

# Tables of Molecular Vibrational Frequencies Part 10

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Takehiko Shimanouchi, Hiroatsu Matsuura, Yoshiki Ogawa, and Issei Harada



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# Tables of Molecular Vibrational Frequencies

## Part 10

Takehiko Shimanouchi,\* Hiroatsu Matsuura,\*\* Yoshiki Ogawa,  
and Issei Harada

Department of Chemistry, Faculty of Science, University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113, Japan

Fundamental vibrational frequencies of 94 molecular forms of 23 polyatomic chain molecules of halogenoalkanes and halogenoalkyl ethers consisting of the  $\text{CH}_3$ ,  $\text{CH}_2$ , O, F, Cl, Br, and I groups are given as an extension of tables of molecular vibrational frequencies published in the NSRDS-NBS publication series and in this journal. On preparing the tables in this part, an approach, similar to that in Part 9 but different from that in earlier parts, based on the calculations of normal vibration frequencies was adopted. A set of force constants which explains all the frequencies of small molecules for which the assignments had been established was obtained and then the frequencies of larger molecules were calculated and compared with the frequencies observed in the infrared and Raman spectra. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

Key words: Force constants; fundamental frequencies; infrared spectra; normal vibrations; polyatomic molecules; Raman spectra; vibrational frequencies.

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### 1. Introduction

Establishing the assignment of molecular vibrational frequencies<sup>1</sup> has fundamental importance in elucidating various problems in physics and chemistry. The information

\*Deceased May 19, 1980.

\*\*Present address: Department of Chemistry, Faculty of Science, Hiroshima University, Higashisenda-machi, Hiroshima 730, Japan.

<sup>1</sup> Following common usage, the term "vibrational frequencies" is used in this series, even though numerical values are given for the equivalent wavenumbers in units of  $\text{cm}^{-1}$ .

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concerning the force field and the motion of atoms in a molecule can be most directly derived from its vibrational frequencies. If all the vibrational frequencies of a molecule are known as well as the molecular structure, thermodynamic quantities can be easily computed on the ideal gas model. Thus the need for a tabulation of evaluated reference data on molecular vibrational frequencies has often been felt by many investigators.

A project for producing such tables was initiated in 1964 at the University of Tokyo in cooperation with the National Standard Reference Data System of the National Bureau of Standards. The evaluated data resulting from this project have been published as Tables of Molecular Vibrational Frequencies, Part 1 [1]<sup>2</sup>, Part 2 [2], Part 3 [3], Part 4, Part 5

<sup>2</sup> Figures in brackets indicate literature references in section 6.

[4], Part 6 [5], Part 7 [6], and Part 8 [7], and as the Consolidated Volumes I [8] and II [9].

Succeeding these tables, we adopted in Part 9 [10] and this part a different approach for preparing the further extension of such tables. In the new approach, first we tried to determine a set of force constants which explains all the frequencies of a group of small molecules for which the assignments had already been established. Then we calculated the frequencies of larger molecules and compared them with the observed when they were available. We chose the chain molecules consisting of the  $\text{CH}_3$ ,  $\text{CD}_3$ ,  $\text{CH}_2$ ,  $\text{CD}_2$ ,  $\text{CHD}$ ,  $\text{O}$ ,  $\text{S}$ ,  $\text{F}$ ,  $\text{Cl}$ ,  $\text{Br}$ , and  $\text{I}$  groups. The result was successful as shown in a series of papers entitled "Vibration Spectra and Rotational Isomerism of Chain Molecules" [11–18]. The tables of vibrational frequencies thus compiled for 109 molecular forms of 38 polyatomic chain molecules of alkanes, alkyl ethers, and alkyl sulfides have been published as Part 9 [10].

In the present article, which is the second of the new series, we give the tables of force constants used and tables of the calculated and observed frequencies of basic halogenoalkane and halogenoalkyl ether molecules. We have suitable computer programs for calculating the frequencies of larger molecules, and we are prepared to perform the calculations and make the results available for any molecule upon request, provided that this is within the capacity of our programs.

## 2. Molecules Selected

The present part contains tables of fundamental vibrational frequencies for 94 molecular forms of 23 chain molecules of halogenoalkanes and halogenoalkyl ethers consisting of the  $\text{CH}_3$ ,  $\text{CH}_2$ ,  $\text{O}$ ,  $\text{F}$ ,  $\text{Cl}$ ,  $\text{Br}$ , and  $\text{I}$  groups. The molecules are limited to those with four to six atomic groups and the rotational isomers included have been confirmed to exist.

A list of the molecules covered here is given at the beginning of the tables. The molecules are numbered starting with number 110 succeeding those in Part 9 of the tables.

## 3. Calculation of Vibrational Frequencies

### 3.1. Computer Programs and Calculation

To prepare the tables of molecular vibrational frequencies in Part 9 and this part (Part 10), the computer program system MVIB [10,19] was utilized. The MVIB system uses the structure and force constant data stored in the computer files and calculates the frequencies and other data from the molecular formula with the conformation. The details of the normal coordinate treatment will be found in reference [20].

The calculations were made by the HITAC 8800/8700 Computing System at the Computer Center of the University of Tokyo.

### 3.2. Atomic Masses and Structural Parameters

The atomic masses and the structural parameters listed in table 1 were used in common in the calculations of vibrational frequencies of the molecules treated in this work.

The structural parameters were taken from butane [21], ethyl methyl ether [22], fluoroethane [23], chloroethane [24], bromoethane [25], and iodoethane [26].

The dihedral angles were assumed to be  $180^\circ$  (trans),  $60^\circ$  (gauche<sup>+</sup>), and  $-60^\circ$  (gauche<sup>-</sup>). The symbols t, g<sup>+</sup>, and g<sup>-</sup> are used for the trans, gauche<sup>+</sup>, and gauche<sup>-</sup> conformations, respectively, in the notation of the force constants (section 3.4). The conformations of molecules, as given at the top of each of the tables of vibrational frequencies, are denoted generically by the symbols T, G, and G'. The details will be found in reference [11]. The definition of the dihedral angles will be found in references [27,28].

### 3.3. Local Symmetry Coordinates

The local symmetry coordinates defined in table 2 were adopted as basis coordinates in the calculations. For the coordinate systems of the  $\text{CH}_3$  and  $\text{CH}_2$  groups, the redundant coordinates have been eliminated in accordance with the bond angles given in table 1 (see Appendix of Part 9 [10]). The definition of the coordinates is based on the conventions recommended by IUPAC [28]. It should be noted that the signs of some of the coordinates depend on the direction of taking atomic groups. The signs of the coordinates are important since they are directly related to the signs of the off-diagonal force constants associated with these and other coordinates.

The local symmetry coordinates in a whole molecule are defined on the basis of the following conventions. (1) The signs of the coordinates for all of the non-terminal groups, e.g.,  $\text{CH}_2$  and  $\text{O}$ , in the molecule are positive, when one views the successive atomic groups constituting the molecule, in accordance with the molecular formula given in the tables of vibrational frequencies, from the left to the right. (2) The coordinates of the terminal groups, e.g.,  $\text{CH}_3$ , can be defined uniquely, independent of the position of the groups (left-hand terminal or right-hand terminal) in the molecular formula, on the basis of the definition given in table 2. (3) The symmetry of the whole molecule is not taken into account in defining the basis coordinates for the normal coordinate calculations. The symmetry species of the vibrations are determined from the relative phase relations among the coordinates concerned.

### 3.4. Force Constants

The force constants are given in terms of the local symmetry coordinates [20]. Their values were determined by the least-squares procedure from experimental vibrational frequencies observed in infrared and Raman spectra, except the force constants characteristic of the halogenoalkyl ethers whose values were all assumed to be equivalent to those for the corresponding halogenoalkanes. The force constants for the alkyl and ether groups, not directly associated with the halogen groups, are the same as those given in tables 3 and 4 of Part 9 [10]. Detailed procedures of the least-squares calculations will be found in reference [17]. The force constants which are characteristic of halogenoalkanes and halogenoalkyl ethers are listed in tables 3–7. In these tables only the force constants with non-zero values are given and force constants not found in the tables have zero values. For

the force constants determined by the least-squares procedure, the errors are given in parentheses which apply to the last significant figure(s). Other force constants were

constrained to the values given in the tables or assumed to be equal to the corresponding force constants of similar groups.

Each of the force constants is given by the symbol consisting of four to seven characters which are grouped into the following three parts. The parts are divided by hyphens in the notation of the symbol. (1) The characters denoting the atomic groups to which the coordinates belong, (2) the character(s) denoting the coordinate(s), and (3) the character denoting the skeletal conformation. The symbols of the local symmetry coordinates and of the atomic groups are listed in table 2. The force constants are divided into two categories, the intragroup force constants and the intergroup force constants.

General descriptions of the force constant symbols have been given in Part 9 [10]. Some examples for the molecules treated in this article are given below.

012-2: the diagonal intragroup force constant for the  $\text{CH}_3$  symmetrical deformation in the  $\text{CH}_3$  group of the  $\text{CH}_3\text{CH}_2$  part.

225-46: the off-diagonal intragroup force constant for the  $\text{CH}_2$  rocking and the  $\text{CH}_2$  twisting within the  $\text{C}^b\text{H}_2$  group of the  $\text{C}^a\text{H}_2\text{C}^b\text{H}_2\text{Cl}$  part.

226-SS: the off-diagonal intragroup force constant for the  $\text{C}^a\text{-C}^b$  stretching and the  $\text{C}^b\text{-Br}$  stretching of the  $\text{C}^a\text{H}_2\text{C}^b\text{H}_2\text{Br}$  part.

2250-S: the diagonal intergroup force constant for the  $\text{C}^b\text{-Cl}$  stretching of  $\text{C}^a\text{H}_2\text{C}^b\text{H}_2\text{Cl}$  part.

0123-25: the off-diagonal intergroup force constant for the  $\text{CH}_3$  symmetrical deformation and the  $\text{CH}_2$  wagging of the  $\text{CH}_3\text{CH}_2\text{O}$  part.

2260-5S: the off-diagonal intergroup force constant for the  $\text{C}^b\text{H}_2$  wagging and the  $\text{C}^b\text{-Br}$  stretching of the  $\text{C}^a\text{H}_2\text{C}^b\text{H}_2\text{Br}$  part.

2227-46- $g^+$ : the off-diagonal intergroup force constant for the  $\text{C}^b\text{H}_2$  rocking and the  $\text{C}^b\text{H}_2$  twisting of the  $\text{C}^a\text{H}_2\text{C}^b\text{H}_2\text{C}^b\text{H}_2\text{I}$  part in the gauche<sup>+</sup> conformation.

It should be noted that the signs of some of the force constants are reversed if the force constants are defined by ordering the atomic groups in an opposite direction. Of the force constants listed in tables 3-7, only the following force constants have such sign reverse character: the off-diagonal intragroup or intergroup force constants for which one of the two coordinates is the  $\text{CH}_2$  antisymmetrical stretching, the  $\text{CH}_2$  rocking or the  $\text{CH}_2$  wagging and the other coordinate is

TABLE 1. Relative atomic masses and structural parameters used in the calculations

| Property                               | Quantity  |
|----------------------------------------|-----------|
| Relative atomic masses, <sup>a</sup> u |           |
| Hydrogen (protium)                     | 1.007825  |
| Hydrogen (deuterium)                   | 2.014102  |
| Carbon                                 | 12.011    |
| Oxygen                                 | 15.9994   |
| Fluorine                               | 18.998403 |
| Chlorine                               | 35.453    |
| Bromine                                | 79.904    |
| Iodine                                 | 126.9045  |
| Bond lengths, Å                        |           |
| $r(\text{C-H})$                        | 1.100     |
| $r(\text{C-C})$                        | 1.539     |
| $r(\text{C-O})$                        | 1.410     |
| $r(\text{C-F})$                        | 1.398     |
| $r(\text{C-Cl})$                       | 1.788     |
| $r(\text{C-Br})$                       | 1.950     |
| $r(\text{C-I})$                        | 2.139     |
| Bond angle, degree                     |           |
| $\angle(\text{C-C-C})$                 | 112.2     |
| $\angle(\text{C-C-O})$                 | 108.1     |
| $\angle(\text{C-O-C})$                 | 111.8     |
| $\angle(\text{C-C-F})$                 | 109.7     |
| $\angle(\text{C-C-Cl})$                | 111.0     |
| $\angle(\text{C-C-Br})$                | 111.0     |
| $\angle(\text{C-C-I})$                 | 112.2     |
| $\angle(\text{C-C-H})$                 | 110.4     |
| $\angle(\text{O-C-H})$                 | 109.8     |
| $\angle(\text{F-C-H})$                 | 106.1     |
| $\angle(\text{Cl-C-H})$                | 106.6     |
| $\angle(\text{Br-C-H})$                | 105.4     |
| $\angle(\text{I-C-H})$                 | 105.0     |
| Dihedral angles, degree                |           |
| Trans conformation                     | 180       |
| Gauche <sup>+</sup> conformation       | 60        |
| Gauche <sup>-</sup> conformation       | -60       |

<sup>a</sup>The mean relative atomic mass, i.e., atomic weight (isotope abundance weighted) was used for the atoms other than hydrogen, since the isotopic frequency shifts in these atoms are not considered in this article.

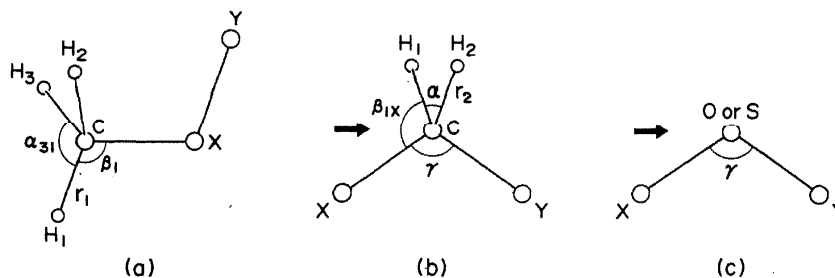


FIGURE 1. Parameters of atomic groups. (a)  $\text{CH}_3\text{-(X)}$ , (b)  $(\text{X})\text{-CH}_2\text{-(Y)}$ , (c)  $(\text{X})\text{-O-(Y)}$  or  $(\text{X})\text{-S-(Y)}$ . Arrows in (b) and (c) indicate the direction of viewing the atomic groups (see text).

TABLE 2. Definition and symbolism of local symmetry coordinates

| Coordinate                                                        | Symbol | Definition                                                                                                        |
|-------------------------------------------------------------------|--------|-------------------------------------------------------------------------------------------------------------------|
| (a) CH <sub>3</sub> -(X) group <sup>a</sup> (see figure 1(a))     |        |                                                                                                                   |
| CH <sub>3</sub> symmetrical stretching                            | 1      | $(\Delta r_1 + \Delta r_2 + \Delta r_3)/\sqrt{3}$                                                                 |
| CH <sub>3</sub> symmetrical deformation                           | 2      | $a(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12}) - b(\Delta\beta_1 + \Delta\beta_2 + \Delta\beta_3)$ |
| CH <sub>3</sub> degenerate stretching                             | 3      | $(2\Delta r_1 - \Delta r_2 - \Delta r_3)/\sqrt{6}$                                                                |
| CH <sub>3</sub> degenerate deformation                            | 4      | $(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{6}$                                           |
| CH <sub>3</sub> rocking                                           | 5      | $(2\Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3)/\sqrt{6}$                                                       |
| CH <sub>3</sub> degenerate stretching                             | 6      | $(\Delta r_2 - \Delta r_3)/\sqrt{2}$                                                                              |
| CH <sub>3</sub> degenerate deformation                            | 7      | $(\Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{2}$                                                                |
| CH <sub>3</sub> rocking                                           | 8      | $(\Delta\beta_2 - \Delta\beta_3)/\sqrt{2}$                                                                        |
| (b) (X)-CH <sub>2</sub> -(Y) group <sup>a</sup> (see figure 1(b)) |        |                                                                                                                   |
| CH <sub>2</sub> symmetrical stretching                            | 1      | $(\Delta r_1 + \Delta r_2)/\sqrt{2}$                                                                              |
| CH <sub>2</sub> scissors                                          | 2      | $c\Delta\alpha - d(\Delta\beta_{1X} + \Delta\beta_{2X}) - e(\Delta\beta_{1Y} + \Delta\beta_{2Y})$                 |
| CH <sub>2</sub> antisymmetrical stretching <sup>b</sup>           | 3      | $(\Delta r_1 - \Delta r_2)/\sqrt{2}$                                                                              |
| CH <sub>2</sub> rocking <sup>b</sup>                              | 4      | $(\Delta\beta_{1X} - \Delta\beta_{2X} + \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$                                   |
| CH <sub>2</sub> wagging <sup>b</sup>                              | 5      | $f(\Delta\beta_{1X} + \Delta\beta_{2Y}) - g(\Delta\beta_{1Y} + \Delta\beta_{2X})$                                 |
| CH <sub>2</sub> twisting                                          | 6      | $(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y})/2$                                   |
| X-CH <sub>2</sub> -Y deformation                                  | D      | $h\Delta\gamma - i\Delta\alpha - j(\Delta\beta_{1X} + \Delta\beta_{2X}) - k(\Delta\beta_{1Y} + \Delta\beta_{2Y})$ |
| (c) (X)-O-(Y) group <sup>a</sup> (see figure 1(c))                |        |                                                                                                                   |
| X-O-Y bending                                                     | B      | $\Delta\gamma$                                                                                                    |
| (d) Skeleton -X-Y-                                                |        |                                                                                                                   |
| Stretching                                                        | S      | $\Delta r_{XY}$                                                                                                   |
| Torsion <sup>c</sup>                                              | T      | $\Delta t_{XY}$                                                                                                   |

$a = 0.414957$  and  $b = 0.401428$  for  $X = C$ ;  $a = 0.410693$  and  $b = 0.405789$  for  $X = O$ .  $c = 0.906922$ ,  $d = e = 0.210650$ ,  $f = g = 1/2$ ,  $h = 0.893737$ ,  $i = 0.188991$  and  $j = k = 0.203418$  for  $X = Y = C$ ;  $c = 0.891960$ ,  $d = 0.227321$ ,  $e = 0.224785$ ,  $f = 0.497188$ ,  $g = 0.502797$ ,  $h = 0.911899$ ,  $i = 0.185554$ ,  $j = 0.184061$  and  $k = 0.182007$  for  $X = C$  and  $Y = O$ ;  $c = 0.890837$ ,  $d = 0.236949$ ,  $e = 0.216935$ ,  $f = 0.477488$ ,  $g = 0.521541$ ,  $h = 0.923376$ ,  $i = 0.174413$ ,  $j = 0.178361$  and  $k = 0.163296$  for  $X = C$  and  $Y = F$ ;  $c = 0.895960$ ,  $d = 0.229861$ ,  $e = 0.213993$ ,  $f = 0.481817$ ,  $g = 0.517544$ ,  $h = 0.916937$ ,  $i = 0.177225$ ,  $j = 0.185030$  and  $k = 0.172258$  for  $X = C$  and  $Y = Cl$ ;  $c = 0.893813$ ,  $d = 0.235095$ ,  $e = 0.212793$ ,  $f = 0.474515$ ,  $g = 0.524248$ ,  $h = 0.922575$ ,  $i = 0.173017$ ,  $j = 0.180786$  and  $k = 0.163636$  for  $X = C$  and  $Y = Br$ ;  $c = 0.896985$ ,  $d = 0.232153$ ,  $e = 0.209319$ ,  $f = 0.473504$ ,  $g = 0.525161$ ,  $h = 0.920673$ ,  $i = 0.172553$ ,  $j = 0.183872$  and  $k = 0.165786$  for  $X = C$  and  $Y = I$ . For redundant coordinates, see Appendix of Part 9 [10].

<sup>a</sup> Symbols of atomic groups are 1 for CH<sub>3</sub>, 1' for CD<sub>3</sub>, 2 for CH<sub>2</sub>, 2' for CD<sub>2</sub>, 2'' for CHD, 3 for O, 4 for S, 5 for Cl, 6 for Br, 7 for I, and 8 for F. The group CHD (2'') is defined in such a way that H<sub>1</sub> and H<sub>2</sub> in figure 1(b) are protium (H) and deuterium (D), respectively.

<sup>b</sup> The signs of the CH<sub>2</sub> antisymmetrical stretching, CH<sub>2</sub> rocking and CH<sub>2</sub> wagging coordinates of the (Y)-CH<sub>2</sub>-(X) group (viewing the Y-CH<sub>2</sub>-X group from the direction perpendicular to the HCH plane with the atom Y nearer to the observer) are opposite to those of the corresponding coordinates of the (X)-CH<sub>2</sub>-(Y) group (viewing the X-CH<sub>2</sub>-Y group with the atom X nearer to the observer) [28]. The signs of the other coordinates are independent of the direction of viewing the atomic groups.

<sup>c</sup> The definition of the torsional coordinate will be found in references [27,28].

Table 3. Force constants of fluoroalkanes

| Constant <sup>a</sup> | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> |
|-----------------------|--------------------|---------------------------------------------------|--------------------|---------------------------------------------------|--------------------|
| 228-1                 | 4.840              | 1228-DD-t = 2228-DD-t                             |                    | 2228-55-t                                         | -0.077(53)         |
| 228-2                 | 0.523(16)          | 1228-44-g <sup>+</sup> = 2228-44-g <sup>+</sup>   |                    | 2228-5D-t = 2222-5D-t                             |                    |
| 228-3                 | 4.752              | *1228-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2228-64-t = -2222-46-t                            |                    |
| 228-4                 | 0.787(101)         | 1228-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    | 2228-66-t                                         | -0.045(118)        |
| 228-5                 | 0.716(58)          | *1228-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    | 2228-D2-t = 2222-2D-t                             |                    |
| 228-6                 | 0.744(124)         | *1228-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2228-D5-t = -2222-5D-t                            |                    |
| 228-D                 | 1.373(84)          | 1228-55-g <sup>+</sup> = 2228-55-g <sup>+</sup>   |                    | 2228-DD-t                                         | 0.217(38)          |
| 228-25                | 0.056(38)          | *1228-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    | 2228-44-g <sup>+</sup>                            | -0.051(60)         |
| 228-2D                | = 222-2D           | 1228-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    | *2228-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
| 228-46                | -0.024(53)         | 1228-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    | 2228-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    |
| 228-5D                | 0.341(91)          | *1228-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    | *2228-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    |
| 228-SS                | 0.316(69)          | 1228-66-g <sup>+</sup> = 2228-66-g <sup>+</sup>   |                    | *2228-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
|                       |                    | *1228-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2228-55-g <sup>+</sup>                            | 0.023(41)          |
| 1228-S                | = 2228-S           | *1228-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    | *2228-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    |
| 1228-T                | = 2228-T           | 1228-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    | 2228-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    |
| 1228-5S               | = 2222-5S          | *1228-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2228-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    |
| 1228-DS               | = 2222-DS          | 1228-DD-g <sup>+</sup> = 2228-DD-g <sup>+</sup>   |                    | *2228-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    |
| 1228-S5               | = -2222-5S         |                                                   |                    | 2228-66-g <sup>+</sup>                            | -0.014(35)         |
| 1228-SD               | = 2225-SD          | 2228-S                                            | 4.399(72)          | *2228-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1228-2D-t             | = 2222-2D-t        | 2228-T                                            | 0.150              | *2228-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    |
| 1228-44-t             | = 2228-44-t        | 2228-5S                                           | = 2222-5S          | 2228-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    |
| 1228-46-t             | = 2222-46-t        | 2228-DS                                           | = 2222-DS          | *2228-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1228-55-t             | = 2228-55-t        | 2228-S5                                           | = -2222-5S         | 2228-DD-g <sup>+</sup>                            | 0.014(49)          |
| 1228-5D-t             | = 2222-5D-t        | 2228-SD                                           | 0.016(24)          |                                                   |                    |
| 1228-64-t             | = -2222-46-t       | 2228-2D-t                                         | = 2222-2D-t        | 2280-S                                            | 4.781(81)          |
| 1228-66-t             | = 2228-66-t        | 2228-44-t                                         | 0.093(89)          | 2280-5S                                           | -0.282(86)         |
| 1228-D2-t             | = 2222-2D-t        | 2228-46-t                                         | = 2222-46-t        | 2280-DS                                           | 0.261(92)          |
| 1228-D5-t             | = -2222-5D-t       |                                                   |                    |                                                   |                    |

<sup>a</sup> The values of the  $g^-$  interaction constants are the same as those of the corresponding  $g^+$  interaction constants, unless they are marked with \*. For those marked with \*, the absolute values of the  $g^+$  and  $g^-$  interaction constants are the same but their signs are opposite to each other.

<sup>b</sup> Units are  $\text{aJ } \text{\AA}^{-2} = \text{mdyn } \text{\AA}^{-1}$  for the stretching and stretching-stretching constants,  $\text{aJ } \text{\AA}^{-1} = \text{mdyn}$  for the stretching-bending constants, and  $\text{aJ} = \text{mdyn } \text{\AA}$  for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

Table 4. Force constants of chloroalkanes

| Constant <sup>a</sup>  | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> |
|------------------------|--------------------|---------------------------------------------------|--------------------|---------------------------------------------------|--------------------|
| 225-1                  | 4.905              | 1225-DD-t = 2225-DD-t                             |                    | 2225-55-t                                         | -0.049(4)          |
| 225-2                  | 0.537(8)           | 1225-44-g <sup>+</sup> = 2225-44-g <sup>+</sup>   |                    | 2225-5D-t = 2222-5D-t                             |                    |
| 225-3                  | 4.787              | *1225-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2225-64-t = -2222-46-t                            |                    |
| 225-4                  | 0.756(16)          | 1225-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    | 2225-66-t                                         | -0.075(8)          |
| 225-5                  | 0.662(18)          | *1225-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    | 2225-D2-t = 2222-2D-t                             |                    |
| 225-6                  | 0.649(26)          | *1225-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2225-D5-t = -2222-5D-t                            |                    |
| 225-D                  | 0.984(44)          | 1225-55-g <sup>+</sup> = 2225-55-g <sup>+</sup>   |                    | 2225-DD-t                                         | 0.112(40)          |
| 225-25                 | 0.049(5)           | *1225-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    | 2225-44-g <sup>+</sup>                            | 0.005(13)          |
| 225-2D = 222-2D        |                    | 1225-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    | *2225-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
| 225-46                 | -0.031(16)         | 1225-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    | 2225-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    |
| 225-5D                 | 0.059(58)          | *1225-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    | *2225-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    |
| 225-SS                 | 0.388(25)          | 1225-66-g <sup>+</sup> = 2225-66-g <sup>+</sup>   |                    | *2225-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
|                        |                    | *1225-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2225-55-g <sup>+</sup>                            | 0.005(14)          |
| 1225-S = 2225-S        |                    | *1225-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    | *2225-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    |
| 1225-T = 2225-T        |                    | 1225-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    | 2225-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    |
| 1225-5S = 2222-5S      |                    | *1225-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2225-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    |
| 1225-DS = 2222-DS      |                    | 1225-DD-g <sup>+</sup> = 2225-DD-g <sup>+</sup>   |                    | *2225-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    |
| 1225-5S = -2222-5S     |                    |                                                   |                    | 2225-66-g <sup>+</sup>                            | 0.039(21)          |
| 1225-SD = 2225-SD      |                    | 2225-S                                            | 4.314(31)          | *2225-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1225-2D-t = 2222-2D-t  |                    | 2225-T                                            | 0.146(15)          | *2225-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    |
| 1225-44-t = 2225-44-t  |                    | 2225-5S = 2222-5S                                 |                    | 2225-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    |
| 1225-46-t = 2222-46-t  |                    | 2225-DS = 2222-DS                                 |                    | *2225-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1225-55-t = 2225-55-t  |                    | 2225-5S = -2222-5S                                |                    | 2225-DD-g <sup>+</sup>                            | 0.025(22)          |
| 1225-5D-t = 2222-5D-t  |                    | 2225-SD                                           | -0.071(46)         |                                                   |                    |
| 1225-64-t = -2222-46-t |                    | 2225-2D-t = 2222-2D-t                             |                    | 2250-S                                            | 2.983(22)          |
| 1225-66-t = 2225-66-t  |                    | 2225-44-t                                         | 0.068(9)           | 2250-5S                                           | -0.177(56)         |
| 1225-D2-t = 2222-2D-t  |                    | 2225-46-t = 2222-46-t                             |                    | 2250-DS                                           | 0.333(21)          |
| 1225-D5-t = -2222-5D-t |                    |                                                   |                    |                                                   |                    |

<sup>a</sup> The values of the  $g^-$  interaction constants are the same as those of the corresponding  $g^+$  interaction constants, unless they are marked with \*. For those marked with \*, the absolute values of the  $g^+$  and  $g^-$  interaction constants are the same but their signs are opposite to each other.

<sup>b</sup> Units are  $\text{aJ } \text{\AA}^{-2} = \text{mdyn } \text{\AA}^{-1}$  for the stretching and stretching-stretching constants,  $\text{aJ } \text{\AA}^{-1} = \text{mdyn}$  for the stretching-bending constants, and  $\text{aJ} = \text{mdyn } \text{\AA}$  for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

Table 5. Force constants of bromoalkanes

| Constant <sup>a</sup>  | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> |
|------------------------|--------------------|---------------------------------------------------|--------------------|---------------------------------------------------|--------------------|
| 226-1                  | 4.920              | 1226-DD-t = 2226-DD-t                             |                    | 2226-55-t                                         | -0.052(6)          |
| 226-2                  | 0.535(2)           | 1226-44-g <sup>+</sup> = 2226-44-g <sup>+</sup>   |                    | 2226-5D-t = 2222-5D-t                             |                    |
| 226-3                  | 4.770              | *1226-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2226-64-t = -2222-46-t                            |                    |
| 226-4                  | 0.700(30)          | 1226-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    | 2226-66-t                                         | -0.070(15)         |
| 226-5                  | 0.621(11)          | *1226-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    | 2226-D2-t = 2222-2D-t                             |                    |
| 226-6                  | 0.613(22)          | *1226-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2226-D5-t = -2222-5D-t                            |                    |
| 226-D                  | 0.977(19)          | 1226-55-g <sup>+</sup> = 2226-55-g <sup>+</sup>   |                    | 2226-DD-t                                         | 0.022(19)          |
| 226-25                 | 0.038(9)           | *1226-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    | 2226-44-g <sup>+</sup>                            | 0.002(44)          |
| 226-2D = 222-2D        |                    | 1226-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    | *2226-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
| 226-46                 | 0.002(20)          | 1226-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    | 2226-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    |
| 226-5D                 | 0.132(16)          | *1226-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    | *2226-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    |
| 226-SS                 | 0.541(34)          | 1226-66-g <sup>+</sup> = 2226-66-g <sup>+</sup>   |                    | *2226-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
|                        |                    | *1226-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2226-55-g <sup>+</sup>                            | -0.004(21)         |
| 1226-S = 2226-S        |                    | *1226-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    | *2226-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    |
| 1226-T = 2226-T        |                    | 1226-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    | 2226-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    |
| 1226-5S = 2222-5S      |                    | *1226-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2226-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    |
| 1226-DS = 2222-DS      |                    | 1226-DD-g <sup>+</sup> = 2226-DD-g <sup>+</sup>   |                    | *2226-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    |
| 1226-S5 = -2222-5S     |                    |                                                   |                    | 2226-66-g <sup>+</sup>                            | 0.045(13)          |
| 1226-SD = 2226-SD      |                    | 2226-S                                            | 4.314(34)          | *2226-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1226-2D-t = 2222-2D-t  |                    | 2226-I                                            | 0.147(20)          | *2226-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    |
| 1226-44-t = 2226-44-t  |                    | 2226-5S = 2222-5S                                 |                    | 2226-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    |
| 1226-46-t = 2222-46-t  |                    | 2226-DS = 2222-DS                                 |                    | *2226-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1226-55-t = 2226-55-t  |                    | 2226-S5 = -2222-5S                                |                    | 2226-DD-g <sup>+</sup>                            | 0.045(16)          |
| 1226-5D-t = 2222-5D-t  |                    | 2226-SD = -0.098(34)                              |                    |                                                   |                    |
| 1226-64-t = -2222-46-t |                    | 2226-2D-t = 2222-2D-t                             |                    | 2260-S                                            | 2.609(47)          |
| 1226-66-t = 2226-66-t  |                    | 2226-44-t = 0.066(22)                             |                    | 2260-5S                                           | -0.171(37)         |
| 1226-D2-t = 2222-2D-t  |                    | 2226-46-t = 2222-46-t                             |                    | 2260-DS                                           | 0.328(25)          |
| 1226-D5-t = -2222-5D-t |                    |                                                   |                    |                                                   |                    |

<sup>a</sup> The values of the g<sup>-</sup> interaction constants are the same as those of the corresponding g<sup>+</sup> interaction constants, unless they are marked with \*. For those marked with \*, the absolute values of the g<sup>+</sup> and g<sup>-</sup> interaction constants are the same but their signs are opposite to each other.

<sup>b</sup> Units are aJ Å<sup>-2</sup> = mdyn Å<sup>-1</sup> for the stretching and stretching-stretching constants, aJ Å<sup>-1</sup> = mdyn for the stretching-bending constants, and aJ = mdyn Å for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).



Table 6. Force constants of iodoalkanes

| Constant <sup>a</sup>  | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> | Constant <sup>a</sup>                             | Value <sup>b</sup> |
|------------------------|--------------------|---------------------------------------------------|--------------------|---------------------------------------------------|--------------------|
| 227-1                  | 4.942              | 1227-DD-t = 2227-DD-t                             |                    | 2227-55-t                                         | -0.059(4)          |
| 227-2                  | 0.528(3)           | 1227-44-g <sup>+</sup> = 2227-44-g <sup>+</sup>   |                    | 2227-5D-t = 2222-5D-t                             |                    |
| 227-3                  | 4.758              | *1227-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2227-64-t = -2222-46-t                            |                    |
| 227-4                  | 0.641(14)          | 1227-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    | 2227-66-t                                         | -0.050(9)          |
| 227-5                  | 0.571(15)          | *1227-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    | 2227-D2-t = 2222-2D-t                             |                    |
| 227-6                  | 0.547(10)          | *1227-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    | 2227-D5-t = -2222-5D-t                            |                    |
| 227-D                  | 0.919(14)          | 1227-55-g <sup>+</sup> = 2227-55-g <sup>+</sup>   |                    | 2227-DD-t                                         | -0.028(22)         |
| 227-25                 | 0.077(8)           | *1227-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    | 2227-44-g <sup>+</sup>                            | 0.014(21)          |
| 227-2D = 222-2D        |                    | 1227-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    | *2227-45-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
| 227-46                 | 0.003(12)          | 1227-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    | 2227-46-g <sup>+</sup> = 2222-46-g <sup>+</sup>   |                    |
| 227-5D                 | 0.196(25)          | *1227-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    | *2227-4D-g <sup>+</sup> = 2222-4D-g <sup>+</sup>  |                    |
| 227-SS                 | 0.424(6)           | 1227-66-g <sup>+</sup> = 2227-66-g <sup>+</sup>   |                    | *2227-54-g <sup>+</sup> = 2222-45-g <sup>+</sup>  |                    |
|                        |                    | *1227-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2227-55-g <sup>+</sup>                            | 0.012(14)          |
| 1227-S = 2227-S        |                    | *1227-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    | *2227-56-g <sup>+</sup> = 2222-56-g <sup>+</sup>  |                    |
| 1227-T = 2227-T        |                    | 1227-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    | 2227-5D-g <sup>+</sup> = 2222-5D-g <sup>+</sup>   |                    |
| 1227-5S = 2222-5S      |                    | *1227-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    | 2227-64-g <sup>+</sup> = -2222-46-g <sup>+</sup>  |                    |
| 1227-DS = 2222-DS      |                    | 1227-DD-g <sup>+</sup> = 2227-DD-g <sup>+</sup>   |                    | *2227-65-g <sup>+</sup> = -2222-56-g <sup>+</sup> |                    |
| 1227-S5 = -2222-5S     |                    |                                                   |                    | 2227-66-g <sup>+</sup>                            | 0.034(12)          |
| 1227-SD = 2227-SD      |                    | 2227-S                                            | 4.327(51)          | *2227-6D-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1227-2D-t = 2222-2D-t  |                    | 2227-T                                            | 0.148(25)          | *2227-D4-g <sup>+</sup> = -2222-4D-g <sup>+</sup> |                    |
| 1227-44-t = 2227-44-t  |                    | 2227-5S = 2222-5S                                 |                    | 2227-D5-g <sup>+</sup> = -2222-5D-g <sup>+</sup>  |                    |
| 1227-46-t = 2222-46-t  |                    | 2227-DS = 2222-DS                                 |                    | *2227-D6-g <sup>+</sup> = 2222-6D-g <sup>+</sup>  |                    |
| 1227-55-t = 2227-55-t  |                    | 2227-S5 = -2222-5S                                |                    | 2227-DD-g <sup>+</sup>                            | 0.063(42)          |
| 1227-5D-t = 2222-5D-t  |                    | 2227-SD                                           | -0.158(56)         |                                                   |                    |
| 1227-64-t = -2222-46-t |                    | 2227-2D-t = 2222-2D-t                             |                    | 2270-S                                            | 2.198(31)          |
| 1227-66-t = 2227-66-t  |                    | 2227-44-t                                         | 0.073(13)          | 2270-5S                                           | -0.038(64)         |
| 1227-D2-t = 2222-2D-t  |                    | 2227-46-t = 2222-46-t                             |                    | 2270-DS                                           | 0.328(40)          |
| 1227-D5-t = -2222-5D-t |                    |                                                   |                    |                                                   |                    |

<sup>a</sup> The values of the  $g^-$  interaction constants are the same as those of the corresponding  $g^+$  interaction constants, unless they are marked with \*. For those marked with \*, the absolute values of the  $g^+$  and  $g^-$  interaction constants are the same but their signs are opposite to each other.

<sup>b</sup> Units are  $\text{aJ } \text{\AA}^{-2} = \text{mdyn } \text{\AA}^{-1}$  for the stretching and stretching-stretching constants,  $\text{aJ } \text{\AA}^{-1} = \text{mdyn}$  for the stretching-bending constants, and  $\text{aJ} = \text{mdyn } \text{\AA}$  for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

Table 7. Force constants of halogenoalkyl ethers

| Constant <sup>a</sup>   | Value <sup>b</sup>        | Constant <sup>a</sup>   | Value <sup>b</sup>        | Constant <sup>a</sup>   | Value <sup>b</sup>        |
|-------------------------|---------------------------|-------------------------|---------------------------|-------------------------|---------------------------|
| 3225-S                  | = 2225-S                  | 3226-S                  | = 2226-S                  | 3227-S                  | = 2227-S                  |
| 3225-T                  | = 2225-T                  | 3226-T                  | = 2226-T                  | 3227-T                  | = 2227-T                  |
| 3225-5S                 | = 2222-5S                 | 3226-5S                 | = 2222-5S                 | 3227-5S                 | = 2222-5S                 |
| 3225-DS                 | = 2222-DS                 | 3226-DS                 | = 2222-DS                 | 3227-DS                 | = 2222-DS                 |
| 3225-S5                 | = -2222-5S                | 3226-S5                 | = -2222-5S                | 3227-S5                 | = -2222-5S                |
| 3225-SD                 | = 2225-SD                 | 3226-SD                 | = 2226-SD                 | 3227-SD                 | = 2227-SD                 |
| 3225-2D-t               | = 2222-2D-t               | 3226-2D-t               | = 2222-2D-t               | 3227-2D-t               | = 2222-2D-t               |
| 3225-44-t               | = 2225-44-t               | 3226-44-t               | = 2226-44-t               | 3227-44-t               | = 2227-44-t               |
| 3225-46-t               | = 2222-46-t               | 3226-46-t               | = 2222-46-t               | 3227-46-t               | = 2222-46-t               |
| 3225-55-t               | = 2225-55-t               | 3226-55-t               | = 2226-55-t               | 3227-55-t               | = 2227-55-t               |
| 3225-5D-t               | = 2222-5D-t               | 3226-5D-t               | = 2222-5D-t               | 3227-5D-t               | = 2222-5D-t               |
| 3225-64-t               | = -2222-46-t              | 3226-64-t               | = -2222-46-t              | 3227-64-t               | = -2222-46-t              |
| 3225-66-t               | = 2225-66-t               | 3226-66-t               | = 2226-66-t               | 3227-66-t               | = 2227-66-t               |
| 3225-D2-t               | = 2222-2D-t               | 3226-D2-t               | = 2222-2D-t               | 3227-D2-t               | = 2222-2D-t               |
| 3225-D5-t               | = -2222-5D-t              | 3226-D5-t               | = -2222-5D-t              | 3227-D5-t               | = -2222-5D-t              |
| 3225-DD-t               | = 2225-DD-t               | 3226-DD-t               | = 2226-DD-t               | 3227-DD-t               | = 2227-DD-t               |
| 3225-44-g <sup>+</sup>  | = 2225-44-g <sup>+</sup>  | 3226-44-g <sup>+</sup>  | = 2226-44-g <sup>+</sup>  | 3227-44-g <sup>+</sup>  | = 2227-44-g <sup>+</sup>  |
| *3225-45-g <sup>+</sup> | = 2222-45-g <sup>+</sup>  | *3226-45-g <sup>+</sup> | = 2222-45-g <sup>+</sup>  | *3227-45-g <sup>+</sup> | = 2222-45-g <sup>+</sup>  |
| 3225-46-g <sup>+</sup>  | = 2222-46-g <sup>+</sup>  | 3226-46-g <sup>+</sup>  | = 2222-46-g <sup>+</sup>  | 3227-46-g <sup>+</sup>  | = 2222-46-g <sup>+</sup>  |
| *3225-4D-g <sup>+</sup> | = 2222-4D-g <sup>+</sup>  | *3226-4D-g <sup>+</sup> | = 2222-4D-g <sup>+</sup>  | *3227-4D-g <sup>+</sup> | = 2222-4D-g <sup>+</sup>  |
| *3225-54-g <sup>+</sup> | = 2222-45-g <sup>+</sup>  | *3226-54-g <sup>+</sup> | = 2222-45-g <sup>+</sup>  | *3227-54-g <sup>+</sup> | = 2222-45-g <sup>+</sup>  |
| 3225-55-g <sup>+</sup>  | = 2225-55-g <sup>+</sup>  | 3226-55-g <sup>+</sup>  | = 2226-55-g <sup>+</sup>  | 3227-55-g <sup>+</sup>  | = 2227-55-g <sup>+</sup>  |
| *3225-56-g <sup>+</sup> | = 2222-56-g <sup>+</sup>  | *3226-56-g <sup>+</sup> | = 2222-56-g <sup>+</sup>  | *3227-56-g <sup>+</sup> | = 2222-56-g <sup>+</sup>  |
| 3225-5D-g <sup>+</sup>  | = 2222-5D-g <sup>+</sup>  | 3226-5D-g <sup>+</sup>  | = 2222-5D-g <sup>+</sup>  | 3227-5D-g <sup>+</sup>  | = 2222-5D-g <sup>+</sup>  |
| 3225-64-g <sup>+</sup>  | = -2222-46-g <sup>+</sup> | 3226-64-g <sup>+</sup>  | = -2222-46-g <sup>+</sup> | 3227-64-g <sup>+</sup>  | = -2222-46-g <sup>+</sup> |
| *3225-65-g <sup>+</sup> | = -2222-56-g <sup>+</sup> | *3226-65-g <sup>+</sup> | = -2222-56-g <sup>+</sup> | *3227-65-g <sup>+</sup> | = -2222-56-g <sup>+</sup> |
| 3225-66-g <sup>+</sup>  | = 2225-66-g <sup>+</sup>  | 3226-66-g <sup>+</sup>  | = 2226-66-g <sup>+</sup>  | 3227-66-g <sup>+</sup>  | = 2227-66-g <sup>+</sup>  |
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| *3225-D4-g <sup>+</sup> | = -2222-4D-g <sup>+</sup> | *3226-D4-g <sup>+</sup> | = -2222-4D-g <sup>+</sup> | *3227-D4-g <sup>+</sup> | = -2222-4D-g <sup>+</sup> |
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| *3225-D6-g <sup>+</sup> | = 2222-6D-g <sup>+</sup>  | *3226-D6-g <sup>+</sup> | = 2222-6D-g <sup>+</sup>  | *3227-D6-g <sup>+</sup> | = 2222-6D-g <sup>+</sup>  |
| 3225-DD-g <sup>+</sup>  | = 2225-DD-g <sup>+</sup>  | 3226-DD-g <sup>+</sup>  | = 2226-DD-g <sup>+</sup>  | 3227-DD-g <sup>+</sup>  | = 2227-DD-g <sup>+</sup>  |

<sup>a</sup> The values of the  $g^-$  interaction constants are the same as those of the corresponding  $g^+$  interaction constants, unless they are marked with \*. For those marked with \*, the absolute values of the  $g^+$  and  $g^-$  interaction constants are the same but their signs are opposite to each other.

<sup>b</sup> Units are  $\text{aJ } \text{\AA}^{-2} = \text{mdyn } \text{\AA}^{-1}$  for the stretching and stretching-stretching constants,  $\text{aJ } \text{\AA}^{-1} = \text{mdyn}$  for the stretching-bending constants, and  $\text{aJ} = \text{mdyn } \text{\AA}$  for the bending, bending-bending and torsional constants. Errors in the force constants, given in parentheses, apply to the last significant figure(s).

not any of these three coordinates. Thus, for example,  $225-5D = -522-5D$ ,  $0123-S5 = -3210-5S$ ,  $2226-46-t = -6222-64-t$ ,  $2227-S5 = -7222-5S$ , etc.

Most of the intergroup force constants for the gauche<sup>-</sup> conformation are equivalent to the corresponding force constants for the gauche<sup>+</sup> conformation. For some of the force constants, however, the absolute values of the gauche<sup>+</sup> and gauche<sup>-</sup> constants are the same but their signs are opposite to each other. These force constants are marked with \* in tables 3-7.

## 4. Description of Tables

### 4.1. Symmetry

The symmetry (point group) of each molecule is given by the Schoenflies notation. Detailed discussions of symmetry properties will be found in references [29,30].

### 4.2. Symmetry Number

The symmetry number,  $\sigma$ , is used in the calculation of thermodynamic quantities. It is the number of indistinguishable positions into which the molecule can be transformed by simple rigid rotations. A general discussion and pertinent formulas may be found in reference [30], page 508.

### 4.3. Symmetry Species

In the tables the normal modes are divided into the symmetry species of the point group to which the molecule belongs. The ordering of species in each point group is given in table I of reference [8], which is a summary of tables 12-30 of reference [30]. When a molecule has two or three planes of symmetry, the relationship between the vibrational modes and symmetry species cannot be defined uniquely. In such cases we generally follow the notation adopted in reference [30].

### 4.4. Observed Frequencies

The sources of the observed frequencies are given at the bottom of each of the tables. The infrared and Raman spectra of most of the molecules covered in this part were remeasured or newly measured in our laboratory. The abbreviations IR and R stand for infrared and Raman, respectively.

The observed frequencies used in the refinement of the force field are, as a general rule, those observed in the liquid state or in solution. For the cases where the bands of the liquid state or solution are not well resolved, the frequencies observed in the solid state, or in rarer cases, in the gaseous state are used. The following abbreviations are used in the column for observed frequency to indicate the state of aggregation in which the frequency is observed. If no indication is given, the frequency is that observed in the liquid state or in solution.

- (s) Observed in the solid state.
- (g) Observed in the gaseous state.

## 4.5. Vibrational Assignment

Assignments of the vibrations are given by the calculated potential-energy distributions (P.E.D.) [31,32] in terms of the local symmetry coordinates. The values in parentheses are the potential-energy distributions given by percent, and the signs denote relative phase relations among the coordinates associated with the normal vibration. In the tables, the potential-energy distributions more than 10 percent are given with a maximum of four coordinates, but, if the total of these distributions is less than 70 percent and if the number of the coordinates so far listed is smaller than four, additional distributions are also given until the total exceeds 70 percent.

The coordinates are given by the symbols which have the same format as that of the corresponding diagonal force constants. The arranging order of the atomic groups in the coordinate symbols is in accordance with the molecular formulas given in the tables. The symbols of the deuterated atomic groups are not distinguished from those of the corresponding undeuterated atomic groups. Thus the symbol 1 is used for the CH<sub>3</sub> and CD<sub>3</sub> groups in common and the symbol 2 for the CH<sub>2</sub>, CD<sub>2</sub>, and CHD groups.

## 5. Acknowledgments

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| 169. 1-Iodopropane $\text{CH}_3\text{CH}_2\text{CH}_2\text{I}$ (trans form) .....                                       | 1220 |
| 170. 1-Iodopropane $\text{CH}_3\text{CH}_2\text{CH}_2\text{I}$ (gauche form).....                                       | 1221 |
| 171. 1-Iodobutane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-trans form).....                        | 1222 |
| 172. 1-Iodobutane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-gauche form).....                       | 1223 |
| 173. 1-Iodobutane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-trans form).....                       | 1224 |
| 174. 1-Iodobutane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-gauche form).....                      | 1225 |
| 175. 1-Iodopentane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-trans-trans form) .....     | 1226 |
| 176. 1-Iodopentane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-trans-gauche form) .....    | 1227 |
| 177. 1-Iodopentane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-gauche-trans form) .....    | 1228 |
| 178. 1-Iodopentane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-trans-trans form) .....    | 1229 |
| 179. 1-Iodopentane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-gauche-gauche form) .....   | 1230 |
| 180. 1-Iodopentane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-trans-gauche form) .....   | 1231 |
| 181. 1-Iodopentane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-trans-gauche' form) .....  | 1232 |
| 182. 1,3-Diiodopropane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-trans form) .....                            | 1233 |
| 183. 1,3-Diiodopropane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-gauche form) .....                           | 1234 |
| 184. 1,3-Diiodopropane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-gauche form) .....                          | 1235 |
| 185. 1,4-Diiodobutane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-trans-trans form) .....            | 1236 |
| 186. 1,4-Diiodobutane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-trans-gauche form) .....           | 1237 |
| 187. 1,4-Diiodobutane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-gauche-trans form) .....           | 1238 |
| 188. 1,4-Diiodobutane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (trans-gauche-gauche form) .....          | 1239 |
| 189. 1,4-Diiodobutane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-trans-gauche form) .....          | 1240 |
| 190. 1,4-Diiodobutane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-trans-gauche' form).....          | 1241 |
| 191. 1,4-Diiodobutane $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$ (gauche-gauche-gauche form).....          | 1242 |
| 192. 2-Chloroethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Cl}$ (trans-trans form) .....                  | 1243 |
| 193. 2-Chloroethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Cl}$ (trans-gauche form) .....                 | 1244 |
| 194. 2-Chloroethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Cl}$ (gauche-trans form) .....                 | 1245 |
| 195. 2-Chloroethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Cl}$ (gauche-gauche form) .....                | 1246 |
| 196. 2-Bromoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Br}$ (trans-trans form).....                    | 1247 |
| 197. 2-Bromoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Br}$ (trans-gauche form) .....                  | 1248 |
| 198. 2-Bromoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Br}$ (gauche-trans form).....                   | 1249 |
| 199. 2-Bromoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Br}$ (gauche-gauche form).....                  | 1250 |
| 200. 2-Iodoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{I}$ (trans-trans form) .....                     | 1251 |
| 201. 2-Iodoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{I}$ (trans-gauche form).....                     | 1252 |
| 202. 2-Iodoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{I}$ (gauche-trans form).....                     | 1253 |
| 203. 2-Iodoethyl methyl ether $\text{CH}_3\text{OCH}_2\text{CH}_2\text{I}$ (gauche-gauche form).....                    | 1254 |

## No. 110

Molecule: 1228-T  $\text{CH}_3\text{CH}_2\text{CH}_2\text{F}$  (trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           | 1474*                               | 1479                                  | 122-2 (58+)           | 012-4 (26+) |             |             |
|              | 1456*                               | 1453                                  | 012-4 (56+)           | 122-2 (35-) |             |             |
|              | 1441*                               | 1428                                  | 228-2 (87+)           |             |             |             |
|              | 1397*                               | 1397                                  | 228-5 (62-)           | 122-5 (26+) | 1228-S(17+) |             |
|              | 1377*                               | 1378                                  | 012-2 (102+)          |             |             |             |
|              | 1290                                | 1290                                  | 122-5 (60+)           | 228-5 (30+) |             |             |
|              | 1156*                               | 1139                                  | 012-5 (27+)           | 122-D (12+) | 1228-S(12-) | 228-D (11+) |
|              | 1037                                | 1045                                  | 0122-S(45+)           | 1228-S(35-) | 2280-S(17+) |             |
|              | 1002                                | 999                                   | 2280-S(63+)           | 0122-S(33-) |             |             |
|              | 894                                 | 891                                   | 012-5 (48-)           | 1228-S(25-) | 122-5 (13-) |             |
|              | 452                                 | 457                                   | 228-D (39+)           | 122-D (16+) | 1228-S(12+) | 0122-S(10+) |
|              |                                     | 272                                   | 122-D (80+)           | 228-D (62-) | 228-5 (20+) |             |
| a''          | 1469*                               | 1463                                  | 012-7 (80+)           | 012-8 (14+) |             |             |
|              | 1308                                | 1307                                  | 228-6 (71+)           | 122-6 (14-) |             |             |
|              | 1277                                | 1270                                  | 122-6 (57+)           | 012-8 (11-) | 228-6 (9+)  |             |
|              | 1127                                | 1138                                  | 228-4 (31-)           | 122-4 (20-) | 012-8 (18+) | 228-6 (15+) |
|              | 894                                 | 897                                   | 012-8 (43+)           | 228-4 (42+) | 122-6 (27+) |             |
|              |                                     | 746                                   | 122-4 (65+)           | 228-4 (21-) | 012-8 (17+) |             |
|              |                                     | 227                                   | 0122-T(96+)           |             |             |             |
|              |                                     | 152                                   | 1228-T(89+)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3000 2962 2962 2934 2905 2880 2869

All the observed frequencies given are those in the unannealed solid state.

\* Not used in the force constant determination.

## Reference

- [1] I.R.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **18**, 33 (1973).

## No. 111

Molecule: 1228-G  $\text{CH}_3\text{CH}_2\text{CH}_2\text{F}$  (gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474                                | 1480                                  | 122-2 (69+)           | 012-4 (17+) |             |             |
|              | 1469                                | 1464                                  | 012-7 (79+)           | 012-8 (14+) |             |             |
|              | 1456                                | 1457                                  | 012-4 (65+)           | 122-2 (17-) |             |             |
|              | 1441                                | 1437                                  | 228-2 (74+)           |             |             |             |
|              | 1397                                | 1392                                  | 228-5 (53+)           | 122-5 (16+) | 012-2 (11-) |             |
|              | 1377                                | 1378                                  | 012-2 (93+)           |             |             |             |
|              | 1331                                | 1334                                  | 122-5 (36+)           | 228-5 (27-) | 228-6 (17+) | 1228-S(17+) |
|              | 1277*                               | 1283                                  | 228-6 (37+)           | 122-6 (26-) | 122-5 (10-) |             |
|              | 1252                                | 1250                                  | 122-6 (39+)           | 228-6 (30+) | 122-5 (5-)  |             |
|              | 1156                                | 1151                                  | 122-4 (23-)           | 228-4 (17+) | 012-8 (15+) | 122-6 (6+)  |
|              | 1102                                | 1104                                  | 012-5 (24+)           | 2280-S(15+) | 228-4 (10+) | 122-D (9+)  |
|              | 1059                                | 1063                                  | 0122-S(42-)           | 1228-S(27+) | 2280-S(8-)  |             |
|              | 948                                 | 948                                   | 2280-S(57-)           | 012-5 (17+) |             |             |
|              | 911                                 | 908                                   | 228-4 (37-)           | 012-8 (24+) | 012-5 (18+) | 122-5 (11+) |
|              | 868                                 | 862                                   | 0122-S(38-)           | 1228-S(26-) | 228-4 (9-)  |             |
|              | 764                                 | 766                                   | 122-4 (52+)           | 012-8 (26+) | 228-4 (10+) |             |
|              | 482                                 | 475                                   | 228-D (60+)           | 122-D (31-) | 228-5 (16-) | 122-4 (10+) |
|              | 324                                 | 320                                   | 122-D (52-)           | 228-D (24-) | 1228-T(13+) |             |
|              |                                     | 213                                   | 0122-T(81+)           | 228-D (11-) |             |             |
|              |                                     | 148                                   | 1228-T(78+)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3000 2962 2962 2934 2905 2880 2868

All the observed frequencies given are those in the unannealed solid state.

\* Not used in the force constant determination.

## Reference

- [1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **18**, 33 (1973).

## No. 112

Molecule: 12228-TT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (trans-trans form)Symmetry  $\text{C}_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           | 1480*                               | 1484                                  | 122-2 (42-)           | 222-2 (32+) | 012-4 (16-) |             |
|              | 1457*                               | 1462                                  | 222-2 (59+)           | 012-4 (18+) | 122-2 (12+) |             |
|              | 1457*                               | 1453                                  | 012-4 (51-)           | 122-2 (37+) |             |             |
|              | 1433*                               | 1428                                  | 228-2 (85+)           |             |             |             |
|              | 1394*                               | 1395                                  | 228-5 (59+)           | 222-5 (27-) | 2228-S(15-) |             |
|              | 1387*                               | 1379                                  | 012-2 (105+)          |             |             |             |
|              | 1344*                               | 1340                                  | 122-5 (63+)           | 228-5 (19-) | 1222-S(12+) |             |
|              | 1255*                               | 1259                                  | 222-5 (63+)           | 122-5 (15+) | 228-5 (14+) |             |
|              | 1150*                               | 1142                                  | 012-5 (20+)           | 1222-S(18-) | 222-D (11+) | 122-D (10+) |
|              | 1064*                               | 1056                                  | 1222-S(32+)           | 2228-S(28-) | 0122-S(24-) |             |
|              | 1037                                | 1029                                  | 2280-S(35-)           | 2228-S(31+) | 0122-S(24-) |             |
|              | 989                                 | 988                                   | 2280-S(44-)           | 0122-S(29+) | 012-5 (11-) |             |
|              | 904                                 | 905                                   | 012-5 (40+)           | 1222-S(28+) | 0122-S( 9+) |             |
|              | 442                                 | 446                                   | 228-D (62+)           | 122-D (32-) | 228-5 (13-) |             |
|              | 394                                 | 395                                   | 222-D (28+)           | 122-D (26+) | 2228-S( 9+) | 0122-S( 7+) |
|              | 187                                 | 187                                   | 222-D (64+)           | 228-D (41-) | 122-D (36-) | 228-5 (12+) |
| a''          | 1467*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1309*                               | 1310                                  | 228-6 (67-)           | 122-6 (14+) |             |             |
|              | 1296*                               | 1298                                  | 222-6 (42+)           | 122-6 (35-) |             |             |
|              | 1229*                               | 1236                                  | 222-6 (28-)           | 122-6 (18-) | 012-8 (15+) | 122-4 (10-) |
|              | 1150*                               | 1142                                  | 228-4 (26-)           | 222-4 (17-) | 228-6 (14+) | 122-4 (13-) |
|              | 949*                                | 947                                   | 228-4 (30+)           | 012-8 (29+) | 122-6 (27+) | 222-6 (20+) |
|              | 795                                 | 798                                   | 228-4 (29-)           | 122-4 (26+) | 012-8 (25+) | 222-4 (21+) |
|              | 740*                                | 734                                   | 122-4 (42+)           | 222-4 (40-) |             |             |
|              |                                     | 234                                   | 0122-T(88-)           |             |             |             |
|              |                                     | 147                                   | 2228-T(66+)           | 1222-T(20+) |             |             |
|              |                                     | 113                                   | 1222-T(70+)           | 2228-T(14-) |             |             |

352

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3000 2962 2962 2935 2909 2901 2880 2873 2865

\* Not used in the force constant determination.

## Reference

[1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **23**, 161 (1974).



No. 113

Molecule: 12228-TG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (trans-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1480                                | 1486                                  | 222-2 (40+)           | 122-2 (36-) | 012-4 (12-) |             |
|              | 1467                                | 1464                                  | 222-2 (46+)           | 012-4 (24+) | 122-2 (17+) |             |
|              | 1457                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1457                                | 1452                                  | 012-4 (49-)           | 122-2 (41+) |             |             |
|              | 1433                                | 1436                                  | 228-2 (73+)           |             |             |             |
|              | 1394                                | 1395                                  | 228-5 (49-)           | 222-5 (24-) | 228-2 (11+) |             |
|              | 1387                                | 1379                                  | 012-2 (105+)          |             |             |             |
|              | 1344                                | 1352                                  | 122-5 (35+)           | 228-5 (30+) | 222-5 (16-) | 2228-S(14-) |
|              | 1309                                | 1313                                  | 228-6 (33-)           | 122-5 (25-) | 122-6 (11-) | 228-5 ( 5+) |
|              | 1296                                | 1295                                  | 122-6 (36-)           | 222-6 (22+) | 122-5 (12+) | 222-5 (10+) |
|              | 1255                                | 1252                                  | 228-6 (33+)           | 222-5 (21-) | 122-6 (14-) | 012-8 ( 5+) |
|              | 1229                                | 1232                                  | 222-6 (37+)           | 228-6 (12+) | 012-8 ( 9-) | 122-6 ( 7+) |
|              | 1150                                | 1151                                  | 222-4 (22-)           | 122-4 (13-) | 228-4 (12+) | 012-8 (11+) |
|              | 1122                                | 1117                                  | 012-5 (21+)           | 1222-S(20-) | 228-4 ( 9+) | 222-D ( 8+) |
|              | 1064                                | 1069                                  | 2228-S(31+)           | 1222-S(18-) | 2280-S(17-) | 0122-S(13+) |
|              | 1025                                | 1020                                  | 0122-S(65-)           | 2228-S(17+) | 2280-S(11-) |             |
|              | 970                                 | 963                                   | 228-4 (32-)           | 012-8 (15+) | 012-5 (15+) | 122-6 (15+) |
|              | 949                                 | 952                                   | 2280-S(36+)           | 012-5 (15-) | 012-8 ( 7+) | 222-6 ( 7+) |
|              | 841                                 | 845                                   | 2280-S(21-)           | 222-4 (18+) | 012-8 (15+) | 2228-S(11-) |
|              | 832                                 | 820                                   | 1222-S(30-)           | 228-4 (25-) | 012-8 (11-) | 012-5 ( 9-) |
|              | 740                                 | 740                                   | 122-4 (55+)           | 222-4 (23-) | 012-8 (14+) |             |
|              | 513                                 | 514                                   | 228-D (48+)           | 222-D (21-) | 228-5 (13-) | 122-D (11-) |
|              | 350                                 | 343                                   | 228-D (38+)           | 122-D (36+) | 2228-S(15+) |             |
|              | 265                                 | 265                                   | 222-D (44-)           | 122-D (38+) | 2228-T(18+) |             |
|              |                                     | 227                                   | 0122-T(83+)           |             |             |             |
|              |                                     | 134                                   | 2228-T(67+)           | 222-D (12+) |             |             |
|              |                                     | 99                                    | 1222-T(86+)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3000 2962 2962 2934 2909 2901 2880 2873 2865

## Reference

[1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **23**, 161 (1974).

## No. 114

Molecule: 12228-GT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (gauche-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1480*                               | 1484                                  | 122-2 (48+)           | 222-2 (36+) |             |             |
|              | 1467*                               | 1471                                  | 222-2 (44-)           | 012-4 (25+) | 122-2 (14+) |             |
|              | 1457*                               | 1463                                  | 012-7 (77+)           | 012-8 (13+) |             |             |
|              | 1457*                               | 1453                                  | 012-4 (51-)           | 122-2 (30+) |             |             |
|              | 1433*                               | 1429                                  | 228-2 (90+)           |             |             |             |
|              | 1394*                               | 1396                                  | 228-5 (58-)           | 222-5 (26+) | 2228-S(14+) |             |
|              | 1387*                               | 1379                                  | 012-2 (103+)          |             |             |             |
|              | 1344*                               | 1347                                  | 122-5 (68+)           | 1222-S( 9+) |             |             |
|              | 1309*                               | 1306                                  | 228-6 (63+)           | 222-6 (19-) |             |             |
|              | 1296*                               | 1299                                  | 222-5 (41+)           | 228-5 (28+) | 122-6 (21-) |             |
|              | 1255*                               | 1264                                  | 122-6 (38+)           | 222-5 (18+) | 012-8 ( 8-) | 012-7 ( 6+) |
|              | 1229*                               | 1232                                  | 222-6 (46+)           | 228-6 (14+) | 122-6 ( 5-) | 012-5 ( 5+) |
|              | 1150*                               | 1144                                  | 228-4 (13+)           | 122-4 (13-) | 012-8 (10+) | 1222-S( 9-) |
|              | 1122*                               | 1121                                  | 012-5 (16+)           | 2228-S(12+) | 228-4 ( 8+) | 122-D ( 7+) |
|              | 1064*                               | 1079                                  | 0122-S(31-)           | 1222-S(29+) | 2228-S(14-) |             |
|              | 1004                                | 1010                                  | 2280-S(67+)           | 2228-S(15-) |             |             |
|              | 970*                                | 970                                   | 012-5 (24-)           | 2228-S(16+) | 122-5 (13-) | 228-4 (11+) |
|              | 949*                                | 952                                   | 012-8 (21-)           | 122-6 (20-) | 228-4 (19+) | 222-6 (13+) |
|              | 880                                 | 889                                   | 0122-S(31-)           | 1222-S(28-) | 012-5 (20-) |             |
|              | 795*                                | 793                                   | 222-4 (26-)           | 122-4 (25+) | 228-4 (23+) | 012-8 (17+) |
|              | 740*                                | 749                                   | 122-4 (37+)           | 222-4 (29+) | 012-8 (15+) | 228-4 (13-) |
|              | 483                                 | 483                                   | 122-D (26+)           | 228-D (19-) | 222-D (17-) | 2228-S(10-) |
|              | 350*                                | 355                                   | 122-D (49+)           | 228-D (40+) |             |             |
|              |                                     | 285                                   | 222-D (40-)           | 0122-T(33-) | 228-D (27+) |             |
|              |                                     | 194                                   | 0122-T(62+)           | 222-D (27-) | 228-D (11+) |             |
|              |                                     | 124                                   | 2228-T(73-)           | 1222-T(15-) |             |             |
|              |                                     | 115                                   | 1222-T(66+)           | 222-4 ( 8-) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3000 2962 2962 2935 2907 2903 2880 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct.,
- 23**
- , 161 (1974).

## No. 115

Molecule: 12228-GG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1480*                               | 1486                                  | 222-2 (46+)           | 122-2 (38+) |             |             |
|              | 1467*                               | 1472                                  | 222-2 (32-)           | 012-4 (26+) | 122-2 (24+) |             |
|              | 1457*                               | 1463                                  | 012-7 (78+)           | 012-8 (14+) |             |             |
|              | 1457*                               | 1453                                  | 012-4 (52+)           | 122-2 (30-) |             |             |
|              | 1433*                               | 1436                                  | 228-2 (71+)           |             |             |             |
|              | 1394*                               | 1395                                  | 228-5 (51+)           | 222-5 (24+) | 228-2 (12-) |             |
|              | 1387*                               | 1380                                  | 012-2 (102+)          |             |             |             |
|              | 1344*                               | 1349                                  | 122-5 (62-)           | 1222-S(12-) |             |             |
|              | 1344*                               | 1340                                  | 222-5 (32-)           | 228-5 (29+) | 2228-S(17-) | 228-6 (10-) |
|              |                                     | 1272                                  | 122-6 (52+)           | 228-6 (18+) | 222-6 (6+)  |             |
|              | 1255*                               | 1254                                  | 228-6 (48+)           | 222-5 (16-) | 222-6 (7-)  |             |
|              | 1229*                               | 1230                                  | 222-6 (54+)           | 012-8 (7+)  | 122-4 (5-)  | 122-6 (5-)  |
|              | 1150*                               | 1147                                  | 222-4 (20-)           | 012-5 (15-) | 1222-S(15+) | 122-D (7-)  |
|              | 1122*                               | 1110                                  | 228-4 (16-)           | 122-4 (15+) | 012-8 (14-) | 222-D (9-)  |
|              |                                     | 1083                                  | 0122-S(25-)           | 1222-S(18+) | 2228-S(11-) | 2280-S(11+) |
|              | 989*                                | 989                                   | 2228-S(22-)           | 2280-S(21+) | 012-5 (14+) | 012-8 (11-) |
|              | 970*                                | 973                                   | 0122-S(35+)           | 228-4 (17-) | 2280-S(17+) | 222-6 (13+) |
|              | 949*                                | 940                                   | 2280-S(16-)           | 0122-S(16+) | 228-4 (15-) | 012-5 (14+) |
|              | 841*                                | 848                                   | 012-8 (23-)           | 2280-S(19-) | 222-4 (19+) | 122-4 (10-) |
|              | 813                                 | 813                                   | 1222-S(41-)           | 228-4 (13-) | 0122-S(12-) | 012-5 (7-)  |
|              | 740*                                | 743                                   | 122-4 (45+)           | 222-4 (22+) | 012-8 (16+) | 228-4 (11+) |
|              |                                     | 502                                   | 228-D (43+)           | 222-D (36-) | 122-D (13+) | 228-5 (11-) |
|              | 394*                                | 402                                   | 122-D (48-)           | 228-D (28+) | 2228-T(12-) |             |
|              | 265*                                | 263                                   | 222-D (28+)           | 0122-T(27+) | 228-D (21+) | 122-D (18+) |
|              |                                     | 211                                   | 0122-T(56+)           | 222-D (16-) | 122-D (11-) | 2228-T(10+) |
|              |                                     | 155                                   | 2228-T(42-)           | 1222-T(24+) | 0122-T(11+) | 222-4 (11-) |
|              |                                     | 79                                    | 1222-T(60-)           | 2228-T(29-) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3000 2962 2962 2934 2907 2903 2880 2870 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **23**, 161 (1974).

## No. 116

Molecule: 122228-TTT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (trans-trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           |                                     | 1484                                  | 122-2 (38-)           | 222-2 (34+) | 012-4 (15-) |             |
|              | 1469*                               | 1475                                  | 222-2 (67+)           | 122-2 (14-) | 222-2 (10-) |             |
|              | 1463*                               | 1458                                  | 012-4 (44+)           | 222-2 (33+) | 222-2 (11+) |             |
|              | 1446*                               | 1449                                  | 122-2 (41+)           | 012-4 (23-) | 222-2 (15+) | 222-2 (10+) |
|              | 1435*                               | 1427                                  | 228-2 (83+)           |             |             |             |
|              | 1394*                               | 1396                                  | 228-5 (57-)           | 222-5 (27+) | 2228-S(15+) |             |
|              | 1385*                               | 1379                                  | 012-2 (104+)          |             |             |             |
|              |                                     | 1359                                  | 122-5 (44-)           | 222-5 (35+) | 1222-S(16-) | 228-5 (10-) |
|              | 1303*                               | 1305                                  | 122-5 (33+)           | 222-5 (24-) | 228-5 (19-) | 222-5 (18+) |
|              | 1243*                               | 1244                                  | 222-5 (43+)           | 222-5 (34+) |             |             |
|              | 1151*                               | 1142                                  | 012-5 (16+)           | 1222-S(14-) | 2222-S(10-) | 222-D (10+) |
|              | 1075*                               | 1061                                  | 2222-S(39+)           | 1222-S(28-) | 0122-S(11+) |             |
|              | 1051*                               | 1047                                  | 2228-S(42-)           | 0122-S(20-) | 2280-S(10+) |             |
|              | 1029*                               | 1015                                  | 0122-S(28-)           | 012-5 (17+) | 2228-S(15+) | 2280-S(13+) |
|              | 1005                                | 1002                                  | 2280-S(55-)           | 0122-S(20-) | 2222-S(15+) |             |
|              | 886*                                | 891                                   | 012-5 (36+)           | 1222-S(34+) | 0122-S( 9+) |             |
|              | 516                                 | 512                                   | 228-D (39+)           | 122-D (22-) | 222-D (16-) |             |
|              | 357                                 | 366                                   | 222-D (35-)           | 222-D (28-) | 1222-S( 7-) | 122-D ( 5+) |
|              | 317                                 | 311                                   | 122-D (48+)           | 228-D (38+) | 2222-S(12+) |             |
|              |                                     | 138                                   | 222-D (51+)           | 222-D (45-) | 228-D (23-) | 122-D (18+) |
| a''          | 1463*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1303*                               | 1312                                  | 228-6 (52-)           | 222-6 (23+) |             |             |
|              | 1295*                               | 1301                                  | 222-6 (30-)           | 222-6 (26+) | 228-6 (18+) | 122-6 (10-) |
|              | 1278*                               | 1283                                  | 122-6 (46+)           | 222-6 (23-) | 222-4 ( 6-) |             |
|              | 1214*                               | 1216                                  | 222-6 (18+)           | 222-6 (18+) | 012-8 (16-) | 122-4 (15+) |
|              | 1151*                               | 1144                                  | 228-4 (24+)           | 222-4 (16+) | 228-6 (13-) | 222-4 (12+) |
|              | 979*                                | 977                                   | 222-6 (26+)           | 228-4 (22+) | 012-8 (20+) | 122-6 (20+) |
|              | 841                                 | 850                                   | 222-4 (31-)           | 012-8 (25-) | 228-4 (25+) | 122-6 (12-) |
|              | 743                                 | 759                                   | 222-4 (40-)           | 122-4 (30+) | 228-4 (18+) | 012-8 (12+) |
|              | 733*                                | 729                                   | 222-4 (39-)           | 122-4 (31+) | 222-4 (19+) |             |
|              |                                     | 231                                   | 0122-T(91+)           |             |             |             |
|              |                                     | 171                                   | 2228-T(63+)           | 1222-T(28-) |             |             |
|              |                                     | 121                                   | 2222-T(67+)           | 1222-T(21+) |             |             |
|              |                                     | 78                                    | 1222-T(42+)           | 2228-T(21+) | 2222-T(19-) |             |

Calculated frequencies higher than 2000  $\text{cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3000 | 2962 | 2962 | 2935 | 2911 | 2905 | 2899 | 2880 | 2875 | 2869 |
| 2864 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

[1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **23**, 161 (1974).

## No. 117

Molecule: 122220-TTG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (trans-trans-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1484                                  | 222-2 (37+)           | 122-2 (31-) | 012-4 (13-) | 222-2 (10-) |
|              | 1469                                | 1478                                  | 222-2 (61+)           | 122-2 (21-) |             |             |
|              | 1463                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1463                                | 1457                                  | 012-4 (47+)           | 222-2 (36+) |             |             |
|              | 1446                                | 1449                                  | 122-2 (42-)           | 222-2 (21-) | 012-4 (21+) |             |
|              | 1435                                | 1436                                  | 228-2 (71+)           |             |             |             |
|              | 1394                                | 1396                                  | 228-5 (47+)           | 222-5 (24+) | 228-2 (11-) |             |
|              | 1385                                | 1379                                  | 012-2 (104+)          |             |             |             |
|              |                                     | 1360                                  | 222-5 (33+)           | 122-5 (32-) | 228-5 (20+) | 1222-S(13-) |
|              | 1346                                | 1333                                  | 122-5 (28-)           | 222-5 (26+) | 228-5 (17-) | 228-6 (15+) |
|              | 1303                                | 1307                                  | 222-6 (41+)           | 222-6 (13-) | 122-6 (12-) | 228-6 ( 8+) |
|              | 1278                                | 1291                                  | 122-6 (34+)           | 228-6 (20+) | 222-5 (11+) | 122-5 ( 7+) |
|              | 1268                                | 1275                                  | 222-6 (22-)           | 222-5 (20-) | 122-6 (16+) | 228-6 ( 9-) |
|              | 1243                                | 1235                                  | 228-6 (29+)           | 222-5 (23-) | 222-5 (18-) | 222-6 ( 5-) |
|              | 1214                                | 1217                                  | 222-6 (28+)           | 222-6 (14+) | 012-8 (13-) | 122-4 (12+) |
|              | 1151                                | 1153                                  | 222-4 (20+)           | 222-4 (12+) | 228-4 (11-) | 122-4 ( 9+) |
|              | 1123                                | 1123                                  | 012-5 (17-)           | 1222-S(16+) | 122-D ( 7-) | 222-D ( 7-) |
|              | 1075                                | 1072                                  | 2222-S(35-)           | 2228-S(22+) | 2280-S( 8-) | 1222-S( 7+) |
|              | 1051                                | 1050                                  | 0122-S(36+)           | 1222-S(25-) | 2228-S(15+) |             |
|              | 1029                                | 1015                                  | 0122-S(36-)           | 228-4 (15-) | 2280-S(12-) | 012-5 (10+) |
|              | 979                                 | 983                                   | 2280-S(22-)           | 222-6 (22-) | 012-8 (16-) | 122-6 (16-) |
|              | 911                                 | 922                                   | 012-5 (23-)           | 1222-S(16-) | 0122-S(14-) | 228-4 ( 9+) |
|              | 886                                 | 885                                   | 2280-S(33-)           | 012-8 (13+) | 222-4 (12+) | 2228-S(10-) |
|              | 863                                 | 859                                   | 228-4 (26+)           | 012-5 (14+) | 2222-S(14+) | 1222-S(12+) |
|              | 781                                 | 779                                   | 222-4 (31-)           | 122-4 (26+) | 012-8 (16+) |             |
|              | 733                                 | 730                                   | 222-4 (40-)           | 122-4 (39+) |             |             |
|              | 501                                 | 503                                   | 228-D (54+)           | 222-D (22-) | 228-5 (14-) | 222-4 (10+) |
|              | 402                                 | 402                                   | 122-D (52-)           | 222-D (14-) | 222-D ( 9+) |             |
|              | 322                                 | 321                                   | 228-D (35-)           | 222-D (19-) | 222-D (15-) | 2228-S(11-) |
|              |                                     | 230                                   | 0122-T(93+)           |             |             |             |
|              |                                     | 203                                   | 222-D (35+)           | 2228-T(33+) | 122-D (23-) | 222-D (11-) |
|              |                                     | 141                                   | 1222-T(33+)           | 222-D (22-) | 2228-T(19-) | 222-D (14+) |
|              |                                     | 94                                    | 2222-T(51+)           | 1222-T(22+) | 2228-T(19+) |             |
|              |                                     | 87                                    | 2222-T(32-)           | 1222-T(30+) | 2228-T(10+) |             |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3000 | 2962 | 2962 | 2934 | 2911 | 2905 | 2899 | 2880 | 2875 | 2869 |
| 2864 |      |      |      |      |      |      |      |      |      |

## Reference

[1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **23**, 161 (1974).

## No. 118

Molecule: 122228-TGT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (trans-gauche-trans form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1489                                  | 222-2 (38+)           | 122-2 (24-) | 222-2 (21+) |             |
|              | 1469*                               | 1474                                  | 222-2 (50+)           | 122-2 (25+) | 012-4 (14+) |             |
|              | 1463*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1463*                               | 1459                                  | 222-2 (50+)           | 012-4 (22+) | 222-2 (18-) |             |
|              | 1446*                               | 1452                                  | 122-2 (44+)           | 012-4 (41-) |             |             |
|              | 1435*                               | 1429                                  | 228-2 (90+)           |             |             |             |
|              | 1394*                               | 1396                                  | 228-5 (58-)           | 222-5 (27+) | 2228-S(14+) |             |
|              | 1385*                               | 1379                                  | 012-2 (103+)          |             |             |             |
|              |                                     | 1364                                  | 222-5 (43-)           | 122-5 (37+) | 1222-S(16+) |             |
|              | 1303*                               | 1313                                  | 228-6 (52+)           | 122-5 (18+) | 222-5 (7+)  |             |
|              | 1303*                               | 1301                                  | 222-6 (31-)           | 222-5 (21+) | 228-5 (17+) | 122-6 (11+) |
|              | 1303*                               | 1297                                  | 122-5 (19+)           | 222-6 (16+) | 222-5 (16+) | 222-5 (14+) |
|              | 1303*                               | 1293                                  | 122-6 (40-)           | 222-5 (12+) | 222-6 (8-)  | 122-5 (6-)  |
|              | 1243*                               | 1239                                  | 222-6 (20+)           | 222-5 (11+) | 122-6 (10+) | 222-6 (9+)  |
|              | 1214*                               | 1218                                  | 222-6 (31+)           | 228-6 (13+) | 222-6 (10-) | 012-8 (7+)  |
|              | 1151*                               | 1144                                  | 222-4 (15-)           | 122-4 (10-) | 228-4 (8+)  | 012-8 (8+)  |
|              | 1123*                               | 1128                                  | 012-5 (16+)           | 1222-S(16-) | 228-4 (11+) | 222-4 (8+)  |
|              | 1075*                               | 1082                                  | 2222-S(35-)           | 2228-S(22+) | 1222-S(16+) |             |
|              | 1029*                               | 1027                                  | 0122-S(62-)           | 2228-S(11-) | 2280-S(11+) |             |
|              | 1005*                               | 1009                                  | 2280-S(45+)           | 012-5 (11-) | 228-4 (10+) | 0122-S(7+)  |
|              | 995                                 | 997                                   | 2280-S(23+)           | 012-5 (13+) | 228-4 (12-) | 2222-S(11-) |
|              | 979*                                | 980                                   | 222-6 (23-)           | 2228-S(19-) | 012-8 (18-) | 122-6 (18-) |
|              | 863*                                | 867                                   | 1222-S(32-)           | 012-5 (25-) | 228-4 (17-) |             |
|              | 841*                                | 843                                   | 222-4 (32+)           | 012-8 (26+) | 122-6 (12+) | 122-4 (8+)  |
|              | 774                                 | 769                                   | 222-4 (44-)           | 228-4 (24+) | 122-4 (13-) |             |
|              | 733*                                | 733                                   | 122-4 (46+)           | 222-4 (28-) | 012-8 (10+) |             |
|              |                                     | 535                                   | 228-D (17+)           | 222-D (17-) | 122-D (13-) | 222-D (13+) |
|              | 344                                 | 347                                   | 228-D (40-)           | 222-D (18-) | 2222-S(13-) | 122-D (11-) |
|              | 290*                                | 304                                   | 122-D (45-)           | 222-D (36-) | 228-D (20+) | 222-D (14+) |
|              |                                     | 261                                   | 222-D (22-)           | 222-D (18-) | 122-D (17+) | 228-D (16+) |
|              |                                     | 225                                   | 0122-T(82-)           |             |             |             |
|              |                                     | 120                                   | 2228-T(47+)           | 2222-T(41+) |             |             |
|              |                                     | 96                                    | 2222-T(37-)           | 2228-T(23+) | 222-D (16-) | 222-4 (11+) |
|              |                                     | 86                                    | 1222-T(75+)           | 222-D (11-) |             |             |

Calculated frequencies higher than 2000  $\text{cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3000 | 2962 | 2962 | 2935 | 2910 | 2905 | 2900 | 2880 | 2873 | 2870 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

[1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **23**, 161 (1974).

## No. 119

Molecule: 122228-GTT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{F}$  (gauche-trans-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1485                                  | 122-2 (39+)           | 222-2 (38+) | 222-2 (12-) |             |
|              | 1469*                               | 1475                                  | 222-2 (35+)           | 122-2 (24+) | 012-4 (18+) | 222-2 (12-) |
|              | 1463*                               | 1464                                  | 012-7 (48+)           | 222-2 (20+) | 222-2 (10+) |             |
|              | 1463*                               | 1461                                  | 012-7 (31+)           | 222-2 (23-) | 222-2 (18-) | 012-4 (14+) |
|              | 1446*                               | 1453                                  | 012-4 (44-)           | 122-2 (29+) | 222-2 (13-) |             |
|              | 1435*                               | 1428                                  | 228-2 (86+)           |             |             |             |
|              | 1394*                               | 1396                                  | 228-5 (55-)           | 222-5 (27+) | 2228-S(15+) |             |
|              | 1385*                               | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1346*                               | 1350                                  | 122-5 (42+)           | 222-5 (32+) | 228-5 (10-) |             |
|              | 1346*                               | 1339                                  | 122-5 (32-)           | 222-5 (26+) | 1222-S(16-) | 228-5 (10-) |
|              | 1303*                               | 1309                                  | 228-6 (72-)           |             |             |             |
|              | 1303*                               | 1296                                  | 222-6 (45-)           | 222-6 (31+) |             |             |
|              | 1268*                               | 1273                                  | 122-6 (46-)           | 222-5 (23+) | 228-5 (8+)  |             |
|              | 1243*                               | 1252                                  | 222-5 (37+)           | 222-5 (18+) | 122-6 (12+) | 012-8 (7-)  |
|              | 1214*                               | 1204                                  | 222-6 (27+)           | 222-6 (20+) | 228-6 (11+) | 012-5 (7+)  |
|              | 1151*                               | 1145                                  | 228-4 (14+)           | 122-4 (9-)  | 222-4 (9+)  | 228-6 (8-)  |
|              | 1123*                               | 1127                                  | 2222-S(15-)           | 012-5 (13-) | 228-4 (6-)  | 122-D (6-)  |
|              | 1075*                               | 1083                                  | 1222-S(27+)           | 0122-S(24-) | 2222-S(14-) | 122-5 (6-)  |
|              | 1029*                               | 1037                                  | 2228-S(52+)           | 2280-S(22-) |             |             |
|              | 1005*                               | 1008                                  | 2280-S(39-)           | 0122-S(14-) | 222-5 (10-) | 012-8 (9-)  |
|              | 979*                                | 989                                   | 012-5 (23+)           | 222-6 (17-) | 228-4 (16-) | 122-5 (11+) |
|              | 979*                                | 968                                   | 2222-S(29-)           | 122-6 (16-) | 012-8 (15-) | 0122-S(11+) |
|              | 886*                                | 880                                   | 1222-S(33-)           | 012-5 (23-) | 0122-S(18-) |             |
|              | 841*                                | 844                                   | 222-4 (36-)           | 228-4 (27+) | 0122-S(12-) | 222-6 (12+) |
|              | 774                                 | 775                                   | 122-4 (47-)           | 012-8 (26-) | 222-4 (13-) |             |
|              | 733*                                | 739                                   | 222-4 (44+)           | 222-4 (26-) | 228-4 (10-) |             |
|              | 462                                 | 471                                   | 222-D (40+)           | 228-D (34-) | 122-D (23-) |             |
|              | 425                                 | 423                                   | 228-D (25+)           | 122-D (18-) | 222-D (13+) | 2228-S(11+) |
|              | 322*                                | 319                                   | 122-D (41+)           | 222-D (15+) | 222-D (10+) | 1222-T(6-)  |
|              |                                     | 237                                   | 0122-T(61+)           | 222-D (23-) | 228-D (18+) |             |
|              |                                     | 176                                   | 2228-T(25+)           | 0122-T(25-) | 1222-T(21-) | 222-D (16-) |
|              |                                     | 151                                   | 2228-T(42-)           | 222-D (22+) | 222-D (20-) | 228-D (12+) |
|              |                                     | 98                                    | 2222-T(66+)           | 1222-T(25+) |             |             |
|              |                                     | 85                                    | 1222-T(35+)           | 2222-T(18-) | 2228-T(16+) | 222-4 (9-)  |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3000 | 2963 | 2962 | 2935 | 2910 | 2905 | 2900 | 2880 | 2874 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct.,
- 23**
- , 161 (1974).

## No. 120

Molecule: 1225-T CH3CH2CH2Cl (trans form)  
 Symmetry  $C_s$  Symmetry number  $\sigma = 1$

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           | 1464                                | 1478                                  | 122-2 (56+)           | 012-4 (28+) |             |             |
|              | 1457                                | 1452                                  | 012-4 (55+)           | 122-2 (37-) |             |             |
|              | 1442                                | 1430                                  | 225-2 (86+)           |             |             |             |
|              | 1381                                | 1379                                  | 012-2 (105+)          |             |             |             |
|              | 1339                                | 1342                                  | 122-5 (59+)           | 225-5 (30-) | 1225-S(15+) |             |
|              | 1266                                | 1269                                  | 225-5 (67+)           | 122-5 (24+) |             |             |
|              | 1104                                | 1101                                  | 012-5 (27+)           | 1225-S(27-) | 122-5 (14+) | 122-D (9+)  |
|              | 1027                                | 1031                                  | 0122-S(79-)           | 1225-S(20+) |             |             |
|              | 899                                 | 899                                   | 012-5 (39+)           | 1225-S(39+) |             |             |
|              | 723                                 | 728                                   | 2250-S(80-)           | 225-D (11+) | 122-D (11+) |             |
|              | 364                                 | 364                                   | 122-D (35+)           | 2250-S(19+) | 225-D (17+) |             |
|              | 248                                 | 230                                   | 225-D (71+)           | 122-D (49-) |             |             |
| a''          | 1457                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1288                                | 1295                                  | 122-6 (56-)           | 225-6 (23+) |             |             |
|              | 1217                                | 1228                                  | 225-6 (40+)           | 012-8 (17-) | 122-4 (14+) | 122-6 (11+) |
|              | 1078                                | 1077                                  | 225-6 (32+)           | 225-4 (21-) | 012-8 (16+) | 122-4 (14-) |
|              | 863(s)                              | 864                                   | 225-4 (45+)           | 012-8 (41+) | 122-6 (23+) |             |
|              | 746                                 | 743                                   | 122-4 (60+)           | 225-4 (26-) | 012-8 (13+) |             |
|              | 231                                 | 227                                   | 0122-T(96+)           |             |             |             |
|              | 140                                 | 129                                   | 1225-T(88+)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$

3005 2962 2962 2956 2905 2880 2869

## References

- [1] IR. K. Radcliffe and J. L. Wood, Trans. Faraday Soc., **62**, 1678 (1966).  
 [2] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).



## No. 121

Molecule: 1225-G  $\text{CH}_3\text{CH}_2\text{CH}_2\text{Cl}$  (gauche form)  
 Symmetry  $C_1$  Symmetry number  $\sigma = 1$

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |              |              |              |
|--------------|-------------------------------------|---------------------------------------|-----------------------|--------------|--------------|--------------|
| a            | 1464*                               | 1479                                  | 122-2 (68+)           | 012-4 (19+)  |              |              |
|              | 1457*                               | 1463                                  | 012-7 (80+)           | 012-8 (14+)  |              |              |
|              | 1457*                               | 1456                                  | 012-4 (62+)           | 122-2 (18-)  |              |              |
|              | 1436                                | 1439                                  | 225-2 (70+)           | 122-2 (6-)   |              |              |
|              | 1381                                | 1380                                  | 012-2 (105+)          |              |              |              |
|              | 1347                                | 1355                                  | 122-5 (56+)           | 225-5 (17+)  | 225-2 (11-)  |              |
|              | 1306                                | 1307                                  | 225-5 (44+)           | 122-6 (26-)  | 1225-S (9-)  |              |
|              | 1260                                | 1258                                  | 122-6 (35+)           | 225-5 (24+)  | 012-8 (10-)  | 012-7 (7+)   |
|              | 1209                                | 1210                                  | 225-6 (57+)           | 012-5 (8+)   | 012-8 (6+)   |              |
|              | 1090                                | 1092                                  | 1225-S (23+)          | 225-6 (14+)  | 122-4 (10+)  | 122-6 (9-)   |
|              | 1063                                | 1067                                  | 0122-S (28-)          | 012-5 (24+)  | 225-4 (9+)   | 122-D (7+)   |
|              | 1038                                | 1040                                  | 0122-S (23-)          | 1225-S (16+) | 012-8 (12+)  | 122-6 (11+)  |
|              | 895                                 | 884                                   | 012-5 (32+)           | 1225-S (28+) | 225-4 (16-)  |              |
|              | 856                                 | 854                                   | 225-4 (39-)           | 0122-S (31-) | 1225-S (12-) |              |
|              | 789                                 | 792                                   | 122-4 (43+)           | 012-8 (31+)  | 225-4 (11+)  |              |
|              | 648                                 | 652                                   | 2250-S (89+)          | 122-4 (10-)  |              |              |
|              | 424                                 | 420                                   | 122-D (59-)           | 225-D (29+)  |              |              |
|              | 292                                 | 292                                   | 225-D (32-)           | 122-D (23-)  | 0122-T (23-) | 1225-T (16+) |
|              | 214                                 | 200                                   | 0122-T (71+)          | 225-D (20-)  |              |              |
|              | 126                                 | 122                                   | 1225-T (74+)          |              |              |              |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$

3005 2962 2962 2956 2905 2880 2868

\* Not used in the force constant determination.

## References

- [1] IR. K. Radcliffe and J. L. Wood, Trans. Faraday Soc., **62**, 1678 (1966).
- [2] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 122

Molecule: 12225-TT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym.<br>species | Observed<br>frequency<br>cm <sup>-1</sup> | Calculated<br>frequency<br>cm <sup>-1</sup> | Assignment<br>(P.E.D. %) |             |             |             |
|-----------------|-------------------------------------------|---------------------------------------------|--------------------------|-------------|-------------|-------------|
| a'              | 1476                                      | 1483                                        | 122-2 (45-)              | 222-2 (28+) | 012-4 (16-) |             |
|                 | 1460                                      | 1461                                        | 222-2 (62+)              | 012-4 (19+) |             |             |
|                 | 1447                                      | 1453                                        | 012-4 (49-)              | 122-2 (36+) |             |             |
|                 | 1434                                      | 1430                                        | 225-2 (81+)              |             |             |             |
|                 | 1383                                      | 1379                                        | 012-2 (105+)             |             |             |             |
|                 | 1358                                      | 1358                                        | 122-5 (42+)              | 222-5 (40-) | 1222-S(16+) |             |
|                 | 1316                                      | 1315                                        | 225-5 (50-)              | 122-5 (31+) | 222-5 (10+) |             |
|                 | 1248                                      | 1242                                        | 222-5 (46+)              | 225-5 (38+) |             |             |
|                 | 1107                                      | 1111                                        | 1222-S(23-)              | 012-5 (22+) | 122-D ( 9+) | 122-5 ( 8+) |
|                 | 1051                                      | 1052                                        | 0122-S(32-)              | 1222-S(29+) | 2225-S(25-) |             |
|                 | 1017                                      | 1012                                        | 0122-S(47+)              | 2225-S(46-) |             |             |
|                 | 896                                       | 903                                         | 012-5 (44-)              | 1222-S(30-) | 122-5 (11-) |             |
|                 | 727                                       | 728                                         | 2250-S(83-)              |             |             |             |
|                 | 401                                       | 406                                         | 122-D (63-)              | 225-D (24+) |             |             |
|                 | 334                                       | 333                                         | 222-D (28+)              | 225-D (20+) | 2250-S(16+) | 1222-S( 6+) |
|                 | a''                                       | 161                                         | 159                      | 222-D (48-) | 225-D (46+) | 122-D (29+) |
| 1467            |                                           | 1463                                        | 012-7 (81+)              | 012-8 (14+) |             |             |
| 1302            |                                           | 1303                                        | 222-6 (48+)              | 122-6 (26-) |             |             |
| 1280(s)         |                                           | 1278                                        | 122-6 (38-)              | 225-6 (28+) | 222-6 ( 7-) |             |
| 1205(s)         |                                           | 1210                                        | 225-6 (25-)              | 012-8 (17+) | 122-4 (17-) | 222-6 (12-) |
| 1084            |                                           | 1085                                        | 225-6 (33+)              | 225-4 (17-) | 222-6 (15+) | 222-4 (10-) |
| 920(s)          |                                           | 920                                         | 012-8 (31+)              | 225-4 (29+) | 122-6 (26+) | 222-4 (14+) |
| 783             |                                           | 784                                         | 225-4 (37-)              | 122-4 (29+) | 012-8 (20+) | 222-4 (12+) |
| 738             |                                           | 734                                         | 222-4 (41-)              | 122-4 (39+) | 225-4 (10+) |             |
| 237(s)          |                                           | 232                                         | 0122-T(90-)              |             |             |             |
| 125             |                                           | 132                                         | 1222-T(52+)              | 2225-T(40+) |             |             |
|                 |                                           | 105                                         | 2225-T(42+)              | 1222-T(38-) | 222-4 (11+) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 2962 2962 2956 2909 2900 2880 2873 2865

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 123

Molecule: 12225-TG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.F.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1476*                               | 1486                                  | 222-2 (38+)           | 122-2 (37-) | 012-4 (13-) |             |
|              | 1467*                               | 1464                                  | 222-2 (44+)           | 012-4 (24+) | 122-2 (15+) |             |
|              | 1460*                               | 1463                                  | 012-7 (80+)           | 012-8 (14+) |             |             |
|              | 1447*                               | 1452                                  | 012-4 (48-)           | 122-2 (42+) |             |             |
|              | 1434*                               | 1438                                  | 225-2 (71+)           | 222-2 (10-) |             |             |
|              | 1383*                               | 1380                                  | 012-2 (101+)          |             |             |             |
|              | 1369                                | 1369                                  | 222-5 (42-)           | 122-5 (28+) | 1222-S(14+) |             |
|              | 1319                                | 1318                                  | 225-5 (49+)           | 122-5 (28+) |             |             |
|              | 1302*                               | 1303                                  | 222-6 (29+)           | 122-6 (22-) | 122-5 (15+) | 222-5 ( 8+) |
|              | 1291                                | 1287                                  | 122-6 (36-)           | 222-5 (14-) | 225-5 (13+) | 122-5 ( 9-) |
|              | 1234                                | 1231                                  | 222-6 (23+)           | 225-5 (15+) | 012-8 (13-) | 122-4 (10+) |
|              | 1198                                | 1198                                  | 225-6 (48+)           | 222-5 (10-) | 122-4 ( 5-) | 012-8 ( 5+) |
|              | 1107*                               | 1102                                  | 1222-S(25+)           | 2225-S(12-) | 012-5 (11-) | 122-5 ( 8-) |
|              | 1084*                               | 1089                                  | 225-6 (22+)           | 225-4 (11-) | 012-5 (10-) | 222-6 (10-) |
|              | 1051*                               | 1050                                  | 0122-S(36+)           | 1222-S(16-) | 2225-S(11+) | 222-6 ( 7+) |
|              | 1000                                | 1006                                  | 0122-S(42-)           | 2225-S(37+) |             |             |
|              | 932                                 | 931                                   | 225-4 (35+)           | 012-5 (26-) | 122-5 ( 9-) | 222-5 ( 7-) |
|              | 875                                 | 877                                   | 222-4 (31+)           | 012-8 (27+) | 122-6 (17+) |             |
|              | 811                                 | 807                                   | 225-4 (36-)           | 1222-S(32-) | 012-5 ( 9-) |             |
|              | 746                                 | 746                                   | 122-4 (60+)           | 012-8 (17+) | 222-4 (16-) |             |
|              | 653                                 | 655                                   | 2250-S(92-)           |             |             |             |
|              | 474                                 | 474                                   | 222-D (29-)           | 225-D (21+) | 122-D (20-) | 0122-S( 6-) |
|              | 302                                 | 302                                   | 225-D (41+)           | 122-D (40+) | 2225-S(10+) |             |
|              | 265                                 | 260                                   | 222-D (38-)           | 122-D (26+) | 2225-T(20+) | 0122-T(14-) |
|              |                                     | 222                                   | 0122-T(77-)           |             |             |             |
|              |                                     | 107                                   | 2225-T(66+)           | 222-D ( 8+) |             |             |
|              |                                     | 90                                    | 1222-T(74+)           | 225-D (12-) |             |             |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

3005 2962 2962 2956 2909 2901 2880 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 124

Molecule: 12225-GT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (gauche-trans form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1476*                               | 1483                                  | 122-2 (54+)           | 222-2 (29+) |             |             |
|              | 1467*                               | 1470                                  | 222-2 (49-)           | 012-4 (24+) |             |             |
|              | 1460*                               | 1463                                  | 012-7 (75+)           | 012-8 (13+) |             |             |
|              | 1447*                               | 1453                                  | 012-4 (49-)           | 122-2 (30+) | 222-2 (11-) |             |
|              | 1434*                               | 1432                                  | 225-2 (88+)           |             |             |             |
|              | 1383*                               | 1380                                  | 012-2 (104+)          |             |             |             |
|              | 1349                                | 1352                                  | 222-5 (38+)           | 122-5 (34+) | 225-5 (13-) |             |
|              | 1344*                               | 1340                                  | 122-5 (40+)           | 222-5 (19-) | 1222-S(15+) | 225-5 (14+) |
|              | 1291*                               | 1292                                  | 222-6 (39-)           | 225-6 (24+) | 225-5 (9+)  |             |
|              | 1285*                               | 1278                                  | 225-5 (34+)           | 122-6 (31-) | 225-6 (12-) |             |
|              | 1248*                               | 1252                                  | 225-5 (26+)           | 122-6 (22-) | 222-5 (20+) | 012-8 (11-) |
|              | 1190                                | 1193                                  | 225-6 (29+)           | 222-6 (21+) | 012-5 (11+) | 222-4 (8+)  |
|              | 1107*                               | 1099                                  | 2225-S(20-)           | 122-4 (15-) | 012-8 (14+) | 222-5 (13+) |
|              | 1084*                               | 1094                                  | 225-6 (20-)           | 1222-S(20-) | 012-5 (12+) | 225-4 (8+)  |
|              | 1058*                               | 1064                                  | 0122-S(45-)           | 1222-S(21+) | 225-4 (7+)  |             |
|              | 973*                                | 969                                   | 2225-S(47-)           | 012-5 (15+) | 012-8 (11-) | 122-6 (11-) |
|              | 927*                                | 929                                   | 225-4 (29+)           | 222-4 (15+) | 0122-S(13+) | 222-6 (12+) |
|              | 896*                                | 884                                   | 0122-S(32-)           | 1222-S(30-) | 012-5 (16-) |             |
|              | 800*                                | 792                                   | 122-4 (35-)           | 012-8 (25-) | 225-4 (14-) |             |
|              | 755*                                | 758                                   | 222-4 (33-)           | 225-4 (28+) | 2250-S(16-) |             |
|              | 718                                 | 715                                   | 2250-S(57-)           | 122-4 (23+) |             |             |
|              | 437                                 | 435                                   | 122-D (52-)           | 222-D (19+) | 2250-S(12+) |             |
|              | 302*                                | 302                                   | 122-D (29-)           | 225-D (14-) | 222-D (11-) | 0122-T(7-)  |
|              | 265*                                | 264                                   | 225-D (52+)           | 0122-T(35-) | 222-D (15-) |             |
|              |                                     | 187                                   | 0122-T(53+)           | 222-D (28-) | 225-D (17+) |             |
|              |                                     | 114                                   | 1222-T(79-)           |             |             |             |
|              |                                     | 98                                    | 2225-T(79-)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 2962 2962 2956 2907 2903 2880 2870 2867

\* Not used in the force constant determination.

## Reference

- [1] I.R.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 125

Molecule: 12225-GG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (gauche-gauche form)Symmetry  $C_1$ Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1476*                               | 1486                                  | 222-2 (43+)           | 122-2 (40+) |             |             |
|              | 1467*                               | 1472                                  | 222-2 (34-)           | 012-4 (27+) | 122-2 (21+) |             |
|              | 1460*                               | 1463                                  | 012-7 (78-)           | 012-8 (14+) |             |             |
|              | 1447*                               | 1454                                  | 012-4 (50+)           | 122-2 (29-) |             |             |
|              | 1434*                               | 1437                                  | 225-2 (69+)           | 222-2 (11-) |             |             |
|              | 1383*                               | 1381                                  | 012-2 (100+)          |             |             |             |
|              | 1360*                               | 1362                                  | 222-5 (49+)           | 225-5 (12+) | 122-5 (12+) |             |
|              | 1344                                | 1342                                  | 122-5 (62-)           | 1222-S(14-) |             |             |
|              | 1316*                               | 1307                                  | 225-5 (54+)           | 222-6 (15-) | 2225-S(10-) |             |
|              | 1285*                               | 1274                                  | 122-6 (51+)           | 222-6 (11+) | 225-6 (6+)  | 012-8 (5-)  |
|              | 1230                                | 1232                                  | 222-6 (21-)           | 225-5 (15-) | 012-8 (11-) | 225-6 (10-) |
|              | 1178                                | 1177                                  | 225-6 (51+)           | 222-6 (17-) | 012-5 (10-) |             |
|              | 1107*                               | 1121                                  | 1222-S(25+)           | 2225-S(20-) | 012-5 (8-)  | 222-6 (8-)  |
|              | 1080                                | 1084                                  | 012-8 (17-)           | 122-4 (16+) | 122-6 (12-) | 225-4 (10-) |
|              | 1058                                | 1052                                  | 0122-S(35-)           | 222-6 (11-) | 222-4 (10+) | 1222-S(9+)  |
|              | 973                                 | 969                                   | 2225-S(38-)           | 012-5 (28+) | 122-5 (15+) |             |
|              | 927                                 | 927                                   | 225-4 (39+)           | 0122-S(38-) |             |             |
|              | 875*                                | 878                                   | 222-4 (29-)           | 012-8 (23+) | 122-6 (13+) | 012-5 (12+) |
|              | 800                                 | 806                                   | 1222-S(39+)           | 225-4 (17+) | 2225-S(9+)  | 0122-S(9+)  |
|              | 755                                 | 755                                   | 122-4 (51+)           | 012-8 (20+) | 225-4 (12+) | 222-4 (11+) |
|              | 653*                                | 655                                   | 2250-S(88-)           |             |             |             |
|              | 458                                 | 463                                   | 222-D (47-)           | 122-D (28+) | 225-D (12+) |             |
|              | 370                                 | 372                                   | 122-D (39+)           | 225-D (29-) | 1222-T(9-)  |             |
|              | 243                                 | 237                                   | 0122-T(38+)           | 225-D (32+) | 222-D (13+) | 122-D (10+) |
|              |                                     | 208                                   | 0122-T(46-)           | 222-D (20+) | 122-D (13+) |             |
|              |                                     | 136                                   | 1222-T(36+)           | 2225-T(28-) | 225-D (14-) | 222-4 (12-) |
|              |                                     | 65                                    | 1222-T(46+)           | 2225-T(42-) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 2962 2962 2956 2907 2903 2880 2870 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 126

Molecule: 122225-TTT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |  |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|--|
| a'           | 1475                                | 1484                                  | 122-2 (39-)           | 222-2 (34+) | 012-4 (15-) |             |  |
|              | 1467                                | 1473                                  | 222-2 (65+)           | 122-2 (15-) | 222-2 (13-) |             |  |
|              | 1455                                | 1457                                  | 012-4 (45+)           | 222-2 (29+) | 222-2 (12+) |             |  |
|              | 1447                                | 1449                                  | 122-2 (40+)           | 012-4 (22-) | 222-2 (15+) | 222-2 (12+) |  |
|              | 1433                                | 1429                                  | 225-2 (79+)           |             |             |             |  |
|              | 1388(s)                             | 1380                                  | 012-2 (103+)          |             |             |             |  |
|              | 1368                                | 1366                                  | 222-5 (42-)           | 122-5 (25+) | 222-5 (21+) | 1222-S(14+) |  |
|              | 1343                                | 1337                                  | 222-5 (34+)           | 122-5 (32-) | 225-5 (26-) |             |  |
|              | 1293                                | 1293                                  | 225-5 (44-)           | 222-5 (26+) | 122-5 (22+) |             |  |
|              | 1228                                | 1227                                  | 222-5 (39+)           | 222-5 (26+) | 225-5 (24+) |             |  |
|              | 1112                                | 1117                                  | 012-5 (19+)           | 1222-S(16-) | 222-D (9+)  | 122-D (8+)  |  |
|              | 1057                                | 1060                                  | 2222-S(35-)           | 1222-S(29+) | 0122-S(18-) |             |  |
|              | 1037                                | 1039                                  | 2225-S(44+)           | 2222-S(21-) | 0122-S(17+) |             |  |
|              | 1006                                | 1006                                  | 0122-S(43+)           | 2225-S(26-) | 2222-S(14-) |             |  |
|              | 895                                 | 901                                   | 012-5 (40-)           | 1222-S(29-) | 0122-S(9-)  |             |  |
|              | 727                                 | 726                                   | 2250-S(82-)           |             |             |             |  |
|              | 452                                 | 462                                   | 122-D (32-)           | 222-D (21-) | 225-D (19+) |             |  |
|              | 348                                 | 352                                   | 222-D (32-)           | 222-D (26-) | 122-D (16+) | 2250-S(11-) |  |
|              | 266                                 | 256                                   | 225-D (38+)           | 122-D (32+) | 2222-S(11+) |             |  |
|              |                                     | 119                                   | 222-D (45+)           | 222-D (40-) | 225-D (28-) | 122-D (13+) |  |
| a''          | 1460                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |  |
|              | 1309                                | 1305                                  | 222-6 (38+)           | 222-6 (30-) | 122-6 (10-) |             |  |
|              | 1301                                | 1296                                  | 122-6 (34-)           | 222-6 (25+) | 225-6 (14-) |             |  |
|              | 1257(s)                             | 1260                                  | 225-6 (27+)           | 122-6 (23-) | 222-6 (17-) | 222-4 (8+)  |  |
|              | 1188                                | 1198                                  | 122-4 (18-)           | 012-8 (16+) | 225-6 (16-) | 222-4 (13-) |  |
|              | 1090                                | 1089                                  | 225-6 (34+)           | 222-6 (16+) | 225-4 (15-) | 222-6 (8+)  |  |
|              | 962                                 | 956                                   | 012-8 (23+)           | 122-6 (22+) | 222-6 (22+) | 225-4 (20+) |  |
|              | 838                                 | 833                                   | 225-4 (29+)           | 222-4 (29-) | 012-8 (23-) | 222-6 (13+) |  |
|              | 759(s)                              | 755                                   | 222-4 (36-)           | 122-4 (27+) | 225-4 (25+) | 012-8 (10+) |  |
|              | 731                                 | 729                                   | 222-4 (38-)           | 122-4 (31+) | 222-4 (19+) |             |  |
|              |                                     | 231                                   | 0122-T(92+)           |             |             |             |  |
|              |                                     | 157                                   | 2225-T(50-)           | 1222-T(42+) |             |             |  |
|              |                                     | 120                                   | 2222-T(74+)           | 1222-T(12+) |             |             |  |
|              |                                     | 67                                    | 1222-T(37+)           | 2225-T(32+) | 2222-T(12-) |             |  |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3005 | 2962 | 2962 | 2956 | 2911 | 2905 | 2899 | 2880 | 2875 | 2869 |
| 2864 |      |      |      |      |      |      |      |      |      |

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 127

Molecule: 122225-TTG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-trans-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1475*                               | 1484                                  | 222-2 (36+)           | 122-2 (33-) | 012-4 (13-) |             |
|              | 1467*                               | 1478                                  | 222-2 (61+)           | 122-2 (20-) |             |             |
|              | 1460*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1455*                               | 1457                                  | 012-4 (47+)           | 222-2 (35+) |             |             |
|              | 1447*                               | 1449                                  | 122-2 (40+)           | 222-2 (21+) | 012-4 (20-) |             |
|              | 1433*                               | 1438                                  | 225-2 (68+)           | 222-2 (12-) |             |             |
|              | 1381                                | 1380                                  | 012-2 (98+)           |             |             |             |
|              | 1381                                | 1373                                  | 222-5 (31-)           | 222-5 (31+) | 122-5 (13+) | 2222-S(12-) |
|              | 1343*                               | 1342                                  | 122-5 (46-)           | 222-5 (21+) | 225-5 (13+) |             |
|              | 1313                                | 1310                                  | 225-5 (37+)           | 222-6 (28-) | 222-6 (7+)  |             |
|              | 1301*                               | 1302                                  | 222-6 (39-)           | 122-6 (28+) | 225-5 (10+) |             |
|              | 1278                                | 1281                                  | 122-6 (24+)           | 222-5 (18-) | 222-6 (15-) | 225-5 (9-)  |
|              | 1268                                | 1265                                  | 222-5 (28+)           | 122-6 (12+) | 225-6 (12+) | 122-5 (8+)  |
|              | 1214                                | 1214                                  | 222-6 (14+)           | 012-8 (12-) | 122-4 (11+) | 222-6 (11+) |
|              | 1188                                | 1191                                  | 225-6 (40+)           | 222-5 (9-)  | 122-4 (6-)  | 012-8 (6+)  |
|              | 1108                                | 1107                                  | 1222-S(19+)           | 012-5 (19-) | 225-6 (10+) | 122-5 (8-)  |
|              | 1095                                | 1100                                  | 222-6 (17-)           | 2225-S(17+) | 222-4 (10+) | 2222-S(9-)  |
|              | 1063                                | 1061                                  | 2222-S(32-)           | 1222-S(15+) | 0122-S(7-)  | 225-6 (6-)  |
|              | 1037*                               | 1042                                  | 0122-S(50+)           | 2225-S(16+) | 1222-S(12-) |             |
|              | 988                                 | 987                                   | 2225-S(25+)           | 0122-S(17-) | 225-4 (15-) | 2222-S(10+) |
|              | 927                                 | 928                                   | 222-4 (22+)           | 012-8 (21+) | 122-6 (18+) | 222-6 (11+) |
|              | 913                                 | 916                                   | 012-5 (32-)           | 1222-S(20-) | 0122-S(10-) | 225-4 (7+)  |
|              | 838                                 | 838                                   | 225-4 (40-)           | 2222-S(13-) | 222-4 (10-) | 1222-S(8-)  |
|              | 788                                 | 791                                   | 222-4 (26-)           | 122-4 (21+) | 012-8 (17+) | 222-4 (11+) |
|              | 731                                 | 732                                   | 122-4 (44+)           | 222-4 (38-) |             |             |
|              | 653                                 | 655                                   | 2250-S(92-)           |             |             |             |
|              | 455                                 | 456                                   | 222-D (36-)           | 225-D (26+) | 222-D (10-) |             |
|              | 400                                 | 401                                   | 122-D (51+)           | 222-D (15+) | 2222-S(8+)  |             |
|              | 280                                 | 282                                   | 225-D (45-)           | 2225-T(13+) | 222-D (9-)  | 2225-S(8-)  |
|              |                                     | 229                                   | 0122-T(92-)           |             |             |             |
|              |                                     | 196                                   | 222-D (42-)           | 122-D (27+) | 2225-T(21-) | 222-D (17+) |
|              |                                     | 129                                   | 1222-T(51-)           | 2225-T(13-) | 222-D (12+) |             |
|              |                                     | 86                                    | 2222-T(64-)           | 2225-T(15-) | 1222-T(12-) |             |
|              |                                     | 70                                    | 2225-T(27+)           | 1222-T(22+) | 2222-T(15-) | 222-4 (9+)  |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 2963 2962 2956 2911 2905 2899 2880 2875 2869  
2864

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 128

Molecule: 122225-TGT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-gauche-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1475*                               | 1488                                  | 222-2 (39+)           | 122-2 (26-) | 222-2 (17+) |             |
|              | 1467*                               | 1472                                  | 222-2 (50+)           | 122-2 (24+) | 012-4 (14+) |             |
|              | 1460*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1455*                               | 1458                                  | 222-2 (46+)           | 222-2 (24-) | 012-4 (21+) |             |
|              | 1447*                               | 1452                                  | 122-2 (43+)           | 012-4 (41-) |             |             |
|              | 1433*                               | 1432                                  | 225-2 (88+)           |             |             |             |
|              | 1381*                               | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1368*                               | 1365                                  | 222-5 (44-)           | 122-5 (35+) | 1222-S(16+) |             |
|              | 1346                                | 1347                                  | 222-5 (54+)           | 225-5 (26-) | 2225-S(13+) |             |
|              | 1301*                               | 1302                                  | 122-5 (28+)           | 222-6 (19+) | 222-5 (15+) | 222-6 (14+) |
|              | 1293*                               | 1295                                  | 122-6 (40-)           | 222-6 (16+) | 122-5 (9-)  | 222-5 (8-)  |
|              | 1285                                | 1288                                  | 225-6 (28+)           | 222-6 (23-) | 222-5 (11+) | 225-5 (9+)  |
|              | 1278*                               | 1274                                  | 225-5 (50+)           | 222-5 (12+) | 222-6 (9-)  |             |
|              | 1228*                               | 1228                                  | 222-6 (23+)           | 012-8 (14-) | 222-5 (12+) | 122-4 (12+) |
|              | 1180                                | 1183                                  | 225-6 (26+)           | 222-6 (19+) | 012-5 (7+)  | 222-5 (7-)  |
|              | 1112*                               | 1109                                  | 222-5 (12+)           | 2225-S(11-) | 222-4 (11-) | 1222-S(8+)  |
|              | 1095*                               | 1093                                  | 225-6 (27-)           | 222-6 (14-) | 012-5 (11+) | 225-4 (11+) |
|              | 1074                                | 1078                                  | 2222-S(40-)           | 1222-S(18+) | 2225-S(17+) |             |
|              | 1023                                | 1023                                  | 0122-S(69+)           | 2222-S(13-) |             |             |
|              | 974                                 | 980                                   | 2225-S(22+)           | 012-5 (15-) | 225-4 (8+)  | 222-5 (8-)  |
|              | 974                                 | 968                                   | 225-4 (16-)           | 222-6 (15+) | 222-4 (14-) | 012-8 (13+) |
|              | 855                                 | 856                                   | 1222-S(34-)           | 012-5 (21-) | 225-4 (19-) |             |
|              | 855                                 | 852                                   | 222-4 (29+)           | 012-8 (25+) | 122-6 (13+) | 2225-S(13-) |
|              | 767                                 | 762                                   | 222-4 (37+)           | 225-4 (32-) | 122-4 (12+) |             |
|              | 745                                 | 748                                   | 122-4 (35+)           | 2250-S(32-) | 012-8 (11+) |             |
|              | 712                                 | 713                                   | 2250-S(43+)           | 222-4 (25-) | 122-4 (14+) |             |
|              | 494                                 | 491                                   | 222-D (25-)           | 122-D (19-) | 222-D (11+) | 2250-S(11-) |
|              | 302                                 | 301                                   | 122-D (50-)           | 222-D (29-) |             |             |
|              | 280*                                | 281                                   | 222-D (38+)           | 225-D (26+) | 122-D (8-)  |             |
|              |                                     | 243                                   | 225-D (42+)           | 0122-T(23-) | 222-D (13-) |             |
|              | 218                                 | 222                                   | 0122-T(68-)           | 222-D (9+)  |             |             |
|              |                                     | 110                                   | 2222-T(66+)           | 2225-T(17+) | 1222-T(10+) |             |
|              |                                     | 82                                    | 1222-T(33+)           | 222-D (17-) | 2225-T(13+) | 222-D (12-) |
|              |                                     | 79                                    | 2225-T(45-)           | 1222-T(34+) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ :

3005 2962 2962 2956 2910 2905 2900 2880 2873 2869  
2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).



## No. 129

Molecule: 122225-TGG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1475*                               | 1490                                  | 222-2 (36+)           | 222-2 (28+) | 122-2 (19-) |             |
|              | 1467*                               | 1476                                  | 222-2 (41+)           | 122-2 (30+) | 012-4 (14+) |             |
|              | 1460*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1455*                               | 1459                                  | 222-2 (50+)           | 012-4 (24+) | 222-2 (13-) |             |
|              | 1447*                               | 1451                                  | 122-2 (44+)           | 012-4 (40-) |             |             |
|              | 1433*                               | 1438                                  | 225-2 (71+)           | 222-2 (11-) |             |             |
|              | 1381*                               | 1380                                  | 012-2 (102+)          |             |             |             |
|              | 1368*                               | 1368                                  | 222-5 (33-)           | 222-5 (24-) | 122-5 (20+) | 1222-S(10+) |
|              | 1358                                | 1357                                  | 222-5 (33+)           | 122-5 (21+) | 2222-S(12-) | 222-5 (11-) |
|              | 1309*                               | 1307                                  | 225-5 (51+)           | 222-6 (17-) | 2225-S(10-) |             |
|              | 1301*                               | 1301                                  | 122-5 (26+)           | 222-6 (19+) | 222-5 (16+) | 122-6 (13-) |
|              | 1293*                               | 1293                                  | 122-6 (38-)           | 222-5 (13-) | 122-5 (12-) | 222-6 (8+)  |
|              | 1263*                               | 1255                                  | 222-6 (19+)           | 225-6 (13+) | 222-6 (12+) | 122-6 (12+) |
|              | 1215*                               | 1216                                  | 012-8 (14+)           | 122-4 (14-) | 222-6 (13-) | 222-6 (10+) |
|              | 1174                                | 1174                                  | 225-6 (41+)           | 222-6 (17-) | 1222-S(7+)  | 012-5 (7-)  |
|              | 1112*                               | 1112                                  | 2222-S(24-)           | 2225-S(21+) | 012-5 (8+)  | 222-4 (7+)  |
|              | 1095*                               | 1097                                  | 225-6 (14-)           | 222-6 (10+) | 222-4 (10-) | 1222-S(9+)  |
|              | 1074                                | 1075                                  | 1222-S(17-)           | 222-6 (15-) | 2222-S(9+)  | 2225-S(7-)  |
|              | 1027                                | 1028                                  | 0122-S(75+)           | 1222-S(10-) |             |             |
|              | 974                                 | 979                                   | 225-4 (21-)           | 012-5 (17-) | 222-4 (11+) | 2225-S(11+) |
|              | 927*                                | 928                                   | 222-4 (21+)           | 012-8 (19-) | 122-6 (17-) | 2225-S(10-) |
|              | 878                                 | 886                                   | 225-4 (33+)           | 1222-S(20-) | 2225-S(10+) | 012-5 (8-)  |
|              | 842                                 | 845                                   | 222-4 (16+)           | 2225-S(15-) | 012-8 (14+) | 012-5 (12-) |
|              | 788*                                | 791                                   | 222-4 (21+)           | 225-4 (16+) | 122-4 (15+) | 012-8 (12+) |
|              | 731*                                | 733                                   | 122-4 (47+)           | 222-4 (31-) | 012-8 (10+) |             |
|              | 653*                                | 656                                   | 2250-S(88+)           |             |             |             |
|              | 488                                 | 486                                   | 222-D (37+)           | 222-D (22-) | 122-D (9-)  | 225-D (7-)  |
|              | 387                                 | 384                                   | 225-D (31+)           | 122-D (15-) | 222-D (12-) | 222-D (10-) |
|              | 302                                 | 305                                   | 122-D (52+)           | 222-D (15-) | 2225-T(13-) | 225-D (11+) |
|              |                                     | 233                                   | 0122-T(82-)           |             |             |             |
|              |                                     | 201                                   | 222-D (28+)           | 225-D (24+) | 222-D (21+) | 0122-T(10-) |
|              |                                     | 138                                   | 2225-T(34+)           | 2222-T(17-) | 1222-T(14+) | 222-D (12-) |
|              |                                     | 90                                    | 1222-T(57-)           | 2222-T(32-) |             |             |
|              |                                     | 52                                    | 2225-T(39-)           | 2222-T(30-) | 1222-T(12+) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3005 | 2963 | 2962 | 2956 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 130

Molecule: 122225-GTG CH3CH2CH2CH2CH2Cl (gauche-trans-gauche form)Symmetry  $C_1$ Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1475*                               | 1485                                  | 222-2 (38+)           | 122-2 (31+) | 222-2 (20-) |             |
|              | 1467*                               | 1477                                  | 222-2 (34+)           | 122-2 (31+) | 012-4 (17+) |             |
|              | 1460*                               | 1465                                  | 012-7 (45+)           | 222-2 (16+) | 222-2 (15+) |             |
|              | 1455*                               | 1461                                  | 012-7 (35+)           | 222-2 (20-) | 012-4 (16+) | 222-2 (14-) |
|              | 1447*                               | 1452                                  | 012-4 (42+)           | 122-2 (29-) | 222-2 (17+) |             |
|              | 1433*                               | 1438                                  | 225-2 (72+)           | 222-2 (10-) |             |             |
|              | 1381*                               | 1381                                  | 012-2 (90+)           |             |             |             |
|              | 1368*                               | 1371                                  | 222-5 (35-)           | 222-5 (27+) | 012-2 (15+) | 2222-S(11+) |
|              | 1346                                | 1345                                  | 122-5 (71+)           |             |             |             |
|              | 1313*                               | 1320                                  | 225-5 (44+)           | 222-5 (27+) |             |             |
|              | 1308*                               | 1305                                  | 222-6 (32+)           | 222-6 (16-) | 222-5 (10+) | 225-6 ( 9+) |
|              | 1278*                               | 1278                                  | 222-6 (27-)           | 225-5 (15+) | 222-5 (14-) | 222-5 ( 8-) |
|              | 1263                                | 1266                                  | 122-6 (49+)           | 012-8 ( 9-) | 222-5 ( 8+) | 012-7 ( 7+) |
|              | 1214*                               | 1215                                  | 225-6 (18+)           | 222-6 (13+) | 225-5 (12+) | 222-5 (10-) |
|              | 1174                                | 1175                                  | 225-6 (34+)           | 222-6 (11-) | 012-5 (11-) | 222-6 ( 8-) |
|              | 1106*                               | 1103                                  | 2222-S(16+)           | 122-4 (11+) | 012-8 (10-) | 222-6 ( 9+) |
|              | 1090*                               | 1090                                  | 1222-S(14-)           | 225-6 (13+) | 222-6 (11-) | 012-5 (10+) |
|              | 1090*                               | 1084                                  | 0122-S(26-)           | 1222-S(17+) | 2225-S(13+) | 225-4 ( 4-) |
|              | 1027                                | 1026                                  | 2225-S(37-)           | 0122-S(18-) | 1222-S( 7+) | 2222-S( 6+) |
|              | 974                                 | 981                                   | 225-4 (21-)           | 012-5 (16-) | 2222-S(12+) | 0122-S( 9+) |
|              | 927*                                | 928                                   | 222-4 (19+)           | 012-8 (18-) | 122-6 (14-) | 222-4 (10+) |
|              | 895*                                | 900                                   | 0122-S(26+)           | 012-5 (23+) | 1222-S(20+) | 225-4 ( 9-) |
|              | 822                                 | 823                                   | 225-4 (41-)           | 2222-S(14-) | 1222-S(10-) | 0122-S( 8-) |
|              | 788*                                | 794                                   | 222-4 (23-)           | 122-4 (23+) | 222-4 (21+) | 012-8 (15+) |
|              | 745                                 | 743                                   | 122-4 (34+)           | 222-4 (21+) | 012-8 (13+) | 2222-S(11-) |
|              | 653*                                | 655                                   | 2250-S(92-)           |             |             |             |
|              | 494                                 | 496                                   | 222-D (21+)           | 122-D (19-) | 222-D (18+) | 225-D (13-) |
|              | 372                                 | 369                                   | 122-D (50-)           | 225-D (24+) | 222-D (15-) |             |
|              | 288                                 | 291                                   | 222-D (29+)           | 0122-T(26+) | 122-D (13+) | 225-D (10+) |
|              | 266*                                | 264                                   | 222-D (31+)           | 225-D (26+) | 2225-T(23-) |             |
|              |                                     | 196                                   | 0122-T(65-)           | 222-D (20+) |             |             |
|              |                                     | 127                                   | 1222-T(40+)           | 2225-T(21-) | 222-D (12-) | 222-D (11+) |
|              |                                     | 90                                    | 2225-T(39+)           | 1222-T(29+) | 222-4 ( 8+) |             |
|              |                                     | 55                                    | 2222-T(73-)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3005 | 2963 | 2962 | 2956 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 131

Molecule: 122225-GTG' CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl (gauche-trans-gauche' form)Symmetry C<sub>1</sub>Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1475*                               | 1485                                  | 222-2 (38+)           | 122-2 (31+) | 222-2 (20-) |             |
|              | 1467*                               | 1477                                  | 222-2 (34+)           | 122-2 (31+) | 012-4 (17+) |             |
|              | 1460*                               | 1465                                  | 012-7 (45+)           | 222-2 (15+) | 222-2 (15+) |             |
|              | 1455*                               | 1461                                  | 012-7 (34+)           | 222-2 (20-) | 012-4 (16+) | 222-2 (14-) |
|              | 1447*                               | 1452                                  | 012-4 (42+)           | 122-2 (29-) | 222-2 (17+) |             |
|              | 1433*                               | 1438                                  | 225-2 (72+)           |             |             |             |
|              | 1381*                               | 1381                                  | 012-2 (89+)           |             |             |             |
|              | 1368*                               | 1371                                  | 222-5 (34-)           | 222-5 (26+) | 012-2 (16+) | 222-2 (11+) |
|              | 1346                                | 1345                                  | 122-5 (71+)           |             |             |             |
|              | 1313*                               | 1319                                  | 225-5 (43+)           | 222-5 (25+) | 122-6 ( 7-) |             |
|              | 1301*                               | 1302                                  | 222-6 (30+)           | 222-5 (15-) | 222-5 (14-) | 225-6 (13+) |
|              | 1285                                | 1287                                  | 222-6 (36-)           | 225-5 (19-) | 122-6 ( 9-) | 222-5 ( 8+) |
|              | 1263*                               | 1261                                  | 122-6 (44+)           | 012-8 (10-) | 222-5 ( 9+) | 012-7 ( 8+) |
|              | 1205                                | 1202                                  | 225-6 (34+)           | 222-5 (18+) | 225-5 (13-) | 222-6 ( 9+) |
|              | 1188*                               | 1189                                  | 222-6 (16+)           | 225-6 (14-) | 222-6 (12+) | 222-4 ( 9+) |
|              | 1108*                               | 1109                                  | 2222-S(17+)           | 1222-S(13-) | 222-6 (12-) | 2225-S(11-) |
|              | 1095*                               | 1094                                  | 225-6 (20+)           | 012-8 (11+) | 122-4 (11-) | 2222-S(10-) |
|              | 1063*                               | 1065                                  | 0122-S(42-)           | 1222-S(22+) | 222-4 ( 6+) | 222-4 ( 6+) |
|              | 1037*                               | 1036                                  | 2225-S(42-)           | 012-5 (10-) | 2222-S( 9+) | 122-5 ( 7-) |
|              | 962*                                | 968                                   | 225-4 (23-)           | 012-8 (20-) | 122-6 (19-) | 2222-S(12-) |
|              | 938                                 | 938                                   | 222-4 (23+)           | 012-5 (20-) | 122-5 (12-) | 2225-S(10+) |
|              | 895*                                | 897                                   | 0122-S(36-)           | 1222-S(20-) | 012-5 (15-) |             |
|              | 842                                 | 839                                   | 225-4 (31-)           | 012-8 (18+) | 222-4 (11-) | 122-4 ( 9+) |
|              | 767*                                | 774                                   | 222-4 (21-)           | 222-4 (18+) | 225-4 (15-) | 2222-S(12+) |
|              | 745                                 | 750                                   | 122-4 (40+)           | 222-4 (23+) | 012-8 (16+) |             |
|              | 653*                                | 654                                   | 2250-S(91+)           |             |             |             |
|              | 488                                 | 486                                   | 222-D (23-)           | 222-D (21-) | 122-D (16+) | 225-D (12+) |
|              | 400*                                | 393                                   | 122-D (49-)           | 225-D (26+) | 222-D (10-) |             |
|              | 288                                 | 283                                   | 0122-T(28-)           | 222-D (26-) | 122-D (13-) | 1222-T(13+) |
|              | 266*                                | 260                                   | 222-D (31+)           | 2225-T(25+) | 225-D (24+) |             |
|              |                                     | 194                                   | 0122-T(61+)           | 222-D (24-) |             |             |
|              |                                     | 126                                   | 1222-T(40-)           | 2225-T(23+) | 225-D (11-) |             |
|              |                                     | 83                                    | 2225-T(26+)           | 2222-T(19-) | 1222-T(17+) | 222-4 (10+) |
|              |                                     | 57                                    | 2222-T(59+)           | 1222-T(19+) | 2225-T(14+) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3005 | 2963 | 2962 | 2956 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 132

Molecule: 52225-TT ClCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl (trans-trans form)Symmetry C<sub>2v</sub> Symmetry number  $\sigma = 2$ 

| Sym. species   | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %)                           |
|----------------|-------------------------------------|---------------------------------------|-------------------------------------------------|
| a <sub>1</sub> | 1455*                               | 1468                                  | 222-2 (93+)                                     |
|                | 1421*                               | 1424                                  | 225-2 (44+) 522-2 (44+)                         |
|                | 1305                                | 1300                                  | 225-5 (49+) 522-5 (49-)                         |
|                | 1064                                | 1054                                  | 5222-S(34-) 2225-S(34-) 222-D (11+)             |
|                | 784                                 | 778                                   | 0522-S(36-) 2250-S(36-) 222-D (14+)             |
|                | 300                                 | 298                                   | 222-D (35+) 2250-S(15+) 0522-S(15+) 2225-S( 5+) |
|                | 138                                 | 132                                   | 222-D (44-) 225-D (41+) 522-D (41+)             |
|                | 1305                                | 1302                                  | 222-6 (57-) 522-6 (13+) 225-6 (13+)             |
| a <sub>2</sub> | 1136                                | 1128                                  | 225-6 (36+) 522-6 (36+) 222-6 (27+)             |
|                |                                     | 827                                   | 225-4 (45+) 522-4 (45-) 222-6 (20+)             |
|                |                                     | 146                                   | 2225-T(48+) 5222-T(48+)                         |
| b <sub>1</sub> | 1443*                               | 1438                                  | 522-2 (45-) 225-2 (45+)                         |
|                | 1352                                | 1343                                  | 222-5 (51+) 522-5 (23-) 225-5 (23-) 5222-S(11-) |
|                | 1227                                | 1217                                  | 222-5 (52+) 225-5 (29+) 522-5 (29+)             |
|                | 1035                                | 1027                                  | 2225-S(47+) 5222-S(47-)                         |
|                | 679*                                | 679                                   | 2250-S(51+) 0522-S(51-)                         |
|                | 372                                 | 380                                   | 522-D (48-) 225-D (48+)                         |
| b <sub>2</sub> | 1270                                | 1262                                  | 225-6 (37-) 522-6 (37+) 222-4 (12-)             |
|                | 1035                                | 1033                                  | 522-4 (25+) 225-4 (25+) 222-4 (24+)             |
|                |                                     | 747                                   | 222-4 (55-) 522-4 (19+) 225-4 (19+)             |
|                |                                     | 108                                   | 5222-T(40+) 2225-T(40-) 222-4 (12-)             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3005 3005 2956 2956 2905 2870

\* Not used in the force constant determination.

## References

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torgrimsen, J. Mol. Struct., **15**, 61 (1973).
- [2] IR.R. J. E. Gustavsen, P. Klaboe, and R. Stølevik, J. Mol. Struct., **50**, 285 (1978).

## No. 133

Molecule: 52225-TG  $\text{ClCH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (*trans-gauche form*)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1455*                               | 1474                                  | 222-2 (85+)           |             |             |             |
|              | 1443*                               | 1438                                  | 225-2 (72+)           |             |             |             |
|              | 1421*                               | 1431                                  | 522-2 (85+)           |             |             |             |
|              | 1352                                | 1357                                  | 222-5 (51+)           | 522-5 (17-) | 225-5 (16+) | 5222-S(11-) |
|              | 1316*                               | 1311                                  | 225-5 (45+)           | 222-6 (25-) | 522-5 (9+)  |             |
|              | 1280*                               | 1289                                  | 522-5 (32+)           | 222-6 (20+) | 522-6 (20-) | 225-5 (11+) |
|              | 1270                                | 1269                                  | 522-5 (33+)           | 522-6 (19+) | 225-6 (15+) | 222-5 (12+) |
|              | 1194                                | 1190                                  | 225-6 (38+)           | 222-5 (25-) | 225-5 (13+) |             |
|              | 1136                                | 1139                                  | 522-6 (34+)           | 222-6 (34+) | 225-6 (21-) |             |
|              | 1064                                | 1060                                  | 5222-S(36-)           | 2225-S(35+) |             |             |
|              | 1035                                | 1034                                  | 225-4 (23-)           | 5222-S(18+) | 222-4 (11+) | 2225-S(10+) |
|              | 967*                                | 980                                   | 2225-S(27-)           | 522-4 (22+) | 222-4 (19+) | 225-5 (7-)  |
|              | 861                                 | 857                                   | 225-4 (49-)           | 5222-S(25-) |             |             |
|              | 784                                 | 779                                   | 522-4 (46+)           | 222-4 (30-) |             |             |
|              | 727                                 | 721                                   | 0522-S(69-)           | 225-4 (13-) | 522-D (10+) |             |
|              | 657                                 | 656                                   | 2250-S(92-)           |             |             |             |
|              | 431                                 | 431                                   | 225-D (34+)           | 222-D (23-) | 0522-S(15-) |             |
|              | 271                                 | 270                                   | 225-D (36+)           | 522-D (22+) | 2225-T(10-) | 2225-S(10+) |
|              | 220*                                | 239                                   | 522-D (56+)           | 222-D (41-) | 2225-T(15+) |             |
|              |                                     | 112                                   | 2225-T(60+)           | 5222-T(22+) |             |             |
|              | 79                                  | 84                                    | 5222-T(56-)           | 225-D (17+) | 222-4 (12+) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 3005 2956 2956 2905 2869

\* Not used in the force constant determination.

## References

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torgriksen, *J. Mol. Struct.*, **15**, 61 (1973).
- [2] IR.R. J. E. Gustavsen, P. Klaboe, and R. Stølevik, *J. Mol. Struct.*, **50**, 285 (1978).

## No. 134

Molecule: 52225-GG ClCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl (gauche-gauche form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1455                                | 1480                                  | 222-2 (78+)           |             |             |             |
|              | 1421                                | 1433                                  | 225-2 (37+)           | 522-2 (37+) | 222-2 (17-) |             |
|              | 1316                                | 1315                                  | 522-5 (31+)           | 225-5 (31-) | 222-6 (25+) |             |
|              | 1258                                | 1254                                  | 522-6 (22+)           | 225-6 (22+) | 222-6 (17+) | 225-5 (13+) |
|              | 1148(s)                             | 1143                                  | 222-6 (48-)           | 225-6 (22+) | 522-6 (22+) |             |
|              | 1001                                | 1005                                  | 225-4 (27-)           | 522-4 (27+) | 222-D (12-) | 2225-S( 9+) |
|              | 867                                 | 857                                   | 2225-S(32+)           | 5222-S(32+) | 225-4 (11+) | 522-4 (11-) |
|              | 679                                 | 674                                   | 0522-S(46-)           | 2250-S(46-) |             |             |
|              | 460                                 | 452                                   | 222-D (52-)           | 522-D (15+) | 225-D (15+) |             |
|              | 220                                 | 204                                   | 222-D (31-)           | 225-D (30-) | 522-D (30-) |             |
|              | 65                                  | 55                                    | 2225-T(43+)           | 5222-T(43+) |             |             |
| b            | 1443                                | 1444                                  | 522-2 (37-)           | 225-2 (37+) |             |             |
|              | 1357                                | 1368                                  | 222-5 (49+)           | 225-2 (11-) | 522-2 (11+) | 522-5 (10+) |
|              | 1280                                | 1296                                  | 225-5 (29+)           | 522-5 (29+) | 222-5 (15-) |             |
|              | 1156(s)                             | 1163                                  | 225-6 (37+)           | 522-6 (37-) | 222-5 (18-) |             |
|              | 1077                                | 1092                                  | 5222-S(37+)           | 2225-S(37-) |             |             |
|              | 967                                 | 971                                   | 222-4 (41-)           | 522-4 (12+) | 225-4 (12+) | 222-5 ( 7-) |
|              | 793                                 | 798                                   | 225-4 (32+)           | 522-4 (32+) | 222-4 (18+) | 222-5 (11-) |
|              | 641                                 | 645                                   | 2250-S(45+)           | 0522-S(45-) | 222-4 (10-) |             |
|              | 354                                 | 353                                   | 522-D (33+)           | 225-D (33-) | 5222-T(12-) | 2225-T(12+) |
|              | 138*                                | 144                                   | 2225-T(32+)           | 5222-T(32-) | 222-4 (16+) | 522-D (12-) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3006 3004 2956 2956 2905 2869

\* Not used in the force constant determination.

## References

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torggrimsen, J. Mol. Struct., **15**, 61 (1973).
- [2] IR.R. J. E. Gustavsen, P. Klaboe, and R. Stølevik, J. Mol. Struct., **50**, 285 (1978).

## No. 135

Molecule: 522225-TTT  $\text{ClCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-trans-trans form)Symmetry  $\text{C}_{2h}$  Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| $a_g$        | 1444*                               | 1461                                  | 222-2 (41+)           | 222-2 (41+) |             |             |
|              | 1434*                               | 1427                                  | 225-2 (38+)           | 522-2 (30+) |             |             |
|              | 1363                                | 1357                                  | 222-5 (39-)           | 222-5 (39+) | 2222-S(14+) |             |
|              | 1272*                               | 1279                                  | 225-5 (40+)           | 522-5 (40-) |             |             |
|              | 1067                                | 1069                                  | 5222-S(23-)           | 2225-S(23-) | 2222-S(14-) | 222-D (11+) |
|              | 1043                                | 1047                                  | 2222-S(66-)           | 5222-S(11+) | 2225-S(11+) |             |
|              | 743                                 | 739                                   | 0522-S(41-)           | 2250-S(41-) |             |             |
|              | 340                                 | 345                                   | 222-D (30-)           | 222-D (30-) | 522-D (12+) | 225-D (12+) |
|              | 230                                 | 214                                   | 225-D (34+)           | 522-D (34+) | 2222-S(10+) |             |
|              | 1291*                               | 1290                                  | 522-6 (20-)           | 225-6 (20-) | 222-6 (20+) | 222-6 (20+) |
| $a_u$        | 1113                                | 1118                                  | 522-6 (28+)           | 225-6 (28+) | 222-6 (21+) | 222-6 (21+) |
|              | 888                                 | 888                                   | 522-4 (32-)           | 225-4 (32+) | 222-6 (16+) | 222-6 (16+) |
|              | 730                                 | 738                                   | 222-4 (37+)           | 222-4 (37-) | 225-4 (10-) | 522-4 (10+) |
|              |                                     | 129                                   | 2222-T(79+)           |             |             |             |
| $b_g$        |                                     | 61                                    | 5222-T(34+)           | 2225-T(34+) | 2222-T(12-) |             |
|              | 1305                                | 1305                                  | 222-6 (37+)           | 222-6 (37-) |             |             |
|              | 1241                                | 1240                                  | 225-6 (30-)           | 522-6 (30+) | 222-4 (11-) | 222-4 (11-) |
|              | 1052*                               | 1054                                  | 522-4 (17+)           | 225-4 (17+) | 222-4 (16+) | 222-4 (16+) |
| $b_u$        | 768                                 | 771                                   | 225-4 (29-)           | 522-4 (29-) | 222-4 (18+) | 222-4 (18+) |
|              |                                     | 164                                   | 2225-T(46+)           | 5222-T(46-) |             |             |
|              | 1458*                               | 1476                                  | 222-2 (49-)           | 222-2 (49+) |             |             |
|              | 1433                                | 1432                                  | 522-2 (45+)           | 225-2 (45-) |             |             |
|              | 1323*                               | 1324                                  | 522-5 (33-)           | 225-5 (33-) | 222-5 (16+) | 222-5 (16+) |
|              | 1193*                               | 1207                                  | 222-5 (36+)           | 222-5 (36+) | 225-5 (18+) | 522-5 (18+) |
|              | 1022                                | 1012                                  | 2225-S(45+)           | 5222-S(45-) |             |             |
|              | 724                                 | 723                                   | 2250-S(41-)           | 0522-S(41+) |             |             |
|              | 414                                 | 428                                   | 522-D (22-)           | 225-D (22+) | 222-D (10-) | 222-D (10+) |
|              |                                     | 105                                   | 222-D (43+)           | 222-D (43-) | 225-D (22-) | 522-D (22+) |

Calculated frequencies higher than 2000  $\text{cm}^{-1}$ 

3005 3005 2956 2956 2909 2900 2873 2866

\* Not used in the force constant determination.

## Reference

- [1] I.R.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 136

Molecule: 522225-TTG ClCH2CH2CH2CH2Cl (trans-trans-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1480                                  | 222-2 (59+)           | 222-2 (32-) |             |             |
|              | 1458*                               | 1462                                  | 222-2 (61+)           | 222-2 (24+) |             |             |
|              | 1444*                               | 1439                                  | 225-2 (70+)           | 522-2 (6+)  |             |             |
|              | 1434*                               | 1429                                  | 522-2 (78-)           |             |             |             |
|              | 1370                                | 1368                                  | 222-5 (45-)           | 222-5 (27+) | 2222-S(13+) |             |
|              | 1323*                               | 1325                                  | 522-5 (39-)           | 222-5 (24+) | 225-5 (22+) |             |
|              | 1305                                | 1309                                  | 222-6 (31-)           | 225-5 (20+) | 222-6 (14+) | 225-6 (7-)  |
|              | 1291                                | 1298                                  | 222-6 (42+)           | 225-5 (16-) | 522-6 (14-) |             |
|              | 1266                                | 1266                                  | 522-6 (22+)           | 222-6 (18-) | 522-5 (16-) | 225-5 (12-) |
|              | 1250                                | 1246                                  | 222-5 (25+)           | 522-5 (22+) | 225-6 (16+) | 522-6 (13+) |
|              | 1190                                | 1184                                  | 225-6 (39+)           | 222-5 (21-) | 222-5 (15-) |             |
|              | 1126                                | 1127                                  | 222-6 (28+)           | 522-6 (27+) | 222-6 (21+) | 225-6 (12-) |
|              | 1067                                | 1073                                  | 2225-S(28+)           | 2222-S(28-) | 522-6 (8+)  | 522-4 (6+)  |
|              | 1052*                               | 1058                                  | 5222-S(31-)           | 225-4 (15+) | 2222-S(13-) | 225-6 (10-) |
|              | 1043                                | 1036                                  | 5222-S(27-)           | 222-4 (12+) | 222-4 (11+) | 522-4 (11+) |
|              | 974                                 | 988                                   | 2225-S(39+)           | 5222-S(18-) | 2222-S(8+)  | 522-4 (5-)  |
|              | 885                                 | 872                                   | 225-4 (34+)           | 522-4 (18+) | 222-4 (12-) | 222-6 (10-) |
|              | 822                                 | 823                                   | 225-4 (28+)           | 222-4 (24+) | 522-4 (23-) |             |
|              | 740                                 | 747                                   | 222-4 (54+)           | 522-4 (25-) | 222-4 (10-) |             |
|              | 730                                 | 729                                   | 0522-S(81+)           |             |             |             |
|              | 652*                                | 655                                   | 2250-S(91-)           |             |             |             |
|              | 452                                 | 456                                   | 222-D (43+)           | 225-D (24-) | 522-D (12-) |             |
|              | 340                                 | 339                                   | 522-D (33-)           | 222-D (16-) | 0522-S(11-) | 222-D (8+)  |
|              | 274                                 | 279                                   | 225-D (41+)           | 2225-T(14-) | 222-D (12+) | 2225-S(9+)  |
|              | 175                                 | 181                                   | 222-D (32+)           | 522-D (30-) | 2225-T(29+) |             |
|              | 135                                 | 127                                   | 5222-T(49+)           | 222-D (15-) | 522-D (11-) | 222-D (11+) |
|              |                                     | 95                                    | 2222-T(71+)           | 2225-T(14+) |             |             |
|              |                                     | 62                                    | 2225-T(30+)           | 5222-T(19+) | 222-D (11+) | 2222-T(10-) |

Calculated frequencies higher than 2000  $\text{cm}^{-1}$ 

3005 3005 2956 2956 2909 2901 2873 2866

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).



## No. 137

Molecule: 522225-TGG  $\text{ClCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Cl}$  (trans-gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1486                                  | 222-2 (53+)           | 222-2 (34+) |             |             |
|              | 1458*                               | 1463                                  | 222-2 (57+)           | 222-2 (29-) |             |             |
|              | 1444*                               | 1438                                  | 225-2 (69+)           | 222-2 (12-) |             |             |
|              | 1434*                               | 1431                                  | 522-2 (87+)           |             |             |             |
|              | 1370                                | 1364                                  | 222-5 (51+)           | 222-5 (13+) | 225-5 (12+) | 225-2 (10-) |
|              | 1349                                | 1345                                  | 222-5 (46-)           | 522-5 (26+) | 5222-S(11+) | 2222-S(11-) |
|              | 1311                                | 1307                                  | 225-5 (54+)           | 222-6 (14-) | 2225-S(10-) |             |
|              | 1288                                | 1291                                  | 222-6 (40+)           | 522-6 (22-) | 522-5 (10+) |             |
|              | 1266                                | 1273                                  | 522-5 (47+)           | 522-6 (12+) | 222-5 (11+) | 222-6 (9+)  |
|              | 1241*                               | 1240                                  | 225-6 (24+)           | 225-5 (13+) | 222-6 (11+) | 522-5 (11-) |
|              | 1161                                | 1157                                  | 225-6 (47+)           | 222-6 (22-) | 222-5 (14+) |             |
|              | 1142                                | 1142                                  | 522-6 (37-)           | 222-6 (31-) | 222-6 (12+) |             |
|              | 1083*                               | 1094                                  | 2222-S(43+)           | 2225-S(32-) |             |             |
|              | 1055                                | 1053                                  | 5222-S(35-)           | 225-4 (12-) | 225-6 (8+)  | 222-4 (8+)  |
|              | 1024                                | 1027                                  | 222-4 (23-)           | 522-4 (21-) | 222-4 (9+)  | 5222-S(8-)  |
|              | 925                                 | 932                                   | 225-4 (32+)           | 5222-S(29-) | 222-4 (11-) |             |
|              | 888                                 | 891                                   | 2225-S(38-)           | 2222-S(17-) | 522-4 (13+) | 222-4 (8+)  |
|              | 822                                 | 825                                   | 225-4 (25+)           | 222-4 (20+) | 522-4 (19+) | 2222-S(13+) |
|              | 748*                                | 754                                   | 222-4 (38-)           | 522-4 (28+) | 0522-S(11+) |             |
|              | 730                                 | 728                                   | 0522-S(65-)           | 222-D (9+)  |             |             |
|              | 652*                                | 654                                   | 2250-S(86+)           |             |             |             |
|              | 467                                 | 464                                   | 222-D (49-)           | 225-D (14+) | 222-D (11+) |             |
|              | 347                                 | 357                                   | 225-D (33+)           | 222-D (20-) | 0522-S(9-)  | 2225-T(8-)  |
|              | 274                                 | 273                                   | 522-D (63+)           | 2225-T(11-) | 222-D (10+) |             |
|              |                                     | 198                                   | 225-D (31+)           | 222-D (28+) | 222-D (19+) | 522-D (12-) |
|              | 135*                                | 137                                   | 2225-T(32-)           | 222-D (19+) | 2222-T(17+) | 222-4 (11-) |
|              |                                     | 96                                    | 5222-T(51+)           | 2222-T(39+) |             |             |
|              |                                     | 46                                    | 2225-T(38-)           | 2222-T(23-) | 5222-T(17+) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 3005 2956 2956 2907 2903 2871 2868

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 138

Molecule: 522225-GTG ClCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl (gauche-trans-gauche form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1458*                               | 1464                                  | 222-2 (41+)           | 222-2 (41+) |             |             |
|              | 1434*                               | 1439                                  | 522-2 (33+)           | 225-2 (33+) | 222-2 ( 6-) |             |
|              | 1383                                | 1375                                  | 222-5 (34+)           | 222-5 (34-) | 2222-S(12+) |             |
|              | 1316*                               | 1308                                  | 522-5 (29+)           | 225-5 (29-) | 222-6 ( 9+) | 222-6 ( 9+) |
|              | 1220                                | 1230                                  | 522-6 (23+)           | 225-6 (23+) | 522-5 ( 9-) | 225-5 ( 9+) |
|              | 1133                                | 1140                                  | 222-6 (28-)           | 222-6 (28-) | 522-6 (10+) | 225-6 (10+) |
|              | 1067                                | 1067                                  | 2222-S(34+)           | 2225-S(14-) | 5222-S(14-) | 522-6 ( 4+) |
|              | 1024                                | 1033                                  | 225-4 (16-)           | 522-4 (16+) | 2225-S(11+) | 5222-S(11+) |
|              | 821                                 | 828                                   | 222-4 (16+)           | 222-4 (16-) | 2222-S(16-) | 225-4 (12-) |
|              | 768                                 | 771                                   | 222-4 (20+)           | 222-4 (20-) | 2222-S(20+) | 225-4 (12+) |
|              | 652*                                | 653                                   | 2250-S(44-)           | 0522-S(44-) |             |             |
|              | 505                                 | 504                                   | 222-D (22-)           | 222-D (22-) | 522-D (13+) | 225-D (13+) |
|              | 256*                                | 258                                   | 225-D (22-)           | 522-D (22-) | 2222-T(14-) | 222-D ( 8-) |
|              |                                     | 87                                    | 5222-T(35+)           | 2225-T(35+) | 222-4 ( 7+) |             |
|              |                                     | 46                                    | 2222-T(74+)           |             |             |             |
|              |                                     | 1482                                  | 222-2 (44+)           | 222-2 (44-) |             |             |
| b            |                                     | 1437                                  | 225-2 (39-)           | 522-2 (39+) |             |             |
|              | 1434*                               | 1437                                  | 225-2 (39-)           | 522-2 (39+) |             |             |
|              | 1323*                               | 1330                                  | 522-5 (27+)           | 225-5 (27+) | 222-5 (15+) | 222-5 (15+) |
|              | 1311                                | 1307                                  | 222-6 (27+)           | 222-6 (27-) | 222-5 ( 6+) | 222-5 ( 6+) |
|              | 1266                                | 1268                                  | 522-5 (12+)           | 225-5 (12+) | 222-5 (12-) | 222-5 (12-) |
|              | 1161                                | 1164                                  | 225-6 (33-)           | 522-6 (33+) | 222-5 (12+) | 222-5 (12+) |
|              | 1055                                | 1053                                  | 5222-S(21-)           | 2225-S(21+) | 222-4 (15+) | 222-4 (15+) |
|              | 985                                 | 984                                   | 5222-S(20-)           | 2225-S(20+) | 222-4 (11-) | 222-4 (11-) |
|              | 870                                 | 864                                   | 522-4 (35+)           | 225-4 (35+) | 222-5 ( 7-) |             |
|              | 652*                                | 657                                   | 0522-S(48+)           | 2250-S(48-) |             |             |
|              | 347                                 | 344                                   | 522-D (35-)           | 225-D (35+) | 222-D (11-) | 222-D (11+) |
|              | 256*                                | 261                                   | 222-D (31+)           | 222-D (31-) | 5222-T(19-) | 2225-T(19+) |
|              |                                     | 121                                   | 2225-T(27-)           | 5222-T(27+) | 222-D (14+) | 222-D (14-) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3005 3005 2956 2956 2909 2901 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 139

Molecule: 522225-GTG' ClCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl (gauche-trans-gauche' form)Symmetry C<sub>i</sub>Symmetry number  $\sigma = 1$ 

| Sym. species   | Observed frequency<br>cm <sup>-1</sup> | Calculated frequency<br>cm <sup>-1</sup> | Assignment<br>(P.E.D. %) |             |             |             |
|----------------|----------------------------------------|------------------------------------------|--------------------------|-------------|-------------|-------------|
| a <sub>g</sub> | 1444                                   | 1464                                     | 222-2 (41+)              | 222-2 (41+) |             |             |
|                | 1434                                   | 1439                                     | 225-2 (33+)              | 522-2 (33+) | 222-2 ( 6-) |             |
|                | 1383                                   | 1376                                     | 222-5 (33+)              | 222-5 (33-) | 2222-S(12+) |             |
|                | 1316                                   | 1312                                     | 222-6 (20-)              | 222-6 (20+) | 522-5 (18-) | 225-5 (18+) |
|                | 1272                                   | 1281                                     | 225-5 (19-)              | 522-5 (19+) | 222-6 (17-) | 222-6 (17+) |
|                | 1220                                   | 1215                                     | 522-6 (33-)              | 225-6 (33+) | 222-5 ( 4+) | 222-5 ( 4-) |
|                | 1083                                   | 1089                                     | 2222-S(28-)              | 5222-S(20+) | 2225-S(20+) | 222-4 ( 5-) |
|                | 1052                                   | 1046                                     | 2222-S(21+)              | 522-4 (17+) | 225-4 (17+) | 522-6 ( 9+) |
|                | 974                                    | 984                                      | 222-4 (20+)              | 222-4 (20+) | 2225-S( 9+) | 5222-S( 9+) |
|                | 803                                    | 795                                      | 2222-S(35-)              | 522-4 (24+) | 225-4 (24+) |             |
|                | 652                                    | 652                                      | 2250-S(49+)              | 0522-S(49+) |             |             |
|                | 494                                    | 495                                      | 222-D (24-)              | 222-D (24-) | 225-D (11+) | 522-D (11+) |
|                | 256                                    | 261                                      | 5222-T(22-)              | 2225-T(22+) | 522-D (19+) | 225-D (19+) |
|                |                                        | 111                                      | 5222-T(25+)              | 2225-T(25-) | 225-D (15+) | 522-D (15+) |
| a <sub>u</sub> |                                        | 1482                                     | 222-2 (44+)              | 222-2 (44-) |             |             |
|                | 1443                                   | 1437                                     | 522-2 (39-)              | 225-2 (39+) |             |             |
|                | 1323                                   | 1330                                     | 522-5 (27+)              | 225-5 (27+) | 222-5 (15+) | 222-5 (15+) |
|                | 1291                                   | 1296                                     | 222-5 (16-)              | 222-5 (16-) | 225-6 (12+) | 522-6 (12+) |
|                | 1193                                   | 1181                                     | 222-5 (15+)              | 222-5 (15+) | 225-6 (13+) | 522-6 (13+) |
|                | 1127                                   | 1128                                     | 222-6 (24-)              | 222-6 (24-) | 522-6 (22+) | 225-6 (22+) |
|                | 1008                                   | 1012                                     | 2225-S(39-)              | 5222-S(39+) |             |             |
|                | 897                                    | 897                                      | 522-4 (36+)              | 225-4 (36-) |             |             |
|                | 777                                    | 785                                      | 222-4 (32-)              | 222-4 (32+) | 0522-S( 6-) | 2250-S( 6+) |
|                | 652                                    | 656                                      | 0522-S(43+)              | 2250-S(43-) |             |             |
|                | 368                                    | 369                                      | 522-D (35-)              | 225-D (35+) | 222-D ( 8-) |             |
|                | 247                                    | 249                                      | 222-D (40-)              | 222-D (40+) |             |             |
|                |                                        | 77                                       | 2225-T(21-)              | 5222-T(21-) | 2222-T(18+) | 222-4 ( 8-) |
|                |                                        | 51                                       | 2222-T(61+)              | 2225-T(15+) | 5222-T(15+) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3005 3005 2956 2956 2909 2901 2873 2865

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 140

Molecule: 522225-GGG ClCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Cl (gauche-gauche-gauche form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1489                                  | 222-2 (42+)           | 222-2 (42+) |             |             |
|              | 1444*                               | 1438                                  | 225-2 (38+)           | 522-2 (38+) |             |             |
|              | 1349                                | 1352                                  | 222-5 (26+)           | 222-5 (26-) | 2222-S(13-) | 225-5 ( 8+) |
|              | 1305                                | 1303                                  | 225-5 (27-)           | 522-5 (27+) | 222-5 ( 6+) | 222-5 ( 6-) |
|              | 1266                                | 1269                                  | 222-6 (24+)           | 222-6 (24+) | 225-5 (10+) | 522-5 (10-) |
|              | 1161                                | 1153                                  | 522-6 (24+)           | 225-6 (24+) | 222-5 (10-) | 222-5 (10+) |
|              | 1113                                | 1104                                  | 2222-S(37+)           | 2225-S(16-) | 5222-S(16-) | 225-6 ( 9+) |
|              | 985                                 | 984                                   | 222-4 (27-)           | 222-4 (27+) | 225-5 ( 6-) | 522-5 ( 6+) |
|              | 909                                 | 923                                   | 522-4 (24-)           | 225-4 (24+) | 2225-S(13-) | 5222-S(13-) |
|              | 797                                 | 798                                   | 2222-S(42+)           | 225-4 (17+) | 522-4 (17-) |             |
|              | 652*                                | 660                                   | 0522-S(48+)           | 2250-S(48+) |             |             |
|              | 393                                 | 400                                   | 522-D (20-)           | 225-D (20-) | 222-D (14+) | 222-D (14+) |
|              |                                     | 204                                   | 222-D (24+)           | 222-D (24+) | 2225-T(15-) | 5222-T(15-) |
|              | 135                                 | 138                                   | 225-D (22+)           | 522-D (22+) | 2225-T(14+) | 5222-T(14+) |
|              |                                     | 41                                    | 2222-T(64-)           | 5222-T(14-) | 2225-T(14-) |             |
| b            | 1458*                               | 1466                                  | 222-2 (40-)           | 222-2 (40+) |             |             |
|              | 1433*                               | 1437                                  | 522-2 (33-)           | 225-2 (33+) | 222-2 ( 9+) |             |
|              | 1370                                | 1369                                  | 222-5 (32+)           | 222-5 (32+) | 522-5 ( 7+) |             |
|              | 1311                                | 1309                                  | 522-5 (27+)           | 225-5 (27+) | 222-6 (12+) | 222-6 (12-) |
|              | 1221*                               | 1209                                  | 225-6 (33+)           | 522-6 (33-) | 225-5 ( 6+) |             |
|              | 1142                                | 1149                                  | 222-6 (34+)           | 222-6 (34-) | 225-5 ( 9+) |             |
|              | 1055                                | 1056                                  | 5222-S(15+)           | 2225-S(15-) | 522-4 (11+) | 225-4 (11+) |
|              | 939                                 | 933                                   | 5222-S(20+)           | 2225-S(20-) | 225-4 (17-) | 522-4 (17-) |
|              | 777*                                | 783                                   | 222-4 (25+)           | 222-4 (25+) | 522-4 (11+) | 225-4 (11+) |
|              | 652*                                | 649                                   | 2250-S(41-)           | 0522-S(41+) |             |             |
|              | 494                                 | 487                                   | 222-D (35+)           | 222-D (35-) | 522-D ( 8-) |             |
|              |                                     | 301                                   | 225-D (35+)           | 522-D (35-) | 222-D ( 6-) |             |
|              |                                     | 75                                    | 2225-T(37-)           | 5222-T(37+) |             |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3005 3005 2956 2956 2907 2903 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 141

Molecule: 1226-T  $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$  (trans form)  
 Symmetry  $C_s$  Symmetry number  $\sigma = 1$

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           | 1464                                | 1478                                  | 122-2 (55+)           | 012-4 (28+) |             |             |
|              | 1458                                | 1452                                  | 012-4 (56+)           | 122-2 (37-) |             |             |
|              | 1435                                | 1430                                  | 226-2 (91+)           |             |             |             |
|              | 1368(s)                             | 1379                                  | 012-2 (105+)          |             |             |             |
|              | 1330                                | 1329                                  | 122-5 (79+)           | 1226-S(13+) | 226-5 (11-) |             |
|              | 1228                                | 1227                                  | 226-5 (90+)           |             |             |             |
|              | 1099                                | 1092                                  | 012-5 (28+)           | 1226-S(26-) | 122-5 (14+) | 012-4 (9-)  |
|              | 1025                                | 1029                                  | 0122-S(80-)           | 1226-S(21+) |             |             |
|              | 897                                 | 892                                   | 1226-S(40-)           | 012-5 (39-) |             |             |
|              | 648                                 | 644                                   | 2260-S(77-)           | 122-D (18+) | 226-D (14+) |             |
|              | 311                                 | 313                                   | 122-D (49+)           | 2260-S(31+) |             |             |
|              | 224                                 | 221                                   | 226-D (83+)           | 122-D (26-) |             |             |
| a''          | 1458                                | 1463                                  | 012-7 (81-)           | 012-8 (14+) |             |             |
|              | 1290                                | 1289                                  | 122-6 (63-)           | 226-6 (15+) |             |             |
|              | 1213                                | 1220                                  | 226-6 (37+)           | 012-8 (18-) | 122-4 (18+) |             |
|              | 1041                                | 1039                                  | 226-6 (45+)           | 012-8 (19+) | 122-6 (16+) | 226-4 (13-) |
|              | 850                                 | 849                                   | 226-4 (46+)           | 012-8 (38+) | 122-6 (19+) |             |
|              | 740                                 | 739                                   | 122-4 (56+)           | 226-4 (31-) | 012-8 (11+) | 1226-T(10-) |
|              | 232(s)                              | 227                                   | 0122-T(96+)           |             |             |             |
|              | 133                                 | 122                                   | 1226-T(87+)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$

3003 2962 2962 2956 2905 2880 2868

## References

- [1] IR. K. Radcliffe and J. L. Wood, Trans. Faraday Soc., **62**, 1678 (1966).  
 [2] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 142

Molecule: 1226-G  $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$  (gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1464*                               | 1479                                  | 122-2 (68+)           | 012-4 (18+) |             |             |
|              | 1458*                               | 1463                                  | 012-7 (80+)           | 012-8 (14+) |             |             |
|              | 1458*                               | 1457                                  | 012-4 (61-)           | 122-2 (16+) | 226-2 (11+) |             |
|              | 1435*                               | 1435                                  | 226-2 (77+)           |             |             |             |
|              | 1382                                | 1379                                  | 012-2 (105+)          |             |             |             |
|              | 1343                                | 1347                                  | 122-5 (72+)           |             |             |             |
|              | 1283                                | 1291                                  | 122-6 (52-)           | 226-5 (25+) |             |             |
|              | 1233                                | 1235                                  | 226-5 (55+)           | 122-6 (11+) | 012-8 (11-) |             |
|              | 1200                                | 1194                                  | 226-6 (46+)           | 012-5 (12+) | 226-5 (7+)  | 1226-S (7-) |
|              | 1082                                | 1080                                  | 1226-S(25+)           | 0122-S(25-) | 122-6 (10-) | 122-4 (10+) |
|              | 1065                                | 1055                                  | 012-5 (31+)           | 122-5 (12+) | 226-6 (10-) | 012-4 (8-)  |
|              | 1032                                | 1025                                  | 0122-S(31-)           | 226-6 (23-) | 122-6 (11+) | 012-8 (9+)  |
|              | 888                                 | 878                                   | 1226-S(34+)           | 012-5 (28+) | 0122-S(12+) |             |
|              | 840                                 | 842                                   | 226-4 (43-)           | 0122-S(22-) | 012-8 (12+) |             |
|              | 778                                 | 781                                   | 122-4 (44+)           | 012-8 (26+) | 226-4 (19+) |             |
|              | 563                                 | 562                                   | 2260-S(97-)           | 226-D (14+) |             |             |
|              | 402                                 | 398                                   | 122-D (70-)           | 226-D (16+) |             |             |
|              | 274                                 | 276                                   | 0122-T(34+)           | 226-D (31+) | 1226-T(16-) | 122-D (11+) |
|              | 205                                 | 191                                   | 0122-T(61+)           | 226-D (28-) |             |             |
|              | 115(g)                              | 109                                   | 1226-T(68+)           | 226-D (15+) |             |             |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

3004 2962 2962 2956 2905 2880 2868

\* Not used in the force constant determination.

## References

- [1] IR. K. Radcliffe and J. L. Wood, *Trans. Faraday Soc.*, **62**, 1678 (1966).  
 [2] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, *Bull. Chem. Soc. Jpn.*, **51**, 748 (1978).

## No. 143

Molecule: 12"26-T  $\text{CH}_3\text{CHDCH}_2\text{Br}$  (trans form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1459                                | 1462                                  | 012-4 (68+)           | 012-7 (12+) | 012-5 (11+) |             |
|              | 1459                                | 1461                                  | 012-7 (70-)           | 012-4 (12+) | 012-8 (11-) |             |
|              | 1437                                | 1432                                  | 226-2 (91+)           |             |             |             |
|              | 1379                                | 1380                                  | 012-2 (104+)          |             |             |             |
|              | 1319(s)                             | 1323                                  | 122-2 (40+)           | 122-5 (25-) | 122-6 (11-) |             |
|              | 1295                                | 1306                                  | 122-2 (39+)           | 122-5 (24+) | 122-6 (13+) |             |
|              | 1230                                | 1229                                  | 226-5 (92+)           |             |             |             |
|              | 1191                                | 1195                                  | 226-6 (56+)           | 122-2 (10+) | 1226-S( 7+) |             |
|              | 1143                                | 1148                                  | 012-8 (23-)           | 122-6 (16+) | 012-5 (15+) | 1226-S(14-) |
|              | 1064                                | 1068                                  | 0122-S(23-)           | 226-6 (16+) | 012-5 (15+) | 122-5 (14+) |
|              | 1017                                | 1022                                  | 0122-S(47-)           | 012-8 (13-) | 1226-S(12+) | 226-6 (11-) |
|              | 948                                 | 938                                   | 226-4 (32-)           | 1226-S(19+) | 122-5 (12-) | 122-6 ( 8+) |
|              | 886                                 | 883                                   | 012-5 (31-)           | 1226-S(30-) | 0122-S(10-) | 122-5 (10-) |
|              | 780                                 | 779                                   | 122-6 (44-)           | 226-4 (28-) | 012-8 (20-) | 122-5 (13+) |
|              | 659                                 | 657                                   | 122-4 (68-)           | 226-4 (17+) | 012-8 (11-) |             |
|              | 641                                 | 641                                   | 2260-S(76+)           | 122-D (18-) | 226-D (13-) |             |
|              | 310(s)                              | 311                                   | 122-D (50+)           | 2260-S(30+) |             |             |
|              |                                     | 225                                   | 0122-T(96-)           |             |             |             |
|              |                                     | 216                                   | 226-D (83+)           | 122-D (25-) |             |             |
|              |                                     | 119                                   | 1226-T(88+)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3003 2962 2962 2956 2887 2879 2140

## Reference

- [1] IR. M. Hayashi, K. Ohno, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 2332 (1973).

## No. 144

Molecule: 12"26-G CH<sub>3</sub>CHDCH<sub>2</sub>Br (*gauche form*)<sup>a</sup>Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency<br>cm <sup>-1</sup> | Calculated frequency<br>cm <sup>-1</sup> | Assignment<br>(P.E.D. %) |             |             |             |
|--------------|----------------------------------------|------------------------------------------|--------------------------|-------------|-------------|-------------|
| a            | 1459*                                  | 1462                                     | 012-7 (43+)              | 012-4 (39+) |             |             |
|              | 1459*                                  | 1461                                     | 012-4 (43+)              | 012-7 (39-) |             |             |
|              | 1437*                                  | 1437                                     | 226-2 (93+)              |             |             |             |
|              | 1379*                                  | 1381                                     | 012-2 (103+)             |             |             |             |
|              |                                        | 1346                                     | 122-5 (33+)              | 122-2 (23-) | 0122-S(12-) | 122-6 (11+) |
|              | 1295*                                  | 1299                                     | 122-2 (55+)              | 122-5 (17+) |             |             |
|              | 1235                                   | 1239                                     | 226-5 (88+)              |             |             |             |
|              | 1191*                                  | 1194                                     | 226-6 (46+)              | 012-5 (10+) | 012-8 ( 8+) | 1226-S( 5-) |
|              | 1143*                                  | 1150                                     | 1226-S(20-)              | 122-6 (19+) | 012-8 (18-) | 012-5 (14+) |
|              | 1064*                                  | 1059                                     | 012-8 (23-)              | 1226-S(21+) | 0122-S(12-) | 226-6 ( 9+) |
|              | 1036                                   | 1038                                     | 226-6 (30+)              | 0122-S(26+) | 012-5 (23-) | 226-4 (12-) |
|              | 886*                                   | 877                                      | 012-5 (27-)              | 1226-S(21-) | 0122-S(16-) | 122-5 (13-) |
|              | 862                                    | 863                                      | 122-6 (40-)              | 122-5 (10+) | 1226-S(10-) | 226-4 ( 8+) |
|              | 830                                    | 829                                      | 226-4 (49-)              | 0122-S(21-) | 1226-S(13-) | 122-5 (11+) |
|              | 703                                    | 701                                      | 122-4 (47+)              | 012-8 (23+) | 122-6 (10+) |             |
|              | 535                                    | 539                                      | 2260-S(87-)              | 122-4 (13+) | 226-D (11+) |             |
|              |                                        | 395                                      | 122-D (71-)              | 226-D (15+) |             |             |
|              |                                        | 266                                      | 0122-T(39+)              | 226-D (31+) | 1226-T(15-) |             |
|              |                                        | 190                                      | 0122-T(56-)              | 226-D (32+) |             |             |
|              |                                        | 108                                      | 1226-T(70+)              | 226-D (13+) |             |             |

<sup>a</sup> The CH<sub>2</sub>Br group and the deuterium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3004 2962 2962 2956 2888 2879 2138

\* Not used in the force constant determination.

## Reference

- [1] IR. M. Hayashi, K. Ohno, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 2332 (1973).



## No. 145

Molecule: 12"26-G' CH<sub>3</sub>CHDCH<sub>2</sub>Br (*gauche'* form)<sup>a</sup>Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1459*                               | 1462                                  | 012-7 (62+)           | 012-4 (19+) | 012-8 (10+) |             |
|              | 1459*                               | 1461                                  | 012 4 (64)            | 012 7 (20+) |             |             |
|              | 1437*                               | 1439                                  | 226-2 (90+)           |             |             |             |
|              | 1379*                               | 1381                                  | 012-2 (104+)          |             |             |             |
|              |                                     | 1336                                  | 122-2 (30-)           | 122-5 (30+) | 0122-S(12-) |             |
|              | 1308                                | 1311                                  | 122-2 (41+)           | 226-5 (21+) | 122-5 (16+) |             |
|              | 1230*                               | 1221                                  | 226-5 (72+)           | 1226-S(18-) |             |             |
|              | 1210                                | 1202                                  | 226-6 (53+)           | 0122-S(12+) | 122-6 (10+) |             |
|              | 1143*                               | 1147                                  | 012-8 (22-)           | 012-5 (15+) | 226-6 (13-) | 1226-S(11-) |
|              | 1053                                | 1053                                  | 012-5 (29+)           | 0122-S(12-) | 226-6 (11+) | 012-8 (10+) |
|              | 1017*                               | 1016                                  | 0122-S(29-)           | 012-8 (19-) | 1226-S(18+) | 226-6 (10+) |
|              | 948*                                | 941                                   | 226-4 (31-)           | 122-6 (19-) | 1226-S(11-) | 122-4 (6+)  |
|              | 858                                 | 858                                   | 1226-S(36-)           | 0122-S(33-) | 012-5 (16-) |             |
|              | 780*                                | 783                                   | 226-4 (42+)           | 122-5 (33+) | 122-6 (20-) | 012-5 (10+) |
|              | 718                                 | 722                                   | 122-4 (49+)           | 012-8 (28+) | 122-6 (11+) |             |
|              | 546                                 | 551                                   | 2260-S(95+)           | 122-4 (11+) |             |             |
|              |                                     | 390                                   | 122-D (74+)           | 226-D (13-) |             |             |
|              |                                     | 263                                   | 0122-T(43-)           | 226-D (30+) | 1226-T(14+) |             |
|              |                                     | 188                                   | 0122-T(52-)           | 226-D (34-) |             |             |
|              |                                     | 108                                   | 1226-T(70-)           | 226-D (13+) |             |             |

<sup>a</sup> The CH<sub>2</sub>Br group and the protium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3003 2962 2962 2956 2887 2879 2141

\* Not used in the force constant determination.

## Reference

- [1] IR. M. Hayashi, K. Ohno, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 2332 (1973).

## No. 146

Molecule: 122"6-T CH<sub>3</sub>CH<sub>2</sub>CHDBr (trans form)Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1461                                | 1476                                  | 122-2 (57+)           | 012-4 (30+) |             |             |
|              | 1455                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1455                                | 1452                                  | 012-4 (55+)           | 122-2 (38-) |             |             |
|              | 1381                                | 1380                                  | 012-2 (105+)          |             |             |             |
|              | 1341                                | 1326                                  | 122-5 (78+)           | 1226-S(14+) |             |             |
|              | 1296                                | 1298                                  | 226-2 (57+)           | 122-6 (19+) |             |             |
|              | 1260                                | 1268                                  | 122-6 (46-)           | 226-2 (25+) |             |             |
|              | 1200*                               | 1220                                  | 226-5 (35+)           | 226-6 (26+) | 122-4 ( 9+) | 012-8 ( 9-) |
|              | 1118                                | 1106                                  | 226-5 (32-)           | 122-4 (19+) | 012-8 (18-) | 122-6 (11-) |
|              |                                     | 1085                                  | 012-5 (31+)           | 1226-S(16-) | 122-5 (13+) | 0122-S(11-) |
|              | 1020                                | 1022                                  | 0122-S(72-)           | 1226-S(18+) |             |             |
|              | 908                                 | 914                                   | 1226-S(26-)           | 226-6 (25-) | 012-5 (17-) | 012-8 (11-) |
|              | 843                                 | 845                                   | 012-5 (19-)           | 226-6 (19+) | 226-5 (16-) | 1226-S(15-) |
|              | 801                                 | 801                                   | 122-4 (30-)           | 012-8 (27-) | 226-4 (22-) | 226-6 (14+) |
|              | 671                                 | 671                                   | 226-4 (56-)           | 122-4 (28+) |             |             |
|              | 616                                 | 611                                   | 2260-S(65-)           | 122-D (15+) | 226-D (13+) |             |
|              | 311(s)                              | 313                                   | 122-D (48+)           | 2260-S(31+) |             |             |
|              |                                     | 225                                   | 0122-T(92+)           |             |             |             |
|              |                                     | 217                                   | 226-D (80+)           | 122-D (26-) |             |             |
|              |                                     | 120                                   | 1226-T(88+)           |             |             |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2981 2962 2962 2905 2880 2868 2200

\* Not used in the force constant determination.

## Reference

- [1] IR. M. Hayashi, K. Ohno, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 2332 (1973).

## No. 147

Molecule: 122"6-G CH<sub>3</sub>CH<sub>2</sub>CHDBr (gauche form)<sup>a</sup>Symmetry C<sub>1</sub>Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1461*                               | 1478                                  | 122-2 (66+)           | 012-4 (22+) |             |             |
|              | 1455*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1455*                               | 1454                                  | 012-4 (63+)           | 122-2 (26-) |             |             |
|              | 1381*                               | 1380                                  | 012-2 (105+)          |             |             |             |
|              | 1341*                               | 1347                                  | 122-5 (75+)           |             |             |             |
|              | 1296*                               | 1305                                  | 226-2 (61+)           | 122-6 (20-) |             |             |
|              | 1260*                               | 1259                                  | 122-6 (48+)           | 226-2 (19+) | 012-8 (10-) |             |
|              | 1200*                               | 1206                                  | 226-5 (55+)           | 226-6 (22+) | 1226-S(10-) |             |
|              | 1118*                               | 1116                                  | 122-4 (23+)           | 012-8 (22-) | 122-6 (11-) | 226-6 ( 9-) |
|              | 1068                                | 1067                                  | 0122-S(47-)           | 1226-S(23+) | 226-5 ( 7-) |             |
|              |                                     | 1046                                  | 012-5 (36+)           | 122-5 (19+) | 1226-S(12-) | 012-4 ( 9-) |
|              | 886                                 | 880                                   | 0122-S(35+)           | 1226-S(25+) | 226-6 (23+) |             |
|              | 843*                                | 841                                   | 012-8 (28-)           | 226-6 (17+) | 1226-S(13-) | 122-6 (12-) |
|              | 778                                 | 779                                   | 122-4 (34+)           | 226-5 (17-) | 012-8 (16+) | 226-6 (15+) |
|              | 745                                 | 742                                   | 226-4 (56+)           | 012-5 ( 9-) | 122-4 ( 9+) |             |
|              | 545                                 | 540                                   | 2260-S(93-)           | 226-D (12+) |             |             |
|              |                                     | 379                                   | 122-D (63-)           | 226-D (21+) | 226-4 (11+) |             |
|              |                                     | 271                                   | 0122-T(34-)           | 226-D (27-) | 1226-T(16+) | 122-D (15-) |
|              |                                     | 191                                   | 0122-T(59+)           | 226-D (29-) |             |             |
|              |                                     | 107                                   | 1226-T(69+)           | 226-D (14+) |             |             |

<sup>a</sup> The CH<sub>2</sub>CH<sub>3</sub> group and the protium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2981 2962 2962 2905 2880 2868 2201

\* Not used in the force constant determination.

## Reference

- [1] IR. M. Hayashi, K. Ohno, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 2332 (1973).

## No. 148

Molecule: 122"6-G' CH<sub>3</sub>CH<sub>2</sub>CHDBr (*gauche'* form)<sup>a</sup>  
 Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1461*                               | 1478                                  | 122-2 (65+)           | 012-4 (23+) |             |             |
|              | 1455*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1455*                               | 1454                                  | 012-4 (62-)           | 122-2 (29+) |             |             |
|              | 1381*                               | 1380                                  | 012-2 (105+)          |             |             |             |
|              | 1341*                               | 1349                                  | 122-5 (61+)           | 226-2 (18+) | 1226-S(12+) |             |
|              | 1289                                | 1295                                  | 122-6 (52+)           | 226-5 (10+) | 226-6 ( 7+) | 226-2 ( 7+) |
|              | 1272                                | 1269                                  | 226-2 (60+)           | 122-5 (18-) | 226-5 (10-) |             |
|              | 1200*                               | 1219                                  | 226-5 (26-)           | 012-8 (16-) | 226-6 (16-) | 122-4 (13+) |
|              | 1118*                               | 1114                                  | 012-5 (29-)           | 1226-S(28+) | 226-5 (15-) |             |
|              | 1068                                | 1072                                  | 0122-S(31-)           | 122-6 (14+) | 122-4 (12-) | 012-8 (12+) |
|              | 1027                                | 1025                                  | 0122-S(39-)           | 122-6 (12-) | 012-8 (12-) | 1226-S(10+) |
|              | 912                                 | 910                                   | 012-5 (34+)           | 1226-S(26+) | 226-6 (25+) | 122-5 (11+) |
|              | 820*                                | 839                                   | 012-8 (29+)           | 122-4 (20+) | 226-6 (15+) | 226-4 (10-) |
|              | 778                                 | 775                                   | 122-4 (23-)           | 226-6 (18+) | 226-5 (17-) | 012-8 (15-) |
|              | 710                                 | 704                                   | 226-4 (62-)           | 122-4 (10-) |             |             |
|              | 550                                 | 548                                   | 2260-S(94-)           | 226-D (15+) |             |             |
|              |                                     | 389                                   | 122-D (64-)           | 226-D (18+) |             |             |
|              |                                     | 270                                   | 0122-T(35+)           | 226-D (28-) | 1226-T(16-) | 122-D (13-) |
|              |                                     | 190                                   | 0122-T(58+)           | 226-D (30+) |             |             |
|              |                                     | 108                                   | 1226-T(69-)           | 226-D (14+) |             |             |

<sup>a</sup> The CH<sub>2</sub>CH<sub>3</sub> group and the deuterium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2981 2962 2962 2905 2880 2868 2201

\* Not used in the force constant determination.

## Reference

- [1] IR. M. Hayashi, K. Ohno, and H. Murata, Bull. Chem. Soc. Jpn., **46**, 2332 (1973).

No. 149

Molecule: 12226-TT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           | 1473                                | 1483                                  | 122-2 (46-)           | 222-2 (27+) | 012-4 (17-) |             |
|              | 1456                                | 1461                                  | 222-2 (63+)           | 012-4 (18+) |             |             |
|              | 1448                                | 1453                                  | 012-4 (50+)           | 122-2 (35-) |             |             |
|              | 1430                                | 1429                                  | 226-2 (84-)           |             |             |             |
|              | 1382                                | 1379                                  | 012-2 (105+)          |             |             |             |
|              | 1360                                | 1355                                  | 122-5 (53+)           | 222-5 (36-) | 1222-S(16+) |             |
|              | 1295                                | 1292                                  | 222-5 (41+)           | 122-5 (27+) | 226-5 (27-) |             |
|              | 1215                                | 1214                                  | 226-5 (72+)           | 222-5 (19+) |             |             |
|              | 1103                                | 1105                                  | 1222-S(25-)           | 012-5 (23+) | 122-5 (10+) | 122-D (9+)  |
|              | 1057                                | 1051                                  | 0122-S(35-)           | 1222-S(27+) | 2226-S(25-) |             |
|              | 1013                                | 1009                                  | 2226-S(49-)           | 0122-S(45+) |             |             |
|              | 893                                 | 898                                   | 012-5 (44-)           | 1222-S(32-) | 122-5 (10-) |             |
|              | 643                                 | 642                                   | 2260-S(79-)           | 222-D (13+) | 226-D (10+) |             |
|              | 393                                 | 401                                   | 122-D (64-)           | 226-D (22+) |             |             |
|              | 279                                 | 279                                   | 222-D (35+)           | 2260-S(24+) | 226-D (17+) |             |
|              | 143                                 | 144                                   | 226-D (54+)           | 222-D (35-) | 122-D (26+) |             |
| a''          | 1465                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1305                                | 1301                                  | 222-6 (44+)           | 122-6 (34-) |             |             |
|              | 1273                                | 1272                                  | 122-6 (32+)           | 226-6 (23-) | 222-6 (16+) |             |
|              | 1198                                | 1204                                  | 226-6 (24+)           | 122-4 (19+) | 012-8 (18-) | 222-4 (12+) |
|              | 1048                                | 1051                                  | 226-6 (44+)           | 222-6 (19+) | 012-8 (10+) | 122-6 (10+) |
|              | 907                                 | 906                                   | 012-8 (31+)           | 226-4 (28+) | 122-6 (23+) | 222-4 (19+) |
|              | 777                                 | 777                                   | 226-4 (41+)           | 122-4 (32-) | 012-8 (19-) |             |
|              | 732                                 | 733                                   | 222-4 (42-)           | 122-4 (35+) | 226-4 (12+) |             |
|              | 224*                                | 232                                   | 0122-T(91-)           |             |             |             |
|              | 115*                                | 129                                   | 1222-T(64+)           | 2226-T(29+) |             |             |
|              |                                     | 101                                   | 2226-T(53+)           | 1222-T(27-) | 222-4 (11+) |             |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

3003 2962 2962 2956 2909 2900 2880 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] I.R.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., 51, 748 (1978).

## No. 150

Molecule: 12226-TG CH3CH2CH2CH2Br (trans-gauche form)  
 Symmetry  $C_1$  Symmetry number  $\sigma = 1$

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1473*                               | 1486                                  | 222-2 (38+)           | 122-2 (36-) | 012-4 (12-) |             |
|              | 1465*                               | 1464                                  | 222-2 (43+)           | 012-4 (24+) | 122-2 (16+) |             |
|              | 1465*                               | 1463                                  | 012-7 (80+)           | 012-8 (14+) |             |             |
|              | 1448*                               | 1452                                  | 012-4 (48+)           | 122-2 (42-) |             |             |
|              | 1437                                | 1434                                  | 226-2 (81+)           | 222-2 (12-) |             |             |
|              | 1382*                               | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1370                                | 1365                                  | 222-5 (45-)           | 122-5 (36+) | 1222-S(16+) |             |
|              | 1305*                               | 1304                                  | 222-6 (33+)           | 122-6 (24-) | 122-5 (12+) | 226-6 ( 6+) |
|              | 1295*                               | 1298                                  | 122-5 (34+)           | 222-5 (24+) | 226-5 (12+) | 122-6 ( 8+) |
|              | 1267                                | 1272                                  | 226-5 (35+)           | 122-6 (32-) | 222-6 ( 8-) |             |
|              | 1220                                | 1219                                  | 226-5 (35+)           | 222-6 (15+) | 012-8 (13-) | 122-4 (12+) |
|              | 1186                                | 1183                                  | 226-6 (38+)           | 222-5 ( 9-) | 012-5 ( 8+) | 226-5 ( 6+) |
|              | 1100                                | 1099                                  | 1222-S(22-)           | 2226-S(14+) | 222-6 ( 9-) | 012-5 ( 8+) |
|              | 1057*                               | 1063                                  | 226-6 (29-)           | 0122-S(19-) | 012-5 (16+) | 2226-S( 8-) |
|              | 1048*                               | 1045                                  | 0122-S(27+)           | 1222-S(18-) | 222-6 (12+) | 226-6 (11-) |
|              | 996                                 | 1003                                  | 2226-S(40+)           | 0122-S(38-) |             |             |
|              | 915                                 | 917                                   | 226-4 (31+)           | 012-5 (23-) | 012-8 ( 9-) | 122-6 ( 7-) |
|              | 868                                 | 873                                   | 222-4 (29+)           | 012-8 (25+) | 122-6 (16+) | 012-5 (11-) |
|              | 799                                 | 797                                   | 226-4 (43-)           | 1222-S(27-) | 012-5 ( 7-) |             |
|              | 742                                 | 743                                   | 122-4 (58+)           | 222-4 (20-) | 012-8 (15+) |             |
|              | 562                                 | 563                                   | 2260-S(98+)           | 226-D (15-) |             |             |
|              | 463                                 | 459                                   | 222-D (29-)           | 122-D (25-) | 226-D (11+) | 0122-S( 6-) |
|              | 279*                                | 280                                   | 122-D (50+)           | 226-D (30+) | 222-D (14-) |             |
|              | 267                                 | 257                                   | 222-D (26-)           | 0122-T(23-) | 2226-T(23+) | 226-D (13-) |
|              | 224                                 | 218                                   | 0122-T(67+)           | 226-D (12-) |             |             |
|              |                                     | 99                                    | 2226-T(52+)           | 1222-T(33+) |             |             |
|              |                                     | 80                                    | 1222-T(46+)           | 226-D (23-) | 2226-T(13-) | 222-4 (12-) |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$

3004 2962 2962 2956 2909 2901 2880 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 151

Molecule: 12226-GT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (gauche-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1473*                               | 1483                                  | 122-2 (55+)           | 222-2 (27+) |             |             |
|              | 1465*                               | 1469                                  | 222-2 (50-)           | 012-4 (24+) |             |             |
|              | 1465*                               | 1463                                  | 012-7 (74+)           | 012-8 (13+) |             |             |
|              | 1448*                               | 1452                                  | 012-4 (49-)           | 122-2 (30+) | 222-2 (12-) |             |
|              | 1437*                               | 1432                                  | 226-2 (93+)           |             |             |             |
|              | 1382*                               | 1380                                  | 012-2 (105+)          |             |             |             |
|              | 1347                                | 1348                                  | 122-5 (61+)           | 222-5 (19+) |             |             |
|              | 1340*                               | 1331                                  | 222-5 (53-)           | 122-5 (13+) | 1222-S(12+) | 122-6 (11+) |
|              | 1288*                               | 1282                                  | 222-6 (45+)           | 226-6 (21-) | 122-6 (4+)  | 226-4 (3-)  |
|              | 1267*                               | 1265                                  | 122-6 (50+)           | 012-8 (9-)  | 226-5 (9-)  | 012-7 (7+)  |
|              | 1220*                               | 1224                                  | 226-5 (78+)           |             |             |             |
|              | 1186*                               | 1186                                  | 226-6 (25-)           | 222-6 (14-) | 012-5 (13-) | 222-4 (11-) |
|              | 1100*                               | 1093                                  | 2226-S(25+)           | 222-5 (15-) | 012-8 (12-) | 122-4 (11+) |
|              | 1080                                | 1080                                  | 1222-S(35-)           | 0122-S(18+) | 226-6 (13-) | 122-5 (8+)  |
|              | 1048*                               | 1047                                  | 0122-S(32-)           | 226-6 (28-) | 012-5 (11+) | 222-6 (11-) |
|              | 970*                                | 964                                   | 2226-S(49+)           | 012-5 (14-) | 012-8 (12+) | 122-6 (12+) |
|              | 907*                                | 913                                   | 226-4 (29+)           | 222-4 (21+) | 012-5 (13-) | 012-8 (10-) |
|              | 868*                                | 880                                   | 0122-S(33+)           | 1222-S(31+) | 012-5 (14+) |             |
|              | 777*                                | 784                                   | 122-4 (40-)           | 012-8 (25-) | 226-4 (18-) |             |
|              | 740*                                | 746                                   | 222-4 (35-)           | 226-4 (32+) | 122-4 (14-) |             |
|              | 643*                                | 642                                   | 2260-S(72-)           | 222-D (16+) | 226-D (13+) |             |
|              | 417                                 | 417                                   | 122-D (64+)           | 2260-S(15-) | 222-D (13-) |             |
|              | 279*                                | 281                                   | 0122-T(30-)           | 222-D (25-) | 122-D (13-) | 2260-S(12-) |
|              | 238                                 | 237                                   | 226-D (63-)           | 0122-T(18+) |             |             |
|              |                                     | 183                                   | 0122-T(47+)           | 222-D (25-) | 226-D (23+) |             |
|              |                                     | 113                                   | 1222-T(77-)           |             |             |             |
|              |                                     | 89                                    | 2226-T(78-)           |             |             |             |

Calculated frequencies higher than 2000  $\text{cm}^{-1}$ 

3003 2962 2962 2956 2907 2903 2880 2870 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 152

Molecule: 12226-GG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1473*                               | 1486                                  | 222-2 (44+)           | 122-2 (39+) |             |             |
|              | 1465*                               | 1472                                  | 222-2 (32-)           | 012-4 (27+) | 122-2 (23+) |             |
|              | 1465*                               | 1463                                  | 012-7 (78+)           | 012-8 (14+) |             |             |
|              | 1448*                               | 1453                                  | 012-4 (51+)           | 122-2 (30-) |             |             |
|              | 1437*                               | 1434                                  | 226-2 (80+)           | 222-2 (12-) |             |             |
|              | 1382*                               | 1380                                  | 012-2 (102+)          |             |             |             |
|              | 1355                                | 1356                                  | 222-5 (55+)           | 122-5 (20+) |             |             |
|              | 1340                                | 1341                                  | 122-5 (54-)           | 1222-S(16-) | 222-5 (13+) |             |
|              | 1288                                | 1286                                  | 222-6 (38-)           | 226-5 (25+) | 226-6 (11-) |             |
|              | 1267*                               | 1266                                  | 122-6 (52+)           | 226-5 (19+) |             |             |
|              | 1215*                               | 1218                                  | 226-5 (41+)           | 222-6 (14+) | 122-4 ( 8-) | 012-8 ( 8+) |
|              | 1160                                | 1158                                  | 226-6 (43+)           | 012-5 (13-) | 222-6 (10-) | 0122-S( 6+) |
|              |                                     | 1116                                  | 1222-S(27+)           | 2226-S(17-) | 222-6 ( 9+) | 122-5 ( 7-) |
|              | 1064                                | 1073                                  | 012-8 (20-)           | 122-4 (17+) | 222-5 (15-) | 122-6 (14-) |
|              | 1048*                               | 1039                                  | 0122-S(40-)           | 226-6 (20+) | 222-6 (12-) | 1222-S(10+) |
|              | 970                                 | 966                                   | 2226-S(38-)           | 012-5 (28+) | 122-5 (14+) |             |
|              | 915*                                | 912                                   | 226-4 (36+)           | 0122-S(34-) | 222-4 (12-) |             |
|              | 868*                                | 874                                   | 012-8 (25+)           | 222-4 (24-) | 122-6 (13+) | 012-5 (11+) |
|              | 799*                                | 800                                   | 1222-S(35+)           | 226-4 (20+) | 2226-S( 9+) | 122-4 ( 7-) |
|              | 740*                                | 747                                   | 122-4 (48+)           | 226-4 (18+) | 012-8 (17+) | 222-4 (14+) |
|              | 562*                                | 567                                   | 2260-S(93-)           | 226-D (16+) |             |             |
|              | 448                                 | 449                                   | 222-D (42-)           | 122-D (35+) |             |             |
|              | 353                                 | 355                                   | 122-D (34+)           | 226-D (24-) | 1222-T(10-) | 222-D (10+) |
|              | 224*                                | 222                                   | 0122-T(56+)           | 226-D (30+) |             |             |
|              |                                     | 206                                   | 0122-T(27-)           | 222-D (24+) | 122-D (18+) | 2226-T(13-) |
|              |                                     | 126                                   | 1222-T(40+)           | 226-D (22-) | 2226-T(19-) | 222-4 (12-) |
|              |                                     | 57                                    | 2226-T(47+)           | 1222-T(40+) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3004 2962 2962 2956 2907 2903 2880 2870 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).



## No. 153

Molecule: 122226-TTT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (trans-trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474                                | 1484                                  | 122-2 (39-)           | 222-2 (34+) | 012-4 (15-) |             |
|              | 1465                                | 1473                                  | 222-2 (63+)           | 122-2 (15-) | 222-2 (14-) |             |
|              | 1454                                | 1457                                  | 012-4 (44+)           | 222-2 (28+) | 222-2 (13+) |             |
|              | 1437                                | 1449                                  | 122-2 (40+)           | 012-4 (23-) | 222-2 (14+) | 222-2 (12+) |
|              | 1429                                | 1429                                  | 226-2 (82+)           |             |             |             |
|              | 1380                                | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1365                                | 1365                                  | 222-5 (44-)           | 122-5 (29+) | 222-5 (17+) | 1222-S(15+) |
|              | 1337                                | 1327                                  | 222-5 (46+)           | 122-5 (39-) |             |             |
|              | 1273                                | 1268                                  | 222-5 (37+)           | 226-5 (34-) | 122-5 (13+) | 222-5 (11+) |
|              | 1210                                | 1207                                  | 226-5 (59+)           | 222-5 (22+) | 222-5 (11+) |             |
|              | 1108                                | 1112                                  | 012-5 (20+)           | 1222-S(16-) | 222-D (8+)  | 122-D (8+)  |
|              | 1053                                | 1059                                  | 2222-S(36-)           | 1222-S(28+) | 0122-S(19-) |             |
|              | 1037                                | 1038                                  | 2226-S(41+)           | 2222-S(21-) | 0122-S(21+) |             |
|              | 999                                 | 1000                                  | 0122-S(37+)           | 2226-S(31-) | 2222-S(15-) |             |
|              | 893                                 | 899                                   | 012-5 (40-)           | 1222-S(30-) | 0122-S(9-)  |             |
|              | 641                                 | 642                                   | 2260-S(78-)           | 222-D (14+) | 226-D (12+) |             |
|              | 437                                 | 446                                   | 122-D (33-)           | 222-D (24-) | 226-D (15+) |             |
|              | 334                                 | 341                                   | 222-D (26-)           | 122-D (25+) | 222-D (24-) | 2260-S(16-) |
|              | 217                                 | 214                                   | 226-D (35+)           | 122-D (22+) | 2260-S(9+)  | 2222-S(9+)  |
|              | 115(s)                              | 110                                   | 222-D (38+)           | 222-D (38-) | 226-D (34-) | 122-D (11+) |
| a''          | 1459                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1303                                | 1304                                  | 222-6 (44+)           | 222-6 (22-) | 122-6 (16-) |             |
|              | 1298                                | 1292                                  | 222-6 (36+)           | 122-6 (33-) | 226-6 (9-)  |             |
|              | 1254                                | 1254                                  | 226-6 (24+)           | 122-6 (19-) | 222-6 (19-) | 222-4 (9+)  |
|              | 1188(s)                             | 1195                                  | 122-4 (18-)           | 012-8 (16+) | 226-6 (16-) | 222-4 (14-) |
|              | 1053                                | 1058                                  | 226-6 (43+)           | 222-6 (20+) | 222-6 (13+) |             |
|              | 947                                 | 944                                   | 012-8 (23+)           | 122-6 (21+) | 222-4 (19+) | 226-4 (18+) |
|              | 828                                 | 825                                   | 226-4 (31+)           | 222-4 (26-) | 012-8 (22-) | 122-4 (12-) |
|              | 753(s)                              | 751                                   | 222-4 (31-)           | 226-4 (30+) | 122-4 (27+) |             |
|              | 729                                 | 729                                   | 222-4 (37-)           | 122-4 (29+) | 222-4 (20+) |             |
|              | 244(s)                              | 231                                   | 0122-T(92+)           |             |             |             |
|              |                                     | 154                                   | 1222-T(47+)           | 2226-T(45-) |             |             |
|              |                                     | 119                                   | 2222-T(76+)           |             |             |             |
|              |                                     | 62                                    | 2226-T(36+)           | 1222-T(35+) | 2222-T(10-) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3003 | 2962 | 2962 | 2956 | 2911 | 2905 | 2899 | 2880 | 2875 | 2869 |
| 2864 |      |      |      |      |      |      |      |      |      |

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 154

Molecule: 122226-TTG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (trans-trans-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474                                | 1484                                  | 222-2 (37+)           | 122-2 (31-) | 012-4 (13-) | 222-2 (10-) |
|              | 1465                                | 1478                                  | 222-2 (59+)           | 122-2 (21-) |             |             |
|              | 1459                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1454                                | 1457                                  | 012-4 (47+)           | 222-2 (35+) |             |             |
|              | 1437                                | 1449                                  | 122-2 (41+)           | 222-2 (22+) | 012-4 (20-) |             |
|              | 1429                                | 1434                                  | 226-2 (79+)           | 222-2 (13-) |             |             |
|              | 1380                                | 1380                                  | 012-2 (101+)          |             |             |             |
|              | 1373                                | 1371                                  | 222-5 (37-)           | 222-5 (30+) | 122-5 (17+) | 2222-S(14-) |
|              | 1337                                | 1337                                  | 122-5 (47-)           | 222-5 (34+) |             |             |
|              | 1303                                | 1305                                  | 222-6 (41+)           | 222-6 (24-) | 122-6 (13-) |             |
|              | 1298                                | 1292                                  | 122-6 (37+)           | 222-6 (25-) | 226-5 (12+) |             |
|              | 1273                                | 1268                                  | 222-5 (50-)           | 122-5 (16-) | 226-5 (13-) |             |
|              | 1254                                | 1258                                  | 226-5 (32+)           | 122-6 (17-) | 222-6 (17-) | 222-4 ( 7+) |
|              | 1210                                | 1206                                  | 226-5 (22+)           | 122-4 (14+) | 012-8 (13-) | 222-6 (13+) |
|              | 1178                                | 1177                                  | 226-6 (34+)           | 222-5 ( 8-) | 012-5 ( 6+) | 226-5 ( 6+) |
|              | 1103                                | 1103                                  | 012-5 (13+)           | 1222-S(11-) | 226-5 ( 8-) | 2222-S( 8-) |
|              | 1078                                | 1087                                  | 226-6 (15+)           | 1222-S(14+) | 2222-S(14-) | 2226-S(12+) |
|              | 1053                                | 1050                                  | 0122-S(32-)           | 1222-S(15+) | 2222-S(15-) | 226-6 (15-) |
|              | 1037                                | 1038                                  | 0122-S(29+)           | 2226-S(20+) | 2222-S( 9-) | 222-6 ( 8+) |
|              | 975                                 | 976                                   | 2226-S(26+)           | 0122-S(16-) | 2222-S(15+) | 226-4 (13-) |
|              | 921                                 | 926                                   | 222-4 (23-)           | 012-8 (23-) | 122-6 (19-) | 222-6 (11-) |
|              | 910                                 | 912                                   | 012-5 (35-)           | 1222-S(23-) | 0122-S(10-) | 122-5 ( 8-) |
|              | 828                                 | 827                                   | 226-4 (39+)           | 222-4 (13-) | 012-8 (10+) | 2222-S( 9+) |
|              | 782                                 | 783                                   | 222-4 (25-)           | 122-4 (21+) | 226-4 (18-) | 012-8 (14+) |
|              | 729                                 | 731                                   | 122-4 (42-)           | 222-4 (40+) |             |             |
|              | 562                                 | 563                                   | 2260-S(98-)           | 226-D (15+) |             |             |
|              | 437                                 | 438                                   | 222-D (37+)           | 226-D (15-) | 222-D (13+) | 1222-S( 6+) |
|              | 398                                 | 400                                   | 122-D (52+)           | 222-D (14+) | 222-D ( 8-) |             |
|              | 253                                 | 260                                   | 226-D (45+)           | 2226-T(17-) | 2222-T( 9+) |             |
|              |                                     | 228                                   | 0122-T(89-)           |             |             |             |
|              |                                     | 193                                   | 222-D (46+)           | 122-D (29-) | 222-D (19-) | 2226-T(15+) |
|              |                                     | 123                                   | 1222-T(57-)           | 2226-T(10+) | 222-D ( 8+) |             |
|              |                                     | 83                                    | 2222-T(61+)           | 2226-T(16+) | 1222-T(13+) |             |
|              |                                     | 59                                    | 2226-T(30+)           | 1222-T(14+) | 2222-T(14-) | 226-D (14+) |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3004 2963 2962 2956 2911 2905 2899 2880 2875 2869  
2864

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

No. 155

Molecule: 122226-TGT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (trans-gauche-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474*                               | 1488                                  | 222-2 (39+)           | 122-2 (27-) | 222-2 (16+) |             |
|              | 1465*                               | 1472                                  | 222-2 (50+)           | 122-2 (24+) | 012-4 (15+) |             |
|              | 1459*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1454*                               | 1458                                  | 222-2 (46+)           | 222-2 (25-) | 012-4 (21+) |             |
|              | 1437*                               | 1452                                  | 122-2 (43+)           | 012-4 (41-) |             |             |
|              | 1429*                               | 1432                                  | 226-2 (92+)           |             |             |             |
|              | 1380*                               | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1365*                               | 1365                                  | 222-5 (44-)           | 122-5 (36+) | 1222-S(16+) |             |
|              | 1337*                               | 1335                                  | 222-5 (69+)           | 2226-S(10+) |             |             |
|              | 1303*                               | 1302                                  | 122-5 (30+)           | 222-5 (17+) | 222-6 (15+) | 222-6 (14+) |
|              | 1298*                               | 1294                                  | 122-6 (44-)           | 222-6 (12+) | 122-5 (9-)  | 222-5 (8-)  |
|              | 1273*                               | 1278                                  | 222-6 (33-)           | 226-6 (27+) | 222-5 (10+) | 222-4 (5+)  |
|              | 1254*                               | 1244                                  | 226-5 (37-)           | 222-6 (25+) | 122-6 (11+) |             |
|              | 1218                                | 1217                                  | 226-5 (51+)           | 012-8 (9-)  | 222-5 (9+)  | 122-4 (9+)  |
|              | 1178*                               | 1176                                  | 226-6 (22-)           | 222-6 (13-) | 012-5 (9-)  | 222-4 (8-)  |
|              | 1108*                               | 1104                                  | 222-5 (12+)           | 222-4 (10-) | 1222-S(9+)  | 2226-S(9-)  |
|              | 1078*                               | 1078                                  | 2222-S(34-)           | 1222-S(22+) | 2226-S(18+) |             |
|              | 1073                                | 1068                                  | 226-6 (35-)           | 222-6 (17-) | 012-5 (12+) | 0122-S(7-)  |
|              | 1023                                | 1023                                  | 0122-S(68+)           | 2222-S(14-) |             |             |
|              | 975*                                | 971                                   | 2226-S(32-)           | 222-6 (10-) | 012-8 (9-)  | 122-6 (9-)  |
|              | 947*                                | 953                                   | 222-4 (23+)           | 226-4 (20+) | 012-5 (15-) | 012-8 (8-)  |
|              | 847                                 | 850                                   | 1222-S(29-)           | 012-5 (21-) | 2222-S(8-)  | 226-4 (7-)  |
|              | 847                                 | 847                                   | 222-4 (27-)           | 012-8 (21-) | 226-4 (15-) | 122-6 (10-) |
|              | 759                                 | 757                                   | 226-4 (33-)           | 222-4 (30+) | 122-4 (18+) |             |
|              | 742                                 | 735                                   | 122-4 (41+)           | 222-4 (19-) | 222-4 (12-) |             |
|              | 641*                                | 646                                   | 2260-S(68-)           | 222-D (17+) | 226-D (14+) |             |
|              | 469                                 | 471                                   | 222-D (27-)           | 122-D (21-) | 2260-S(17+) | 222-D (7+)  |
|              | 287                                 | 295                                   | 122-D (54-)           | 222-D (22-) | 222-D (17+) |             |
|              | 253                                 | 260                                   | 222-D (22-)           | 222-D (17-) | 2222-T(15+) | 0122-T(15-) |
|              |                                     | 224                                   | 0122-T(73+)           |             |             |             |
|              |                                     | 214                                   | 226-D (69+)           | 122-D (7+)  |             |             |
|              |                                     | 108                                   | 2222-T(67-)           | 1222-T(13-) | 2226-T(12-) |             |
|              |                                     | 78                                    | 1222-T(58+)           | 222-D (16-) |             |             |
|              |                                     | 71                                    | 2226-T(64+)           | 222-D (12-) | 222-4 (10+) |             |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3004 | 2962 | 2962 | 2956 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 156

Molecule: 122226-TGG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (trans-gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474*                               | 1490                                  | 222-2 (36+)           | 222-2 (29+) | 122-2 (18-) |             |
|              | 1465*                               | 1476                                  | 222-2 (40+)           | 122-2 (31+) | 012-4 (14+) |             |
|              | 1459*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1454*                               | 1459                                  | 222-2 (50+)           | 012-4 (24+) | 222-2 (13-) |             |
|              | 1437*                               | 1451                                  | 122-2 (44+)           | 012-4 (40-) |             |             |
|              | 1429*                               | 1434                                  | 226-2 (81+)           | 222-2 (12-) |             |             |
|              | 1380*                               | 1380                                  | 012-2 (102+)          |             |             |             |
|              | 1365*                               | 1366                                  | 222-5 (41-)           | 122-5 (29+) | 1222-S(14+) | 222-5 (13-) |
|              | 1355                                | 1352                                  | 222-5 (56+)           | 2222-S(12-) | 122-5 (11+) |             |
|              | 1303*                               | 1302                                  | 122-5 (28+)           | 222-6 (16+) | 222-5 (16+) | 222-6 (15+) |
|              | 1298*                               | 1295                                  | 122-6 (45-)           | 222-6 (13+) | 122-5 (8-)  | 222-5 (7-)  |
|              | 1273*                               | 1281                                  | 226-5 (34+)           | 222-6 (21-) | 222-5 (11+) | 226-6 (11-) |
|              | 1254*                               | 1244                                  | 222-6 (28+)           | 226-5 (23+) | 122-6 (13+) | 012-8 (8-)  |
|              | 1210*                               | 1207                                  | 226-5 (28+)           | 122-4 (11-) | 222-6 (11+) | 012-8 (11+) |
|              | 1162                                | 1159                                  | 226-6 (33+)           | 1222-S(11+) | 222-6 (10-) | 012-5 (10-) |
|              | 1108*                               | 1108                                  | 2222-S(30-)           | 2226-S(20+) | 222-6 (7-)  | 222-4 (6+)  |
|              | 1078*                               | 1083                                  | 222-5 (16+)           | 222-6 (15+) | 226-6 (14-) | 222-4 (11-) |
|              | 1073                                | 1067                                  | 1222-S(23-)           | 226-6 (20+) | 222-6 (17-) | 012-5 (10+) |
|              | 1028                                | 1028                                  | 0122-S(74-)           |             |             |             |
|              | 967                                 | 967                                   | 012-5 (18+)           | 226-4 (16+) | 222-4 (14-) | 2226-S(11-) |
|              | 921*                                | 925                                   | 012-8 (20-)           | 222-4 (19+) | 122-6 (18-) | 2226-S(13-) |
|              | 875                                 | 874                                   | 226-4 (35-)           | 1222-S(21+) | 2226-S(8-)  | 012-5 (8+)  |
|              | 843                                 | 844                                   | 2226-S(17-)           | 222-4 (15+) | 012-8 (13+) | 2222-S(13-) |
|              | 780*                                | 783                                   | 226-4 (22+)           | 122-4 (20+) | 222-4 (20+) | 012-8 (13+) |
|              | 729*                                | 730                                   | 122-4 (43-)           | 222-4 (32+) |             |             |
|              | 562*                                | 568                                   | 2260-S(90-)           | 226-D (16+) |             |             |
|              | 469                                 | 475                                   | 222-D (30+)           | 222-D (23-) | 2260-S(11-) | 122-D (11-) |
|              | 366                                 | 365                                   | 222-D (24+)           | 226-D (22-) | 122-D (18+) | 2222-T(6-)  |
|              | 287                                 | 300                                   | 122-D (49+)           | 222-D (19-) | 2226-T(14-) | 226-D (13+) |
|              |                                     | 231                                   | 0122-T(89-)           |             |             |             |
|              |                                     | 188                                   | 226-D (31+)           | 222-D (30+) | 222-D (18+) |             |
|              |                                     | 131                                   | 2226-T(26+)           | 1222-T(19+) | 2222-T(18-) | 226-D (15+) |
|              |                                     | 89                                    | 1222-T(54-)           | 2222-T(33-) |             |             |
|              |                                     | 43                                    | 2226-T(44-)           | 2222-T(27-) | 1222-T(10+) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3004 | 2963 | 2962 | 2956 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

No. 157

Molecule: 122226-GTG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (gauche-trans-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474*                               | 1486                                  | 222-2 (38+)           | 122-2 (30+) | 222-2 (21-) |             |
|              | 1465*                               | 1477                                  | 222-2 (33+)           | 122-2 (33+) | 012-4 (17+) |             |
|              | 1459*                               | 1465                                  | 012-7 (43+)           | 222-2 (17+) | 222-2 (15+) |             |
|              | 1454*                               | 1461                                  | 012-7 (36+)           | 222-2 (20-) | 012-4 (15+) | 222-2 (13-) |
|              | 1437*                               | 1452                                  | 012-4 (42-)           | 122-2 (29+) | 222-2 (17-) |             |
|              | 1429*                               | 1434                                  | 226-2 (81+)           | 222-2 (11-) |             |             |
|              | 1380*                               | 1381                                  | 012-2 (95+)           |             |             |             |
|              | 1365*                               | 1368                                  | 222-5 (37-)           | 222-5 (35+) | 2222-S(13+) | 012-2 (10+) |
|              | 1345                                | 1345                                  | 122-5 (71+)           | 1222-S(10+) |             |             |
|              | 1303*                               | 1307                                  | 222-5 (21+)           | 222-5 (19+) | 222-6 (14-) | 222-6 (14+) |
|              | 1298*                               | 1297                                  | 222-6 (34+)           | 226-5 (20-) | 222-5 (10-) | 222-5 (9-)  |
|              | 1273*                               | 1268                                  | 122-6 (24+)           | 222-6 (15+) | 222-5 (12+) | 226-6 (9+)  |
|              | 1254*                               | 1258                                  | 226-5 (34+)           | 122-6 (23+) | 222-6 (14-) |             |
|              | 1210*                               | 1203                                  | 226-5 (28+)           | 222-6 (10+) | 222-6 (10+) | 226-6 (8+)  |
|              | 1162                                | 1161                                  | 226-6 (32+)           | 012-5 (12-) | 222-5 (8-)  | 222-4 (7-)  |
|              | 1099*                               | 1100                                  | 2222-S(13+)           | 222-6 (11+) | 122-4 (10+) | 012-8 (9-)  |
|              | 1078*                               | 1086                                  | 1222-S(31-)           | 0122-S(20+) | 2222-S(12+) | 122-5 (8+)  |
|              | 1073                                | 1067                                  | 226-6 (28+)           | 012-5 (10+) | 2226-S(7+)  | 222-6 (7-)  |
|              | 1023                                | 1021                                  | 2226-S(37+)           | 0122-S(20+) | 2222-S(7-)  | 1222-S(6-)  |
|              | 967                                 | 969                                   | 012-5 (17-)           | 226-4 (17-) | 2222-S(15+) | 222-4 (10+) |
|              | 921*                                | 924                                   | 012-8 (19-)           | 222-4 (17+) | 122-6 (15-) | 2226-S(11-) |
|              | 906*                                | 897                                   | 0122-S(27+)           | 1222-S(22+) | 012-5 (22+) |             |
|              | 810                                 | 811                                   | 226-4 (46-)           | 2222-S(11-) | 222-4 (11-) | 1222-S(8-)  |
|              | 780*                                | 791                                   | 122-4 (27+)           | 222-4 (22+) | 222-4 (19-) | 012-8 (17+) |
|              | 742                                 | 741                                   | 122-4 (30+)           | 222-4 (21+) | 222-4 (12-) | 2222-S(11-) |
|              | 562*                                | 563                                   | 2260-S(97+)           | 226-D (15-) |             |             |
|              | 487                                 | 485                                   | 222-D (24-)           | 122-D (23+) | 222-D (16-) | 2260-S(6+)  |
|              | 366                                 | 357                                   | 122-D (52+)           | 222-D (22+) | 226-D (16-) |             |
|              | 268*                                | 285                                   | 0122-T(32+)           | 222-D (31+) | 222-D (12-) |             |
|              | 249                                 | 251                                   | 226-D (30+)           | 2226-T(25-) | 222-D (16+) |             |
|              |                                     | 194                                   | 0122-T(63+)           | 222-D (22-) |             |             |
|              |                                     | 122                                   | 1222-T(50+)           | 2226-T(12-) | 222-D (10+) |             |
|              |                                     | 80                                    | 2226-T(48+)           | 1222-T(21+) | 226-D (11+) |             |
|              |                                     | 49                                    | 2222-T(72-)           | 226-D (10+) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3004 | 2963 | 2962 | 2956 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] I.R.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, *Bull. Chem. Soc. Jpn.*, **52**, 2512 (1979).

## No. 158

Molecule: 122226-GTG' CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (gauche-trans-gauche' form)Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474*                               | 1486                                  | 222-2 (38+)           | 122-2 (30+) | 222-2 (21-) |             |
|              | 1465*                               | 1477                                  | 222-2 (33+)           | 122-2 (33+) | 012-4 (17+) |             |
|              | 1459*                               | 1465                                  | 012-7 (44+)           | 222-2 (16+) | 222-2 (15+) |             |
|              | 1454*                               | 1461                                  | 012-7 (35+)           | 222-2 (20-) | 012-4 (16+) | 222-2 (13-) |
|              | 1437*                               | 1452                                  | 012-4 (42+)           | 122-2 (29-) | 222-2 (17+) |             |
|              | 1429*                               | 1434                                  | 226-2 (81+)           | 222-2 (11-) |             |             |
|              | 1380*                               | 1381                                  | 012-2 (94+)           |             |             |             |
|              | 1365*                               | 1368                                  | 222-5 (37-)           | 222-5 (34+) | 2222-S(13+) | 012-2 (11+) |
|              | 1345                                | 1344                                  | 122-5 (71+)           | 1222-S(11+) |             |             |
|              | 1303*                               | 1305                                  | 222-5 (32+)           | 222-5 (29+) | 122-6 (17-) |             |
|              | 1298*                               | 1301                                  | 222-6 (46+)           | 222-6 (21-) | 226-5 (10+) |             |
|              | 1273*                               | 1266                                  | 226-5 (33+)           | 122-6 (21+) | 222-6 (12+) | 222-5 ( 8+) |
|              | 1254*                               | 1258                                  | 122-6 (26+)           | 226-5 (18-) | 222-6 (15-) | 012-8 ( 7-) |
|              | 1178*                               | 1189                                  | 226-5 (26-)           | 222-6 (15+) | 222-6 (15+) | 012-5 ( 9+) |
|              | 1178*                               | 1181                                  | 226-6 (31+)           | 122-4 (11+) | 012-8 ( 8-) | 222-4 ( 6-) |
|              | 1108*                               | 1106                                  | 2222-S(24+)           | 1222-S(11-) | 2226-S( 9-) | 222-6 ( 8-) |
|              | 1073                                | 1074                                  | 0122-S(21+)           | 226-6 (19+) | 1222-S(12-) | 012-8 ( 9+) |
|              | 1053*                               | 1060                                  | 0122-S(24-)           | 226-6 (16+) | 1222-S(12+) | 222-6 (10-) |
|              | 1031                                | 1031                                  | 2226-S(40-)           | 2222-S(11+) | 012-5 (11-) | 122-5 ( 7-) |
|              | 957                                 | 956                                   | 226-4 (19+)           | 012-8 (19+) | 122-6 (17+) | 2222-S(17+) |
|              | 930                                 | 935                                   | 222-4 (22-)           | 012-5 (20+) | 2226-S(13-) | 122-5 (12+) |
|              | 906*                                | 894                                   | 0122-S(36+)           | 1222-S(22+) | 012-5 (15+) |             |
|              | 828*                                | 831                                   | 226-4 (32-)           | 012-8 (18+) | 222-4 (14-) | 122-4 (12+) |
|              | 766                                 | 767                                   | 226-4 (23+)           | 222-4 (19+) | 2222-S(15-) | 122-4 (12+) |
|              | 742                                 | 747                                   | 122-4 (37+)           | 222-4 (26+) | 012-8 (15+) | 222-4 (11-) |
|              | 562*                                | 563                                   | 2260-S(98-)           | 226-D (15+) |             |             |
|              | 469                                 | 478                                   | 222-D (26+)           | 122-D (22-) | 222-D (18+) | 226-D ( 5-) |
|              | 366                                 | 376                                   | 122-D (49-)           | 226-D (19+) | 222-D (16-) |             |
|              | 268                                 | 280                                   | 0122-T(33-)           | 222-D (28-) | 222-D (16+) | 1222-T(11+) |
|              | 249                                 | 248                                   | 226-D (33+)           | 2226-T(30+) | 222-D (17+) |             |
|              |                                     | 193                                   | 0122-T(61+)           | 222-D (24-) |             |             |
|              |                                     | 116                                   | 1222-T(46-)           | 2226-T(12+) | 226-D (11-) | 122-D ( 9-) |
|              |                                     | 72                                    | 2226-T(34+)           | 226-D (16-) | 2222-T(15-) | 222-4 (11+) |
|              |                                     | 53                                    | 2222-T(59+)           | 1222-T(18+) | 2226-T(14+) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 3004 | 2963 | 2962 | 2956 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 159

Molecule: 62226-TT BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (trans-trans form)Symmetry C<sub>2v</sub> Symmetry number  $\sigma = 2$ 

| Sym. species   | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |
|----------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|
| a <sub>1</sub> | 1465*                               | 1467                                  | 222-2 (93+)           |             |             |
|                | 1417*                               | 1422                                  | 226-2 (46+)           | 622-2 (46+) |             |
|                | 1240*                               | 1243                                  | 622-5 (52-)           | 226-5 (52+) |             |
|                | 1031                                | 1033                                  | 6222-S(35-)           | 2226-S(35-) | 222-D (12+) |
|                | 701                                 | 696                                   | 0622-S(34-)           | 2260-S(34-) | 222-D (22+) |
|                | 230                                 | 231                                   | 222-D (46+)           | 2260-S(20+) | 0622-S(20+) |
|                | 105                                 | 97                                    | 226-D (43+)           | 622-D (43+) | 222-D (22-) |
|                | 1294*                               | 1294                                  | 222-6 (62+)           | 622-6 (10-) | 226-6 (10-) |
|                | 1073*                               | 1089                                  | 226-6 (40+)           | 622-6 (40+) | 222-6 (25+) |
|                |                                     | 804                                   | 226-4 (46+)           | 622-4 (46-) | 222-6 (16+) |
| a <sub>2</sub> |                                     | 138                                   | 2226-T(47+)           | 6222-T(47+) |             |
|                | 1450                                | 1440                                  | 622-2 (47-)           | 226-2 (47+) |             |
|                | 1327                                | 1319                                  | 222-5 (74+)           | 622-5 (14-) | 226-5 (14-) |
|                | 1193                                | 1185                                  | 226-5 (40+)           | 622-5 (40+) | 222-5 (31+) |
|                | 1031                                | 1025                                  | 2226-S(48+)           | 6222-S(48-) |             |
|                | 591*                                | 579                                   | 2260-S(54+)           | 0622-S(54-) |             |
|                | 324*                                | 333                                   | 622-D (47-)           | 226-D (47+) |             |
| b <sub>1</sub> | 1232*                               | 1247                                  | 622-6 (33+)           | 226-6 (33-) | 222-4 (15-) |
|                |                                     | 982                                   | 222-4 (25+)           | 226-4 (22-) | 622-4 (22+) |
|                |                                     | 743                                   | 222-4 (51-)           | 622-4 (20+) | 226-4 (20+) |
|                | 105*                                | 100                                   | 6222-T(40+)           | 2226-T(40-) | 222-4 (12-) |
|                |                                     |                                       |                       |             | 226-6 (15-) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3004 3003 2956 2955 2905 2869

\* Not used in the force constant determination.

## References

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torggrimsen, J. Mol. Struct., **15**, 61 (1973).
- [2] IR.R. J. E. Gustavsen, P. Klaboe, and R. Stølevik, J. Mol. Struct., **50**, 285 (1978).

## No. 160

Molecule: 62226-TG BrCH2CH2CH2Br (trans-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1465*                               | 1474                                  | 222-2 (83+)           | 226-2 (10+) |             |             |
|              | 1440                                | 1434                                  | 226-2 (83+)           | 222-2 (10-) |             |             |
|              | 1417*                               | 1432                                  | 622-2 (92+)           |             |             |             |
|              | 1342                                | 1339                                  | 222-5 (73+)           | 6222-S(10-) |             |             |
|              | 1294*                               | 1295                                  | 222-6 (53-)           | 226-5 (18+) |             |             |
|              | 1240*                               | 1252                                  | 226-5 (48+)           | 622-6 (25-) | 222-4 (11+) |             |
|              | 1232*                               | 1233                                  | 622-5 (80+)           | 226-6 (11+) |             |             |
|              | 1168                                | 1165                                  | 226-6 (27+)           | 226-5 (22+) | 222-5 (19-) | 622-5 (14-) |
|              | 1106*                               | 1108                                  | 222-6 (27-)           | 622-6 (26-) | 226-6 (24+) | 6222-S(10-) |
|              | 1053                                | 1046                                  | 2226-S(37+)           | 6222-S(31-) | 622-6 (11+) |             |
|              | 999                                 | 997                                   | 6222-S(20+)           | 226-4 (19-) | 226-6 (16+) | 2226-S(13+) |
|              | 944*                                | 954                                   | 222-4 (25+)           | 622-4 (23+) | 2226-S(23-) |             |
|              | 834                                 | 833                                   | 226-4 (55-)           | 6222-S(20-) |             |             |
|              | 763*                                | 764                                   | 622-4 (50+)           | 222-4 (32-) |             |             |
|              | 651                                 | 643                                   | 0622-S(70-)           | 222-D (17+) | 622-D (13+) |             |
|              | 564                                 | 563                                   | 2260-S(99-)           | 226-D (13+) |             |             |
|              | 376                                 | 376                                   | 226-D (34+)           | 222-D (25-) | 0622-S(22-) |             |
|              | 230*                                | 238                                   | 2226-T(29+)           | 222-D (26-) | 226-D (22-) |             |
|              | 213                                 | 213                                   | 622-D (78+)           |             |             |             |
|              | 105*                                | 101                                   | 2226-T(51+)           | 6222-T(33+) |             |             |
|              | 65                                  | 59                                    | 6222-T(43-)           | 226-D (26+) | 222-4 (13+) | 2226-T(10+) |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3004 3003 2956 2956 2905 2869

\* Not used in the force constant determination.

## References

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torgimsen, J. Mol. Struct., **15**, 61 (1973).
- [2] IR.R. J. E. Gustavsen, P. Klaboe, and R. Stølevik, J. Mol. Struct., **50**, 285 (1978).



No. 161

Molecule: 62226-GG BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (*gauche-gauche form*)Symmetry C<sub>2</sub>Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1465                                | 1481                                  | 222-2 (76+)           |             |             |             |
|              | 1417                                | 1430                                  | 226-2 (39+)           | 622-2 (39+) | 222-2 (19-) |             |
|              | 1294                                | 1297                                  | 222-6 (47+)           | 226-5 (15-) | 622-5 (15+) |             |
|              | 1232                                | 1221                                  | 622-5 (29-)           | 226-5 (29+) | 622-6 (15+) | 226-6 (15+) |
|              | 1106                                | 1115                                  | 222-6 (44-)           | 226-6 (21+) | 622-6 (21+) |             |
|              | 960                                 | 967                                   | 226-4 (23-)           | 622-4 (23+) | 6222-S(13+) | 2226-S(13+) |
|              | 854                                 | 844                                   | 2226-S(29+)           | 6222-S(29+) | 622-4 (15-) | 226-4 (15+) |
|              | 591                                 | 586                                   | 0622-S(45-)           | 2260-S(45-) | 622-D (11+) | 226-D (11+) |
|              | 424                                 | 417                                   | 222-D (56-)           | 622-D (9+)  | 226-D (9+)  |             |
|              | 185                                 | 176                                   | 622-D (35+)           | 226-D (35+) | 222-D (20+) |             |
|              | 54                                  | 36                                    | 6222-T(42+)           | 2226-T(42+) |             |             |
| b            | 1430                                | 1439                                  | 622-2 (45-)           | 226-2 (45+) |             |             |
|              | 1349                                | 1356                                  | 222-5 (69+)           | 2226-S(4+)  |             |             |
|              | 1240                                | 1256                                  | 226-5 (39+)           | 622-5 (39+) |             |             |
|              | 1122                                | 1127                                  | 622-6 (38-)           | 226-6 (38+) | 222-5 (18-) |             |
|              | 1073                                | 1086                                  | 6222-S(36+)           | 2226-S(36-) |             |             |
|              | 944                                 | 956                                   | 222-4 (43-)           | 622-4 (11+) | 226-4 (11+) | 226-5 (5+)  |
|              | 763                                 | 772                                   | 226-4 (35+)           | 622-4 (35+) | 222-4 (18+) | 222-5 (11-) |
|              | 549                                 | 553                                   | 2260-S(50-)           | 0622-S(50+) |             |             |
|              | 324                                 | 319                                   | 226-D (30-)           | 622-D (30+) | 6222-T(15-) | 2226-T(15+) |
|              |                                     | 128                                   | 2226-T(29+)           | 6222-T(29-) | 222-4 (17+) | 622-D (16-) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3005 3002 2956 2956 2905 2869

## References

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torgrimsen, J. Mol. Struct., **15**, 61 (1973).
- [2] IR.R. J. E. Gustavsen, P. Klaboe, and R. Stølevik, J. Mol. Struct., **50**, 285 (1978).

## No. 162

Molecule: 622226-TTT BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (trans-trans-trans form)Symmetry C<sub>2h</sub> Symmetry number  $\sigma = 2$ 

| Sym. species   | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|----------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a <sub>g</sub> | 1453*                               | 1461                                  | 222-2 (40+)           | 222-2 (40+) |             |             |
|                | 1428*                               | 1426                                  | 226-2 (39+)           | 622-2 (39+) |             |             |
|                | 1353                                | 1349                                  | 222-5 (46+)           | 222-5 (46-) | 2222-S(13+) |             |
|                | 1233                                | 1231                                  | 622-5 (48-)           | 226-5 (48+) |             |             |
|                | 1057                                | 1053                                  | 6222-S(32-)           | 2226-S(32-) | 222-D (10+) | 222-D (10+) |
|                | 1042                                | 1045                                  | 2222-S(82+)           |             |             |             |
|                | 648                                 | 654                                   | 0622-S(38+)           | 2260-S(38+) |             |             |
|                | 325                                 | 331                                   | 222-D (25-)           | 222-D (25-) | 622-D (16+) | 226-D (16+) |
|                | 148                                 | 142                                   | 226-D (31+)           | 622-D (31+) | 2222-S( 9+) |             |
|                | 1273                                | 1280                                  | 222-6 (23+)           | 222-6 (23+) | 226-6 (16-) | 622-6 (16-) |
| a <sub>u</sub> | 1083                                | 1084                                  | 622-6 (32+)           | 226-6 (32+) | 222-6 (22+) | 222-6 (22+) |
|                | 871                                 | 864                                   | 622-4 (32-)           | 226-4 (32+) | 222-6 (12+) | 222-6 (12+) |
|                | 743                                 | 736                                   | 222-4 (35+)           | 222-4 (35-) | 226-4 (11-) | 622-4 (11+) |
|                |                                     | 128                                   | 2222-T(82+)           |             |             |             |
|                |                                     | 50                                    | 2226-T(35+)           | 6222-T(35+) | 2222-T( 9-) |             |
| b <sub>g</sub> | 1308                                | 1302                                  | 222-6 (39-)           | 222-6 (39+) |             |             |
|                | 1223                                | 1228                                  | 622-6 (27+)           | 226-6 (27-) | 222-4 (13-) | 222-4 (13-) |
|                | 1010*                               | 1009                                  | 226-6 (19-)           | 622-6 (19+) | 222-4 (16+) | 222-4 (16+) |
|                | 755                                 | 761                                   | 622-4 (31-)           | 226-4 (31-) | 222-4 (16+) | 222-4 (16+) |
|                |                                     | 158                                   | 2226-T(45+)           | 6222-T(45-) |             |             |
| b <sub>u</sub> | 1460*                               | 1476                                  | 222-2 (49-)           | 222-2 (49+) |             |             |
|                | 1436*                               | 1432                                  | 622-2 (48+)           | 226-2 (48-) |             |             |
|                | 1293                                | 1290                                  | 222-5 (29+)           | 222-5 (29+) | 622-5 (22-) | 226-5 (22-) |
|                | 1196                                | 1184                                  | 226-5 (30+)           | 622-5 (30+) | 222-5 (24+) | 222-5 (24+) |
|                | 1010*                               | 1006                                  | 2226-S(45+)           | 6222-S(45-) |             |             |
|                | 638                                 | 636                                   | 2260-S(40-)           | 0622-S(40+) | 226-D (11+) | 622-D (11-) |
|                | 354                                 | 365                                   | 622-D (20-)           | 226-D (20+) | 0622-S(12-) | 2260-S(12+) |
|                |                                     | 88                                    | 222-D (38-)           | 222-D (38+) | 622-D (22-) | 226-D (22+) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3003 3003 2956 2956 2909 2900 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 163

Molecule: 622226-TTG BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (trans-trans-gauche form)Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.F.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1480                                  | 222-2 (60+)           | 222-2 (29-) |             |             |
|              | 1453*                               | 1462                                  | 222-2 (63+)           | 222-2 (21+) |             |             |
|              | 1437*                               | 1435                                  | 226-2 (74+)           | 622-2 (12+) |             |             |
|              | 1430*                               | 1428                                  | 622-2 (75-)           |             |             |             |
|              | 1368                                | 1361                                  | 222-5 (54-)           | 222-5 (31+) | 2222-S(14+) |             |
|              | 1303                                | 1304                                  | 222-6 (35-)           | 222-6 (33+) | 226-5 (4+)  |             |
|              | 1296*                               | 1295                                  | 222-5 (42+)           | 622-5 (23-) | 222-5 (17+) |             |
|              | 1273*                               | 1279                                  | 226-5 (26+)           | 222-6 (24-) | 622-6 (15+) | 222-6 (14-) |
|              | 1236*                               | 1239                                  | 226-5 (40+)           | 622-6 (22-) | 222-4 (10+) |             |
|              | 1224                                | 1219                                  | 622-5 (63+)           | 222-5 (13+) | 226-6 (12+) |             |
|              | 1169                                | 1163                                  | 226-6 (30+)           | 222-5 (18-) | 226-5 (14+) | 622-5 (12-) |
|              | 1100                                | 1104                                  | 222-6 (24-)           | 622-6 (19-) | 222-6 (14-) | 2222-S(13-) |
|              | 1058                                | 1060                                  | 2226-S(25-)           | 2222-S(24+) | 622-6 (13-) | 6222-S(11-) |
|              | 1043                                | 1034                                  | 6222-S(53-)           | 226-6 (12-) | 222-D (7+)  |             |
|              | 1010*                               | 1011                                  | 2222-S(15-)           | 222-4 (15-) | 622-6 (13-) | 226-6 (13-) |
|              | 968                                 | 976                                   | 2226-S(39-)           | 6222-S(10+) | 2222-S(9-)  | 222-4 (7+)  |
|              | 846                                 | 854                                   | 226-4 (31+)           | 622-4 (22+) | 222-4 (15-) | 222-6 (9-)  |
|              | 802                                 | 804                                   | 226-4 (36+)           | 622-4 (22-) | 222-4 (21+) |             |
|              | 737                                 | 743                                   | 222-4 (51+)           | 622-4 (28-) | 222-4 (11-) |             |
|              | 648                                 | 643                                   | 0622-S(78+)           | 222-D (13-) | 622-D (10-) |             |
|              | 563*                                | 564                                   | 2260-S(98-)           | 226-D (15+) |             |             |
|              | 428                                 | 433                                   | 222-D (47-)           | 622-D (15+) | 226-D (14+) |             |
|              | 289                                 | 289                                   | 622-D (23-)           | 222-D (16-) | 226-D (15+) | 0622-S(13-) |
|              | 237*                                | 251                                   | 226-D (32-)           | 222-D (17-) | 2226-T(14+) | 0622-S(9-)  |
|              | 173                                 | 166                                   | 622-D (35-)           | 222-D (25+) | 2226-T(24+) |             |
|              |                                     | 115                                   | 6222-T(46+)           | 622-D (11-) | 222-D (11-) | 2222-T(9-)  |
|              |                                     | 90                                    | 2222-T(64-)           | 6222-T(14-) | 2226-T(11-) |             |
|              |                                     | 42                                    | 2226-T(31+)           | 6222-T(15+) | 222-D (12+) | 226-D (11+) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3004 3003 2956 2956 2909 2901 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 164

Molecule: 622226-TGT BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (trans-gauche-trans form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1481                                  | 222-2 (46+)           | 222-2 (46+) |             |             |
|              | 1437*                               | 1433                                  | 622-2 (47+)           | 226-2 (47+) |             |             |
|              | 1337                                | 1328                                  | 222-5 (31-)           | 222-5 (31+) | 2222-S(12+) | 222-6 (10+) |
|              | 1273*                               | 1282                                  | 222-6 (22+)           | 222-6 (22+) | 226-6 (10-) | 622-6 (10-) |
|              | 1236*                               | 1232                                  | 622-5 (35-)           | 226-5 (35+) | 226-6 ( 7-) |             |
|              | 1169                                | 1159                                  | 226-6 (15+)           | 622-6 (15+) | 222-5 (13-) | 222-5 (13+) |
|              | 1067                                | 1068                                  | 2222-S(51+)           | 6222-S(20-) | 2226-S(20-) |             |
|              | 1010*                               | 1017                                  | 226-6 (15+)           | 622-6 (15+) | 222-4 (11-) | 222-4 (11+) |
|              | 902                                 | 909                                   | 2226-S(17-)           | 6222-S(17-) | 2222-S(14-) | 622-4 ( 9+) |
|              |                                     | 770                                   | 622-4 (28+)           | 226-4 (28-) | 222-4 (16-) | 222-4 (16+) |
|              | 638                                 | 634                                   | 2260-S(42-)           | 0622-S(42-) |             |             |
|              | 237*                                | 245                                   | 222-D (21-)           | 222-D (21-) | 2222-T(17+) | 6222-T(11-) |
|              | 173                                 | 169                                   | 226-D (36+)           | 622-D (36+) |             |             |
|              |                                     | 112                                   | 2222-T(67+)           | 2226-T(13+) | 6222-T(13+) |             |
|              |                                     | 57                                    | 6222-T(20-)           | 2226-T(20-) | 222-D (16+) | 222-D (16+) |
| b            | 1453*                               | 1460                                  | 222-2 (46-)           | 222-2 (46+) |             |             |
|              | 1430*                               | 1430                                  | 226-2 (47+)           | 622-2 (47-) |             |             |
|              | 1341                                | 1344                                  | 222-5 (41+)           | 222-5 (41+) |             |             |
|              | 1273*                               | 1277                                  | 222-6 (23-)           | 222-6 (23+) | 622-6 (15+) | 226-6 (15-) |
|              | 1224                                | 1230                                  | 226-5 (46-)           | 622-5 (46-) |             |             |
|              | 1120                                | 1113                                  | 622-6 (21-)           | 226-6 (21+) | 222-6 (16-) | 222-6 (16+) |
|              | 1024                                | 1031                                  | 2226-S(23+)           | 6222-S(23-) | 622-6 ( 9+) | 226-6 ( 9-) |
|              | 898                                 | 895                                   | 226-4 (20+)           | 622-4 (20+) | 6222-S(13+) | 2226-S(13-) |
|              | 755                                 | 748                                   | 226-4 (21+)           | 622-4 (21+) | 222-4 (19-) | 222-4 (19-) |
|              | 648                                 | 656                                   | 0622-S(30-)           | 2260-S(30+) | 222-D (11+) | 222-D (11-) |
|              | 391                                 | 398                                   | 2260-S(21+)           | 0622-S(21-) | 222-D (19-) | 222-D (19+) |
|              |                                     | 260                                   | 622-D (41-)           | 226-D (41+) | 222-D (12+) | 222-D (12-) |
|              |                                     | 63                                    | 2226-T(39-)           | 6222-T(39+) |             |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3003 3003 2956 2956 2907 2903 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 165

Molecule: 622226-TGG  $\text{BrCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{Br}$  (trans-gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1486                                  | 222-2 (55+)           | 222-2 (32+) |             |             |
|              | 1460*                               | 1463                                  | 222-2 (60+)           | 222-2 (27-) |             |             |
|              | 1437*                               | 1434                                  | 226-2 (73+)           | 222-2 (12-) |             |             |
|              | 1430*                               | 1431                                  | 622-2 (85+)           |             |             |             |
|              | 1355                                | 1358                                  | 222-5 (63+)           | 222-5 (13+) |             |             |
|              | 1337                                | 1332                                  | 222-5 (59-)           | 2222-S(11-) | 222-6 (10-) |             |
|              | 1293                                | 1285                                  | 222-6 (27-)           | 226-5 (18+) | 222-6 (14-) | 226-6 (10-) |
|              | 1273*                               | 1278                                  | 222-6 (33-)           | 622-6 (21+) | 226-5 (19-) |             |
|              | 1236*                               | 1236                                  | 622-5 (51+)           | 226-5 (25+) |             |             |
|              | 1207*                               | 1215                                  | 622-5 (35-)           | 226-5 (21+) | 226-6 (14+) | 222-5 (7-)  |
|              | 1141                                | 1134                                  | 222-6 (28-)           | 226-6 (24+) | 222-5 (12+) | 6222-S(9+)  |
|              | 1120                                | 1119                                  | 622-6 (33+)           | 222-6 (23+) | 226-6 (22-) | 222-5 (14+) |
|              | 1083                                | 1088                                  | 2222-S(41+)           | 2226-S(33-) |             |             |
|              | 1024                                | 1031                                  | 6222-S(43-)           | 226-6 (17+) | 222-4 (11+) |             |
|              | 1010*                               | 998                                   | 222-4 (25+)           | 622-6 (21+) | 622-4 (19+) | 2226-S(7+)  |
|              | 918                                 | 915                                   | 226-4 (29-)           | 6222-S(28+) | 222-4 (15+) |             |
|              | 873                                 | 878                                   | 2226-S(39-)           | 2222-S(17-) | 622-4 (14+) | 222-4 (7+)  |
|              | 802                                 | 808                                   | 226-4 (30-)           | 622-4 (24-) | 222-4 (17-) | 2222-S(10-) |
|              | 737                                 | 743                                   | 222-4 (41-)           | 622-4 (31+) | 226-4 (11-) |             |
|              | 648                                 | 649                                   | 0622-S(71+)           | 222-D (18-) | 622-D (13-) |             |
|              | 563*                                | 564                                   | 2260-S(93-)           | 226-D (15+) |             |             |
|              | 443                                 | 435                                   | 222-D (54-)           | 0622-S(12+) | 2260-S(9+)  |             |
|              | 318                                 | 322                                   | 226-D (30+)           | 222-D (23-) | 2226-T(13-) | 0622-S(13-) |
|              | 237*                                | 235                                   | 622-D (72+)           |             |             |             |
|              | 173                                 | 179                                   | 226-D (38-)           | 222-D (26-) | 222-D (16-) | 622-D (10+) |
|              |                                     | 128                                   | 2226-T(26+)           | 2222-T(22-) | 222-D (15-) | 222-4 (12+) |
|              |                                     | 89                                    | 6222-T(49+)           | 2222-T(40+) |             |             |
|              |                                     | 31                                    | 2226-T(39-)           | 6222-T(20+) | 2222-T(17-) |             |

Calculated frequencies higher than 2000  $\text{cm}^{-1}$ 

3004 3003 2956 2956 2907 2903 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 166

Molecule: 622226-GTG BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (gauche-trans-gauche form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1460*                               | 1464                                  | 222-2 (41+)           | 222-2 (41+) |             |             |
|              | 1437*                               | 1435                                  | 226-2 (40+)           | 622-2 (40+) |             |             |
|              | 1375                                | 1370                                  | 222-5 (40+)           | 222-5 (40-) | 2222-S(15+) |             |
|              | 1273*                               | 1280                                  | 226-5 (23-)           | 622-5 (23+) | 222-6 (16+) | 222-6 (16+) |
|              | 1196                                | 1207                                  | 622-5 (20-)           | 226-5 (20+) | 622-6 (16+) | 226-6 (16+) |
|              | 1121                                | 1124                                  | 222-6 (22-)           | 222-6 (22-) | 2222-S(16-) | 226-6 (9+)  |
|              | 1057                                | 1057                                  | 2222-S(22-)           | 6222-S(19+) | 2226-S(19+) | 222-6 (8+)  |
|              | 1010*                               | 1000                                  | 2222-S(16+)           | 622-4 (14+) | 226-4 (14-) | 226-6 (11+) |
|              | 817                                 | 820                                   | 222-4 (20+)           | 222-4 (20-) | 2222-S(13-) | 622-4 (11+) |
|              | 755                                 | 761                                   | 2222-S(19+)           | 222-4 (19+) | 222-4 (19-) | 226-4 (16+) |
|              | 558*                                | 566                                   | 0622-S(45+)           | 2260-S(45+) |             |             |
|              | 404                                 | 401                                   | 222-D (23-)           | 222-D (23-) | 622-D (7+)  | 226-D (7+)  |
|              | 237*                                | 234                                   | 226-D (22+)           | 622-D (22+) | 2222-T(17+) | 2226-T(6-)  |
|              |                                     | 72                                    | 6222-T(36+)           | 2226-T(36+) |             |             |
|              |                                     | 31                                    | 2222-T(71-)           |             |             |             |
| b            |                                     | 1483                                  | 222-2 (43+)           | 222-2 (43-) |             |             |
|              | 1430*                               | 1434                                  | 622-2 (43+)           | 226-2 (43-) |             |             |
|              | 1313*                               | 1310                                  | 222-5 (18+)           | 222-5 (18+) | 222-6 (17+) | 222-6 (17-) |
|              | 1303                                | 1300                                  | 222-6 (17-)           | 222-6 (17+) | 222-5 (16-) | 222-5 (16-) |
|              | 1236*                               | 1244                                  | 226-5 (30+)           | 622-5 (30+) | 222-4 (8+)  | 222-4 (8+)  |
|              | 1144                                | 1133                                  | 622-6 (31+)           | 226-6 (31-) | 222-5 (11+) | 222-5 (11+) |
|              | 1043                                | 1042                                  | 2226-S(21+)           | 6222-S(21-) | 222-4 (12+) | 222-4 (12+) |
|              | 968                                 | 973                                   | 2226-S(20-)           | 6222-S(20+) | 222-4 (13+) | 222-4 (13+) |
|              | 846                                 | 838                                   | 226-4 (38+)           | 622-4 (38+) |             |             |
|              | 563*                                | 561                                   | 2260-S(52-)           | 0622-S(52+) |             |             |
|              | 303                                 | 305                                   | 622-D (30-)           | 226-D (30+) | 222-D (17-) | 222-D (17+) |
|              | 240*                                | 258                                   | 222-D (25+)           | 222-D (25-) | 6222-T(21-) | 2226-T(21+) |
|              |                                     | 106                                   | 2226-T(25-)           | 6222-T(25+) | 222-D (12-) | 222-D (12+) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3004 3004 2956 2956 2909 2901 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 167

Molecule: 622226-GTG' BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (gauche-trans-gauche' form)Symmetry C<sub>i</sub> Symmetry number  $\sigma = 1$ 

| Sym. species   | Observed frequency<br>cm <sup>-1</sup> | Calculated frequency<br>cm <sup>-1</sup> | Assignment<br>(P.E.D. %) |             |             |             |
|----------------|----------------------------------------|------------------------------------------|--------------------------|-------------|-------------|-------------|
| a <sub>g</sub> |                                        | 1464                                     | 222-2 (41+)              | 222-2 (41+) |             |             |
|                | 1437                                   | 1435                                     | 226-2 (39+)              | 622-2 (39+) |             |             |
|                | 1366                                   | 1370                                     | 222-5 (40+)              | 222-5 (40-) | 2222-S(15+) |             |
|                | 1296                                   | 1305                                     | 222-6 (34-)              | 222-6 (34+) | 226-5 ( 6+) |             |
|                | 1238                                   | 1245                                     | 226-5 (35+)              | 622-5 (35-) | 222-4 ( 8-) |             |
|                | 1207                                   | 1196                                     | 622-6 (27-)              | 226-6 (27+) | 622-5 ( 5+) | 226-5 ( 5-) |
|                | 1078                                   | 1086                                     | 2222-S(31-)              | 6222-S(19+) | 2226-S(19+) | 222-4 ( 5-) |
|                | 1010                                   | 1007                                     | 2222-S(18-)              | 622-6 (15-) | 226-6 (15+) | 622-4 (12-) |
|                | 959                                    | 976                                      | 222-4 (17+)              | 222-4 (17+) | 2226-S(11+) | 6222-S(11+) |
|                | 787                                    | 782                                      | 2222-S(31-)              | 622-4 (27+) | 226-4 (27+) |             |
|                | 558                                    | 559                                      | 2260-S(49+)              | 0622-S(49+) |             |             |
|                | 481                                    | 475                                      | 222-D (25+)              | 222-D (25+) | 622-D ( 6-) | 226-D ( 6-) |
|                | 237                                    | 244                                      | 2226-T(27+)              | 6222-T(27-) | 226-D (17+) | 622-D (17+) |
|                |                                        | 77                                       | 226-D (21+)              | 622-D (21+) | 2226-T(20-) | 6222-T(20+) |
| a <sub>u</sub> |                                        | 1483                                     | 222-2 (43+)              | 222-2 (43-) |             |             |
|                | 1436                                   | 1433                                     | 622-2 (43+)              | 226-2 (43-) |             |             |
|                | 1313                                   | 1306                                     | 222-5 (35+)              | 222-5 (35+) | 226-6 ( 7-) |             |
|                | 1263                                   | 1279                                     | 622-5 (26+)              | 226-5 (26+) | 222-6 (16+) | 222-6 (16+) |
|                | 1169                                   | 1164                                     | 226-5 (20-)              | 622-5 (20-) | 222-6 (13+) | 222-6 (13+) |
|                | 1092(s)                                | 1092                                     | 226-6 (31+)              | 622-6 (31+) | 222-6 (16-) | 222-6 (16-) |
|                | 1010                                   | 1005                                     | 6222-S(40+)              | 2226-S(40-) |             |             |
|                | 871                                    | 874                                      | 622-4 (34+)              | 226-4 (34-) | 222-4 ( 7+) |             |
|                | 758                                    | 772                                      | 222-4 (33+)              | 222-4 (33-) | 226-4 ( 8+) |             |
|                | 563                                    | 567                                      | 0622-S(49+)              | 2260-S(49-) |             |             |
|                | 322                                    | 326                                      | 622-D (32+)              | 226-D (32-) | 222-D (11+) | 222-D (11-) |
|                | 240                                    | 247                                      | 222-D (36-)              | 222-D (36+) |             |             |
|                |                                        | 63                                       | 6222-T(19+)              | 2226-T(19+) | 2222-T(19-) | 222-4 ( 9-) |
|                |                                        | 42                                       | 2222-T(57+)              | 6222-T(17+) | 2226-T(17+) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3004 3004 2956 2956 2909 2900 2873 2865

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 168

Molecule: 622226-GGG BrCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>Br (gauche-gauche-gauche form)  
 Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1490                                  | 222-2 (42+)           | 222-2 (42+) |             |             |
|              | 1436*                               | 1435                                  | 226-2 (42+)           | 622-2 (42+) |             |             |
|              | 1341                                | 1346                                  | 222-5 (32-)           | 222-5 (32+) | 2222-S(16-) |             |
|              | 1293                                | 1288                                  | 222-6 (23+)           | 222-6 (23+) | 226-5 (9-)  | 622-5 (9+)  |
|              | 1236*                               | 1238                                  | 622-5 (36-)           | 226-5 (36+) |             |             |
|              | 1121                                | 1131                                  | 2222-S(16+)           | 622-6 (13-) | 226-6 (13-) | 222-5 (9-)  |
|              | 1083                                | 1081                                  | 2222-S(24+)           | 226-6 (23+) | 622-6 (23+) | 6222-S(11-) |
|              | 968                                 | 981                                   | 222-4 (28+)           | 222-4 (28-) | 226-5 (6-)  | 622-5 (6+)  |
|              | 902                                 | 904                                   | 622-4 (21-)           | 226-4 (21+) | 2226-S(15-) | 6222-S(15-) |
|              | 787                                 | 787                                   | 2222-S(38+)           | 622-4 (21-) | 226-4 (21+) |             |
|              | 563*                                | 566                                   | 2260-S(50+)           | 0622-S(50+) |             |             |
|              | 368                                 | 372                                   | 222-D (17+)           | 222-D (17+) | 622-D (15-) | 226-D (15-) |
|              | 190                                 | 201                                   | 222-D (21+)           | 222-D (21+) | 2226-T(17-) | 6222-T(17-) |
|              |                                     | 107                                   | 226-D (28-)           | 622-D (28-) | 2222-T(10+) | 2226-T(9-)  |
|              |                                     | 30                                    | 2222-T(61+)           | 6222-T(16+) | 2226-T(16+) |             |
| b            | 1460*                               | 1466                                  | 222-2 (40+)           | 222-2 (40-) |             |             |
|              | 1430*                               | 1433                                  | 622-2 (39-)           | 226-2 (39+) |             |             |
|              | 1368                                | 1362                                  | 222-5 (38+)           | 222-5 (38+) |             |             |
|              | 1273*                               | 1280                                  | 226-5 (26+)           | 622-5 (26+) | 222-6 (16-) | 222-6 (16+) |
|              | 1170                                | 1185                                  | 226-6 (25+)           | 622-6 (25-) | 226-5 (13+) | 622-5 (13+) |
|              | 1144                                | 1139                                  | 222-6 (30-)           | 222-6 (30+) | 226-5 (11+) | 622-5 (11+) |
|              | 1024                                | 1029                                  | 2226-S(17-)           | 6222-S(17+) | 226-6 (12-) | 622-6 (12+) |
|              | 918                                 | 915                                   | 226-4 (18+)           | 622-4 (18+) | 6222-S(18-) | 2226-S(18+) |
|              | 758*                                | 764                                   | 222-4 (27+)           | 222-4 (27+) | 226-4 (15+) | 622-4 (15+) |
|              | 563*                                | 567                                   | 0622-S(42+)           | 2260-S(42-) |             |             |
|              | 474                                 | 464                                   | 222-D (33-)           | 222-D (33+) | 2260-S(9-)  |             |
|              | 289                                 | 271                                   | 226-D (40+)           | 622-D (40-) |             |             |
|              |                                     | 62                                    | 2226-T(37-)           | 6222-T(37+) |             |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3004 3004 2956 2956 2907 2903 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).



## No. 169

Molecule: 1227-T  $\text{CH}_3\text{CH}_2\text{CH}_2\text{I}$  (trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|
| a'           | 1460                                | 1478                                  | 122-2 (55+)           | 012-4 (29+) |             |
|              | 1456                                | 1452                                  | 012-4 (55+)           | 122-2 (38-) |             |
|              | 1428                                | 1421                                  | 227-2 (86+)           |             |             |
|              | 1380                                | 1379                                  | 012-2 (104+)          |             |             |
|              | 1328                                | 1329                                  | 122-5 (79+)           | 1227-S(15+) |             |
|              | 1185                                | 1187                                  | 227-5 (91+)           |             |             |
|              | 1089                                | 1092                                  | 1227-S(28-)           | 012-5 (28+) | 122-5 (15+) |
|              | 1019                                | 1028                                  | 0122-S(82-)           | 1227-S(19+) |             |
|              | 895                                 | 889                                   | 012-5 (38-)           | 1227-S(37-) | 0122-S(10-) |
|              | 593                                 | 590                                   | 2270-S(69-)           | 122-D (26+) | 227-D (18+) |
|              | 288                                 | 289                                   | 122-D (54-)           | 2270-S(37-) |             |
|              | 203                                 | 200                                   | 227-D (94+)           | 227-5 (14-) | 122-D (14-) |
| a''          | 1456                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |
|              | 1285                                | 1274                                  | 122-6 (72+)           |             |             |
|              | 1185                                | 1197                                  | 227-6 (39+)           | 122-4 (21+) | 012-8 (15-) |
|              | 1012                                | 1015                                  | 227-6 (54+)           | 012-8 (21+) | 122-6 (14+) |
|              | 828                                 | 826                                   | 012-8 (39+)           | 227-4 (35+) | 122-4 (20+) |
|              | 726                                 | 719                                   | 227-4 (47-)           | 122-4 (44+) | 1227-T(11-) |
|              | 240(s)                              | 227                                   | 0122-T(96+)           |             |             |
|              | 130                                 | 117                                   | 1227-T(86+)           |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2998 2963 2962 2962 2904 2880 2868

## References

- [1] IR. K. Radcliffe and J. L. Wood, Trans. Faraday Soc., **62**, 1678 (1966).  
 [2] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 170

Molecule: 1227-G CH3CH2CH2I (gauche form)  
 Symmetry  $C_1$  Symmetry number  $\sigma = 1$

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |            |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|------------|
| a            | 1460*                               | 1479                                  | 122-2 (67+)           | 012-4 (20+) |             |            |
|              | 1456*                               | 1463                                  | 012-7 (80+)           | 012-8 (14+) |             |            |
|              | 1456*                               | 1456                                  | 012-4 (62+)           | 122-2 (22-) |             |            |
|              | 1433                                | 1431                                  | 227-2 (73+)           |             |             |            |
|              | 1380*                               | 1379                                  | 012-2 (106+)          |             |             |            |
|              | 1344                                | 1343                                  | 122-5 (72+)           |             |             |            |
|              | 1279                                | 1275                                  | 122-6 (64-)           | 227-5 (7+)  |             |            |
|              | 1195                                | 1206                                  | 227-5 (64+)           | 1227-S(13-) | 122-4 (10+) |            |
|              |                                     | 1167                                  | 227-6 (36+)           | 012-5 (16+) | 1227-S(11-) | 227-5 (6+) |
|              | 1075                                | 1081                                  | 0122-S(33-)           | 1227-S(21+) | 122-6 (10-) | 122-4 (9+) |
|              | 1036                                | 1038                                  | 012-5 (23+)           | 122-5 (16+) | 227-5 (16-) | 012-8 (8-) |
|              | 1012*                               | 1003                                  | 227-6 (41-)           | 0122-S(26-) | 122-6 (9+)  |            |
|              | 880                                 | 875                                   | 1227-S(36+)           | 012-5 (25+) | 0122-S(20+) |            |
|              | 816                                 | 817                                   | 227-4 (31-)           | 012-8 (26+) | 122-4 (25+) |            |
|              | 764                                 | 767                                   | 227-4 (42+)           | 122-4 (29+) | 012-8 (15+) |            |
|              | 503                                 | 505                                   | 2270-S(93-)           | 227-D (21+) |             |            |
|              | 390                                 | 383                                   | 122-D (76-)           |             |             |            |
|              | 263                                 | 265                                   | 0122-T(43+)           | 227-D (28+) | 1227-T(16-) |            |
|              | 189(g)                              | 184                                   | 0122-T(51+)           | 227-D (37-) | 1227-T(11+) |            |
|              | 116(g)                              | 101                                   | 1227-T(62+)           | 227-D (22+) |             |            |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$

2998 2963 2962 2962 2904 2880 2868

\* Not used in the force constant determination.

## References

- [1] IR. K. Radcliffe and J. L. Wood, *Trans. Faraday Soc.*, **62**, 1678 (1966).  
 [2] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, *Bull. Chem. Soc. Jpn.*, **51**, 748 (1978).

## No. 171

Molecule: 12227-TT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           | 1474                                | 1483                                  | 122-2 (46-)           | 222-2 (27+) | 012-4 (16-) |             |
|              | 1453                                | 1461                                  | 222-2 (63+)           | 012-4 (22+) |             |             |
|              | 1446                                | 1452                                  | 012-4 (46-)           | 122-2 (39+) |             |             |
|              | 1419                                | 1420                                  | 227-2 (84+)           |             |             |             |
|              | 1380                                | 1379                                  | 012-2 (105+)          |             |             |             |
|              | 1354                                | 1355                                  | 122-5 (53+)           | 222-5 (35-) | 1222-S(16+) |             |
|              | 1290                                | 1285                                  | 222-5 (48+)           | 122-5 (29+) | 227-5 (13-) |             |
|              | 1183                                | 1180                                  | 227-5 (81+)           | 222-5 (11+) |             |             |
|              | 1093                                | 1103                                  | 1222-S(24-)           | 012-5 (24+) | 122-5 (10+) | 122-D (9+)  |
|              | 1049                                | 1052                                  | 0122-S(33-)           | 1222-S(28+) | 2227-S(26-) |             |
|              | 1008                                | 1008                                  | 0122-S(46-)           | 2227-S(44+) |             |             |
|              | 889                                 | 894                                   | 012-5 (43-)           | 1222-S(34-) | 122-5 (10-) |             |
|              | 593                                 | 591                                   | 2270-S(70-)           | 222-D (20+) | 227-D (12+) |             |
|              | 388                                 | 392                                   | 122-D (65-)           | 227-D (23+) |             |             |
|              | 251                                 | 252                                   | 222-D (39+)           | 2270-S(29+) | 227-D (12+) |             |
|              | 132                                 | 132                                   | 227-D (65+)           | 222-D (26-) | 122-D (22+) | 227-5 (11-) |
| a''          | 1463                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1303                                | 1299                                  | 122-6 (47-)           | 222-6 (33+) |             |             |
|              | 1250                                | 1251                                  | 222-6 (40-)           | 122-6 (20-) | 227-6 (9+)  | 012-8 (8+)  |
|              | 1175                                | 1190                                  | 227-6 (30-)           | 222-4 (18-) | 122-4 (16-) | 012-8 (14+) |
|              | 1032                                | 1031                                  | 227-6 (51+)           | 222-6 (17+) | 122-6 (12+) | 012-8 (12+) |
|              | 889                                 | 890                                   | 012-8 (31+)           | 222-4 (26+) | 122-6 (21+) | 227-4 (20+) |
|              | 772                                 | 759                                   | 122-4 (52+)           | 227-4 (28-) | 012-8 (21+) |             |
|              | 726                                 | 720                                   | 222-4 (42-)           | 227-4 (37+) | 122-4 (13+) | 2227-T(10+) |
|              | 231*                                | 232                                   | 0122-T(91-)           |             |             |             |
|              | 132*                                | 129                                   | 1222-T(69+)           | 2227-T(24+) |             |             |
|              |                                     | 97                                    | 2227-T(57+)           | 1222-T(22-) | 222-4 (11+) |             |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

2998 2963 2962 2962 2909 2900 2880 2872 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 172

Molecule: 12227-TG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474*                               | 1485                                  | 122-2 (39-)           | 222-2 (36+) | 012-4 (13-) |             |
|              | 1463*                               | 1463                                  | 222-2 (43+)           | 012-4 (22+) | 122-2 (12+) |             |
|              | 1463*                               | 1463                                  | 012-7 (73+)           | 012-8 (13+) |             |             |
|              | 1446*                               | 1452                                  | 012-4 (47-)           | 122-2 (42+) |             |             |
|              | 1429                                | 1429                                  | 227-2 (74+)           |             |             |             |
|              | 1380*                               | 1379                                  | 012-2 (104+)          |             |             |             |
|              | 1367                                | 1363                                  | 222-5 (41-)           | 122-5 (39+) | 1222-S(16+) |             |
|              | 1303*                               | 1299                                  | 122-6 (41-)           | 222-6 (29+) | 122-5 ( 5+) |             |
|              | 1295                                | 1296                                  | 122-5 (38+)           | 222-5 (31+) | 012-5 ( 7-) |             |
|              | 1250                                | 1251                                  | 222-6 (29-)           | 122-6 (22-) | 227-5 (15+) | 012-8 ( 8+) |
|              | 1192                                | 1199                                  | 227-5 (48+)           | 122-4 (11+) | 012-8 (10-) | 2227-S(10-) |
|              | 1153                                | 1159                                  | 227-6 (28+)           | 012-5 (12+) | 227-5 (11+) | 2227-S( 9-) |
|              | 1093*                               | 1101                                  | 1222-S(21+)           | 2227-S(20-) | 222-6 (10+) | 222-4 ( 9-) |
|              | 1049*                               | 1048                                  | 0122-S(47+)           | 012-5 ( 9-) | 227-6 ( 9+) | 222-5 ( 9-) |
|              | 1032*                               | 1031                                  | 227-6 (44-)           | 222-6 (12+) | 1222-S( 9-) | 012-5 ( 8+) |
|              | 990                                 | 1000                                  | 2227-S(35+)           | 0122-S(32-) | 227-5 ( 6+) |             |
|              | 896                                 | 898                                   | 012-5 (23+)           | 227-4 (20-) | 1222-S(14+) | 222-4 (11+) |
|              | 863                                 | 871                                   | 222-4 (28+)           | 012-8 (24+) | 122-6 (15+) | 012-5 (11-) |
|              | 779                                 | 773                                   | 227-4 (49-)           | 1222-S(18-) | 122-4 (14-) |             |
|              | 735                                 | 740                                   | 122-4 (50+)           | 222-4 (21-) | 012-8 (12+) | 227-4 (11-) |
|              | 506                                 | 505                                   | 2270-S(92+)           | 227-D (23-) |             |             |
|              | 450                                 | 449                                   | 122-D (29-)           | 222-D (27-) | 2270-S( 9+) | 0122-S( 6-) |
|              | 267                                 | 268                                   | 122-D (59+)           | 222-D (36-) | 227-D (12+) |             |
|              | 251*                                | 252                                   | 0122-T(39-)           | 227-D (24-) | 2227-T(23+) |             |
|              | 212                                 | 213                                   | 0122-T(54+)           | 227-D (21-) |             |             |
|              |                                     | 96                                    | 2227-T(44+)           | 1222-T(43+) |             |             |
|              | 75*                                 | 72                                    | 1222-T(34+)           | 227-D (32-) | 2227-T(18-) | 222-4 (13-) |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2999 2963 2962 2962 2909 2900 2880 2872 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 173

Molecule: 12227-GT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (gauche-trans form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474*                               | 1483                                  | 122-2 (55+)           | 222-2 (27+) |             |             |
|              | 1463*                               | 1469                                  | 222-2 (50-)           | 012-4 (24+) |             |             |
|              | 1463*                               | 1463                                  | 012-7 (74+)           | 012-8 (13+) |             |             |
|              | 1446*                               | 1453                                  | 012-4 (48-)           | 122-2 (30+) | 222-2 (12-) |             |
|              | 1425*                               | 1421                                  | 227-2 (88+)           |             |             |             |
|              | 1380*                               | 1380                                  | 012-2 (105+)          |             |             |             |
|              | 1350                                | 1349                                  | 122-5 (61+)           | 222-5 (18+) |             |             |
|              | 1333                                | 1331                                  | 222-5 (53-)           | 122-6 (13+) | 1222-S(12+) | 122-5 (12+) |
|              | 1272                                | 1267                                  | 122-6 (39-)           | 222-6 (17+) | 222-5 ( 8+) | 012-8 ( 7-) |
|              | 1250*                               | 1250                                  | 222-6 (47-)           | 122-6 (15+) | 227-6 ( 9+) |             |
|              | 1183                                | 1189                                  | 227-5 (73+)           |             |             |             |
|              | 1153*                               | 1174                                  | 227-6 (24-)           | 227-5 (15-) | 222-4 (13-) | 012-5 (13-) |
|              | 1089                                | 1093                                  | 2227-S(27+)           | 222-5 (15-) | 012-8 (11-) | 122-4 (11+) |
|              |                                     | 1074                                  | 1222-S(37-)           | 0122-S(28+) | 227-6 ( 8-) |             |
|              | 1037                                | 1032                                  | 227-6 (39-)           | 0122-S(26-) | 012-5 (15+) | 222-6 (12-) |
|              | 968*                                | 962                                   | 2227-S(45-)           | 012-8 (13+) | 122-6 (13+) | 012-5 (12-) |
|              | 896*                                | 895                                   | 222-4 (26+)           | 227-4 (18+) | 012-5 (18-) | 012-8 (11-) |
|              | 861*                                | 874                                   | 0122-S(36-)           | 1222-S(29-) | 012-5 ( 8-) |             |
|              | 779*                                | 777                                   | 122-4 (51+)           | 012-8 (29+) |             |             |
|              | 726*                                | 724                                   | 227-4 (52+)           | 222-4 (32-) |             |             |
|              | 593*                                | 592                                   | 2270-S(63-)           | 222-D (25+) | 227-D (16+) |             |
|              | 407                                 | 407                                   | 122-D (67+)           | 2270-S(18-) |             |             |
|              | 267*                                | 274                                   | 0122-T(37-)           | 222-D (23-) | 2270-S(13-) | 1222-T(11+) |
|              | 212*                                | 212                                   | 227-D (47-)           | 0122-T(23+) | 2270-S( 7-) |             |
|              | 190                                 | 177                                   | 227-D (43+)           | 0122-T(35+) | 222-D (21-) |             |
|              |                                     | 111                                   | 1222-T(76-)           |             |             |             |
|              |                                     | 84                                    | 2227-T(77-)           |             |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2990 2963 2962 2962 2907 2903 2880 2870 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 174

Molecule: 12227-GG CH3CH2CH2CH2I (gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1474*                               | 1485                                  | 122-2 (42+)           | 222-2 (41+) |             |             |
|              | 1463*                               | 1471                                  | 222-2 (36-)           | 012-4 (26+) | 122-2 (20+) |             |
|              | 1463*                               | 1463                                  | 012-7 (78+)           | 012-8 (14+) |             |             |
|              | 1446*                               | 1454                                  | 012-4 (51-)           | 122-2 (30+) |             |             |
|              | 1425                                | 1429                                  | 227-2 (72+)           | 222-2 (10-) |             |             |
|              | 1380*                               | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1354*                               | 1354                                  | 222-5 (47+)           | 122-5 (29+) |             |             |
|              | 1343                                | 1339                                  | 122-5 (44-)           | 222-5 (21+) | 1222-S(16-) |             |
|              | 1272                                | 1270                                  | 122-6 (44+)           | 222-6 (17+) | 012-8 (6-)  | 012-7 (5+)  |
|              | 1264                                | 1254                                  | 222-6 (35-)           | 227-5 (21+) | 122-6 (15+) |             |
|              | 1191*                               | 1194                                  | 227-5 (56+)           | 2227-S(12-) | 122-4 (8-)  |             |
|              |                                     | 1139                                  | 227-6 (31-)           | 012-5 (16+) | 2227-S(11+) | 222-4 (8+)  |
|              | 1122                                | 1118                                  | 1222-S(28-)           | 2227-S(11+) | 222-6 (10-) | 0122-S(9+)  |
|              | 1059                                | 1057                                  | 012-8 (18-)           | 222-5 (17-) | 227-5 (14+) | 122-6 (13-) |
|              | 1032*                               | 1024                                  | 0122-S(39-)           | 227-6 (35+) | 222-6 (10-) |             |
|              | 968                                 | 965                                   | 2227-S(35-)           | 012-5 (28+) | 122-5 (14+) |             |
|              | 886                                 | 889                                   | 0122-S(30-)           | 222-4 (25-) | 227-4 (24+) |             |
|              | 861*                                | 871                                   | 012-8 (24+)           | 222-4 (17-) | 1222-S(12+) | 012-5 (12+) |
|              | 787                                 | 790                                   | 1222-S(26+)           | 227-4 (19+) | 122-4 (17-) | 012-8 (13-) |
|              | 736*                                | 737                                   | 122-4 (38+)           | 227-4 (32+) | 222-4 (13+) | 012-8 (12+) |
|              | 515                                 | 512                                   | 2270-S(82+)           | 227-D (22-) | 222-D (13+) |             |
|              | 438                                 | 440                                   | 122-D (38+)           | 222-D (34-) | 2270-S(17+) |             |
|              | 339                                 | 342                                   | 122-D (30-)           | 227-D (19+) | 222-D (17-) | 1222-T(10+) |
|              | 223                                 | 214                                   | 0122-T(79+)           | 227-D (16+) |             |             |
|              | 203(g)                              | 202                                   | 227-D (26+)           | 122-D (20+) | 222-D (20+) | 2227-T(18-) |
|              |                                     | 119                                   | 1222-T(41-)           | 227-D (33+) | 2227-T(14+) | 222-4 (13+) |
|              |                                     | 54                                    | 2227-T(48+)           | 1222-T(36+) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2999 2963 2962 2962 2907 2903 2880 2870 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. Y. Ogawa, S. Imazeki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

## No. 175

Molecule: 122227-TTT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1481                                | 1484                                  | 122-2 (39-)           | 222-2 (34+) | 012-4 (15-) |             |
|              | 1474                                | 1473                                  | 222-2 (62+)           | 122-2 (16-) | 222-2 (14-) |             |
|              | 1460                                | 1457                                  | 012-4 (47+)           | 222-2 (27+) | 222-2 (13+) |             |
|              | 1443                                | 1449                                  | 122-2 (39+)           | 012-4 (19-) | 222-2 (18+) | 222-2 (15+) |
|              | 1420                                | 1419                                  | 227-2 (83+)           |             |             |             |
|              | 1380                                | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1365                                | 1365                                  | 222-5 (44-)           | 122-5 (29+) | 222-5 (17+) | 1222-S(15+) |
|              | 1331                                | 1327                                  | 222-5 (44+)           | 122-5 (41-) |             |             |
|              | 1265                                | 1258                                  | 222-5 (44+)           | 222-5 (20+) | 227-5 (14-) | 122-5 (12+) |
|              | 1188                                | 1178                                  | 227-5 (75+)           | 222-5 (12+) |             |             |
|              | 1104                                | 1111                                  | 012-5 (19+)           | 1222-S(15-) | 222-5 (9+)  | 222-D (8+)  |
|              | 1052                                | 1058                                  | 2222-S(36-)           | 1222-S(27+) | 0122-S(21-) |             |
|              | 1036                                | 1038                                  | 2227-S(38+)           | 0122-S(21+) | 2222-S(21-) |             |
|              | 998                                 | 998                                   | 0122-S(36+)           | 2227-S(28-) | 2222-S(17-) |             |
|              | 893                                 | 898                                   | 012-5 (40-)           | 1222-S(31-) |             |             |
|              | 592                                 | 590                                   | 2270-S(69-)           | 222-D (21+) | 227-D (15+) |             |
|              | 427                                 | 438                                   | 122-D (34-)           | 222-D (24-) | 227-D (12+) | 0122-S(6-)  |
|              | 326                                 | 332                                   | 122-D (27+)           | 222-D (25-) | 2270-S(20-) | 222-D (19-) |
|              | 194                                 | 191                                   | 227-D (31+)           | 122-D (20+) | 222-D (13+) | 2270-S(13+) |
|              |                                     | 102                                   | 227-D (43-)           | 222-D (34-) | 222-D (32+) |             |
| a''          | 1466                                | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1303                                | 1304                                  | 222-6 (47+)           | 122-6 (21-) | 222-6 (14-) |             |
|              | 1296                                | 1285                                  | 122-6 (38-)           | 222-6 (37+) |             |             |
|              | 1234                                | 1234                                  | 222-6 (21-)           | 222-6 (19-) | 227-6 (14+) | 122-6 (9-)  |
|              | 1175                                | 1186                                  | 227-6 (23-)           | 122-4 (15-) | 222-4 (15-) | 222-4 (13-) |
|              | 1039(s)                             | 1039                                  | 227-6 (48+)           | 222-6 (18+) | 222-6 (16+) |             |
|              | 927                                 | 930                                   | 012-8 (24+)           | 222-4 (21+) | 122-6 (21+) | 222-6 (13+) |
|              | 808                                 | 811                                   | 222-4 (23-)           | 012-8 (22-) | 227-4 (22+) | 122-4 (17-) |
|              | 738                                 | 736                                   | 122-4 (47-)           | 222-4 (23+) | 227-4 (17-) | 012-8 (11-) |
|              | 727                                 | 720                                   | 222-4 (40+)           | 227-4 (35-) | 222-4 (14-) | 2227-T(10-) |
|              | 235                                 | 231                                   | 0122-T(92+)           |             |             |             |
|              |                                     | 152                                   | 1222-T(49+)           | 2227-T(41-) |             |             |
|              |                                     | 119                                   | 2222-T(76+)           |             |             |             |
|              |                                     | 60                                    | 2227-T(38+)           | 1222-T(33+) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2998 2963 2962 2962 2911 2905 2899 2880 2875 2869  
2864

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 176

Molecule: 122227-TTG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-trans-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1481*                               | 1484                                  | 222-2 (36+)           | 122-2 (34-) | 012-4 (14-) |             |
|              | 1474*                               | 1477                                  | 222-2 (62+)           | 122-2 (19-) |             |             |
|              | 1466*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1460*                               | 1457                                  | 012-4 (48+)           | 222-2 (33+) |             |             |
|              | 1443*                               | 1449                                  | 122-2 (41+)           | 222-2 (23+) | 012-4 (19-) | 222-2 (10+) |
|              | 1433                                | 1429                                  | 227-2 (73+)           |             |             |             |
|              | 1380*                               | 1380                                  | 012-2 (102+)          |             |             |             |
|              | 1365*                               | 1369                                  | 222-5 (38-)           | 222-5 (25+) | 122-5 (20+) | 2222-S(13-) |
|              | 1342                                | 1335                                  | 122-5 (46-)           | 222-5 (37+) |             |             |
|              | 1303*                               | 1304                                  | 222-6 (46+)           | 122-6 (21-) | 222-6 (14-) |             |
|              | 1303*                               | 1285                                  | 122-6 (38+)           | 222-6 (34-) |             |             |
|              | 1265*                               | 1264                                  | 222-5 (53+)           | 122-5 (16+) | 222-5 (12+) |             |
|              | 1234                                | 1235                                  | 227-5 (24+)           | 222-6 (19-) | 222-6 (12-) | 122-6 (9-)  |
|              | 1188                                | 1194                                  | 227-5 (36+)           | 122-4 (12+) | 012-8 (11-) | 222-4 (10+) |
|              | 1155                                | 1157                                  | 227-6 (24+)           | 012-5 (9+)  | 227-5 (9+)  | 2227-S(9-)  |
|              | 1092                                | 1102                                  | 2227-S(17+)           | 2222-S(14-) | 222-6 (12-) | 227-5 (8-)  |
|              | 1076                                | 1077                                  | 1222-S(24+)           | 2222-S(17-) | 227-6 (16+) | 222-5 (11-) |
|              | 1047                                | 1043                                  | 0122-S(61+)           | 1222-S(14-) |             |             |
|              | 1036                                | 1029                                  | 227-6 (22+)           | 2227-S(15-) | 222-6 (14-) | 2222-S(12+) |
|              | 962                                 | 965                                   | 2227-S(24+)           | 2222-S(21+) | 0122-S(16-) | 227-6 (12+) |
|              | 917                                 | 922                                   | 222-4 (25-)           | 012-8 (24-) | 122-6 (20-) | 222-6 (11-) |
|              | 904                                 | 908                                   | 012-5 (38-)           | 1222-S(26-) | 0122-S(9-)  |             |
|              | 808                                 | 808                                   | 227-4 (22+)           | 222-4 (17+) | 012-8 (17+) | 222-4 (15-) |
|              | 769                                 | 769                                   | 227-4 (45+)           | 122-4 (14-) | 222-4 (13+) |             |
|              | 727*                                | 731                                   | 222-4 (40+)           | 122-4 (39-) |             |             |
|              | 506                                 | 506                                   | 2270-S(98-)           | 227-D (22+) |             |             |
|              | 427                                 | 426                                   | 222-D (35+)           | 222-D (18+) | 227-D (9-)  | 2270-S(7-)  |
|              | 395                                 | 399                                   | 122-D (54+)           | 222-D (11+) | 222-D (10-) |             |
|              | 235                                 | 246                                   | 227-D (39+)           | 2227-T(17-) | 0122-T(15-) | 2222-T(11+) |
|              | 235*                                | 227                                   | 0122-T(79-)           |             |             |             |
|              | 194                                 | 191                                   | 222-D (49-)           | 122-D (30+) | 222-D (20+) | 2227-T(10-) |
|              |                                     | 120                                   | 1222-T(57-)           | 227-D (9+)  | 2227-T(8+)  |             |
|              |                                     | 82                                    | 2222-T(58+)           | 2227-T(17+) | 1222-T(15+) |             |
|              |                                     | 52                                    | 2227-T(29+)           | 227-D (20+) | 2222-T(14-) | 1222-T(11+) |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2999 2963 2963 2962 2911 2905 2899 2880 2875 2869  
2864

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).



No. 177

Molecule: 122227-TGT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-gauche-trans form)Symmetry  $\text{C}_1$ Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1481*                               | 1488                                  | 222-2 (39+)           | 122-2 (27-) | 222-2 (16+) |             |
|              | 1474*                               | 1472                                  | 222-2 (50+)           | 122-2 (23+) | 012-4 (14+) |             |
|              | 1466*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1460*                               | 1458                                  | 222-2 (45+)           | 222-2 (25-) | 012-4 (22+) |             |
|              | 1443*                               | 1452                                  | 122-2 (44+)           | 012-4 (40-) |             |             |
|              | 1427                                | 1422                                  | 227-2 (88+)           |             |             |             |
|              | 1380*                               | 1380                                  | 012-2 (103+)          |             |             |             |
|              | 1365*                               | 1365                                  | 222-5 (45-)           | 122-5 (36+) | 1222-S(16+) |             |
|              | 1331*                               | 1335                                  | 222-5 (68+)           | 2227-S(12+) | 222 6 (10 ) |             |
|              | 1303*                               | 1302                                  | 122-5 (31+)           | 222-5 (19+) | 222-6 (14+) | 222-6 (11+) |
|              | 1296                                | 1294                                  | 122-6 (45-)           | 222-6 (11+) | 122-5 ( 9-) | 222-5 ( 9-) |
|              | 1251                                | 1252                                  | 222-6 (46-)           | 222-5 (11+) | 227-6 (10+) | 227-4 ( 3+) |
|              | 1234*                               | 1232                                  | 222-6 (30-)           | 012-8 (13+) | 122-6 (11-) | 122-4 (10-) |
|              | 1188*                               | 1187                                  | 227-5 (77+)           |             |             |             |
|              | 1155*                               | 1166                                  | 227-6 (23-)           | 222-4 (11-) | 012-5 (10-) | 227-5 ( 6-) |
|              | 1104*                               | 1103                                  | 222-5 (14+)           | 2227-S(12-) | 222-4 (10 ) | 1222 S( 8+) |
|              | 1076*                               | 1078                                  | 2222-S(38-)           | 1222-S(23+) | 2227-S(16+) |             |
|              | 1052*                               | 1054                                  | 227-6 (40-)           | 222-6 (15-) | 012-5 (13+) | 0122-S( 8-) |
|              | 1025                                | 1022                                  | 0122-S(66+)           | 2222-S(15-) |             |             |
|              | 962*                                | 968                                   | 2227-S(31+)           | 222-6 (13+) | 012-8 (11+) | 122-6 (11+) |
|              | 943                                 | 937                                   | 222-4 (25+)           | 012-5 (18-) | 227-6 (15-) | 227-4 (13+) |
|              | 850                                 | 848                                   | 222-4 (23+)           | 012-8 (20+) | 2227-S(11-) | 1222-S(11-) |
|              | 837                                 | 837                                   | 1222-S(27+)           | 227-4 (17+) | 012-5 (11+) | 222-4 ( 9+) |
|              | 752                                 | 744                                   | 122-4 (49+)           | 222-4 (17-) | 012-8 (13+) | 227-4 (13-) |
|              | 722                                 | 721                                   | 227-4 (43-)           | 222-4 (28+) |             |             |
|              | 602                                 | 598                                   | 2270-S(57-)           | 222-D (27+) | 227-D (18+) |             |
|              | 453                                 | 457                                   | 222-D (27-)           | 122-D (22-) | 2270-S(22+) |             |
|              | 282                                 | 292                                   | 122-D (55+)           | 222-D (22-) | 222-D (16+) |             |
|              | 253                                 | 255                                   | 0122-T(22-)           | 222-D (18-) | 2222-T(17+) | 222-D (16-) |
|              |                                     | 221                                   | 0122-T(71+)           |             |             |             |
|              | 194*                                | 188                                   | 227-D (80+)           | 227-5 (11-) |             |             |
|              |                                     | 107                                   | 2222-T(67-)           | 1222-T(15-) | 2227-T(10-) |             |
|              |                                     | 76                                    | 1222-T(58+)           | 222-D (16-) |             |             |
|              |                                     | 66                                    | 2227-T(64+)           | 222-D (13-) | 222-4 (11+) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2998 2963 2963 2962 2910 2905 2900 2880 2873 2869  
2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 178

Molecule: 122227-GTT  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (gauche-trans-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1481*                               | 1485                                  | 122-2 (40+)           | 222-2 (38+) | 222-2 (10-) |             |
|              | 1474*                               | 1474                                  | 222-2 (28+)           | 122-2 (23+) | 012-4 (20+) | 222-2 (18-) |
|              | 1466*                               | 1464                                  | 012-7 (65+)           | 222-2 (14+) | 012-8 (12+) |             |
|              | 1460*                               | 1460                                  | 222-2 (39-)           | 222-2 (17-) | 012-4 (17+) | 012-7 (14+) |
|              | 1443*                               | 1452                                  | 012-4 (42-)           | 122-2 (28+) | 222-2 (15-) |             |
|              | 1427                                | 1420                                  | 227-2 (85+)           |             |             |             |
|              | 1380*                               | 1381                                  | 012-2 (101+)          |             |             |             |
|              | 1365*                               | 1361                                  | 222-5 (50+)           | 222-5 (28-) | 2222-S(13+) |             |
|              | 1342*                               | 1344                                  | 122-5 (67+)           | 1222-S(13+) |             |             |
|              | 1303*                               | 1298                                  | 222-6 (29-)           | 222-6 (24+) | 222-5 (14+) | 122-6 (10-) |
|              | 1296                                | 1289                                  | 222-5 (27-)           | 222-6 (22+) | 122-6 (15+) | 222-5 (11-) |
|              | 1251                                | 1260                                  | 122-6 (36-)           | 222-5 (14-) | 012-8 (10+) | 012-7 (7-)  |
|              | 1234*                               | 1233                                  | 222-6 (24+)           | 222-6 (23+) | 227-6 (19-) | 222-4 (8-)  |
|              | 1188*                               | 1183                                  | 227-5 (54+)           | 227-6 (6-)  | 222-5 (6+)  | 122-4 (6+)  |
|              | 1155*                               | 1165                                  | 227-5 (27+)           | 227-6 (12+) | 012-5 (11+) | 222-4 (9+)  |
|              | 1104*                               | 1105                                  | 2222-S(22+)           | 122-4 (11+) | 012-8 (11-) | 222-5 (11-) |
|              | 1076*                               | 1083                                  | 1222-S(30-)           | 0122-S(22+) | 2227-S(8-)  | 2222-S(7+)  |
|              | 1036*                               | 1040                                  | 227-6 (38-)           | 222-6 (14-) | 222-6 (12-) | 0122-S(12-) |
|              | 1025                                | 1021                                  | 2227-S(54+)           | 0122-S(15+) | 2222-S(9-)  |             |
|              | 962*                                | 967                                   | 2222-S(35+)           | 012-5 (15-) | 012-8 (13+) | 122-6 (12+) |
|              | 943                                 | 937                                   | 222-4 (20+)           | 0122-S(12+) | 227-6 (12-) | 227-4 (12+) |
|              | 875                                 | 883                                   | 1222-S(31-)           | 0122-S(28-) | 012-5 (19-) |             |
|              | 808*                                | 805                                   | 222-4 (30-)           | 227-4 (20+) | 122-4 (15+) | 012-8 (12+) |
|              | 752                                 | 759                                   | 122-4 (44-)           | 012-8 (20-) | 222-4 (15-) | 227-4 (13+) |
|              | 722                                 | 721                                   | 222-4 (42+)           | 227-4 (41-) | 2227-T(11-) |             |
|              | 592*                                | 590                                   | 2270-S(69+)           | 222-D (19-) | 227-D (11-) |             |
|              | 453                                 | 449                                   | 122-D (40+)           | 222-D (36-) | 227-D (13+) |             |
|              | 326*                                | 321                                   | 122-D (40-)           | 222-D (20-) | 227-D (12+) |             |
|              | 253                                 | 253                                   | 222-D (42+)           | 2270-S(28+) | 0122-T(9-)  |             |
|              |                                     | 215                                   | 0122-T(66-)           | 227-D (20-) |             |             |
|              |                                     | 156                                   | 1222-T(41-)           | 2227-T(22+) | 227-D (13+) |             |
|              |                                     | 111                                   | 227-D (32-)           | 2227-T(31+) | 222-D (19-) | 222-D (15+) |
|              |                                     | 98                                    | 2222-T(79+)           | 1222-T(10+) |             |             |
|              |                                     | 65                                    | 1222-T(32+)           | 2227-T(30+) | 222-D (8+)  | 227-D (8+)  |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 2998 | 2963 | 2963 | 2962 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 179

Molecule: 122227-TGG  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1481*                               | 1490                                  | 222-2 (37+)           | 222-2 (26+) | 122-2 (20-) |             |
|              | 1474*                               | 1475                                  | 222-2 (44+)           | 122-2 (29+) | 012-4 (14+) |             |
|              | 1466*                               | 1463                                  | 012-7 (81+)           | 012-8 (14+) |             |             |
|              | 1460*                               | 1459                                  | 222-2 (50+)           | 012-4 (24+) | 222-2 (14-) |             |
|              | 1443*                               | 1451                                  | 122-2 (44+)           | 012-4 (40-) |             |             |
|              | 1427                                | 1429                                  | 227-2 (73+)           | 222-2 (10-) |             |             |
|              | 1380*                               | 1380                                  | 012-2 (102+)          |             |             |             |
|              | 1365*                               | 1366                                  | 222-5 (43-)           | 122-5 (32+) | 1222-S(15+) |             |
|              | 1350                                | 1348                                  | 222-5 (60+)           | 2222-S(11-) |             |             |
|              | 1303*                               | 1301                                  | 122-5 (29+)           | 222-5 (18+) | 222-6 (15+) | 222-6 (12+) |
|              | 1296                                | 1295                                  | 122-6 (43-)           | 222-6 (12+) | 122-5 (10-) | 222-5 (9-)  |
|              | 1251                                | 1255                                  | 222-6 (36-)           | 222-5 (12+) | 227-5 (10+) | 227-6 (8-)  |
|              | 1234*                               | 1236                                  | 222-6 (29+)           | 227-5 (20+) | 122-6 (12+) | 012-8 (11-) |
|              | 1188*                               | 1189                                  | 227-5 (46+)           | 2227-S(11-) | 222-6 (8+)  | 122-4 (8-)  |
|              | 1137                                | 1144                                  | 227-6 (26-)           | 1222-S(14-) | 012-5 (11+) | 222-D (5+)  |
|              | 1104*                               | 1112                                  | 2222-S(32-)           | 2227-S(19+) | 222-6 (7-)  | 222-4 (6+)  |
|              | 1068                                | 1067                                  | 227-5 (15+)           | 222-5 (15-) | 222-6 (14-) | 012-8 (8-)  |
|              | 1052*                               | 1052                                  | 227-6 (42+)           | 1222-S(17-) | 222-6 (10-) | 012-5 (10+) |
|              | 1025                                | 1027                                  | 0122-S(72+)           |             |             |             |
|              | 952                                 | 954                                   | 012-5 (18-)           | 222-4 (13+) | 2227-S(11+) | 227-6 (10+) |
|              | 924                                 | 923                                   | 012-8 (20+)           | 222-4 (18-) | 122-6 (17+) | 2227-S(11+) |
|              | 850                                 | 853                                   | 227-4 (28-)           | 1222-S(18+) | 222-4 (11+) | 2227-S(8-)  |
|              | 842                                 | 844                                   | 1222-S(17+)           | 012-5 (15+) | 2227-S(14+) | 222-4 (13-) |
|              | 768*                                | 771                                   | 227-4 (29+)           | 122-4 (28+) | 012-8 (14+) | 222-4 (12+) |
|              | 727*                                | 726                                   | 122-4 (34+)           | 222-4 (33-) | 227-4 (14-) |             |
|              | 525                                 | 516                                   | 2270-S(70+)           | 227-D (21-) | 222-D (17+) |             |
|              | 458                                 | 463                                   | 2270-S(28-)           | 222-D (21-) | 222-D (18+) | 122-D (10-) |
|              | 355                                 | 352                                   | 222-D (33+)           | 122-D (23+) | 227-D (13-) | 2270-S(5-)  |
|              | 282                                 | 295                                   | 122-D (44+)           | 222-D (22-) | 2227-T(15-) | 227-D (14+) |
|              |                                     | 230                                   | 0122-T(91-)           |             |             |             |
|              |                                     | 179                                   | 227-D (34-)           | 222-D (30-) | 222-D (15-) |             |
|              |                                     | 125                                   | 227-D (24+)           | 1222-T(23+) | 2227-T(20+) | 2222-T(16-) |
|              |                                     | 88                                    | 1222-T(52-)           | 2222-T(35-) |             |             |
|              |                                     | 39                                    | 2227-T(45-)           | 2222-T(25-) | 1222-T(10+) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 2999 | 2963 | 2963 | 2962 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 180

Molecule: 122227-GTG CH3CH2CH2CH2CH2I (gauche-trans-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |  |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|--|
| a            | 1481*                               | 1485                                  | 222-2 (38+)           | 122-2 (32+) | 222-2 (19-) |             |  |
|              | 1474*                               | 1476                                  | 222-2 (34+)           | 122-2 (30+) | 012-4 (18+) |             |  |
|              | 1466*                               | 1465                                  | 012-7 (51+)           | 222-2 (15+) | 222-2 (12+) |             |  |
|              | 1460*                               | 1461                                  | 012-7 (29+)           | 222-2 (21-) | 222-2 (19-) | 012-4 (18+) |  |
|              | 1443*                               | 1452                                  | 012-4 (41-)           | 122-2 (29+) | 222-2 (17-) |             |  |
|              | 1427                                | 1429                                  | 227-2 (74+)           |             |             |             |  |
|              | 1380*                               | 1381                                  | 012-2 (97+)           |             |             |             |  |
|              | 1365*                               | 1366                                  | 222-5 (38+)           | 222-5 (34-) | 2222-S(13+) |             |  |
|              | 1342*                               | 1344                                  | 122-5 (71+)           | 1222-S(11+) |             |             |  |
|              | 1303*                               | 1303                                  | 222-5 (26+)           | 222-5 (21+) | 122-6 (16-) | 222-6 (14-) |  |
|              | 1296                                | 1292                                  | 222-6 (36+)           | 222-6 (19-) | 222-5 ( 8-) | 222-5 ( 7-) |  |
|              | 1265*                               | 1263                                  | 122-6 (42+)           | 222-5 (14+) | 012-8 (10-) | 012-7 ( 7+) |  |
|              | 1234*                               | 1232                                  | 227-5 (29+)           | 222-6 (24-) | 222-6 (12-) | 227-6 ( 7-) |  |
|              | 1188*                               | 1188                                  | 227-5 (39+)           | 2227-S(12-) | 222-6 ( 8+) | 222-4 ( 7+) |  |
|              | 1137                                | 1143                                  | 227-6 (28+)           | 012-5 (10-) | 2222-S(10-) | 222-5 ( 5-) |  |
|              | 1104*                               | 1101                                  | 2227-S(17-)           | 2222-S(15+) | 222-6 (11+) | 227-5 ( 8+) |  |
|              | 1076*                               | 1084                                  | 1222-S(33+)           | 0122-S(22-) | 122-5 ( 8-) | 2222-S( 7-) |  |
|              | 1047*                               | 1049                                  | 227-6 (38+)           | 012-5 ( 9+) | 222-5 ( 8-) | 012-8 ( 8-) |  |
|              | 1025                                | 1016                                  | 2227-S(30+)           | 0122-S(23+) | 222-6 ( 8+) | 222-6 ( 7+) |  |
|              | 952                                 | 954                                   | 2222-S(20+)           | 012-5 (19-) | 227-6 (12+) | 222-4 (12+) |  |
|              | 924                                 | 922                                   | 012-8 (19-)           | 222-4 (16+) | 122-6 (15-) | 2227-S(11-) |  |
|              | 885                                 | 891                                   | 0122-S(30+)           | 1222-S(25+) | 012-5 (19+) |             |  |
|              | 799                                 | 791                                   | 222-4 (31-)           | 222-4 (21+) | 122-4 (11+) | 012-8 ( 6+) |  |
|              | 782                                 | 784                                   | 227-4 (42+)           | 122-4 (26+) | 012-8 (17+) |             |  |
|              | 738                                 | 736                                   | 122-4 (24-)           | 222-4 (17-) | 227-4 (17+) | 2222-S(14+) |  |
|              | 506*                                | 508                                   | 2270-S(80+)           | 227-D (23-) |             |             |  |
|              | 481                                 | 477                                   | 222-D (26-)           | 122-D (23+) | 2270-S(20+) | 222-D (10-) |  |
|              | 355                                 | 348                                   | 122-D (52+)           | 222-D (26+) | 227-D (11-) |             |  |
|              | 282                                 | 282                                   | 0122-T(33+)           | 222-D (29+) | 222-D (19-) |             |  |
|              | 235*                                | 238                                   | 227-D (43+)           | 2227-T(26-) | 2222-T(10+) |             |  |
|              |                                     | 192                                   | 0122-T(60-)           | 222-D (23+) |             |             |  |
|              |                                     | 121                                   | 1222-T(53+)           | 222-D ( 9+) | 2227-T( 8-) | 222-D ( 7-) |  |
|              |                                     | 74                                    | 2227-T(50+)           | 1222-T(18+) | 227-D (14+) |             |  |
|              |                                     | 45                                    | 2222-T(69-)           | 227-D (15+) |             |             |  |

Calculated frequencies higher than 2000  $\text{cm}^{-1}$ 

|      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|
| 2999 | 2963 | 2963 | 2962 | 2910 | 2905 | 2900 | 2880 | 2873 | 2869 |
| 2865 |      |      |      |      |      |      |      |      |      |

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 181

Molecule: 122227-GTG' CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (gauche-trans-gauche' form)  
 Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1481*                               | 1485                                  | 222-2 (38+)           | 122-2 (32+) | 222-2 (18-) |             |
|              | 1474*                               | 1476                                  | 222-2 (34+)           | 122-2 (30+) | 012-4 (17+) |             |
|              | 1466*                               | 1464                                  | 012-7 (51+)           | 222-2 (15+) | 222-2 (12+) | 012-8 (10+) |
|              | 1460*                               | 1461                                  | 012-7 (28+)           | 222-2 (21-) | 222-2 (19-) | 012-4 (18+) |
|              | 1443*                               | 1452                                  | 012-4 (41+)           | 122-2 (29-) | 222-2 (18+) |             |
|              | 1427                                | 1429                                  | 227-2 (74+)           |             |             |             |
|              | 1380*                               | 1381                                  | 012-2 (97+)           |             |             |             |
|              | 1365*                               | 1366                                  | 222-5 (37+)           | 222-5 (34-) | 2222-S(13+) |             |
|              | 1342*                               | 1344                                  | 122-5 (70+)           | 1222-S(11+) |             |             |
|              | 1303*                               | 1302                                  | 222-5 (31+)           | 222-5 (23+) | 122-6 (18-) |             |
|              | 1296                                | 1294                                  | 222-6 (41+)           | 222-6 (25-) | 222-5 ( 6-) |             |
|              | 1265*                               | 1262                                  | 122-6 (44+)           | 222-5 (13+) | 012-8 (11-) | 012-7 ( 8+) |
|              | 1234*                               | 1233                                  | 227-5 (34+)           | 222-6 (24+) | 222-6 (12+) | 222-4 ( 6-) |
|              | 1175*                               | 1179                                  | 227-5 (23-)           | 012-5 (10+) | 222-4 (10+) | 222-6 ( 9+) |
|              | 1155*                               | 1158                                  | 227-6 (24+)           | 227-5 (18-) | 2227-S(15+) | 122-4 ( 8+) |
|              | 1104*                               | 1108                                  | 2222-S(26-)           | 1222-S(10+) | 2227-S( 9+) | 012-5 ( 8-) |
|              | 1068                                | 1066                                  | 0122-S(42+)           | 1222-S(24-) | 222-4 ( 4-) | 227-5 ( 4-) |
|              | 1047*                               | 1046                                  | 227-6 (37-)           | 012-8 (10-) | 122-6 ( 8-) | 222-5 ( 7-) |
|              | 1025                                | 1025                                  | 2227-S(28-)           | 012-5 (11-) | 222-6 (10+) | 2222-S(10+) |
|              | 943                                 | 942                                   | 2222-S(26+)           | 012-8 (17+) | 122-6 (15+) | 227-4 (11+) |
|              | 927*                                | 932                                   | 222-4 (26+)           | 012-5 (18-) | 222-4 (12+) | 122-5 (11-) |
|              | 885                                 | 891                                   | 0122-S(34-)           | 1222-S(25-) | 012-5 (16-) |             |
|              | 817                                 | 814                                   | 227-4 (24-)           | 012-8 (18+) | 122-4 (18+) | 222-4 (17-) |
|              | 752                                 | 752                                   | 227-4 (42-)           | 2222-S(15+) | 222-4 (14-) |             |
|              | 738                                 | 747                                   | 122-4 (37+)           | 222-4 (26+) | 012-8 (14+) | 222-4 (12-) |
|              | 506*                                | 505                                   | 2270-S(93-)           | 227-D (22+) |             |             |
|              | 481                                 | 474                                   | 222-D (28+)           | 122-D (25-) | 222-D (15+) | 012-5 ( 5+) |
|              | 355                                 | 365                                   | 122-D (49-)           | 222-D (20-) | 227-D (13+) |             |
|              | 282                                 | 277                                   | 0122-T(35-)           | 222-D (28-) | 222-D (23+) |             |
|              | 235*                                | 238                                   | 227-D (38+)           | 2227-T(32+) | 222-D ( 9+) |             |
|              |                                     | 192                                   | 0122-T(60+)           | 222-D (24-) |             |             |
|              |                                     | 112                                   | 1222-T(46-)           | 227-D (12-) | 122-D ( 9-) | 2222-T( 8+) |
|              |                                     | 65                                    | 2227-T(37-)           | 227-D (22+) | 222-4 (11-) | 2222-T(10+) |
|              |                                     | 51                                    | 2222-T(60+)           | 1222-T(18+) | 2227-T(12+) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2999 2963 2963 2962 2910 2905 2900 2880 2873 2869  
 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. H. Matsuura, S. Imazeki, Y. Ogawa, M. Sakakibara, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **52**, 2512 (1979).

## No. 182

Molecule: 72227-TT ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (trans-trans form)Symmetry C<sub>2v</sub> Symmetry number  $\sigma = 2$ 

| Sym. species   | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|----------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a <sub>1</sub> | 1456                                | 1467                                  | 222-2 (94+)           |             |             |             |
|                | 1418                                | 1411                                  | 227-2 (45+)           | 722-2 (45+) |             |             |
|                | 1209                                | 1202                                  | 722-5 (50-)           | 227-5 (50+) |             |             |
|                | 1019                                | 1024                                  | 7222-S(34-)           | 2227-S(34-) | 222-D (12+) |             |
|                | 646                                 | 644                                   | 222-D (30+)           | 0722-S(30-) | 2270-S(30-) |             |
|                | 195                                 | 200                                   | 222-D (47+)           | 2270-S(23+) | 0722-S(23+) |             |
|                | 82                                  | 74                                    | 227-D (47+)           | 722-D (47+) | 222-D (13-) |             |
|                |                                     |                                       |                       |             |             |             |
| a <sub>2</sub> | 1252(s)                             | 1264                                  | 222-6 (76+)           |             |             |             |
|                | 1040                                | 1059                                  | 227-6 (45+)           | 722-6 (45+) | 222-6 (13+) |             |
|                | 761                                 | 757                                   | 227-4 (47+)           | 722-4 (47-) | 222-6 (13+) |             |
|                |                                     | 135                                   | 2227-T(47+)           | 7222-T(47+) |             |             |
| b <sub>1</sub> | 1435                                | 1430                                  | 722-2 (44-)           | 227-2 (44+) |             |             |
|                | 1311                                | 1313                                  | 222-5 (79+)           | 7222-S(11-) | 2227-S(11+) |             |
|                | 1152                                | 1151                                  | 227-5 (42+)           | 722-5 (42+) | 222-5 (25+) |             |
|                | 1040                                | 1025                                  | 2227-S(46+)           | 7222-S(46-) |             |             |
|                | 521                                 | 516                                   | 2270-S(52+)           | 0722-S(52-) | 227-D (10-) | 722-D (10+) |
|                | 289                                 | 296                                   | 722-D (49-)           | 227-D (49+) |             |             |
| b <sub>2</sub> | 1209                                | 1208                                  | 722-6 (29+)           | 227-6 (29-) | 222-4 (20-) |             |
|                | 960                                 | 941                                   | 222-4 (27+)           | 227-6 (19-) | 722-6 (19+) | 722-4 (17+) |
|                | 720                                 | 718                                   | 222-4 (44-)           | 722-4 (24+) | 227-4 (24+) | 7222-T(10-) |
|                |                                     | 95                                    | 7222-T(39+)           | 2227-T(39-) | 222-4 (12-) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2999 2998 2963 2962 2904 2869

## Reference

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torggrimsen, J. Mol. Struct., **15**, 61 (1973).

No. 183

Molecule: 72227-TG  $\text{ICH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1456*                               | 1472                                  | 222-2 (88+)           |             |             |             |
|              | 1423*                               | 1429                                  | 227-2 (75+)           |             |             |             |
|              | 1423*                               | 1421                                  | 722-2 (86+)           |             |             |             |
|              | 1333                                | 1334                                  | 222-5 (73+)           | 7222-S(12-) |             |             |
|              | 1275*                               | 1267                                  | 222-6 (65-)           | 227-5 (11+) |             |             |
|              | 1195*                               | 1208                                  | 227-5 (47+)           | 722-6 (20-) | 222-4 (11+) |             |
|              | 1188                                | 1188                                  | 722-5 (80-)           |             |             |             |
|              | 1141                                | 1135                                  | 227-5 (26+)           | 2227-S(22-) | 722-6 (15+) | 227-6 (15+) |
|              | 1082                                | 1095                                  | 227-6 (30+)           | 7222-S(22-) | 722-6 (15-) | 222-6 (11-) |
|              | 1040                                | 1035                                  | 2227-S(30+)           | 7222-S(20-) | 722-6 (19+) | 227-6 (11-) |
|              | 960                                 | 969                                   | 7222-S(24+)           | 227-6 (23+) | 2227-S(18+) | 227-4 (11-) |
|              | 938*                                | 928                                   | 222-4 (34+)           | 722-4 (19+) | 722-6 (18+) | 2227-S(12-) |
|              | 794                                 | 795                                   | 227-4 (62+)           | 7222-S(14+) |             |             |
|              | 732*                                | 733                                   | 722-4 (60+)           | 222-4 (27-) |             |             |
|              | 600                                 | 588                                   | 0722-S(62-)           | 222-D (25+) | 722-D (17+) | 227-4 (10-) |
|              | 503                                 | 504                                   | 2270-S(97-)           | 227-D (18+) |             |             |
|              | 340                                 | 338                                   | 227-D (32+)           | 0722-S(28-) | 222-D (27-) |             |
|              | 220                                 | 229                                   | 2227-T(31+)           | 222-D (21-) | 227-D (21-) | 722-D (12+) |
|              | 195                                 | 185                                   | 722-D (78+)           | 722-5 (11+) |             |             |
|              |                                     | 95                                    | 2227-T(46+)           | 7222-T(37+) |             |             |
|              |                                     | 45                                    | 7222-T(36-)           | 227-D (34+) | 222-4 (14+) | 2227-T(11+) |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2998 2998 2963 2963 2904 2869

\* Not used in the force constant determination.

## Reference

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torggrimsen, J. Mol. Struct., **15**, 61 (1973).

## No. 184

Molecule: 72227-GG ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (gauche-gauche form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency<br>cm <sup>-1</sup> | Calculated frequency<br>cm <sup>-1</sup> | Assignment<br>(P.E.D. %) |             |             |             |
|--------------|----------------------------------------|------------------------------------------|--------------------------|-------------|-------------|-------------|
| a            | 1456                                   | 1478                                     | 222-2 (82+)              |             |             |             |
|              | 1418                                   | 1423                                     | 227-2 (38+)              | 722-2 (38+) | 222-2 (14-) |             |
|              | 1275                                   | 1267                                     | 222-6 (57+)              | 722-5 (11+) | 227-5 (11-) |             |
|              | 1195                                   | 1185                                     | 227-5 (30+)              | 722-5 (30-) | 722-6 (11+) | 227-6 (11+) |
|              | 1101                                   | 1093                                     | 222-6 (30-)              | 722-6 (25+) | 227-6 (25+) |             |
|              | 938                                    | 933                                      | 7222-S(19+)              | 2227-S(19+) | 227-4 (14-) | 722-4 (14+) |
|              | 824                                    | 822                                      | 722-4 (22-)              | 227-4 (22+) | 2227-S(19+) | 7222-S(19+) |
|              | 535                                    | 526                                      | 0722-S(41-)              | 2270-S(41-) | 222-D (17-) | 722-D (15+) |
|              | 399                                    | 390                                      | 222-D (58-)              | 2270-S(12+) | 0722-S(12+) |             |
|              | 170                                    | 159                                      | 227-D (41+)              | 722-D (41+) | 222-D (13+) |             |
|              |                                        | 27                                       | 7222-T(42+)              | 2227-T(42+) |             |             |
| b            | 1423                                   | 1436                                     | 722-2 (38-)              | 227-2 (38+) |             |             |
|              | 1342                                   | 1348                                     | 222-5 (67+)              | 227-2 (9-)  |             |             |
|              | 1209                                   | 1212                                     | 722-5 (36+)              | 227-5 (36+) | 7222-S(12+) | 2227-S(12-) |
|              | 1094                                   | 1093                                     | 2227-S(29-)              | 7222-S(29+) | 222-4 (13-) |             |
|              | 1072                                   | 1073                                     | 227-6 (30+)              | 722-6 (30-) | 222-5 (19-) |             |
|              | 917                                    | 928                                      | 222-4 (49-)              | 722-4 (7+)  | 227-4 (7+)  | 227-5 (6+)  |
|              | 732                                    | 739                                      | 227-4 (40+)              | 722-4 (40+) | 222-4 (12+) | 222-5 (10-) |
|              | 491                                    | 496                                      | 2270-S(49-)              | 0722-S(49+) |             |             |
|              | 289                                    | 294                                      | 722-D (27+)              | 227-D (27-) | 7222-T(17-) | 2227-T(17+) |
|              |                                        | 116                                      | 2227-T(26+)              | 7222-T(26-) | 722-D (22-) | 227-D (22+) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

3000 2997 2963 2962 2904 2869

## Reference

- [1] IR.R. J. Thorbjørnsrud, O. H. Ellestad, P. Klaboe, and T. Torggrimsen,  
J. Mol. Struct., **15**, 61 (1973).



## No. 185

Molecule: 722227-TTT ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (trans-trans-trans form)Symmetry C<sub>2h</sub> Symmetry number  $\sigma = 2$ 

| Sym. species   | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|----------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a <sub>g</sub> | 1448*                               | 1460                                  | 222-2 (43+)           | 222-2 (43+) |             |             |
|                | 1425*                               | 1417                                  | 227-2 (40+)           | 722-2 (40+) |             |             |
|                | 1341                                | 1350                                  | 222-5 (46+)           | 222-5 (46-) | 2222-S(13+) |             |
|                | 1189                                | 1187                                  | 722-5 (48-)           | 227-5 (48+) |             |             |
|                | 1052                                | 1053                                  | 7222-S(34-)           | 2227-S(34-) | 222-D (6+)  |             |
|                | 1046                                | 1038                                  | 2222-S(82-)           |             |             |             |
|                | 603                                 | 607                                   | 2270-S(33+)           | 0722-S(33+) | 222-D (10-) | 222-D (10-) |
|                | 305                                 | 313                                   | 222-D (21+)           | 222-D (21+) | 722-D (19-) | 227-D (19-) |
|                | 111                                 | 106                                   | 227-D (33+)           | 722-D (33+) | 2222-S (7+) |             |
|                | 1246*                               | 1246                                  | 222-6 (30+)           | 222-6 (30+) | 722-6 (10-) | 227-6 (10-) |
| a <sub>u</sub> | 1060                                | 1063                                  | 722-6 (36+)           | 227-6 (36+) | 222-6 (17+) | 222-6 (17+) |
|                | 830                                 | 830                                   | 722-4 (26-)           | 227-4 (26+) | 222-4 (16+) | 222-4 (16-) |
|                | 725                                 | 720                                   | 222-4 (28-)           | 222-4 (28-) | 227-4 (18-) | 722-4 (18+) |
|                |                                     | 127                                   | 2222-T(83+)           |             |             |             |
|                |                                     | 44                                    | 2227-T(35+)           | 7222-T(35+) | 222-4 (8+)  |             |
| b <sub>g</sub> | 1300                                | 1297                                  | 222-6 (41+)           | 222-6 (41-) |             |             |
|                | 1189                                | 1196                                  | 227-6 (25-)           | 722-6 (25+) | 222-4 (15-) | 222-4 (15-) |
|                | 1001                                | 976                                   | 227-6 (24-)           | 722-6 (24+) | 222-4 (16+) | 222-4 (16+) |
|                | 725*                                | 728                                   | 722-4 (35-)           | 227-4 (35-) | 222-4 (13+) | 222-4 (13+) |
| b <sub>u</sub> |                                     | 153                                   | 2227-T(44+)           | 7222-T(44-) |             |             |
|                |                                     | 1476                                  | 222-2 (49-)           | 222-2 (49+) |             |             |
|                | 1425*                               | 1422                                  | 722-2 (45-)           | 227-2 (45-) |             |             |
|                | 1285                                | 1276                                  | 222-5 (36+)           | 222-5 (36+) | 722-5 (14-) | 227-5 (14-) |
|                | 1158                                | 1161                                  | 227-5 (35+)           | 722-5 (35+) | 222-5 (17+) | 222-5 (17+) |
|                | 1013                                | 1004                                  | 2227-S(40+)           | 7222-S(40-) |             |             |
|                | 576                                 | 576                                   | 0722-S(37+)           | 2270-S(37-) | 722-D (15-) | 227-D (15+) |
|                | 316                                 | 327                                   | 722-D (19-)           | 227-D (19+) | 0722-S(14-) | 2270-S(14+) |
|                |                                     | 77                                    | 222-D (34-)           | 222-D (34+) | 722-D (25-) | 227-D (25+) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2998 2998 2963 2962 2909 2900 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. M. Sakakibara, H. Matsuura, and H. Murata, J. Mol. Struct., **55**, 21 (1979).

## No. 186

Molecule: 722227-TTG ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (trans-trans-gauche form)Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1479                                  | 222-2 (59+)           | 222-2 (33-) |             |             |
|              | 1448*                               | 1460                                  | 222-2 (61+)           | 222-2 (27+) |             |             |
|              | 1425*                               | 1430                                  | 227-2 (72+)           |             |             |             |
|              | 1425*                               | 1419                                  | 722-2 (81-)           |             |             |             |
|              | 1359                                | 1359                                  | 222-5 (51-)           | 222-5 (32+) | 2222-S(13+) |             |
|              | 1294                                | 1297                                  | 222-6 (39-)           | 222-6 (38+) |             |             |
|              | 1287                                | 1286                                  | 222-5 (49+)           | 222-5 (24+) | 722-5 (13-) |             |
|              | 1235                                | 1245                                  | 222-6 (31-)           | 222-6 (20-) | 227-5 (17+) | 722-6 (10+) |
|              | 1202                                | 1204                                  | 227-5 (42+)           | 722-6 (19-) | 222-4 (11+) |             |
|              | 1189                                | 1181                                  | 722-5 (72+)           |             |             |             |
|              | 1127                                | 1134                                  | 227-6 (20+)           | 227-5 (20+) | 2227-S(14-) | 722-5 (10-) |
|              | 1104                                | 1097                                  | 2222-S(26+)           | 227-6 (17-) | 222-6 (14+) | 722-6 (11+) |
|              | 1052                                | 1052                                  | 7222-S(22-)           | 2222-S(15+) | 722-6 (15-) | 2227-S(13-) |
|              | 1022                                | 1023                                  | 7222-S(46-)           | 227-6 (12-) | 722-6 (10+) | 2227-S( 7+) |
|              | 977                                 | 984                                   | 227-6 (26+)           | 2222-S(21+) | 722-6 (12+) | 222-4 (12+) |
|              | 965                                 | 963                                   | 2227-S(28-)           | 722-6 (11+) | 222-4 (10+) | 222-4 ( 8+) |
|              | 820                                 | 823                                   | 222-4 (26+)           | 722-4 (22-) | 227-4 (20-) | 222-4 (12-) |
|              | 772                                 | 774                                   | 227-4 (52+)           | 222-4 (15+) | 722-4 (10-) |             |
|              | 725                                 | 722                                   | 722-4 (46-)           | 222-4 (41+) | 7222-T(11+) |             |
|              | 596                                 | 593                                   | 0722-S(68+)           | 222-D (20-) | 722-D (11-) |             |
|              | 504                                 | 506                                   | 2270-S(93+)           | 227-D (22-) |             |             |
|              | 409                                 | 411                                   | 222-D (48+)           | 722-D (18-) | 0722-S(11+) |             |
|              | 263                                 | 264                                   | 227-D (22+)           | 222-D (16-) | 722-D (14-) | 0722-S(13-) |
|              | 219                                 | 231                                   | 227-D (24+)           | 222-D (20+) | 0722-S(14+) | 2227-T(12-) |
|              | 164                                 | 153                                   | 722-D (42-)           | 2227-T(21+) | 222-D (19+) | 227-D (13+) |
|              | 111*                                | 108                                   | 7222-T(39+)           | 2222-T(16-) | 722 D (14-) | 222-D ( 9-) |
|              |                                     | 87                                    | 2222-T(56+)           | 7222-T(20+) | 227-D (10-) | 2227-T(10+) |
|              |                                     | 31                                    | 2227-T(29+)           | 227-D (15+) | 7222-T(13+) | 222-D (11+) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2999 2998 2963 2963 2909 2900 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. M. Sakakibara, H. Matsuura, and H. Murata, J. Mol. Struct., **55**, 21 (1979).

## No. 187

Molecule: 722227-TGT  $\text{ICH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{I}$  (trans-gauche-trans form)Symmetry  $\text{C}_2$  Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1480                                  | 222-2 (47+)           | 222-2 (47+) |             |             |
|              | 1425*                               | 1423                                  | 227-2 (45+)           | 722-2 (45+) |             |             |
|              | 1332                                | 1328                                  | 222-5 (31-)           | 222-5 (31+) | 2222-S(11-) | 222-6 (11-) |
|              | 1262                                | 1257                                  | 222-6 (28-)           | 222-6 (28-) | 222-5 ( 7+) | 222-5 ( 7-) |
|              | 1197                                | 1195                                  | 722-5 (32-)           | 227-5 (32+) | 227-6 ( 8-) |             |
|              | 1148                                | 1142                                  | 722-6 (14+)           | 227-6 (14+) | 227-5 (12+) | 722-5 (12-) |
|              | 1067                                | 1067                                  | 2222-S(51-)           | 7222-S(20+) | 2227-S(20+) |             |
|              | 1001                                | 992                                   | 722-6 (19+)           | 227-6 (19+) | 2222-S(13+) | 222-4 ( 9+) |
|              | 892                                 | 893                                   | 7222-S(14-)           | 2227-S(14-) | 2222-S(13-) | 222-4 ( 8-) |
|              | 740                                 | 738                                   | 722-4 (32+)           | 227-4 (32-) | 222-4 (13-) | 222-4 (13+) |
|              | 572                                 | 576                                   | 2270-S(39-)           | 0722-S(39-) |             |             |
|              | 242                                 | 237                                   | 222-D (18-)           | 222-D (18-) | 2222-T(18+) | 7222-T(10-) |
|              | 141                                 | 136                                   | 722-D (36+)           | 227-D (36+) |             |             |
|              |                                     | 109                                   | 2222-T(60-)           | 2227-T(13-) | 7222-T(13-) |             |
|              |                                     | 48                                    | 7222-T(20-)           | 2227-T(20-) | 222-D (16+) | 222-D (16+) |
| b            | 1448*                               | 1460                                  | 222-2 (47-)           | 222-2 (47+) |             |             |
|              | 1425*                               | 1420                                  | 722-2 (44-)           | 227-2 (44+) |             |             |
|              | 1341                                | 1345                                  | 222-5 (41+)           | 222-5 (41+) |             |             |
|              | 1248                                | 1244                                  | 222-6 (30-)           | 222-6 (30+) | 722-6 ( 9+) | 227-6 ( 9-) |
|              | 1189                                | 1188                                  | 227-5 (45+)           | 722-5 (45+) |             |             |
|              | 1104                                | 1100                                  | 227-6 (21+)           | 722-6 (21-) | 222-6 ( 9-) | 222-6 ( 9+) |
|              | 1022                                | 1019                                  | 7222-S(23-)           | 2227-S(23+) | 227-6 (13-) | 722-6 (13+) |
|              | 870                                 | 871                                   | 722-4 (16+)           | 227-4 (16+) | 222-4 (15+) | 222-4 (15+) |
|              | 717                                 | 720                                   | 227-4 (28+)           | 722-4 (28+) | 222-4 (16-) | 222-4 (16-) |
|              | 612                                 | 611                                   | 0722-S(26+)           | 2270-S(26-) | 222-D (17-) | 222-D (17+) |
|              | 367                                 | 364                                   | 0722-S(26-)           | 2270-S(26+) | 222-D (18-) | 222-D (18+) |
|              | 242                                 | 239                                   | 722-D (46-)           | 227-D (46+) |             |             |
|              |                                     | 57                                    | 2227-T(39-)           | 7222-T(39+) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2998 2998 2963 2962 2907 2903 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. M. Sakakibara, H. Matsuura, and H. Murata, J. Mol. Struct., **55**, 21 (1979).

## No. 188

Molecule: 722227-TGG ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (trans-gauche-gauche form)Symmetry C<sub>1</sub> Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1484                                  | 222-2 (55+)           | 222-2 (35+) |             |             |
|              | 1448*                               | 1462                                  | 222-2 (58+)           | 222-2 (31-) |             |             |
|              | 1425*                               | 1429                                  | 227-2 (70+)           | 222-2 (10-) |             |             |
|              | 1425*                               | 1421                                  | 722-2 (87+)           |             |             |             |
|              | 1359                                | 1354                                  | 222-5 (59+)           | 222-5 (16+) |             |             |
|              | 1332                                | 1331                                  | 222-5 (55-)           | 2222-S(11-) | 222-6 (11-) | 222-5 (10+) |
|              | 1262                                | 1260                                  | 222-6 (33-)           | 222-6 (25-) | 222-5 ( 7+) | 227-6 ( 6-) |
|              | 1248                                | 1247                                  | 222-6 (29+)           | 227-5 (23+) | 222-6 (21-) |             |
|              | 1197                                | 1199                                  | 227-5 (39-)           | 722-5 (23-) | 722-6 (12-) |             |
|              | 1189                                | 1182                                  | 722-5 (63-)           | 227-5 ( 8+) |             |             |
|              | 1119                                | 1126                                  | 222-6 (18+)           | 227-6 (14-) | 7222-S(11-) | 2222-S(11+) |
|              | 1104                                | 1091                                  | 227-6 (31+)           | 722-6 (15-) | 2227-S(14-) | 2222-S( 7+) |
|              | 1083                                | 1081                                  | 2222-S(26+)           | 2227-S(15-) | 722-6 (14+) | 222-5 (11+) |
|              | 1022                                | 1018                                  | 7222-S(42-)           | 227-6 (27+) | 222-6 ( 9-) |             |
|              | 972                                 | 971                                   | 722-6 (27-)           | 222-4 (22+) | 722-4 (11+) | 2227-S( 9+) |
|              | 892                                 | 894                                   | 7222-S(21+)           | 222-4 (18+) | 227-4 (17-) | 2222-S(11+) |
|              | 859                                 | 865                                   | 2227-S(30-)           | 222-4 (12+) | 2222-S(12-) | 722-4 (11+) |
|              | 772                                 | 776                                   | 227-4 (43-)           | 722-4 (22+) | 222-4 (13+) |             |
|              | 717                                 | 718                                   | 722-4 (43+)           | 222-4 (36-) | 227-4 (10-) |             |
|              | 599                                 | 598                                   | 0722-S(61-)           | 222-D (26+) | 722-D (16+) |             |
|              | 504                                 | 507                                   | 2270-S(87+)           | 227-D (21-) |             |             |
|              | 416                                 | 414                                   | 222-D (53+)           | 0722-S(15-) | 2270-S(14-) |             |
|              | 305                                 | 302                                   | 227-D (27+)           | 222-D (21-) | 2227-T(15-) | 0722-S(14-) |
|              | 210                                 | 207                                   | 722-D (72+)           |             |             |             |
|              | 175                                 | 165                                   | 227-D (42-)           | 222-D (26-) | 722-D (15+) | 222-D (12-) |
|              | 128                                 | 121                                   | 2222-T(24-)           | 2227-T(21+) | 227-D (19+) | 222-4 (13+) |
|              |                                     | 86                                    | 7222-T(49+)           | 2222-T(38+) |             |             |
|              |                                     | 24                                    | 2227-T(39-)           | 7222-T(20+) | 2222-T(15-) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2999 2998 2963 2963 2907 2903 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. M. Sakakibara, H. Matsuura, and H. Murata, J. Mol. Struct., 55, 21 (1979).

## No. 189

Molecule: 722227-GTG ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (gauche-trans-gauche form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1448*                               | 1462                                  | 222-2 (43+)           | 222-2 (43+) |             |             |
|              | 1425*                               | 1431                                  | 227-2 (34+)           | 722-2 (34+) | 222-2 ( 5-) |             |
|              | 1368                                | 1365                                  | 222-5 (38+)           | 222-5 (38-) | 2222-S(13+) |             |
|              | 1235                                | 1246                                  | 222-6 (21+)           | 222-6 (21+) | 722-5 (16+) | 227-5 (16-) |
|              | 1189                                | 1174                                  | 227-5 (23+)           | 722-5 (23-) | 7222-S(13-) | 2227-S(13-) |
|              | 1119                                | 1121                                  | 2222-S(26-)           | 222-6 (14-) | 222-6 (14-) | 227-6 (11+) |
|              | 1052                                | 1047                                  | 2222-S(14-)           | 7222-S(14+) | 2227-S(14+) | 222-6 ( 9+) |
|              | 951                                 | 966                                   | 2222-S(20+)           | 722-6 (17+) | 227-6 (17+) | 722-4 (10+) |
|              | 793                                 | 804                                   | 222-4 (30-)           | 222-4 (30+) | 227-4 ( 7-) | 722-4 ( 7+) |
|              | 740                                 | 742                                   | 227-4 (23+)           | 722-4 (23-) | 2222-S(21+) | 222-4 (11+) |
|              | 504                                 | 512                                   | 0722-S(38+)           | 2270-S(38+) | 722-D (14-) | 227-D (14-) |
|              | 464                                 | 463                                   | 222-D (23-)           | 222-D (23-) | 2270-S(12+) | 0722-S(12+) |
|              | 219                                 | 219                                   | 227-D (23-)           | 722-D (23-) | 2222-T(20-) | 2227-T( 6+) |
|              |                                     | 66                                    | 7222-T(35+)           | 2227-T(35+) | 722-D ( 6+) |             |
|              |                                     | 23                                    | 2222-T(67-)           | 227-D (12+) | 722-D (12+) |             |
| b            |                                     | 1482                                  | 222-2 (45-)           | 222-2 (45+) |             |             |
|              | 1425*                               | 1428                                  | 722-2 (40+)           | 227-2 (40-) |             |             |
|              | 1294                                | 1300                                  | 222-5 (24+)           | 222-5 (24+) | 222-6 (15+) | 222-6 (15-) |
|              | 1287                                | 1295                                  | 222-6 (22-)           | 222-6 (22+) | 222-5 (13-) | 222-5 (13-) |
|              | 1202                                | 1206                                  | 722-5 (32+)           | 227-5 (32+) | 222-4 ( 8+) |             |
|              | 1104                                | 1097                                  | 722-6 (24+)           | 227-6 (24-) | 2227-S(10+) | 7222-S(10-) |
|              | 1031                                | 1033                                  | 2227-S(17+)           | 7222-S(17-) | 722-6 (14-) | 227-6 (14+) |
|              | 940                                 | 959                                   | 222-4 (16+)           | 222-4 (16+) | 2227-S(15-) | 7222-S(15+) |
|              | 793                                 | 798                                   | 722-4 (40+)           | 227-4 (40+) |             |             |
|              | 504                                 | 502                                   | 2270-S(50-)           | 0722-S(50+) |             |             |
|              | 281                                 | 278                                   | 222-D (30-)           | 222-D (30+) | 722-D (22-) | 227-D (22+) |
|              |                                     | 254                                   | 7222-T(23-)           | 2227-T(23+) | 722-D (14+) | 227-D (14-) |
|              |                                     | 97                                    | 2227-T(23-)           | 7222-T(23+) | 227-D (14-) | 722-D (14+) |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2999 2998 2963 2963 2909 2900 2873 2865

\* Not used in the force constant determination.

## Reference

- [1] IR.R. M. Sakakibara, H. Matsuura, and H. Murata, J. Mol. Struct., **55**, 21 (1979).

## No. 190

Molecule: 722227-GTG' ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (gauche-trans-gauche' form)Symmetry C<sub>i</sub> Symmetry number  $\sigma = 1$ 

| Sym. species   | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|----------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a <sub>g</sub> |                                     | 1462                                  | 222-2 (43+)           | 222-2 (43+) |             |             |
|                | 1425                                | 1431                                  | 227-2 (34+)           | 722-2 (34+) | 222-2 ( 5-) |             |
|                | 1368                                | 1366                                  | 222-5 (38+)           | 222-5 (38-) | 2222-S(13+) |             |
|                | 1287                                | 1297                                  | 222-6 (37-)           | 222-6 (37+) |             |             |
|                | 1197                                | 1209                                  | 227-5 (35+)           | 722-5 (35-) | 222-4 ( 7-) |             |
|                | 1189                                | 1162                                  | 722-6 (24-)           | 227-6 (24+) | 7222-S( 7+) | 2227-S( 7+) |
|                | 1083                                | 1089                                  | 2222-S(32-)           | 7222-S(15+) | 2227-S(15+) | 222-4 ( 6-) |
|                | 977                                 | 977                                   | 222-4 (19+)           | 222-4 (19+) | 227-6 (12+) | 722-6 (12-) |
|                | 940                                 | 962                                   | 2222-S(12+)           | 222-D (10-) | 222-D (10-) | 7222-S(10+) |
|                | 763                                 | 753                                   | 227-4 (30+)           | 722-4 (30+) | 2222-S(26-) |             |
|                | 504                                 | 500                                   | 2270-S(42-)           | 0722-S(42-) | 227-D (13+) | 722-D (13+) |
|                | 464                                 | 460                                   | 222-D (24-)           | 222-D (24-) | 2270-S(11+) | 0722-S(11+) |
|                | 235(s)                              | 234                                   | 2227-T(29+)           | 7222-T(29-) | 227-D (17+) | 722-D (17+) |
|                |                                     | 59                                    | 722-D (26+)           | 227-D (26+) | 2227-T(17-) | 7222-T(17+) |
| a <sub>u</sub> |                                     | 1482                                  | 222-2 (45-)           | 222-2 (45+) |             |             |
|                | 1425                                | 1427                                  | 722-2 (40-)           | 227-2 (40+) |             |             |
|                | 1295                                | 1298                                  | 222-5 (37+)           | 222-5 (37+) |             |             |
|                | 1235                                | 1245                                  | 222-6 (22+)           | 222-6 (22+) | 722-5 (17+) | 227-5 (17+) |
|                | 1140                                | 1141                                  | 227-5 (25-)           | 722-5 (25-) | 222-6 (16+) | 222-6 (16+) |
|                | 1060                                | 1059                                  | 722-6 (40+)           | 227-6 (40+) |             |             |
|                | 999                                 | 1001                                  | 2227-S(34+)           | 7222-S(34-) | 722-5 ( 4+) |             |
|                | 830                                 | 834                                   | 722-4 (27+)           | 227-4 (27-) | 222-4 (14-) | 222-4 (14+) |
|                | 746                                 | 761                                   | 222-4 (27-)           | 222-4 (27+) | 722-4 (15-) | 227-4 (15+) |
|                | 503                                 | 511                                   | 0722-S(47-)           | 2270-S(47+) | 722-D (10+) | 227-D (10-) |
|                |                                     | 295                                   | 722-D (28+)           | 227-D (28-) | 222-D (18+) | 222-D (18-) |
|                |                                     | 244                                   | 222-D (29+)           | 222-D (29-) | 2222-T(10+) | 722-D ( 9+) |
|                |                                     | 55                                    | 2227-T(18+)           | 7222-T(18+) | 2222-T(18-) | 222-4 ( 9+) |
|                |                                     | 37                                    | 2222-T(55+)           | 7222-T(17+) | 2227-T(17+) |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2999 2998 2963 2963 2909 2900 2873 2865

## Reference

- [1] IR.R. M. Sakakibara, H. Matsuura, and H. Murata, J. Mol. Struct., **55**, 21 (1979).

## No. 191

Molecule: 722227-GGG ICH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>I (gauche-gauche-gauche form)Symmetry C<sub>2</sub> Symmetry number  $\sigma = 2$ 

| Sym. species | Observed frequency cm <sup>-1</sup> | Calculated frequency cm <sup>-1</sup> | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1488                                  | 222-2 (43+)           | 222-2 (43+) |             |             |
|              | 1425*                               | 1429                                  | 227-2 (38+)           | 722-2 (38+) |             |             |
|              | 1341                                | 1341                                  | 222-5 (32-)           | 222-5 (32+) | 2222-S(14+) |             |
|              | 1262                                | 1264                                  | 222-6 (29+)           | 222-6 (29+) | 227-6 ( 5+) | 722-6 ( 5+) |
|              | 1197                                | 1207                                  | 227-5 (39+)           | 722-5 (39-) | 2227-S(10-) | 7222-S(10-) |
|              | 1119                                | 1123                                  | 2222-S(29-)           | 2227-S( 9+) | 7222-S( 9+) | 222-5 ( 6+) |
|              | 1052                                | 1053                                  | 227-6 (34+)           | 722-6 (34+) | 2222-S( 9+) |             |
|              | 972                                 | 970                                   | 222-4 (26-)           | 222-4 (26+) | 722-5 ( 8+) | 227-5 ( 8-) |
|              | 880                                 | 883                                   | 2222-S(17+)           | 7222-S(15+) | 2227-S(15+) | 722-4 (13+) |
|              | 763                                 | 760                                   | 722-4 (29-)           | 227-4 (29+) | 2222-S(29+) |             |
|              | 504                                 | 509                                   | 2270-S(47+)           | 0722-S(47+) | 227-D (11-) | 722-D (11-) |
|              | 349                                 | 351                                   | 222-D (20+)           | 222-D (20+) | 722-D (11-) | 227-D (11-) |
|              | 210                                 | 199                                   | 222-D (20+)           | 222-D (20+) | 7222-T(18-) | 2227-T(18-) |
|              |                                     | 89                                    | 227-D (34-)           | 722-D (34-) | 2222-T( 9+) |             |
|              |                                     | 24                                    | 2222-T(59+)           | 7222-T(16+) | 2227-T(16+) |             |
| b            | 1448*                               | 1465                                  | 222-2 (42+)           | 222-2 (42-) |             |             |
|              | 1425*                               | 1429                                  | 722-2 (35-)           | 227-2 (35+) | 222-2 ( 7+) |             |
|              | 1359                                | 1358                                  | 222-5 (37+)           | 222-5 (37+) |             |             |
|              | 1248                                | 1249                                  | 222-6 (22+)           | 222-6 (22-) | 722-5 (20+) | 227-5 (20+) |
|              | 1158                                | 1151                                  | 722-6 (21-)           | 227-6 (21+) | 7222-S(11+) | 2227-S(11-) |
|              | 1119                                | 1122                                  | 222-6 (23-)           | 222-6 (23+) | 227-5 (16+) | 722-5 (16+) |
|              | 1001                                | 1008                                  | 2227-S(16-)           | 7222-S(16+) | 227-6 (16-) | 722-6 (16+) |
|              | 887                                 | 887                                   | 722-4 (16-)           | 227-4 (16-) | 2227-S(13-) | 7222-S(13+) |
|              | 740                                 | 749                                   | 222-4 (23+)           | 222-4 (23+) | 227-4 (20+) | 722-4 (20+) |
|              | 504                                 | 515                                   | 0722-S(33-)           | 2270-S(33+) | 222-D (16-) | 222-D (16+) |
|              | 445                                 | 445                                   | 222-D (26-)           | 222-D (26+) | 2270-S(18-) | 0722-S(18+) |
|              | 242                                 | 245                                   | 722-D (44-)           | 227-D (44+) |             |             |
|              |                                     | 55                                    | 2227-T(36-)           | 7222-T(36+) |             |             |

Calculated frequencies higher than 2000 cm<sup>-1</sup>

2999 2998 2963 2963 2907 2903 2871 2867

\* Not used in the force constant determination.

## Reference

- [1] IR.R. M. Sakakibara, H. Matsuura, and H. Murata, J. Mol. Struct., **55**, 21 (1979).

## No. 192

Molecule: 13225-TT CH3OCH2CH2Cl (trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a'           |                                     | 1491                                  | 322-2 (93-)           |             |             |             |
|              | 1470                                | 1468                                  | 013-4 (84+)           | 013-5 (15+) |             |             |
|              | 1465                                | 1462                                  | 013-2 (104+)          |             |             |             |
|              | 1433                                | 1432                                  | 225-2 (90+)           |             |             |             |
|              | 1390                                | 1374                                  | 322-5 (86+)           |             |             |             |
|              | 1270                                | 1285                                  | 225-5 (91+)           |             |             |             |
|              | 1207                                | 1201                                  | 013-5 (59+)           | 1322-S(20-) | 013-4 (10-) | 322-5 (10+) |
|              | 1130                                | 1110                                  | 0132-S(63+)           | 1322-S(16-) | 3225-S(11+) |             |
|              | 1058                                | 1043                                  | 3225-S(60-)           | 0132-S(8+)  | 013-5 (6-)  |             |
|              | 963                                 | 960                                   | 1322-S(68-)           | 0132-S(23-) |             |             |
|              | 751                                 | 739                                   | 2250-S(80-)           |             |             |             |
|              | 438                                 | 447                                   | 132-B (66-)           | 225-D (19+) |             |             |
|              | 348                                 | 342                                   | 322-D (30+)           | 2250-S(19+) | 225-D (18+) | 3225-S(6+)  |
|              | 180                                 | 175                                   | 225-D (53+)           | 322-D (44-) | 132-B (23+) |             |
| a''          | 1451                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |             |
|              | 1302                                | 1286                                  | 322-6 (66+)           | 225-6 (20-) |             |             |
|              | 1221                                | 1224                                  | 225-6 (49+)           | 322-4 (21+) | 322-6 (14+) |             |
|              | 1154                                | 1152                                  | 013-8 (76+)           | 013-7 (11-) |             |             |
|              | 1043                                | 1039                                  | 322-4 (37+)           | 225-4 (36+) | 225-6 (19-) |             |
|              |                                     | 775                                   | 225-4 (57+)           | 322-4 (38-) | 322-6 (16+) |             |
|              | 229                                 | 222                                   | 0132-T(81-)           | 3225-T(14+) |             |             |
|              |                                     | 141                                   | 1322-T(44+)           | 3225-T(36+) | 0132-T(18+) |             |
|              |                                     | 107                                   | 1322-T(47+)           | 3225-T(40-) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 2989 2988 2964 2956 2865 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).



## No. 193

Molecule: 13225-TG  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Cl}$  (trans-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1486(s)                             | 1496                                  | 322-2 (85+)           |             |             |             |
|              | 1470                                | 1467                                  | 013-4 (84+)           | 013-5 (15+) |             |             |
|              | 1465                                | 1462                                  | 013-2 (104+)          |             |             |             |
|              | 1451                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |             |
|              | 1433                                | 1435                                  | 225-2 (77+)           | 322-2 (10-) |             |             |
|              | 1390                                | 1386                                  | 322-5 (82+)           |             |             |             |
|              | 1302                                | 1305                                  | 225-5 (67+)           | 322-6 (18-) |             |             |
|              | 1258                                | 1268                                  | 322-6 (47+)           | 225-5 (15+) | 225-6 (11+) |             |
|              | 1221                                | 1227                                  | 225-6 (30+)           | 013-5 (22+) | 1322-S(16-) | 322-6 (12-) |
|              | 1176                                | 1178                                  | 013-5 (36-)           | 225-6 (34+) | 322-5 (6-)  |             |
|              | 1154                                | 1152                                  | 013-8 (73+)           | 013-7 (11-) |             |             |
|              | 1130                                | 1115                                  | 0132-S(55+)           | 1322-S(18-) | 3225-S(13+) |             |
|              | 1058                                | 1045                                  | 3225-S(38+)           | 0132-S(22-) | 322-4 (19+) |             |
|              | 1005                                | 1014                                  | 225-4 (32+)           | 1322-S(24-) | 0132-S(12-) | 3225-S(10+) |
|              | 963                                 | 961                                   | 322-4 (40+)           | 3225-S(14-) | 225-5 (9-)  | 1322-S(9-)  |
|              | 816                                 | 812                                   | 1322-S(43-)           | 225-4 (42-) | 322-5 (11+) |             |
|              | 666                                 | 658                                   | 2250-S(95+)           |             |             |             |
|              | 507                                 | 513                                   | 322-D (31-)           | 132-B (25-) | 225-D (16+) |             |
|              | 329                                 | 324                                   | 132-B (52+)           | 225-D (30+) | 322-D (12-) |             |
|              | 272                                 | 270                                   | 322-D (32+)           | 3225-T(26-) | 225-D (24+) | 132-B (10-) |
|              | 229                                 | 211                                   | 0132-T(81-)           |             |             |             |
|              |                                     | 117                                   | 3225-T(55-)           | 1322-T(23-) | 0132-T(11-) |             |
|              |                                     | 95                                    | 1322-T(60+)           | 225-D (15-) | 3225-T(12-) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 2989 2988 2965 2955 2865 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 194

Molecule: 13225-GT CH3OCH2CH2Cl (gauche-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %)                           |
|--------------|-------------------------------------|---------------------------------------|-------------------------------------------------|
| a            |                                     | 1486                                  | 322-2 (96+)                                     |
|              | 1470                                | 1467                                  | 013-4 (84+) 013-5 (15+)                         |
|              | 1465                                | 1462                                  | 013-2 (103+)                                    |
|              | 1451                                | 1454                                  | 013-7 (86+) 013-8 (16+)                         |
|              | 1433                                | 1432                                  | 225-2 (88+)                                     |
|              | 1390                                | 1372                                  | 322-5 (85+)                                     |
|              | 1302                                | 1302                                  | 322-6 (71-)                                     |
|              | 1270                                | 1283                                  | 225-5 (91+)                                     |
|              | 1255                                | 1245                                  | 225-6 (58+) 322-4 (20+)                         |
|              | 1198                                | 1195                                  | 013-5 (55+) 1322-S(19-)                         |
|              | 1154                                | 1157                                  | 013-8 (80+) 013-7 (12-)                         |
|              | 1105                                | 1085                                  | 0132-S(41-) 1322-S(23+) 225-6 (12-) 322-6 (11-) |
|              | 1043                                | 1033                                  | 225-4 (28+) 322-4 (28+) 1322-S(14-) 225-6 (13-) |
|              | 1043                                | 1031                                  | 3225-S(80-)                                     |
|              | 923                                 | 929                                   | 1322-S(53-) 0132-S(44-)                         |
|              |                                     | 773                                   | 225-4 (56-) 322-4 (38+) 322-6 (16-)             |
|              | 751                                 | 750                                   | 2250-S(76-) 322-D (15+)                         |
|              | 463                                 | 457                                   | 132-B (64-) 322-D (22+) 2250-S(12+)             |
|              | 348                                 | 343                                   | 322-D (24-) 132-B (23-) 2250-S(13-) 1322-T( 8+) |
|              | 282                                 | 276                                   | 225-D (75+) 322-D (13-) 0132-T(12-)             |
|              |                                     | 180                                   | 0132-T(78+) 322-D (15-) 225-D (10+)             |
|              |                                     | 118                                   | 1322-T(85-)                                     |
|              |                                     | 104                                   | 3225-T(82+)                                     |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3005 2989 2988 2965 2956 2865 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 195

Molecule: 13225-GG  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Cl}$  (gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1491                                  | 322-2 (89+)           |             |             |             |
|              | 1470                                | 1467                                  | 013-4 (84+)           | 013-5 (15+) |             |             |
|              | 1465                                | 1462                                  | 013-2 (104+)          |             |             |             |
|              | 1451                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |             |
|              | 1433                                | 1435                                  | 225-2 (78+)           |             |             |             |
|              | 1390                                | 1383                                  | 322-5 (83+)           |             |             |             |
|              | 1302                                | 1307                                  | 225-5 (51+)           | 322-6 (33-) |             |             |
|              | 1270                                | 1291                                  | 322-6 (33+)           | 225-5 (28+) | 322-4 (12+) |             |
|              | 1221                                | 1230                                  | 225-6 (52+)           | 1322-S(20-) | 0132-S(10+) |             |
|              | 1198                                | 1189                                  | 013-5 (50-)           | 225-6 (16+) | 013-4 (8+)  |             |
|              | 1154                                | 1156                                  | 013-8 (79+)           | 013-7 (12-) |             |             |
|              | 1105                                | 1074                                  | 0132-S(38-)           | 1322-S(25+) | 225-6 (15+) | 322-6 (10-) |
|              | 1058                                | 1053                                  | 3225-S(46+)           | 322-4 (21+) | 225-4 (7-)  |             |
|              | 963                                 | 970                                   | 0132-S(46-)           | 225-4 (28+) |             |             |
|              | 963                                 | 950                                   | 322-4 (34+)           | 3225-S(23-) | 322-D (9+)  | 225-5 (8-)  |
|              | 835                                 | 822                                   | 1322-S(48+)           | 225-4 (33+) |             |             |
|              | 666                                 | 657                                   | 2250-S(92+)           |             |             |             |
|              | 493                                 | 502                                   | 322-D (60-)           | 132-B (25+) | 225-D (11+) |             |
|              | 418                                 | 409                                   | 132-B (55+)           | 225-D (16-) |             |             |
|              | 257                                 | 246                                   | 225-D (51+)           | 322-D (21+) | 132-B (10+) |             |
|              |                                     | 203                                   | 0132-T(71-)           |             |             |             |
|              |                                     | 142                                   | 1322-T(33-)           | 3225-T(26+) | 0132-T(20-) | 225-D (11+) |
|              |                                     | 69                                    | 1322-T(47+)           | 3225-T(44+) |             |             |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

3005 2989 2988 2966 2955 2864 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 196

Molecule: 13226-TT CH3OCH2CH2Br (trans-trans form)Symmetry  $C_s$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |                         |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------------------|
| a'           |                                     | 1490                                  | 322-2 (93+)           |                         |
|              | 1467                                | 1467                                  | 013-4 (84+)           | 013-5 (15+)             |
|              | 1458                                | 1462                                  | 013-2 (104+)          |                         |
|              | 1424                                | 1433                                  | 226-2 (96+)           |                         |
|              | 1372                                | 1372                                  | 322-5 (90+)           |                         |
|              | 1224                                | 1233                                  | 226-5 (93+)           |                         |
|              | 1190                                | 1200                                  | 013-5 (56+)           | 1322-S(20-) 322-5 (10+) |
|              | 1096                                | 1108                                  | 0132-S(63+)           | 1322-S(16-) 3226-S(10+) |
|              | 1044                                | 1034                                  | 3226-S(64+)           | 0132-S(9-)              |
|              | 952                                 | 955                                   | 1322-S(72-)           | 0132-S(23-)             |
|              | 658                                 | 656                                   | 2260-S(74-)           | 322-D (17+) 3226-S(11+) |
|              | 434                                 | 441                                   | 132-B (66-)           | 226-D (20+)             |
|              | 295                                 | 288                                   | 322-D (38+)           | 2260-S(28+) 226-D (11+) |
|              | 160                                 | 158                                   | 226-D (62+)           | 322-D (30-) 132-B (20+) |
| a''          | 1450                                | 1454                                  | 013-7 (86+)           | 013-8 (16+)             |
|              | 1279                                | 1281                                  | 322-6 (74+)           | 226-6 (12-)             |
|              | 1212                                | 1213                                  | 226-6 (47+)           | 322-4 (25+)             |
|              | 1154                                | 1151                                  | 013-8 (74+)           | 013-7 (11-)             |
|              | 988                                 | 996                                   | 322-4 (37+)           | 226-6 (32-) 226-4 (29+) |
|              | 778                                 | 765                                   | 226-4 (62+)           | 322-4 (33-) 322-6 (15+) |
|              | 223                                 | 222                                   | 0132-T(82-)           | 3226-T(12+)             |
|              |                                     | 138                                   | 1322-T(53+)           | 3226-T(29+) 0132-T(15+) |
|              |                                     | 103                                   | 3226-T(48+)           | 1322-T(38-)             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3004 2989 2988 2964 2956 2865 2820

Force constants for this molecule were not adjusted

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 197

Molecule: 13226-TG  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Br}$  (trans-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1479(s)                             | 1496                                  | 322-2 (86-)           |             |             |             |
|              | 1467                                | 1467                                  | 013-4 (84+)           | 013-5 (15+) |             |             |
|              | 1458                                | 1462                                  | 013-2 (104+)          |             |             |             |
|              | 1450                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |             |
|              | 1424                                | 1432                                  | 226-2 (87+)           |             |             |             |
|              | 1385                                | 1382                                  | 322-5 (91+)           |             |             |             |
|              | 1279                                | 1284                                  | 322-6 (61-)           | 226-5 (21+) |             |             |
|              | 1236                                | 1243                                  | 226-5 (64+)           | 322-4 (8+)  |             |             |
|              | 1212                                | 1220                                  | 013-5 (30+)           | 1322-S(18-) | 226-6 (18+) | 322-6 (8-)  |
|              | 1164                                | 1165                                  | 226-6 (29+)           | 013-8 (22+) | 013-5 (21-) |             |
|              | 1154                                | 1148                                  | 013-8 (56-)           | 226-6 (16+) |             |             |
|              | 1128                                | 1113                                  | 0132-S(55+)           | 1322-S(19-) | 3226-S(10+) | 013-5 (10-) |
|              | 1044                                | 1039                                  | 3226-S(45+)           | 0132-S(27-) | 322-4 (14+) |             |
|              | 988                                 | 984                                   | 226-4 (25+)           | 1322-S(20-) | 322-4 (18-) | 226-6 (17-) |
|              | 952                                 | 954                                   | 322-4 (31+)           | 3226-S(15-) | 1322-S(15-) | 322-D (11+) |
|              | 802                                 | 800                                   | 226-4 (49-)           | 1322-S(37-) |             |             |
|              | 571                                 | 567                                   | 2260-S(93+)           | 226-D (17-) |             |             |
|              | 500                                 | 498                                   | 132-B (30-)           | 322-D (27-) | 2260-S(10+) | 226-D (7+)  |
|              | 307                                 | 307                                   | 132-B (56+)           | 322-D (29-) | 226-D (15+) |             |
|              | 262                                 | 259                                   | 226-D (34-)           | 3226-T(28+) | 322-D (15-) | 0132-T(14-) |
|              | 223                                 | 207                                   | 0132-T(75+)           | 1322-T(10-) |             |             |
|              |                                     | 112                                   | 1322-T(42-)           | 3226-T(41-) | 0132-T(10-) |             |
|              |                                     | 83                                    | 1322-T(38+)           | 226-D (25-) | 3226-T(23-) | 322-4 (10-) |

Calculated frequencies higher than  $2000\text{ cm}^{-1}$ 

3004 2989 2988 2964 2955 2865 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 198

Molecule: 13226-GT  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Br}$  (gauche-trans form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|
| a            |                                     | 1485                                  | 322-2 (96+)           |             |             |
|              | 1467                                | 1467                                  | 013-4 (84+)           | 013-5 (15+) |             |
|              | 1458                                | 1462                                  | 013-2 (103+)          |             |             |
|              | 1450                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |
|              | 1424                                | 1432                                  | 226-2 (95+)           |             |             |
|              | 1372                                | 1370                                  | 322-5 (90+)           |             |             |
|              | 1299                                | 1299                                  | 322-6 (72-)           |             |             |
|              | 1224                                | 1233                                  | 226-6 (44+)           | 322-4 (19+) | 013-5 (9+)  |
|              | 1224                                | 1229                                  | 226-5 (88+)           |             |             |
|              | 1190                                | 1194                                  | 013-5 (51-)           | 1322-S(18+) | 013-4 (9+)  |
|              | 1164                                | 1156                                  | 013-8 (80+)           | 013-7 (12-) |             |
|              | 1056                                | 1075                                  | 0132-S(50-)           | 1322-S(30+) | 013-5 (10+) |
|              | 1036                                | 1023                                  | 3226-S(82-)           |             |             |
|              | 988                                 | 997                                   | 322-4 (31+)           | 226-6 (29-) | 226-4 (25+) |
|              | 918                                 | 925                                   | 1322-S(53-)           | 0132-S(43-) |             |
|              | 778                                 | 764                                   | 226-4 (61+)           | 322-4 (33-) | 322-6 (15+) |
|              | 668                                 | 670                                   | 2260-S(69-)           | 322-D (26+) | 226-D (11+) |
|              | 445                                 | 442                                   | 132-B (75-)           | 2260-S(13+) | 322-D (13+) |
|              | 316                                 | 321                                   | 322-D (34-)           | 2260-S(21-) | 0132-T(13-) |
|              |                                     | 240                                   | 226-D (74+)           |             | 1322-T(12+) |
|              |                                     | 178                                   | 0132-T(75+)           | 322-D (14-) | 226-D (12+) |
|              |                                     | 117                                   | 1322-T(84-)           |             |             |
|              |                                     | 95                                    | 3226-T(82+)           |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3004 2989 2988 2965 2956 2864 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 199

Molecule: 13226-GG  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{Br}$  (gauche-gauche form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            |                                     | 1491                                  | 322-2 (89+)           |             |             |             |
|              | 1467                                | 1467                                  | 013-4 (84+)           | 013-5 (15+) |             |             |
|              | 1458                                | 1462                                  | 013-2 (104+)          |             |             |             |
|              | 1450                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |             |
|              | 1424                                | 1433                                  | 226-2 (87+)           |             |             |             |
|              | 1385                                | 1379                                  | 322-5 (92+)           |             |             |             |
|              | 1299                                | 1300                                  | 322-6 (67+)           | 226-5 (5-)  |             |             |
|              | 1236                                | 1254                                  | 226-5 (76+)           | 322-4 (12+) |             |             |
|              | 1218                                | 1218                                  | 226-6 (32+)           | 1322-S(27-) | 013-5 (17+) | 0132-S(12+) |
|              | 1174                                | 1181                                  | 013-5 (38-)           | 226-6 (22+) | 226-5 (10+) | 013-8 (8+)  |
|              | 1164                                | 1155                                  | 013-8 (75+)           | 013-7 (11-) |             |             |
|              | 1056                                | 1063                                  | 0132-S(30-)           | 1322-S(27+) | 3226-S(26-) | 013-5 (12+) |
|              | 1044                                | 1037                                  | 3226-S(24+)           | 226-6 (19+) | 0132-S(18-) | 322-4 (17+) |
|              | 952                                 | 955                                   | 0132-S(30-)           | 322-4 (23-) | 226-4 (17+) | 3226-S(13+) |
|              | 952                                 | 939                                   | 3226-S(19-)           | 322-4 (17+) | 1322-S(17-) | 226-4 (17+) |
|              | 802                                 | 811                                   | 226-4 (41+)           | 1322-S(41+) |             |             |
|              | 571                                 | 571                                   | 2260-S(84-)           | 226-D (18+) | 322-D (11-) |             |
|              | 483                                 | 484                                   | 322-D (50-)           | 132-B (32+) | 2260-S(18+) |             |
|              |                                     | 398                                   | 132-B (48+)           | 226-D (12-) | 322-D (9+)  | 1322-T(8-)  |
|              | 223                                 | 223                                   | 226-D (51-)           | 322-D (16-) | 3226-T(13+) | 132-B (11-) |
|              | 189                                 | 201                                   | 0132-T(79-)           |             |             |             |
|              |                                     | 134                                   | 1322-T(39+)           | 3226-T(19-) | 226-D (19-) | 0132-T(15+) |
|              |                                     | 61                                    | 3226-T(49+)           | 1322-T(40+) |             |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

3004 2989 2988 2966 2955 2864 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 200

Molecule: 13227-TT CH3OCH2CH2I (trans-trans form)Symmetry  $C_2$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|
| a'           |                                     | 1491                                  | 322-2 (93+)           |             |             |
|              | 1468                                | 1468                                  | 013-4 (84-)           | 013-5 (15-) |             |
|              | 1458                                | 1462                                  | 013-2 (104+)          |             |             |
|              | 1416                                | 1422                                  | 227-2 (89+)           |             |             |
|              | 1365                                | 1372                                  | 322-5 (88+)           |             |             |
|              | 1200                                | 1205                                  | 013-5 (54+)           | 227-5 (18-) | 1322-S(14-) |
|              | 1189                                | 1188                                  | 227-5 (77+)           |             |             |
|              | 1108                                | 1107                                  | 0132-S(61+)           | 1322-S(16-) | 3227-S(12+) |
|              | 1030                                | 1033                                  | 3227-S(60+)           | 0132-S(10-) | 322-D (6-)  |
|              | 950                                 | 951                                   | 1322-S(74-)           | 0132-S(22-) | 322-D (10+) |
|              | 619                                 | 609                                   | 2270-S(63-)           | 322-D (24+) | 227-D (10+) |
|              | 427                                 | 431                                   | 132-B (67-)           | 227-D (22+) | 2270-S(10-) |
|              | 266                                 | 262                                   | 322-D (41+)           | 2270-S(34+) |             |
|              | 140                                 | 143                                   | 227-D (73+)           | 322-D (21-) | 132-B (16+) |
|              |                                     |                                       |                       |             | 227-5 (12-) |
| a''          | 1450                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |
|              | 1265                                | 1269                                  | 322-6 (83+)           |             |             |
|              | 1189                                | 1186                                  | 227-6 (43+)           | 322-4 (25+) | 013-8 (14-) |
|              | 1148                                | 1148                                  | 013-8 (67+)           | 227-6 (11+) | 013-7 (10-) |
|              | 967                                 | 965                                   | 227-6 (42-)           | 322-4 (39+) | 227-4 (19+) |
|              | 753                                 | 732                                   | 227-4 (70+)           | 322-4 (27-) | 322-6 (12+) |
|              | 200                                 | 221                                   | 0132-T(83-)           | 3227-T(11+) |             |
|              |                                     | 137                                   | 1322-T(57+)           | 3227-T(26+) | 0132-T(14+) |
|              |                                     | 100                                   | 3227-T(51+)           | 1322-T(33-) |             |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2999 2989 2988 2963 2962 2865 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977)



## No. 201

Molecule: 13227-TG  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{I}$  (trans-gauche form)Symmetry  $C_1$ Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %) |             |             |             |
|--------------|-------------------------------------|---------------------------------------|-----------------------|-------------|-------------|-------------|
| a            | 1482(s)                             | 1496                                  | 322-2 (86+)           |             |             |             |
|              | 1468                                | 1467                                  | 013-4 (84-)           | 013-5 (15-) |             |             |
|              | 1458                                | 1462                                  | 013-2 (104+)          |             |             |             |
|              | 1450                                | 1454                                  | 013-7 (86+)           | 013-8 (16+) |             |             |
|              | 1416                                | 1426                                  | 227-2 (76+)           | 322-2 (10-) |             |             |
|              | 1381                                | 1381                                  | 322-5 (86+)           |             |             |             |
|              | 1265                                | 1270                                  | 322-6 (76+)           |             |             |             |
|              | 1220                                | 1219                                  | 013-5 (40+)           | 227-5 (24+) | 1322-S(17-) |             |
|              | 1189                                | 1203                                  | 227-5 (49-)           | 322-4 (11-) | 3227-S(10+) | 013-5 (9+)  |
|              | 1161                                | 1155                                  | 013-8 (66+)           | 013-7 (10-) |             |             |
|              | 1124                                | 1130                                  | 227-6 (42+)           | 0132-S(14-) | 013-8 (9-)  | 3227-S(8-)  |
|              | 1124                                | 1111                                  | 0132-S(42+)           | 1322-S(21-) | 013-5 (17-) |             |
|              | 1037                                | 1039                                  | 3227-S(41+)           | 0132-S(30-) | 322-4 (13+) |             |
|              | 967                                 | 959                                   | 322-4 (41+)           | 227-6 (16+) | 322-6 (9-)  | 227-5 (9-)  |
|              | 933                                 | 940                                   | 1322-S(32-)           | 322-D (14+) | 227-4 (13+) | 227-6 (10-) |
|              | 775                                 | 773                                   | 227-4 (58+)           | 1322-S(28+) |             |             |
|              | 516                                 | 513                                   | 2270-S(64+)           | 227-D (26-) | 322-D (17+) |             |
|              | 489                                 | 486                                   | 2270-S(35+)           | 132-B (30-) | 322-D (16-) |             |
|              | 304                                 | 298                                   | 132-B (54+)           | 322-D (40-) |             |             |
|              | 248                                 | 249                                   | 227-D (37-)           | 3227-T(28+) | 0132-T(24-) |             |
|              | 200                                 | 203                                   | 0132-T(66+)           | 227-D (15-) | 1322-T(13-) |             |
|              |                                     | 110                                   | 1322-T(47-)           | 3227-T(36-) | 0132-T(10-) |             |
|              |                                     | 75                                    | 227-D (33-)           | 1322-T(30+) | 3227-T(25-) | 322-4 (11-) |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2999 2989 2988 2965 2961 2865 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

No. 202

Molecule: 13227-GT  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{I}$  (gauche-trans form)Symmetry  $C_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %)                           |
|--------------|-------------------------------------|---------------------------------------|-------------------------------------------------|
| a            |                                     | 1486                                  | 322-2 (96+)                                     |
|              | 1468                                | 1467                                  | 013-4 (84+) 013-5 (15+)                         |
|              | 1458                                | 1462                                  | 013-2 (103+)                                    |
|              | 1450                                | 1454                                  | 013-7 (86-) 013-8 (16-)                         |
|              | 1416                                | 1422                                  | 227-2 (87+)                                     |
|              | 1365                                | 1369                                  | 322-5 (87+)                                     |
|              | 1293                                | 1296                                  | 322-6 (71+)                                     |
|              | 1200                                | 1206                                  | 013-5 (41+) 227-6 (13+) 1322-S(12-) 227-5 (8-)  |
|              | 1189                                | 1191                                  | 227-5 (55+) 227-6 (19+) 322-4 (10+)             |
|              | 1189                                | 1183                                  | 227-5 (29-) 013-5 (18-) 227-6 (16+) 322-4 (9+)  |
|              | 1161                                | 1155                                  | 013-8 (75+) 013-7 (11-)                         |
|              | 1088                                | 1071                                  | 0132-S(52-) 1322-S(31+) 013-5 (11+)             |
|              | 1019                                | 1022                                  | 3227-S(78-)                                     |
|              | 967                                 | 969                                   | 227-6 (38-) 322-4 (30+) 227-4 (16+) 1322-S(13-) |
|              | 909                                 | 920                                   | 1322-S(50+) 0132-S(41+)                         |
|              | 753                                 | 731                                   | 227-4 (69+) 322-4 (27-) 322-6 (12+)             |
|              | 619                                 | 623                                   | 2270-S(57-) 322-D (36+) 227-D (14+)             |
|              | 440                                 | 434                                   | 132-B (78+) 2270-S(15-)                         |
|              | 304                                 | 309                                   | 322-D (31-) 2270-S(26-) 0132-T(15-) 1322-T(12+) |
|              | 223                                 | 213                                   | 227-D (66+) 0132-T(15-)                         |
|              |                                     | 174                                   | 0132-T(67+) 227-D (23+) 322-D (13-)             |
|              |                                     | 115                                   | 1322-T(83-)                                     |
|              |                                     | 90                                    | 3227-T(81-)                                     |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2999 2989 2988 2965 2963 2864 2820

Force constants for this molecule were not adjusted.

## Reference

- [1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).

## No. 203

Molecule: 13227-GG  $\text{CH}_3\text{OCH}_2\text{CH}_2\text{I}$  (gauche-gauche form)Symmetry  $\text{C}_1$  Symmetry number  $\sigma = 1$ 

| Sym. species | Observed frequency $\text{cm}^{-1}$ | Calculated frequency $\text{cm}^{-1}$ | Assignment (P.E.D. %)                           |
|--------------|-------------------------------------|---------------------------------------|-------------------------------------------------|
| a            |                                     | 1490                                  | 322-2 (90+)                                     |
|              | 1468                                | 1467                                  | 013-4 (84+) 013-5 (15+)                         |
|              | 1458                                | 1462                                  | 013-2 (104+)                                    |
|              | 1450                                | 1454                                  | 013-7 (86-) 013-8 (16-)                         |
|              | 1416                                | 1426                                  | 227-2 (77+)                                     |
|              | 1381                                | 1378                                  | 322-5 (87+)                                     |
|              | 1293                                | 1295                                  | 322-6 (68+) 322-4 (6+)                          |
|              | 1220                                | 1219                                  | 227-5 (50+) 013-5 (25+)                         |
|              | 1189                                | 1202                                  | 1322-S(22-) 227-5 (21-) 013-5 (18+) 227-6 (15+) |
|              | 1161                                | 1164                                  | 013-8 (51+) 227-6 (14+) 013-7 (8-)              |
|              | 1148                                | 1146                                  | 013-8 (31-) 227-6 (21+) 227-5 (12+) 013-5 (11-) |
|              | 1052                                | 1062                                  | 3227-S(36-) 1322-S(23+) 0132-S(18-) 013-5 (12+) |
|              | 1030                                | 1026                                  | 0132-S(36-) 227-6 (30+) 322-6 (14-) 3227-S(11+) |
|              | 933                                 | 941                                   | 322-4 (42-) 3227-S(19+) 0132-S(13-) 227-5 (11+) |
|              | 909                                 | 921                                   | 1322-S(33-) 227-4 (21+) 0132-S(17-)             |
|              | 775                                 | 786                                   | 227-4 (52+) 1322-S(30+)                         |
|              | 516                                 | 521                                   | 2270-S(57-) 322-D (30-) 227-D (23+)             |
|              | 468                                 | 468                                   | 2270-S(40+) 132-B (33+) 322-D (29-)             |
|              | 393                                 | 389                                   | 132-B (40+) 322-D (15+) 227-D (8-) 1322-T(8-)   |
|              | 200                                 | 211                                   | 227-D (35-) 3227-T(21+) 322-D (14-) 132-B (13-) |
|              | 200                                 | 198                                   | 0132-T(78-) 227-D (19-)                         |
|              |                                     | 128                                   | 1322-T(40+) 227-D (29-) 3227-T(14-) 0132-T(12+) |
|              |                                     | 57                                    | 3227-T(50+) 1322-T(37+)                         |

Calculated frequencies higher than  $2000 \text{ cm}^{-1}$ 

2999 2990 2988 2966 2962 2864 2820

Force constants for this molecule were not adjusted.

## Reference

- 1] IR.R. H. Matsuura, M. Kono, H. Iizuka, Y. Ogawa, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **50**, 2272 (1977).