F. F. Cleveland, J. Chem. Phys. **23,** 544 (1955).
[2] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38,** 443 (1965).
[3] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22,** 639 (1966).

**Molecule: Methylchloride $CH_3Cl$** No. 93

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CH_3$ sym. stretch..... | 2937 E | 2966.7 M<br>2878.7 M | 2955 VS, p<br>2861 M | FR($2\nu_5$). |
| | $\nu_2$ | $CH_3$ sym. deform..... | 1355 A | 1354.9 S | 1370 VW, p | |
| | $\nu_3$ | CCl stretch..... | 732 A | 732.1 S | 709 VS, p | |
| $e$ | $\nu_4$ | $CH_3$ deg. stretch..... | 3042 A | 3042.4 S | 3036 M, dp | |
| | $\nu_5$ | $CH_3$ deg. deform..... | 1452 A | 1452.1 M | 1446 W, dp | |
| | $\nu_6$ | $CH_3$ rock..... | 1017 A | 1017.3 M | 1016 W, dp | |

**References**


[1] R. J. Wagner, Z. Physik. Chem. **B40**, 439 (1938).
[2] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) **A222**, 443 (1954).
[3] IR. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1964).
[4] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[5] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22**, 669 (1966).


**Molecule: Methylchloride-$d_3$ $CD_3Cl$** No. 94

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CD_3$ sym. stretch..... | 2141 E | 2161 S<br>2103 M | ..... | FR($2\nu_5$). |
| | $\nu_2$ | $CD_3$ sym. deform..... | 1029 A | 1029 S | | |
| | $\nu_3$ | CCl stretch..... | 695 A | 695 S | | |
| $e$ | $\nu_4$ | $CD_3$ deg. stretch..... | 2283 A | 2283.4 S | | |
| | $\nu_5$ | $CD_3$ deg. deform..... | 1060 A | 1059.9 M | | |
| | $\nu_6$ | $CD_3$ rock..... | 768 A | 767.7 M | | |

**References**


[1] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) **A222**, 443 (1954).
[2] IR. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1964).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[4] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Spectrochim. Acta **22**, 659 (1966).

**Molecule: Methylfluoride $CH_3F$** No. 95

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CH_3$ sym. stretch..... | 2930 E | 2964 VS<br>2863 S | ..... | FR($2\nu_5$). |
| | $\nu_2$ | $CH_3$ sym. deform..... | 1464 A | 1464 S | | |
| | $\nu_3$ | CF stretch..... | 1049 A | 1048.6 S | | |
| $e$ | $\nu_4$ | $CH_3$ deg. stretch..... | 3006 A | 3005.8 S | | |
| | $\nu_5$ | $CH_3$ deg. deform..... | 1467 A | 1466.5 M | | |
| | $\nu_6$ | $CH_3$ rock..... | 1182 A | 1182.4 M | | |

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[1] IR. K. P. Yates and H. H. Nielsen, Phys. Rev. **71,** 349 (1947).
[2] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) **A222,** 443 (1954).
[3] IR. F. A. Anderson, B. Bak, and S. Brodersen, J. Chem. Phys. **24,** 989 (1956).
[4] IR. W. L. Smith and I. M. Mills, J. Mol. Spectry. **11,** 11 (1963).
[5] IR. E. W. Jones, E. J. L. Popplewell, and H. W. Thompson, Proc. Roy. Soc. (London) **A290,** 490 (1966).


**Molecule: Methylfluoride-$d_3$ $CD_3F$** No. 96

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CD_3$ sym. stretch..... | 2110 E | 2090<br>2150 | ..... | FR($2\nu_5$). |
| | $\nu_2$ | $CD_3$ sym. deform..... | 1136 A | 1136 | | |
| | $\nu_3$ | CF stretch..... | 991 A | 991 | | |
| $e$ | $\nu_4$ | $CD_3$ deg. stretch..... | 2258 A | 2258 | | |
| | $\nu_5$ | $CD_3$ deg. deform..... | 1072 A | 1072 | | |
| | $\nu_6$ | $CD_3$ rock..... | 903 A | 903 | | |

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[1] IR. J. Pickworth and H. W. Thompson, Proc. Roy. Soc. (London) **A222,** 443 (1954).
[2] IR. W. F. Edgell and L. Parts, J. Am. Chem. Soc. **78,** 2358 (1956).
[3] IR. E. W. Jones, E. J. L. Popplewell, and H. W. Thompson, Proc. Roy. Soc. (London) **A290,** 490 (1966).

**Molecule: Methyliodide $CH_3I$** No. 97

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CH_3$ sym. stretch..... | 2933 E | 2969.8 M<br>2861.0 M | ..... | FR($2\nu_5$). |
| | $\nu_2$ | $CH_3$ sym. deform..... | 1252 A | 1251.5 S | | |
| | $\nu_3$ | Cl stretch..... | 533 A | 532.8 S | | |
| $e$ | $\nu_4$ | $CH_3$ deg. stretch..... | 3060 A | 3060.3 S | | |
| | $\nu_5$ | $CH_3$ deg. deform..... | 1437 A | 1437.4 M | | |
| | $\nu_6$ | $CH_3$ rock..... | 882 A | 882.4 M | | |

**References**


[1] Th. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1957).
[2] IR. E. W. Jones and H. W. Thompson, Proc. Roy. Soc. (London) **A288**, 50 (1965).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[4] IR. Y. Morino, J. Nakamura, and S. Yamamoto, to be published.


**Molecule: Methyliodide-$d_3$ $CD_3I$** No. 98

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CD_3$ sym. stretch..... | 2130 E | 2155.1<br>2081.0 | ..... | FR($2\nu_5$). |
| | $\nu_2$ | $CD_3$ sym. deform..... | 951 A | 950.7 | | |
| | $\nu_3$ | CI stretch..... | 501 A | 501.4 | | |
| $e$ | $\nu_4$ | $CD_3$ deg. stretch..... | 2298 E | 2298 | | |
| | $\nu_5$ | $CD_3$ deg. deform..... | 1049 A | 1049.3 | | |
| | $\nu_6$ | $CD_3$ rock..... | 656 A | 655.9 | | |

**References**


[1] Th. W. T. King, I. M. Mills, and B. Crawford, Jr., J. Chem. Phys. **27**, 455 (1957).
[2] IR. E. W. Jones, R. J. L. Popplewell, and H. W. Thompson, Proc. Roy. Soc. (London) **A288**, 39 (1965).
[3] IR. Y. Morino and J. Nakamura, Bull. Chem. Soc. Japan **38**, 443 (1965).
[4] IR. Y. Morino, J. Nakamura, and S. Yamamoto, to be published.

**Molecule: Methylamine $CH_3NH_2$** No. 99

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | | Infrared [2] | Raman [1] | Comments |
|---|---|---|---|---|---|---|---|
| | | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a'$ | $\nu_1$ | $NH_2$ sym. stretch | 3361 | B | 3361 W | 3360 VS | |
| | $\nu_2$ | $CH_3$ deg. stretch | 2961 | B | 2961 VS | 2960 VS | |
| | $\nu_3$ | $CH_3$ sym. stretch | 2820 | B | 2820 VS | 2820 S | |
| | $\nu_4$ | $NH_2$ scissors | 1623 | B | 1623 S | | |
| | $\nu_5$ | $CH_3$ deg. deform | 1473 | B | 1473 S | 1460 M | |
| | $\nu_6$ | $CH_3$ sym. deform | 1430 | B | 1430 M | | |
| | $\nu_7$ | $CH_3$ rock | 1130 | A | 1130 M | | |
| | $\nu_8$ | CN stretch | 1044.2 | A | 1044 S | 1044 S | |
| | $\nu_9$ | $NH_2$ wag | 780.1 | A [3] | 780 VS | 781 W | |
| $a''$ | $\nu_{10}$ | $NH_2$ anti. stretch | 3427 | C | 3427 W | 3470 W | |
| | $\nu_{11}$ | $CH_3$ deg. stretch | 2985 | C | 2985 VS | | |
| | $\nu_{12}$ | $CH_3$ deg. deform | 1485 | D | [a] 1485 | | |
| | $\nu_{13}$ | $NH_2$ twist | 1419 | D | ..... | ..... | CF.[b] |
| | $\nu_{14}$ | $CH_3$ rock | 1195 | D | [a] 1195 | | |
| | $\nu_{15}$ | CN torsion | 268 | A | 200 ~ 330 | | |

[a] Estimated from $^RQ$ branch frequency.

[b] Calculated from the force constants which correlate the frequencies of $CH_3NH_2$, $CH_3ND_2$, $CD_3NH_2$, and $CD_3ND_2$ including the $ND_2$ twisting frequency of $CD_3NH_2$.

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[1] R. J. S. Kirby-Smith and L. G. Booner, J. Chem. Phys. **7**, 880 (1939).
[2] IR. A. P. Gray and R. C. Lord, J. Chem. Phys. **26**, 690 (1957).
[3] IR. M. Tsuboi, A. Y. Hirakawa, T. Ino, T. Sasaki, and K. Tamagake, J. Chem. Phys.
[4] IR. M. Tsuboi, A. Y. Hirakawa, and K. Tamagake, to be published.

**Molecule:** **Methylamine-$d_2$** **$CH_3ND_2$ (gas)** No. 100

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared [2] | Raman [1] | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a'$ | $\nu_1$ | $ND_2$ sym. stretch | 2479 B | 2479 W | 2450 S | |
| | $\nu_2$ | $CH_3$ deg. stretch | 2961 B | 2961 VS | 2969 M | |
| | $\nu_3$ | $CH_3$ sym. stretch | 2817 B | 2817 S | 2824 M | |
| | $\nu_4$ | $ND_2$ scissors ($\nu_7$, $\nu_9$) | 1234 B | 1234 S | 1214 M | |
| | $\nu_5$ | $CH_3$ deg. deform | 1468 B | 1468 S | 1473 M | |
| | $\nu_6$ | $CH_2$ sym. deform | 1430 B | 1430 M | | |
| | $\nu_7$ | $CH_3$ rock. ($\nu_4$) | 1117 A | 1117 S | | |
| | $\nu_8$ | CN stretch. ($\nu_4$) | 997 A | 997 S | 995 S | |
| | $\nu_9$ | $ND_2$ wag | 625.4 [3] | 624 VS | | |
| $a''$ | $\nu_{10}$ | $ND_2$ anti. stretch | 2556 B | 2556 M | 2527 M | |
| | $\nu_{11}$ | $CH_3$ deg. stretch | 2985 C | 2985 VS | | |
| | $\nu_{12}$ | $CH_3$ deg. deform | 1485 D | [a] 1485 | | |
| | $\nu_{13}$ | $ND_2$ twist. ($\nu_{14}$) | 1058 D | ..... | ..... | CF.[b] |
| | $\nu_{14}$ | $CH_3$ rock. ($\nu_{13}$) | 1187 C | 1187 M | | |
| | $\nu_{15}$ | CN torsion | 228 | 180 ~ 280 S | | |

[a] Estimated from $^RQ$ branch frequency.

[b] Calculated from the force constants which correlate the frequencies of $CH_3NH_2$, $CH_3ND_2$, $CD_3NH_2$, and $CD_3ND_2$ including the $ND_2$ twisting frequency of $CD_3NH_2$.

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[3] IR. M. Tsuboi. A. Y. Hirakawa. T. Sasaki. and K. Tamagake. to be published.
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**Molecule:** **Methylamine-$d_3$** **$CD_3NH_2$ (gas)** No. 101

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | | Infrared [1] | Raman | Comments |
|---|---|---|---|---|---|---|---|
| | | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a'$ | $\nu_1$ | $NH_2$ sym. stretch | 3361 | B | 3361 W | | |
| | $\nu_2$ | $CD_3$ deg. stretch | 2203 | B | 2203 VS | | |
| | $\nu_3$ | $CD_3$ sym. stretch | 2077 | A | 2077 VS | | |
| | $\nu_4$ | $NH_2$ scissors ($\nu_9$) | 1624 | B | 1624 S | | |
| | $\nu_5$ | $CD_3$ deg. deform | 1065 | D | | | CF.[a] |
| | $\nu_6$ | $CD_3$ sym. deform | 1142 | A | 1142 S | | |
| | $\nu_7$ | $CD_3$ rock. ($\nu_9$) | 913 | A | 913 S | | |
| | $\nu_8$ | CN stretch. ($\nu_6$) | 973 | B | 973 M | | |
| | $\nu_9$ | $NH_2$ wag. ($\nu_7$) | 740.4 | A [2] | 740 VS | | |
| $a''$ | $\nu_{10}$ | $NH_2$ anti. stretch | 3427 | C | 3427 W | | |
| | $\nu_{11}$ | $CD_3$ deg. stretch | 2236 | C | 2236 VS | | |
| | $\nu_{12}$ | $CD_3$ deg. deform | 1077 | C | 1077 W | | |
| | $\nu_{13}$ | $NH_2$ twist | 1416 | C | 1416 W | | |
| | $\nu_{14}$ | $CD_3$ rock | 926 | D | | | CF.[a] |
| | $\nu_{15}$ | CN torsion | 247 | D | | | CF.[a] |

[a] Calculated from the force constants which correlate the frequencies of $CH_3NH_2$, $CH_3ND_2$, $CD_3NH_2$, and $CD_3ND_2$.

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**Molecule: Methylamine-$d_5$ $CD_3ND_2$(Gas)** No. 102

**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared [1] | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a'$ | $\nu_1$ | $ND_2$ sym. stretch | 2477 B | 2477 W | | |
| | $\nu_2$ | $CD_3$ deg. stretch | 2202 B | 2202 VS | | |
| | $\nu_3$ | $CD_3$ sym. stretch | 2073 B | 2073 VS | | |
| | $\nu_4$ | $ND_2$ scissors ($\nu_7$, $\nu_9$) | 1227 B | 1227 S | | |
| | $\nu_5$ | $CD_3$ deg. deform | 1065 D | | | CF.[a] |
| | $\nu_6$ | $CD_3$ sym. deform | 1123 B | 1123 M | | |
| | $\nu_7$ | $CD_3$ rock. ($\nu_8$, $\nu_9$) | 880 B | 880 M | | |
| | $\nu_8$ | CN stretch ($\nu_6$, $\nu_7$) | 942 A | 942 S | | |
| | $\nu_9$ | $ND_2$ wag | 601 A | 601 VS | | |
| $a''$ | $\nu_{10}$ | $ND_2$ anti. stretch | 2556 C | 2556 W | | |
| | $\nu_{11}$ | $CD_3$ deg. stretch | 2238 C | 2238 VS | | |
| | $\nu_{12}$ | $CD_3$ deg. deform | 1077 C | 1077 W | | |
| | $\nu_{13}$ | $ND_2$ twist ($\nu_{14}$) | 1072 D | | | CF.[a] |
| | $\nu_{14}$ | $CD_3$ rock | 910 B | 910 M | | |
| | $\nu_{15}$ | CN torsion | 201 D | | | CF.[a] |

[a] Calculated from the force constants which correlate the frequencies of $CH_3NH_2$. $CH_3ND_2$. $CD_3NH_2$. and $CD_3ND_2$.

**References**


[1] IR. A. P. Gray and R. C. Lord. J. Chem. Phys. **26**, 690 (1957).


**Molecule: Methylcyanide $CH_3CN$** No. 103

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CH_3$ sym. stretch | 2965 A | 2965.3 M | 2942 VS | |
| | $\nu_2$ | CN stretch | 2267 A | 2267.3 M | 2249 S | |
| | $\nu_3$ | $CH_3$ sym. deform | 1400 C | 1400.0 S | 1376 M | |
| | $\nu_4$ | CC stretch | 920 A | 919.9 S | 918 S | |
| $e$ | $\nu_5$ | $CH_3$ deg. stretch | 3009 A | 3009.0 S | 2999 S | |
| | $\nu_6$ | $CH_3$ deg. deform | 1454 A | 1454.0 S | 1440 M. b | |
| | $\nu_7$ | $CH_3$ rock | 1041 A | 1041.0 M | 1124 VW | |
| | $\nu_8$ | CCN bend | 361 A | 361.0 S | 380 S | |

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**Molecule: Methylcyanide-$d_3$ $CD_3CN$** No. 104

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ | |
| $a_1$ | $\nu_1$ | $CD_3$ sym. stretch..... | 2107 A | 2106.9 | | |
| | $\nu_2$ | CN stretch..... | 2278 A | 2277.5 | | |
| | $\nu_3$ | $CD_3$ sym. deform..... | 1112 A | 1112.2 | | |
| | $\nu_4$ | CC stretch..... | 831 A | 831.4 | | |
| $e$ | $\nu_5$ | $CD_3$ deg. stretch..... | 2258 A | 2258.4 | | |
| | $\nu_6$ | $CD_3$ deg. deform..... | 1046 A | 1045.7 | | |
| | $\nu_7$ | $CD_3$ rock..... | 847 A | 846.6 | | |
| | $\nu_8$ | CCN bend..... | 333 A | 333.2 | | |

**References**


[1] IR. Y. Morino and J. Nakamura, to be published.


**Molecule: Ethylene oxide $C_2H_4O$** No. 105

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CH_2$ sym. stretch..... | 3006 C | 3006 S | 3005 S, p | SF($\nu_9$). |
| | $\nu_2$ | $CH_2$ scissors..... | 1498 B | 1498 W | 1490 W, p | |
| | $\nu_3$ | Ring stretch. (ring breath)..... | 1271 B | 1271 S | 1266 S, p | |
| | $\nu_4$ | $CH_2$ wag..... | 1130 D | 1118 W ($CS_2$ soln.) | 1120 M, p | |
| | $\nu_5$ | Ring stretch+deform..... | 877 B | 877 VS | 867 M, dp | |
| $a_2$ | $\nu_6$ | $CH_2$ anti. stretch..... | 3065 D | ia | 3063 W, dp | SF($\nu_{13}$). |
| | $\nu_7$ | $CH_2$ twist..... | 1300 E | ia | | |
| | $\nu_8$ | $CH_2$ rock..... | 860 E | ia | | |
| $b_1$ | $\nu_9$ | $CH_2$ sym. stretch..... | 3006 C | 3006 S | 3005 S, p | SF($\nu_1$). |
| | $\nu_{10}$ | $CH_2$ scissors..... | 1472 B | 1472 W | | |
| | $\nu_{11}$ | $CH_2$ wag..... | 1151 D | 1151 M | 1150 W, dp | |
| | $\nu_{12}$ | Ring stretch+deform..... | 890 E | ..... | ..... | CF [4]. |
| $b_2$ | $\nu_{13}$ | $CH_2$ anti. stretch..... | 3065 B | 3065 S | 3063 W, dp | SF($\nu_6$). |
| | $\nu_{14}$ | $CH_2$ twist..... | 1142 D | 1142 M | 1150 W, dp | |
| $b_2$ | $\nu_{15}$ | $CH_2$ rock..... | 822 B | 822 M | 807 M, dp | |

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[4] IR. R. C. Lord and B. Nolin, J. Chem. Phys. **24**, 656 (1956).
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**Molecule:** **Ethylene oxide-$d_4$** $C_2D_4O$ No. 106

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a_1$ | $\nu_1$ | $CD_2$ sym. stretch..... | 2204 C | ..... | 2204 S | |
| | $\nu_2$ | $CD_2$ scissors..... | 1311 C | 1311 M | 1301 VS | |
| | $\nu_3$ | Ring stretch. (ring breath)..... | 1013 C | 1014 W | 1013 S | |
| | $\nu_4$ | $CD_2$ wag..... | 970 C | 970 VS | 952 M | |
| | $\nu_5$ | Ring stretch. + deform..... | 755 C | 755 VS | 755 M | |
| $a_2$ | $\nu_6$ | $CD_2$ anti. stretch..... | 2250 C | ia | 2250 W | |
| | $\nu_7$ | $CD_2$ twist..... | 1083 D | ia | 1083 VW | |
| | $\nu_8$ | $CD_2$ rock..... | 581 C | ia | 581 W | |
| $b_1$ | $\nu_9$ | $CD_2$ sym. stretch..... | 2174 C | 2174 VS | 2157 M | |
| | $\nu_{10}$ | $CD_2$ scissors..... | 1145 D | 1145 VW | | |
| | $\nu_{11}$ | $CD_2$ wag..... | 952 D | ..... | 952 M | |
| | $\nu_{12}$ | Ring stretch. + deform..... | 809 C | 809 S | 786 M | |
| $b_2$ | $\nu_{13}$ | $CD_2$ anti. stretch..... | 2317 C | 2317 VS | 2319 S | |
| | $\nu_{14}$ | $CD_2$ twist..... | 896 C | 896 S | 896 W | |
| | $\nu_{15}$ | $CD_2$ rock..... | 577 C | 577 W | | |

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**Symmetry $C_s$** **Symmetry number $\sigma = 1$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a'$ | $\nu_1$ | NH stretch | 3338 B | 3338 W | 3302 M, p | |
| | $\nu_2$ | $CH_2$ anti. stretch | 3079 D | 3079 S | 3059 M, dp | SF($\nu_{11}$). |
| | $\nu_3$ | $CH_2$ sym. stretch | 3015 D | 3015 S | 2999 VS, p | SF($\nu_{12}$). |
| | $\nu_4$ | $CH_2$ scissors | 1482 B | 1482 W | 1471 W, p | |
| | $\nu_5$ | Ring stretch. (ring breath) | 1211 B | 1211 S | 1212 VS, p | |
| | $\nu_6$ | $CH_2$ twist | 1095 D | 1095 S | 1088 W, p | |
| | $\nu_7$ | $CH_2$ wag | 1090 D | 1090 S | 1088 W, p | |
| | $\nu_8$ | NH bend | 998 C | 998 M | 1028 W | |
| | $\nu_9$ | Ring stretch. + deform. | 856 B | 856 VS | 855 M, dp | |
| | $\nu_{10}$ | $CH_2$ rock | 773 B | 773 S | 787 W, dp | |
| $a''$ | $\nu_{11}$ | $CH_2$ anti. stretch | 3079 D | 3079 S | 3059 M, dp | SF($\nu_2$). |
| | $\nu_{12}$ | $CH_2$ sym. stretch | 3015 D | 3015 S | 2999 VS, p | SF($\nu_3$). |
| | $\nu_{13}$ | $CH_2$ scissors | 1463 B | 1463 W | 1452 W, dp | |
| | $\nu_{14}$ | $CH_2$ twist | 1268 C | 1268 M | 1276 VW | |
| $a''$ | $\nu_{15}$ | NH bend | 1237 C | 1237 M | 1297 W, p | |
| | $\nu_{16}$ | $CH_2$ wag | 1131 B | 1131 M | 1130 VW | |
| | $\nu_{17}$ | Ring stretch. + deform. | 904 B | 904 S | | |
| | $\nu_{18}$ | $CH_2$ rock | 817 D | ..... | 817 M, dp | |

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[2] IR. H. T. Hoffman, Jr., G. E. Evans, and G. Glockler, J. Am. Chem. Soc. **73**, 3028 (1951).
[3] R.IR. W. J. Potts, Spectrochim. Acta **21**, 511 (1965).

**Molecule: Cyclopropane $C_3H_6$** No. 108

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ | |
| $a_1'$ | $\nu_1$ | $CH_2$ sym. stretch | 3038 C | ia | 3038 S, p | |
| | $\nu_2$ | $CH_2$ scissors | 1475 D | ia | 1504 W, p<br>1453 W, p | FR($2\nu_{14}$). |
| | $\nu_3$ | Ring stretch. (ring breath) | 1188 C | ia | 1188 S, p | |
| $a_1''$ | $\nu_4$ | $CH_2$ twist | 1133 D | ia | ia | |
| $a_2'$ | $\nu_5$ | $CH_2$ wag | 1078 D | ia | ia | |
| $a_2''$ | $\nu_6$ | $CH_2$ anti. stretch | 3101 C | 3101 S | ia | |
| | $\nu_7$ | $CH_2$ rock | 852 C | 852 S | ia | |
| $e'$ | $\nu_8$ | $CH_2$ sym. stretch | 3025 C | 3025 VS | 3019 VS, p | |
| | $\nu_9$ | $CH_2$ scissors | 1442 C | 1442 M | 1443 M, dp | |
| | $\nu_{10}$ | $CH_2$ wag | 1028 C | 1028 S | 1023 VW (liquid). | |
| | $\nu_{11}$ | Ring stretch. + deform. | 866 C | 866 VS | 866 S, dp | |
| $e''$ | $\nu_{12}$ | $CH_2$ anti. stretch | 3082 C | ia | 3090 S, dp | |
| | $\nu_{13}$ | $CH_2$ twist | 1178 C | ia | 1178 M | |
| | $\nu_{14}$ | $CH_2$ rock | 739 C | ia | 739 W, dp | |

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[5] IR. C. Brecher, E. Krikorian, J. Blanc, and R. S. Halford, J. Chem. Phys. **35**, 1097 (1961).

**Molecule:** **Cyclopropane-$d_6$** **$C_3D_6$** No. 109

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ | $cm^{-1}$ (Liquid) | |
| $a_1'$ | $\nu_1$ | $CD_2$ sym. stretch..... | 2236 C | ia | 2236 VS, p | |
| | $\nu_2$ | $CD_2$ scissors..... | 1274 C | ia | 1274 S, p | |
| | $\nu_3$ | Ring stretch. (ring breath)..... | 956 C | ia | 956 S, p | |
| $a_1''$ | $\nu_4$ | $CD_2$ twist..... | 801 E | ia | ia | CF. |
| $a_2'$ | $\nu_5$ | $CD_2$ wag..... | 873 E | ia | ia | CF. |
| $a_2''$ | $\nu_6$ | $CD_2$ anti. stretch..... | 2336 C | 2336 VS | ia | |
| | $\nu_7$ | $CD_2$ rock..... | 614 C | 614 W | ia | |
| $e'$ | $\nu_8$ | $CD_2$ sym. stretch..... | 2211 C | 2211 VS | 2204 W, dp | |
| | $\nu_9$ | $CD_2$ scissors..... | 1074 C | 1074 S | 1068 W, dp | |
| | $\nu_{10}$ | $CD_2$ wag..... | 887 C | 887 M | 884 M, dp | |
| | $\nu_{11}$ | Ring stretch. + deform..... | 720 C | 720 VS | 721 M, dp | |
| $e''$ | $\nu_{12}$ | $CD_2$ anti. stretch..... | 2329 C | ia | 2329 S, p | |
| | $\nu_{13}$ | $CD_2$ twist..... | 928 E | ia | ..... | CF. |
| | $\nu_{14}$ | $CD_2$ rock..... | 528 C | ia | 528 W, dp | |

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**Molecule: Cyclobutane $C_4H_8$** No. 110

**Symmetry $D_{2d}(D_{4h})$** **Symmetry number $\sigma = 4(8)$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1(a_{1g})$ | $\nu_1$ | $CH_2$ sym. stretch..... | [a] 2895 D | ia | 2916 p<br>2866 p | FR($2\nu_2$, $2\nu_{13}$). |
| | $\nu_2$ | $CH_2$ scissors..... | 1443 C | ia | 1443 p | SF($\nu_{13}$). |
| | $\nu_3$ | CC stretch. (ring breathing)..... | 1001 C | ia | 1001 p | SF($\nu_{14}$). |
| $a_1(b_{1u})$ | $\nu_4$ | $CH_2$ anti. stretch..... | 2975 E | ia | ..... | CF [3]. |
| | $\nu_5$ | $CH_2$ rock..... | 741 C | ia | 741 dp | |
| | $\nu_6$ | Ring puckering..... | 200 E | ia | ..... | CF [3]. |
| $a_2(a_{2g})$ | $\nu_7$ | $CH_2$ wag..... | 1260 E | ia | ia | CF [3]. |
| $a_2(b_{2u})$ | $\nu_8$ | $CH_2$ twist..... | 1257 E | ia | ia | CF [3]. |
| $b_1(b_{1g})$ | $\nu_9$ | $CH_2$ wag..... | 1219 C | ia | 1219 dp | |
| | $\nu_{10}$ | CC stretch. (ring deform.)..... | 926 C | ia | 926 dp | |
| $b_1(a_{1u})$ | $\nu_{11}$ | $CH_2$ twist..... | 1222 E | ia | ..... | CF [3]. |
| $b_2(b_{2g})$ | $\nu_{12}$ | $CH_2$ sym. stretch..... | 2893 E | ..... | ..... | CF [3]. |
| | $\nu_{13}$ | $CH_2$ scissors..... | 1443 C | ..... | 1443 dp | SF($\nu_2$). |
| | $\nu_{14}$ | CCC deform. (ring deform.)..... | 1001 D | ..... | (1001 p) | SF($\nu_3$). |
| $b_2(a_{2u})$ | $\nu_{15}$ | $CH_2$ anti. stretch..... | 2987 C | 2987 S | | |
| | $\nu_{16}$ | $CH_2$ rock..... | 627 C | 627 S | | |
| $e(e_g)$ | $\nu_{17}$ | $CH_2$ anti. stretch..... | 2952 C | ..... | 2952 dp? | |
| | $\nu_{18}$ | $CH_2$ twist..... | 1223 C | 1223 W | | |
| | $\nu_{19}$ | $CH_2$ rock..... | 749 C | 749 W | | |
| $e(e_u)$ | $\nu_{20}$ | $CH_2$ sym. stretch..... | 2887 D | 2997<br>2878 | | |
| | $\nu_{21}$ | $CH_2$ scissors..... | 1447 C | 1447 S | | |
| | $\nu_{22}$ | $CH_2$ wag..... | 1257 C | 1257 S | | |
| | $\nu_{23}$ | CC stretch. and CCC deform. (ring deform.)..... | 898 C | 898 S | | |

[a] Corrected for a presumed shift due to Fermi resonance.

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**Molecule:** **Cyclobutane-$d_8$** $C_4D_8$ No. 111

**Symmetry $D_{2d}(D_{4h})$** **Symmetry number $\sigma = 4(8)$**

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared [1] | Raman [1] | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Gas) | $cm^{-1}$ (Liquid) | |
| $a_1(a_{1g})$ | $\nu_1$ | $CD_2$ sym. stretch | 2124 E | ia | ..... | CF [2]. |
| | $\nu_2$ | $CD_2$ scissors | 1160 C | ia | 1160 p | |
| | $\nu_3$ | CC stretch. (ring breathing) | 882 C | ia | 882 p | |
| $a_1(b_{1u})$ | $\nu_4$ | $CD_2$ anti. stretch | 2224 E | ia | ..... | CF [2]. |
| | $\nu_5$ | $CD_2$ rock | 632 E | ia | ..... | CF [2]. |
| | $\nu_6$ | Ring puckering | 151 E | ia | ..... | CF [2]. |
| $a_2(a_{2g})$ | $\nu_7$ | $CD_2$ wag | 1010 E | ia | ia | CF [2]. |
| $a_2(b_{2u})$ | $\nu_8$ | $CD_2$ twist | 889 E | ia | ia | CF [2]. |
| $b_1(b_{1g})$ | $\nu_9$ | $CD_2$ wag | 1078 C | ia | 1078 dp | |
| | $\nu_{10}$ | CC stretch. (ring deform.) | 746 C | ia | 746 dp | |
| $b_1(a_{1u})$ | $\nu_{11}$ | $CD_2$ twist | 864 E | ia | ..... | CF [2]. |
| $b_2(b_{2g})$ | $\nu_{12}$ | $CD_2$ sym. stretch | 2115 E | ..... | ..... | CF [2]. |
| | $\nu_{13}$ | $CD_2$ scissors | 1040 D | ..... | 1040 dp | |
| | $\nu_{14}$ | CCC deform. (ring deform.) | 938 D | ..... | 938 dp | SF($\nu_{18}$). |
| $b_2(a_{2u})$ | $\nu_{15}$ | $CD_2$ anti. stretch | 2242 C | 2242 S | | |
| | $\nu_{16}$ | $CD_2$ rock | 483 C | 483 S | | |
| $e(e_g)$ | $\nu_{17}$ | $CD_2$ anti. stretch | 2230 C | ..... | 2230 dp? | |
| | $\nu_{18}$ | $CD_2$ twist | 938 D | ..... | 938 dp | SF($\nu_{14}$). |
| | $\nu_{19}$ | $CD_2$ rock | 556 C | 556 W | | |
| $e(e_g)$ | $\nu_{20}$ | $CD_2$ sym. stretch | 2103 E | ..... | ..... | CF [2]. |
| | $\nu_{21}$ | $CD_2$ scissors | 1078 C | 1078 S | | |
| | $\nu_{22}$ | $CD_2$ wag | 1048 C | 1048 S | | |
| | $\nu_{23}$ | CC stretch. and CCC deform. (ring. deform.) | 734 C | 734 S | | |

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**Molecule: Polyethylene $(CH_2)_n$** No. 112

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Solid) | $cm^{-1}$ (Solid) | |
| $a_g$ | $\nu_1$ | $CH_2$ sym. stretch..... | 2848 C | ia | 2848 S | |
| | $\nu_2$ | $CH_2$ scissors..... | 1440 C | ia | 1440 M | |
| | $\nu_3$ | CC stretch. + CCC deform..... | 1131 C | ia | 1131 M | |
| $b_{1g}$ | $\nu_4$ | $CH_2$ wag..... | 1415 C | ia | 1415 W | |
| | $\nu_5$ | CC stretch..... | 1061 C | ia | 1061 M | |
| $b_{2g}$ | $\nu_6$ | $CH_2$ twist..... | 1295 C | ia | 1295 M | |
| $b_{3g}$ | $\nu_7$ | $CH_2$ anti. stretch..... | 2883 C | ia | 2883 S | |
| | $\nu_8$ | $CH_2$ rock..... | 1168 C | ia | 1168 W | |
| $a_u$ | $\nu_9$ | $CH_2$ twist..... | 1050 D | ia | ia | [a]. |
| $b_{1u}$ | $\nu_{10}$ | $CH_2$ anti. stretch..... | 2919 C | 2919 S | ia | |
| | $\nu_{11}$ | $CH_2$ rock..... | 725 C | 731 S<br>720 S | ia | [b]. |
| $b_{2u}$ | $\nu_{12}$ | $CH_2$ sym. stretch..... | 2851 C | 2851 S | ia | |
| | $\nu_{13}$ | $CH_2$ scissors..... | 1468 C | 1473 S<br>1463 S | ia | [b]. |
| $b_{3u}$ | $\nu_{14}$ | $CH_2$ wag..... | 1176 C | 1176 VW | ia | |

[a] 1063 $cm^{-1}$ is given to this frequency in reference 6.

[b] Doublet due to the crystal field effect [1, 8].

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**Molecule: Perdeuterated Polyethylene $(CD_2)_n$** No. 113

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

| Sym. class | No. | Approximate type of mode | Selected value of frequency | Infrared | Raman | Comments |
|---|---|---|---|---|---|---|
| | | | | $cm^{-1}$ (Solid) | $cm^{-1}$ (Solid) | |
| $a_g$ | $\nu_1$ | $CD_2$ sym. stretch..... | 2102 C | ia | 2102 S | |
| | $\nu_2$ | $CD_2$ scissors..... | 1146 C | ia | 1146 M | |
| | $\nu_3$ | CC stretch. + CCC deform..... | 966 E | ia | 966 VW | |
| $b_{1g}$ | $\nu_4$ | $CD_2$ wag..... | 1249 C | ia | 1249 W | |
| | $\nu_5$ | CC stretch..... | 820 E | ia | ..... | CF [5]. |
| $b_{2g}$ | $\nu_6$ | $CD_2$ twist..... | 916 C | ia | 916 M | |
| $b_{3g}$ | $\nu_7$ | $CD_2$ anti. stretch..... | 2197 C | ia | 2197 M | |
| | $\nu_8$ | $CD_2$ rock..... | 991 C | ia | 991 M | |
| $a_u$ | $\nu_9$ | $CD_2$ twist..... | 743 E | ia | ia | CF [5]. |
| $b_{1u}$ | $\nu_{10}$ | $CD_2$ anti. stretch..... | 2192 C | 2192 S | ia | |
| | $\nu_{11}$ | $CD_2$ rock..... | 526 C | 528 M<br>522 M | ia | [a]. |
| $b_{2u}$ | $\nu_{12}$ | $CD_2$ sym. stretch..... | 2088 C | 2088 S | ia | |
| | $\nu_{13}$ | $CD_2$ scissors..... | 1090 C | 1092 S<br>1087 S | ia | [a]. |
| $b_{3u}$ | $\nu_{14}$ | $CD_2$ wag..... | 889 E | ..... | ia | CF [5]. |

[a] Doublet due to the crystal field effect [5].

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