Tables of Molecular Vibrational Frequencies

Part 10

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Fundamental vibrational frequencies of 94 molecular forms of 23 polyatomic chain molecules of halogenoalkanes and halogenoalkyl ethers consisting of the CH_3, 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[1] has fundamental importance in elucidating various problems in physics and chemistry. The information 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][2], Part 2 [2], Part 3 [3], Part 4, Part 5

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[1] 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 cm^{-1}.

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[2] 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 CH_3, CD_3, CH_2, CD_2, CHD, O, S, F, Cl, Br, and 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 CH_3, CH_2, O, F, Cl, Br, and 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° (trans), 60° (gauche$^+$), and −60° (gauche$^-$). The symbols t, g^+, and g^- are used for the trans, gauche$^+$, and gauche$^-$ 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 CH_3 and 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., CH_2 and 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., 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.

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

Property	Quantity
Relative atomic masses,[a] 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(C–H)	1.100
r(C–C)	1.539
r(C–O)	1.410
r(C–F)	1.398
r(C–Cl)	1.788
r(C–Br)	1.950
r(C–I)	2.139
Bond angles, degree	
∠(C–C–C)	112.2
∠(C–C–O)	108.1
∠(C–O–C)	111.8
∠(C–C–F)	109.7
∠(C–C–Cl)	111.0
∠(C–C–Br)	111.0
∠(C–C–I)	112.2
∠(C–C–H)	110.4
∠(O–C–H)	109.8
∠(F–C–H)	106.1
∠(Cl–C–H)	106.6
∠(Br–C–H)	105.4
∠(I–C–H)	105.0
Dihedral angles, degree	
Trans conformation	180
Gauche$^+$ conformation	60
Gauche$^-$ conformation	-60

[a] 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.

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 CH_3 symmetrical deformation in the CH_3 group of the CH_3CH_2 part.

225–46: the off-diagonal intragroup force constant for the CH_2 rocking and the CH_2 twisting within the C^bH_2 group of the $C^aH_2C^bH_2Cl$ part.

226–SS: the off-diagonal intragroup force constant for the C^a–C^b stretching and the C^b–Br stretching of the $C^aH_2C^bH_2Br$ part.

2250–S: the diagonal intergroup force constant for the C^b–Cl stretching of $C^aH_2C^bH_2Cl$ part.

0123–25: the off-diagonal intergroup force constant for the CH_3 symmetrical deformation and the CH_2 wagging of the CH_3CH_2O part.

2260–5S: the off-diagonal intergroup force constant for the C^bH_2 wagging and the C^b–Br stretching of the $C^aH_2C^bH_2Br$ part.

2227–46–g$^+$: the off-diagonal intergroup force constant for the C^bH_2 rocking and the C^cH_2 twisting of the $C^aH_2C^bH_2C^cH_2I$ part in the gauche$^+$ 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 CH_2 antisymmetrical stretching, the CH_2 rocking or the CH_2 wagging and the other coordinate is

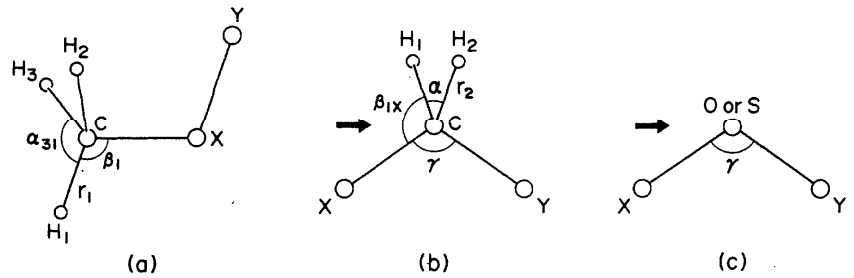

FIGURE 1. Parameters of atomic groups. (a) CH_3–(X), (b) (X)–CH_2–(Y), (c) (X)–O–(Y) or (X)–S–(Y). Arrows in (b) and (c) indicate the direction of viewing the atomic groups (see text).

TABLE 2. Definition and symbolism of local symmetry coordinates

	Coordinate	Symbol	Definition
(a)	CH_3–(X) group[a] (see figure 1(a))		
	CH_3 symmetrical stretching	1	$(\Delta r_1 + \Delta r_2 + \Delta r_3)/\sqrt{3}$
	CH_3 symmetrical deformation	2	$a(\Delta\alpha_{23} + \Delta\alpha_{31} + \Delta\alpha_{12}) - b(\Delta\beta_1 + \Delta\beta_2 + \Delta\beta_3)$
	CH_3 degenerate stretching	3	$(2\Delta r_1 - \Delta r_2 - \Delta r_3)/\sqrt{6}$
	CH_3 degenerate deformation	4	$(2\Delta\alpha_{23} - \Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{6}$
	CH_3 rocking	5	$(2\Delta\beta_1 - \Delta\beta_2 - \Delta\beta_3)/\sqrt{6}$
	CH_3 degenerate stretching	6	$(\Delta r_2 - \Delta r_3)/\sqrt{2}$
	CH_3 degenerate deformation	7	$(\Delta\alpha_{31} - \Delta\alpha_{12})/\sqrt{2}$
	CH_3 rocking	8	$(\Delta\beta_2 - \Delta\beta_3)/\sqrt{2}$
(b)	(X)–CH_2–(Y) group[a] (see figure 1(b))		
	CH_2 symmetrical stretching	1	$(\Delta r_1 + \Delta r_2)/\sqrt{2}$
	CH_2 scissors	2	$c\Delta\alpha - d(\Delta\beta_{1X} + \Delta\beta_{2X}) - e(\Delta\beta_{1Y} + \Delta\beta_{2Y})$
	CH_2 antisymmetrical stretching[b]	3	$(\Delta r_1 - \Delta r_2)/\sqrt{2}$
	CH_2 rocking[b]	4	$(\Delta\beta_{1X} - \Delta\beta_{2X} + \Delta\beta_{1Y} - \Delta\beta_{2Y})/2$
	CH_2 wagging[b]	5	$f(\Delta\beta_{1X} + \Delta\beta_{2X}) - g(\Delta\beta_{1Y} + \Delta\beta_{2Y})$
	CH_2 twisting	6	$(\Delta\beta_{1X} - \Delta\beta_{2X} - \Delta\beta_{1Y} + \Delta\beta_{2Y})/2$
	X–CH_2–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[a] (see figure 1(c))		
	X–O–Y bending	B	$\Delta\gamma$
(d)	Skeleton –X–Y–		
	Stretching	S	Δr_{XY}
	Torsion[c]	T	Δt_{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].

[a] Symbols of atomic groups are 1 for CH_3, 1′ for CD_3, 2 for CH_2, 2′ for CD_2, 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_1 and H_2 in figure 1(b) are protium (H) and deuterium (D), respectively.

[b] The signs of the CH_2 antisymmetrical stretching, CH_2 rocking and CH_2 wagging coordinates of the(Y)–CH_2–(X) group (viewing the Y–CH_2–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_2–(Y) group (viewing the X–CH_2–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.

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

Table 3. Force constants of fluoroalkanes

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
228–1	4.840	1228–DD–t =	2228–DD–t	2228–55–t	–0.077(53)
228–2	0.523(16)	1228–44–g^+=	2228–44–g^+	2228–5D–t =	2222–5D–t
228–3	4.752	*1228–45–g^+=	2222–45–g^+	2228–64–t =	–2222–46–t
228–4	0.787(101)	1228–46–g^+=	2222–46–g^+	2228–66–t	–0.045(118)
228–5	0.716(58)	*1228–4D–g^+=	2222–4D–g^+	2228–D2–t =	2222–2D–t
228–6	0.744(124)	*1228–54–g^+=	2222–45–g^+	2228–D5–t =	–2222–5D–t
228–D	1.373(84)	1228–55–g^+=	2228–55–g^+	2228–DD–t	0.217(38)
228–25	0.056(38)	*1228–56–g^+=	2222–56–g^+	2228–44–g^+	–0.051(60)
228–2D =	222–2D	1228–5D–g^+=	2222–5D–g^+	*2228–45–g^+=	2222–45–g^+
228–46	–0.024(53)	1228–64–g^+=	–2222–46–g^+	2228–46–g^+=	2222–46–g^+
228–5D	0.341(91)	*1228–65–g^+=	–2222–56–g^+	*2228–4D–g^+=	2222–4D–g^+
228–SS	0.316(69)	1228–66–g^+=	2228–66–g^+	*2228–54–g^+=	2222–45–g^+
		*1228–6D–g^+=	2222–6D–g^+	2228–55–g^+	0.023(41)
1228–S =	2228–S	*1228–D4–g^+=	–2222–4D–g^+	*2228–56–g^+=	2222–56–g^+
1228–T =	2228–T	1228–D5–g^+=	–2222–5D–g^+	2228–5D–g^+=	2222–5D–g^+
1228–5S =	2222–5S	*1228–D6–g^+=	2222–6D–g^+	2228–64–g^+=	–2222–46–g^+
1228–DS =	2222–DS	1228–DD–g^+=	2228–DD–g^+	*2228–65–g^+=	–2222–56–g^+
1228–S5 =	–2222–5S			2228–66–g^+	–0.014(35)
1228–SD =	2225–SD	2228–S	4.399(72)	*2228–6D–g^+=	2222–6D–g^+
1228–2D–t =	2222–2D–t	2228–T	0.150	*2228–D4–g^+=	–2222–4D–g^+
1228–44–t =	2228–44–t	2228–5S =	2222–5S	2228–D5–g^+=	–2222–5D–g^+
1228–46–t =	2222–46–t	2228–DS =	2222–DS	*2228–D6–g^+=	2222–6D–g^+
1228–55–t =	2228–55–t	2228–S5 =	–2222–5S	2228–DD–g^+	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				

[a] 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.

[b] Units are aJ $Å^{-2}$ = mdyn $Å^{-1}$ for the stretching and stretching–stretching constants, aJ $Å^{-1}$ = 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 4. Force constants of chloroalkanes

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
225–1	4.905	1225–DD–t =	2225–DD–t	2225–55–t	–0.049(4)
225–2	0.537(8)	1225–44–g^+ =	2225–44–g^+	2225–5D–t =	2222–5D–t
225–3	4.787	*1225–45–g^+ =	2222–45–g^+	2225–64–t =	–2222–46–t
225–4	0.756(16)	1225–46–g^+ =	2222–46–g^+	2225–66–t	–0.075(8)
225–5	0.662(18)	*1225–4D–g^+ =	2222–4D–g^+	2225–D2–t =	2222–2D–t
225–6	0.649(26)	*1225–54–g^+ =	2222–45–g^+	2225–D5–t =	–2222–5D–t
225–D	0.984(44)	1225–55–g^+ =	2225–55–g^+	2225–DD–t	0.112(40)
225–25	0.049(5)	*1225–56–g^+ =	2222–56–g^+	2225–44–g^+	0.005(13)
225–2D =	222–2D	1225–5D–g^+ =	2222–5D–g^+	*2225–45–g^+ =	2222–45–g^+
225–46	–0.031(16)	1225–64–g^+ =	–2222–46–g^+	2225–46–g^+ =	2222–46–g^+
225–5D	0.059(58)	*1225–65–g^+ =	–2222–56–g^+	*2225–4D–g^+ =	2222–4D–g^+
225–SS	0.388(25)	1225–66–g^+ =	2225–66–g^+	*2225–54–g^+ =	2222–45–g^+
		*1225–6D–g^+ =	2222–6D–g^+	2225–55–g^+	0.005(14)
1225–S =	2225–S	*1225–D4–g^+ =	–2222–4D–g^+	*2225–56–g^+ =	2222–56–g^+
1225–T =	2225–T	1225–D5–g^+ =	–2222–5D–g^+	2225–5D–g^+ =	2222–5D–g^+
1225–5S =	2222–5S	*1225–D6–g^+ =	2222–6D–g^+	2225–64–g^+ =	–2222–46–g^+
1225–DS =	2222–DS	1225–DD–g^+ =	2225–DD–g^+	*2225–65–g^+ =	–2222–56–g^+
1225–S5 =	–2222–5S			2225–66–g^+	0.039(21)
1225–SD =	2225–SD	2225–S	4.314(31)	*2225–6D–g^+ =	2222–6D–g^+
1225–2D–t =	2222–2D–t	2225–T	0.146(15)	*2225–D4–g^+ =	–2222–4D–g^+
1225–44–t =	2225–44–t	2225–5S =	2222–5S	2225–D5–g^+ =	–2222–5D–g^+
1225–46–t =	2222–46–t	2225–DS =	2222–DS	*2225–D6–g^+ =	2222–6D–g^+
1225–55–t =	2225–55–t	2225–S5 =	–2222–5S	2225–DD–g^+	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				

[a] 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.

[b] Units are aJ $Å^{-2}$ = mdyn $Å^{-1}$ for the stretching and stretching–stretching constants, aJ $Å^{-1}$ = 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 5. Force constants of bromoalkanes

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
226–1	4.920	1226–DD–t	= 2226–DD–t	2226–55–t	–0.052(6)
226–2	0.535(2)	1226–44–g^+	= 2226–44–g^+	2226–5D–t	= 2222–5D–t
226–3	4.770	*1226–45–g^+	= 2222–45–g^+	2226–64–t	=–2222–46–t
226–4	0.700(30)	1226–46–g^+	= 2222–46–g^+	2226–66–t	–0.070(15)
226–5	0.621(11)	*1226–4D–g^+	= 2222–4D–g^+	2226–D2–t	= 2222–2D–t
226–6	0.613(22)	*1226–54–g^+	= 2222–45–g^+	2226–D5–t	=–2222–5D–t
226–D	0.977(19)	1226–55–g^+	= 2226–55–g^+	2226–DD–t	0.022(19)
226–25	0.038(9)	*1226–56–g^+	= 2222–56–g^+	2226–44–g^+	0.002(44)
226–2D	= 222–2D	1226–5D–g^+	= 2222–5D–g^+	*2226–45–g^+	= 2222–45–g^+
226–46	0.002(20)	1226–64–g^+	=–2222–46–g^+	2226–46–g^+	= 2222–46–g^+
226–5D	0.132(16)	*1226–65–g^+	=–2222–56–g^+	*2226–4D–g^+	= 2222–4D–g^+
226–SS	0.541(34)	1226–66–g^+	= 2226–66–g^+	*2226–54–g^+	= 2222–45–g^+
		*1226–6D–g^+	= 2222–6D–g^+	2226–55–g^+	–0.004(21)
1226–S	= 2226–S	*1226–D4–g^+	=–2222–4D–g^+	*2226–56–g^+	= 2222–56–g^+
1226–T	= 2226–T	1226–D5–g^+	=–2222–5D–g^+	2226–5D–g^+	= 2222–5D–g^+
1226–5S	= 2222–5S	*1226–D6–g^+	= 2222–6D–g^+	2226–64–g^+	=–2222–46–g^+
1226–DS	= 2222–DS	1226–DD–g^+	= 2226–DD–g^+	*2226–65–g^+	=–2222–56–g^+
1226–S5	=–2222–5S			2226–66–g^+	0.045(13)
1226–SD	= 2226–SD	2226–S	4.314(34)	*2226–6D–g^+	= 2222–6D–g^+
1226–2D–t	= 2222–2D–t	2226–T	0.147(20)	*2226–D4–g^+	=–2222–4D–g^+
1226–44–t	= 2226–44–t	2226–5S	= 2222–5S	2226–D5–g^+	=–2222–5D–g^+
1226–46–t	= 2222–46–t	2226–DS	= 2222–DS	*2226–D6–g^+	= 2222–6D–g^+
1226–55–t	= 2226–55–t	2226–S5	=–2222–5S	2226–DD–g^+	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				

[a] 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.

[b] Units are aJ $Å^{-2}$ = mdyn $Å^{-1}$ for the stretching and stretching–stretching constants, aJ $Å^{-1}$ = 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[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
227–1	4.942	1227–DD–t =	2227–DD–t	2227–55–t	–0.059(4)
227–2	0.528(3)	1227–44–g^+=	2227–44–g^+	2227–5D–t =	2222–5D–t
227–3	4.758	*1227–45–g^+=	2222–45–g^+	2227–64–t =	–2222–46–t
227–4	0.641(14)	1227–46–g^+=	2222–46–g^+	2227–66–t	–0.050(9)
227–5	0.571(15)	*1227–4D–g^+=	2222–4D–g^+	2227–D2–t =	2222–2D–t
227–6	0.547(10)	*1227–54–g^+=	2222–45–g^+	2227–D5–t =	–2222–5D–t
227–D	0.919(14)	1227–55–g^+=	2227–55–g^+	2227–DD–t	–0.028(22)
227–25	0.077(8)	*1227–56–g^+=	2222–56–g^+	2227–44–g^+	0.014(21)
227–2D =	222–2D	1227–5D–g^+=	2222–5D–g^+	*2227–45–g^+=	2222–45–g^+
227–46	0.003(12)	1227–64–g^+=	–2222–46–g^+	2227–46–g^+=	2222–46–g^+
227–5D	0.196(25)	*1227–65–g^+=	–2222–56–g^+	*2227–4D–g^+=	2222–4D–g^+
227–SS	0.424(6)	1227–66–g^+=	2227–66–g^+	*2227–54–g^+=	2222–45–g^+
		*1227–6D–g^+=	2222–6D–g^+	2227–55–g^+	0.012(14)
1227–S =	2227–S	*1227–D4–g^+=	–2222–4D–g^+	*2227–56–g^+=	2222–56–g^+
1227–T =	2227–T	1227–D5–g^+=	–2222–5D–g^+	2227–5D–g^+=	2222–5D–g^+
1227–5S =	2222–5S	*1227–D6–g^+=	2222–6D–g^+	2227–64–g^+=	–2222–46–g^+
1227–DS =	2222–DS	1227–DD–g^+=	2227–DD–g^+	*2227–65–g^+=	–2222–56–g^+
1227–S5 =	–2222–5S			2227–66–g^+	0.034(12)
1227–SD =	2227–SD	2227–S	4.327(51)	*2227–6D–g^+=	2222–6D–g^+
1227–2D–t =	2222–2D–t	2227–T	0.148(25)	*2227–D4–g^+=	–2222–4D–g^+
1227–44–t =	2227–44–t	2227–5S =	2222–5S	2227–D5–g^+=	–2222–5D–g^+
1227–46–t =	2222–46–t	2227–DS =	2222–DS	*2227–D6–g^+=	2222–6D–g^+
1227–55–t =	2227–55–t	2227–S5 =	–2222–5S	2227–DD–g^+	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				

[a] 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.

[b] Units are aJ $Å^{-2}$ = mdyn $Å^{-1}$ for the stretching and stretching–stretching constants, aJ $Å^{-1}$ = 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 7. Force constants of halogenoalkyl ethers

Constant[a]	Value[b]	Constant[a]	Value[b]	Constant[a]	Value[b]
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^+	= 2225–44–g^+	3226–44–g^+	= 2226–44–g^+	3227–44–g^+	= 2227–44–g^+
*3225–45–g^+	= 2222–45–g^+	*3226–45–g^+	= 2222–45–g^+	*3227–45–g^+	= 2222–45–g^+
3225–46–g^+	= 2222–46–g^+	3226–46–g^+	= 2222–46–g^+	3227–46–g^+	= 2222–46–g^+
*3225–4D–g^+	= 2222–4D–g^+	*3226–4D–g^+	= 2222–4D–g^+	*3227–4D–g^+	= 2222–4D–g^+
*3225–54–g^+	= 2222–45–g^+	*3226–54–g^+	= 2222–45–g^+	*3227–54–g^+	= 2222–45–g^+
3225–55–g^+	= 2225–55–g^+	3226–55–g^+	= 2226–55–g^+	3227–55–g^+	= 2227–55–g^+
*3225–56–g^+	= 2222–56–g^+	*3226–56–g^+	= 2222–56–g^+	*3227–56–g^+	= 2222–56–g^+
3225–5D–g^+	= 2222–5D–g^+	3226–5D–g^+	= 2222–5D–g^+	3227–5D–g^+	= 2222–5D–g^+
3225–64–g^+	=–2222–46–g^+	3226–64–g^+	=–2222–46–g^+	3227–64–g^+	=–2222–46–g^+
*3225–65–g^+	=–2222–56–g^+	*3226–65–g^+	=–2222–56–g^+	*3227–65–g^+	=–2222–56–g^+
3225–66–g^+	= 2225–66–g^+	3226–66–g^+	= 2226–66–g^+	3227–66–g^+	= 2227–66–g^+
*3225–6D–g^+	= 2222–6D–g^+	*3226–6D–g^+	= 2222–6D–g^+	*3227–6D–g^+	= 2222–6D–g^+
*3225–D4–g^+	=–2222–4D–g^+	*3226–D4–g^+	=–2222–4D–g^+	*3227–D4–g^+	=–2222–4D–g^+
3225–D5–g^+	=–2222–5D–g^+	3226–D5–g^+	=–2222–5D–g^+	3227–D5–g^+	=–2222–5D–g^+
*3225–D6–g^+	= 2222–6D–g^+	*3226–D6–g^+	= 2222–6D–g^+	*3227–D6–g^+	= 2222–6D–g^+
3225–DD–g^+	= 2225–DD–g^+	3226–DD–g^+	= 2226–DD–g^+	3227–DD–g^+	= 2227–DD–g^+

[a] 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.

[b] Units are aJ $Å^{-2}$ = mdyn $Å^{-1}$ for the stretching and stretching–stretching constants, aJ $Å^{-1}$ = 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).

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$^-$ conformation are equivalent to the corresponding force constants for the gauche$^+$ conformation. For some of the force constants, however, the absolute values of the gauche$^+$ and gauche$^-$ 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, σ, is used in the calculation of thermodynamic quantities. It is the number of indistinguishable positions into which the molecule can be transformed by simple rigid rotations. A general discussion and pertinent formulas may be found in 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_3 and CD_3 groups in common and the symbol 2 for the CH_2, CD_2, and CHD groups.

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7. List of Tables of Molecular Vibrational Frequencies

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114.	1-Fluorobutane $CH_3CH_2CH_2CH_2F$ (gauche-trans form)	1165
115.	1-Fluorobutane $CH_3CH_2CH_2CH_2F$ (gauche-gauche form)	1166
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118.	1-Fluoropentane $CH_3CH_2CH_2CH_2CH_2F$ (trans-gauche-trans form)	1169
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120.	1-Chloropropane $CH_3CH_2CH_2Cl$ (trans form)	1171
121.	1-Chloropropane $CH_3CH_2CH_2Cl$ (gauche form)	1172
122.	1-Chlorobutane $CH_3CH_2CH_2CH_2Cl$ (trans-trans form)	1173
123.	1-Chlorobutane $CH_3CH_2CH_2CH_2Cl$ (trans-gauche form)	1174
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139.	1,4-Dichlorobutane $ClCH_2CH_2CH_2CH_2Cl$ (gauche-trans-gauche' form)	1190
140.	1,4-Dichlorobutane $ClCH_2CH_2CH_2CH_2Cl$ (gauche-gauche-gauche form)	1191
141.	1-Bromopropane $CH_3CH_2CH_2Br$ (trans form)	1192
142.	1-Bromopropane $CH_3CH_2CH_2Br$ (gauche form)	1193
143.	1-Bromopropane CH_3CHDCH_2Br (trans form)	1194
144.	1-Bromopropane CH_3CHDCH_2Br (gauche form)	1195
145.	1-Bromopropane CH_3CHDCH_2Br (gauche' form)	1196
146.	1-Bromopropane CH_3CH_2CHDBr (trans form)	1197
147.	1-Bromopropane CH_3CH_2CHDBr (gauche form)	1198
148.	1-Bromopropane CH_3CH_2CHDBr (gauche' form)	1199
149.	1-Bromobutane $CH_3CH_2CH_2CH_2Br$ (trans-trans form)	1200
150.	1-Bromobutane $CH_3CH_2CH_2CH_2Br$ (trans-gauche form)	1201
151.	1-Bromobutane $CH_3CH_2CH_2CH_2Br$ (gauche-trans form)	1202
152.	1-Bromobutane $CH_3CH_2CH_2CH_2Br$ (gauche-gauche form)	1203
153.	1-Bromopentane $CH_3CH_2CH_2CH_2CH_2Br$ (trans-trans-trans form)	1204
154.	1-Bromopentane $CH_3CH_2CH_2CH_2CH_2Br$ (trans-trans-gauche form)	1205
155.	1-Bromopentane $CH_3CH_2CH_2CH_2CH_2Br$ (trans-gauche-trans form)	1206
156.	1-Bromopentane $CH_3CH_2CH_2CH_2CH_2Br$ (trans-gauche-gauche form)	1207

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157. 1-Bromopentane $CH_3CH_2CH_2CH_2CH_2Br$ (gauche-trans-gauche form) ... 1208
158. 1-Bromopentane $CH_3CH_2CH_2CH_2CH_2Br$ (gauche-trans-gauche' form) ... 1209
159. 1,3-Dibromopropane $BrCH_2CH_2CH_2Br$ (trans-trans form) ... 1210
160. 1,3-Dibromopropane $BrCH_2CH_2CH_2Br$ (trans-gauche form) ... 1211
161. 1,3-Dibromopropane $BrCH_2CH_2CH_2Br$ (gauche-gauche form) ... 1212
162. 1,4-Dibromobutane $BrCH_2CH_2CH_2CH_2Br$ (trans-trans-trans form) ... 1213
163. 1,4-Dibromobutane $BrCH_2CH_2CH_2CH_2Br$ (trans-trans-gauche form) ... 1214
164. 1,4-Dibromobutane $BrCH_2CH_2CH_2CH_2Br$ (trans-gauche-trans form) ... 1215
165. 1,4-Dibromobutane $BrCH_2CH_2CH_2CH_2Br$ (trans-gauche-gauche form) ... 1216
166. 1,4-Dibromobutane $BrCH_2CH_2CH_2CH_2Br$ (gauche-trans-gauche form) ... 1217
167. 1,4-Dibromobutane $BrCH_2CH_2CH_2CH_2Br$ (gauche-trans-gauche' form) ... 1218
168. 1,4-Dibromobutane $BrCH_2CH_2CH_2CH_2Br$ (gauche-gauche-gauche form) ... 1219
169. 1-Iodopropane $CH_3CH_2CH_2I$ (trans form) ... 1220
170. 1-Iodopropane $CH_3CH_2CH_2I$ (gauche form) ... 1221
171. 1-Iodobutane $CH_3CH_2CH_2CH_2I$ (trans-trans form) ... 1222
172. 1-Iodobutane $CH_3CH_2CH_2CH_2I$ (trans-gauche form) ... 1223
173. 1-Iodobutane $CH_3CH_2CH_2CH_2I$ (gauche-trans form) ... 1224
174. 1-Iodobutane $CH_3CH_2CH_2CH_2I$ (gauche-gauche form) ... 1225
175. 1-Iodopentane $CH_3CH_2CH_2CH_2CH_2I$ (trans-trans-trans form) ... 1226
176. 1-Iodopentane $CH_3CH_2CH_2CH_2CH_2I$ (trans-trans-gauche form) ... 1227
177. 1-Iodopentane $CH_3CH_2CH_2CH_2CH_2I$ (trans-gauche-trans form) ... 1228
178. 1-Iodopentane $CH_3CH_2CH_2CH_2CH_2I$ (gauche-trans-trans form) ... 1229
179. 1-Iodopentane $CH_3CH_2CH_2CH_2CH_2I$ (trans-gauche-gauche form) ... 1230
180. 1-Iodopentane $CH_3CH_2CH_2CH_2CH_2I$ (gauche-trans-gauche form) ... 1231
181. 1-Iodopentane $CH_3CH_2CH_2CH_2CH_2I$ (gauche-trans-gauche' form) ... 1232
182. 1,3-Diiodopropane $ICH_2CH_2CH_2I$ (trans-trans form) ... 1233
183. 1,3-Diiodopropane $ICH_2CH_2CH_2I$ (trans-gauche form) ... 1234
184. 1,3-Diiodopropane $ICH_2CH_2CH_2I$ (gauche-gauche form) ... 1235
185. 1,4-Diiodobutane $ICH_2CH_2CH_2CH_2I$ (trans-trans-trans form) ... 1236
186. 1,4-Diiodobutane $ICH_2CH_2CH_2CH_2I$ (trans-trans-gauche form) ... 1237
187. 1,4-Diiodobutane $ICH_2CH_2CH_2CH_2I$ (trans-gauche-trans form) ... 1238
188. 1,4-Diiodobutane $ICH_2CH_2CH_2CH_2I$ (trans-gauche-gauche form) ... 1239
189. 1,4-Diiodobutane $ICH_2CH_2CH_2CH_2I$ (gauche-trans-gauche form) ... 1240
190. 1,4-Diiodobutane $ICH_2CH_2CH_2CH_2I$ (gauche-trans-gauche' form) ... 1241
191. 1,4-Diiodobutane $ICH_2CH_2CH_2CH_2I$ (gauche-gauche-gauche form) ... 1242
192. 2-Chloroethyl methyl ether $CH_3OCH_2CH_2Cl$ (trans-trans form) ... 1243
193. 2-Chloroethyl methyl ether $CH_3OCH_2CH_2Cl$ (trans-gauche form) ... 1244
194. 2-Chloroethyl methyl ether $CH_3OCH_2CH_2Cl$ (gauche-trans form) ... 1245
195. 2-Chloroethyl methyl ether $CH_3OCH_2CH_2Cl$ (gauche-gauche form) ... 1246
196. 2-Bromoethyl methyl ether $CH_3OCH_2CH_2Br$ (trans-trans form) ... 1247
197. 2-Bromoethyl methyl ether $CH_3OCH_2CH_2Br$ (trans-gauche form) ... 1248
198. 2-Bromoethyl methyl ether $CH_3OCH_2CH_2Br$ (gauche-trans form) ... 1249
199. 2-Bromoethyl methyl ether $CH_3OCH_2CH_2Br$ (gauche-gauche form) ... 1250
200. 2-Iodoethyl methyl ether $CH_3OCH_2CH_2I$ (trans-trans form) ... 1251
201. 2-Iodoethyl methyl ether $CH_3OCH_2CH_2I$ (trans-gauche form) ... 1252
202. 2-Iodoethyl methyl ether $CH_3OCH_2CH_2I$ (gauche-trans form) ... 1253
203. 2-Iodoethyl methyl ether $CH_3OCH_2CH_2I$ (gauche-gauche form) ... 1254

No. 110
Molecule: 1228-T $CH_3CH_2CH_2F$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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] IR.R. G. A. Crowder and H.-K. Mao, J. Mol. Struct., **18**, 33 (1973).

No. 111
Molecule: 1228-G $CH_3CH_2CH_2F$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2F$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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–)		

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Calculated frequencies higher than 2000 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 $CH_3CH_2CH_2CH_2F$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2F$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2F$ (gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2F$ (trans-trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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: 122228-TTG $CH_3CH_2CH_2CH_2F$ (trans-trans-gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2F$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2F$ (gauche-trans-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2Cl$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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	238	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 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 $CH_3CH_2CH_2Cl$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2Cl$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (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+)
	161	159	222-D (48-)	225-D (46+)	122-D (29+)	
a″	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 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 $CH_3CH_2CH_2CH_2Cl$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.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 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 $CH_3CH_2CH_2CH_2Cl$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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. 125
Molecule: 12225-GG $CH_3CH_2CH_2CH_2Cl$ (gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Cl$ (trans-trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Cl$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Cl$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Cl$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Cl$ (gauche-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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′ $CH_3CH_2CH_2CH_2CH_2Cl$ (gauche–trans–gauche′ form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 (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+)	2222–S(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^{-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. 132
Molecule: 52225-TT $ClCH_2CH_2CH_2Cl$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	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+)	
a_2	1305	1302	222–6 (57–)	522–6 (13+)	225–6 (13+)	
	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_1	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_2	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^{-1}
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 $ClCH_2CH_2CH_2Cl$ (*trans-gauche form*)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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. 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. 134
Molecule: 52225-GG $ClCH_2CH_2CH_2Cl$ (gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}
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. 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. 135
Molecule: 522225-TTT $ClCH_2CH_2CH_2CH_2Cl$ (trans-trans-trans form)
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	1444*	1461	222-2 (41+)	222-2 (41+)		
	1434*	1427	225-2 (38+)	522-2 (38+)		
	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+)	
a_u	1291*	1290	522-6 (20-)	225-6 (20-)	222-6 (20+)	222-6 (20+)
	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+)			
		61	5222-T(34+)	2225-T(34+)	2222-T(12-)	
b_g	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+)
	768	771	225-4 (29-)	522-4 (29-)	222-4 (18+)	222-4 (18+)
		164	2225-T(46+)	5222-T(46-)		
b_u	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 cm^{-1}
3005 3005 2956 2956 2909 2900 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. 136
Molecule: 522225-TTG $ClCH_2CH_2CH_2CH_2Cl$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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-)	
	748	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 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 $ClCH_2CH_2CH_2CH_2Cl$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $ClCH_2CH_2CH_2CH_2Cl$ (gauche-trans-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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+)			
b		1482	222–2 (44+)	222–2 (44–)		
	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^{-1}
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′ $ClCH_2CH_2CH_2CH_2Cl$ (gauche-trans-gauche′ form)
Symmetry C_i Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	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_u		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^{-1}
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 $ClCH_2CH_2CH_2CH_2Cl$ (gauche-gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}

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 $CH_3CH_2CH_2Br$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2Br$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 CH_3CHDCH_2Br (trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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_3CHDCH_2Br (gauche form)[a]
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (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+)		

[a] The CH_2Br group and the deuterium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm^{-1}

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_3CHDCH_2Br (gauche′ form)[a]
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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+)		

[a] The CH_2Br group and the protium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm^{-1}

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_3CH_2CHDBr (trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}
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_3CH_2CHDBr (gauche form)[a]
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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+)		

[a] The CH_2CH_3 group and the protium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm^{-1}

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_3CH_2CHDBr (gauche' form)[a]
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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+)		

[a] The CH_2CH_3 group and the deuterium of the CHD group are in the trans conformation.

Calculated frequencies higher than 2000 cm^{-1}

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 $CH_3CH_2CH_2CH_2Br$ (trans-trans form)

Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 cm^{-1}

3003 2962 2962 2956 2909 2900 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. 150
Molecule: 12226-TG $CH_3CH_2CH_2CH_2Br$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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. Imazcki, H. Yamaguchi, H. Matsuura, I. Harada, and T. Shimanouchi, Bull. Chem. Soc. Jpn., **51**, 748 (1978).

No. 151
Molecule: 12226-GT $CH_3CH_2CH_2CH_2Br$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2Br$ (gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Br$ (trans-trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Br$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Br$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2Br$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2Br$ (gauche-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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. 158
Molecule: 122226-GTG′ $CH_3CH_2CH_2CH_2CH_2Br$ (gauche-trans-gauche′ form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 (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^{-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. 159
Molecule: 62226-TT $BrCH_2CH_2CH_2Br$ (*trans-trans form*)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	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–)	
a_2	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+)	
		138	2226–T(47+)	6222–T(47+)		
b_1	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_2	1232*	1247	622–6 (33+)	226–6 (33–)	222–4 (15–)	
		982	222–4 (25+)	226–4 (22–)	622–4 (22+)	226–6 (15–)
		743	222–4 (51–)	622–4 (20+)	226–4 (20+)	
	105*	100	6222–T(40+)	2226–T(40–)	222–4 (12–)	

Calculated frequencies higher than 2000 cm^{-1}
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. 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. 160
Molecule: 62226-TG $BrCH_2CH_2CH_2Br$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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. 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. 161
Molecule: 62226-GG $BrCH_2CH_2CH_2Br$ (*gauche-gauche form*)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}
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 $BrCH_2CH_2CH_2CH_2Br$ (trans-trans-trans form)
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	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+)	
a_u	1273	1280	222-6 (23+)	222-6 (23+)	226-6 (16-)	622-6 (16-)
	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_g	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_u	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^{-1}

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 $BrCH_2CH_2CH_2CH_2Br$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.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^{-1}

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 $BrCH_2CH_2CH_2CH_2Br$ (trans-gauche-trans form)

Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}

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 $BrCH_2CH_2CH_2CH_2Br$ (*trans-gauche-gauche form*)
Symmetry C_1 **Symmetry number** $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $BrCH_2CH_2CH_2CH_2Br$ (gauche-trans-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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+)		
	484	481	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^{-1}

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′ $BrCH_2CH_2CH_2CH_2Br$ (gauche-trans-gauche′ form)
Symmetry C_i Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g		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_u		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^{-1}
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 $BrCH_2CH_2CH_2CH_2Br$ (gauche-gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}
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 $CH_3CH_2CH_2I$ (trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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+)	122–6 (14+)
	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 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 $CH_3CH_2CH_2I$ (gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2I$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2I$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2I$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 cm^{-1}
2998 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 $CH_3CH_2CH_2CH_2I$ (gauche-gauche form)

Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2I$ (trans-trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a	1481	1484	122-2 (39-)	222-2 (34+)	012-4 (15-)	
	1474	1478	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 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 $CH_3CH_2CH_2CH_2CH_2I$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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(93-)	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 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 $CH_3CH_2CH_2CH_2CH_2I$ (trans-gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2I$ (gauche-trans-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2I$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3CH_2CH_2CH_2CH_2I$ (gauche-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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′ $CH_3CH_2CH_2CH_2CH_2I$ (gauche–trans–gauche′ form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-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. 182
Molecule: 72227-TT $ICH_2CH_2CH_2I$ (trans-trans form)
Symmetry C_{2v} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_1	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_2	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_1	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_2	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^{-1}
2999 2998 2963 2962 2904 2869

Reference

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

No. 183
Molecule: 72227-TG $ICH_2CH_2CH_2I$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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. Torgrimsen, J. Mol. Struct., **15**, 61 (1973).

No. 184
Molecule: 72227-GG $ICH_2CH_2CH_2I$ (gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (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^{-1}
3000 2997 2963 2962 2904 2869

Reference

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

No. 185
Molecule: 722227-TTT $ICH_2CH_2CH_2CH_2I$ (trans-trans-trans form)
Symmetry C_{2h} Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g	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+)	
a_u	1246*	1246	222-6 (30+)	222-6 (30+)	722-6 (10-)	227-6 (10-)
	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_g	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+)
		153	2227-T(44+)	7222-T(44-)		
b_u		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^{-1}

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 $ICH_2CH_2CH_2CH_2I$ (trans-trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}
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 $ICH_2CH_2CH_2CH_2I$ (trans-gauche-trans form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $ICH_2CH_2CH_2CH_2I$ (trans-gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}
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 $ICH_2CH_2CH_2CH_2I$ (gauche-trans-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}

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′ $ICH_2CH_2CH_2CH_2I$ (gauche-trans-gauche′ form)
Symmetry C_i **Symmetry number** $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignment (P.E.D. %)			
a_g		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_u		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^{-1}

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 $ICH_2CH_2CH_2CH_2I$ (gauche-gauche-gauche form)
Symmetry C_2 Symmetry number $\sigma = 2$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	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^{-1}
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 $CH_3OCH_2CH_2Cl$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2Cl$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2Cl$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2Cl$ (gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2Br$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2Br$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2Br$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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+)	3226-S(11+)
	445	442	132-B (75-)	2260-S(13+)	322-D (13+)	
	316	321	322-D (34-)	2260-S(21-)	0132-T(13-)	1322-T(12+)
		240	226-D (74+)			
		178	0132-T(75+)	322-D (14-)	226-D (12+)	
		117	1322-T(84-)			
		95	3226-T(82+)			

Calculated frequencies higher than 2000 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 $CH_3OCH_2CH_2Br$ (gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2I$ (trans-trans form)
Symmetry C_s Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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+)	3227-S(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 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 $CH_3OCH_2CH_2I$ (trans-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2I$ (gauche-trans form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency 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 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 $CH_3OCH_2CH_2I$ (gauche-gauche form)
Symmetry C_1 Symmetry number $\sigma = 1$

Sym. species	Observed frequency cm^{-1}	Calculated frequency cm^{-1}	Assignmen (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 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).