

Vibrational Contributions to Molecular Dipole Polarizabilities

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An often overlooked, but nonetheless important, contribution to molecular dipole polarizabilities is that which comes from molecular vibration. This contribution, which was formerly called the atomic polarization, may be related to the intensities of the infrared-active bands. In this paper we have collected the best available intensity data for some hundred or so molecules and evaluated their vibrational polarizabilities. We have also given estimates of the probable errors of the final numbers.

Key words: Atomic polarization; dipole polarizabilities; infrared intensities; molecular polarizabilities; vibrational polarizabilities.

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Introduction

When a molecule is placed in an electric field it exhibits molecular polarization [1]¹, a property which, in principle, has three components: orientation polarization, electronic polarization and vibrational polarization. In this paper we are concerned with the last component. Vibrational polarization is due to a distortion of the vibrational motion of the molecule by the field, and it exists for all molecules having infrared-active transitions. The measure of this polarization is called vibrational polarizability, or in the older literature "atomic polarizability" (a name first introduced by Ebert [2]). However, this phrase may be confused with the polarizability of an atom, and the expression vibrational polarizability is to be preferred [3]. To be precise we will discuss only the dipole polarizability of a molecule in its vibrational ground state and that only for static fields. A similar contribution exists for the higher order polarizabilities and for dynamic fields. Compared with the electronic polarizability, the vibrational polarizability is often quite large, e.g., for CHF₃ it is 25% of the former.

There are two ways of determining vibrational polarizabilities: (a) directly from dielectric constants and molar refractivities, (b) indirectly from the measured intensities of the molecule's infrared-active bands. The first method is usually of low

accuracy and so we will consider only the second. This approach has been used in the past by several workers [4] and has been discussed in detail and applied to an extensive group of molecules by Illinger and Smyth [5]. Since this last work was published (1960–61), much more experimental intensity data has become available; this paper gives an up-to-date compendium of vibrational polarizabilities which can now be determined.

Since the infrared intensities are related to transition dipole moments, the vibrational polarizabilities may also be derived from calculated values of the latter, e.g., Pandey and Santry's calculation for CO, HCN, and H₂O [6] and Bishop and Cheung's calculation [7] for HeH⁺ (this last calculation shows the importance of vibrational polarizability, in that, because of the charge and the weakness of the bond, the contribution is greater than the electronic contribution). Most purely theoretical calculations of polarizability completely neglect the vibrational contribution (since they are usually fixed nuclei calculations), and one use of the tables we present here is the indication they give of whether such a neglect is reasonable or not. It must be recognized that theoretical predictions of transition dipole moments are often very unreliable.

2. Calculation of Polarizability

Our basic working formula is

$$\bar{\alpha} = \frac{2}{3} \sum_n' g_n \mu_n^2 / h c \omega_n \quad (1)$$

where $\bar{\alpha}$ is the static isotropic vibrational dipole polarizability

¹Figures in brackets indicate literature references at the end of this paper.

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for the molecule in its vibrational ground state, the summation is over the fundamental vibrational modes, g_n is the degeneracy of the n^{th} mode, μ_n is the transition dipole moment (from the ground state) of the n^{th} mode and ω_n the corresponding frequency (in wavenumbers). This formula may be derived from the Kramers-Heisenberg dispersion formula with the proviso that rotational spacings are much smaller than vibrational spacings and closure over rotation can be carried out [3,7]. Contributions to $\bar{\alpha}$ from multiply-excited vibrational levels have been discarded as being inconsequentially small [5]. These approximations are equivalent to working in the harmonic oscillator approximation and taking the transition frequencies to be the harmonic frequencies.

The transition dipole moments are determined from the absolute integrated intensities by way of

$$A_n = 2\pi^2 N_A g_n \omega_n \mu_n^2 / 3\epsilon_0 h c \quad (2)$$

where N_A is Avogadro's number and ϵ_0 the permittivity of empty space. If A_n is in km mol^{-1} and ω_n in cm^{-1} , then

$$\mu_n = 2.1069(A_n / g_n \omega_n)^{1/2} 10^{-30} \text{C m} \quad (3)$$

These formulas are approximate to the extent that it is assumed that the excited vibrational states are not populated [8].

3. Source of Intensity Data

Our survey of intensity data was taken up to the end of 1980; a major source was reference [9]. The conversion factors for converting, where necessary, the A_n to the units of km mol^{-1} were taken from this reference. Often the intensities were originally given as $\Gamma_n = A_n / \omega_n$ (Crawford's alternate definition [8]). In most cases we have used the most recent sources unless the values conflict with several other workers. As well, we have preferred to take the intensity data for a given molecule from a single source. In all cases where error limits on the intensities have been given by the authors, we have categorized the error in $\bar{\alpha}$ (the same as the error in the weighted sum of the intensities) by one of the three following classes: (a) less than or equal to 5%, (b) between 5 and 10%, (c) more than 10%. Where our results are the same as the earlier tabulation by Illinger and Smyth [5] we have so indicated.

It is almost certainly true that the error limits on the intensities given by the authors of the articles surveyed in the review

are unduly optimistic. Often in intensity experiments there are systematic errors much larger than the random errors. An example of such an error is the inaccuracy in the pressure measurement, to which the intensities are very sensitive. Consequently, it is not unusual for the results from two different laboratories to differ by 100%. Further inaccuracies arise from instrumental distortion of the bands, inadequate resolution and, most importantly, band overlapping. With the information available, we have often found it difficult to choose one source of data over another and have simply taken the more recent values. We do, however, feel that the errors given by the authors are probably too small and that more realistically, the error classes a, b, and c given above, should be defined: (a) less than or equal to 10%, (b) between 10 and 50%, (c) greater than 50%.

One check on the accuracy that is available where there is information for a series of isotopic molecules is Crawford's F -sum rule [8]. This rule implies that $\bar{\alpha}$ should, within certain constraints, be approximately constant for such a series. There are many places in the following tables where this rule applies and where the constancy is within the given error bounds. However, two places where this is not so are (a) HCOF/DCOF, where the authors must have underestimated their error, and (b) the value for CD_3Br , which is out of line with that for CH_3Br , CH_2DBr , and CHD_2Br ; this discrepancy is also apparent when alternative intensity data for CD_3Br is used. In both of these cases further intensity measurements are called for.

4. Results

Combination of eqs (1) and (2) allows $\bar{\alpha}$ to be found from the experimental frequencies (ω_n) and intensities (A_n), and these values are listed in tables 1-7. We have also evaluated the contribution of each infrared-active normal mode to the sum in eq (1), by calculating the molar vibrational polarization (P_n) of each mode. The total P and $\bar{\alpha}$ are related by

$$\bar{\alpha} = 3\epsilon_0 P / N_A = 0.441 P \times 10^{-40} \text{C}^2 \text{m}^2 \text{J}^{-1}. \quad (4)$$

Values of individual contributions allow the anisotropic vibrational polarizabilities to be easily found.

The error estimates given in the tables are based on the uncertainties given by the original authors. However, as discussed in section 3, these estimates should be at least doubled to take into account the possible systematic errors in the intensity measurements.

Table 1. Diatomic molecules

Molecule	$\omega(\text{cm}^{-1})$	A(km/mol)	P(cm^3/mol)	$\bar{\alpha}(10^{-40}\text{C}_m^2\text{J}^{-1})$
AlO	964 [9]	177. [10]	0.64	0.28 ^d
BrCl	430 [9]	1.05 [11]	0.019	0.0085 ^d
CO	2143 [9]	61.2 [12]	0.045	0.020 ^b
ClO($^2\Pi_{1/2}$)	842 [13]	2.2 [13]	0.011	0.0047
ClO($^2\Pi_{3/2}$)	844 [13]	2.91 [13]	0.014	0.0061 ^d
FeO	870 [9]	101. [14]	0.45	0.20 ^d
HBr	2559 [9]	8.6 [15]	0.0044	0.0019 ^c
HCl	2886 [9]	33.2 [16]	0.014	0.0059 ^b
DCl	2091 [9]	16.4 [17]	0.013	0.0056 ^{a,c}
HF	3962 [9]	77.5 [18]	0.017	0.0074 ^a
HI	2230 [9]	0.091[19]	0.000062	0.000027 ^b
ICl	381 [9]	6.50 [11]	0.15	0.067 ^{a,d}
NO	1876 [9]	27.3 [20]	0.026	0.012 ^b

^aSame result as reference [5].

^bThe estimated error is 5%.

^cThe estimated error is between 5 and 10%.

^dThe estimated error is more than 10%.

Table 2. Triatomic molecules

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$
BrCN	$\nu_1(\sigma^+)$	589 [21]	1.06 [21]	0.010	0.049 ^c
	$\nu_2(\pi)$	342	3.30	0.095	
	$\nu_3(\sigma^+)$	2198	7.70	0.0054	
ClCN	$\nu_1(\sigma^+)$	744 [21]	9.08 [21]	0.055	0.077 ^c
	$\nu_2(\pi)$	378	4.55	0.11	
	$\nu_3(\sigma^+)$	2216	18.2	0.013	
CO ₂	$\nu_2(\pi_u)$	667 [9]	47.8 [22]	0.36	0.29 ^c
	$\nu_3(\sigma_u^+)$	2349	498.7 [23]	0.31	
CS ₂	$\nu_2(\pi_u)$	397 [9]	5.00 [24]	0.11	0.39 ^c
	$\nu_3(\sigma_u^+)$	1535	550.	0.79	
HCN	$\nu_1(\sigma^+)$	2097 [9]	0.16 [25]	0.00012	0.16 ^{a,d}
	$\nu_2(\pi)$	712	50.2	0.33	
	$\nu_3(\sigma^+)$	3311	59.3	0.018	
DCN	$\nu_1(\sigma^+)$	1925 [9]	3.0 [25]	0.0027	0.078 ^{a,d}
	$\nu_2(\pi)$	569	15.	0.16	
	$\nu_3(\sigma^+)$	2630	33.5	0.016	
H ₂ O	$\nu_1(a_1)$	3657 [9]	2.93 [26]	0.00074	0.041
	$\nu_2(a_1)$	1595	62.5	0.083	
	$\nu_3(b_1)$	3756	41.7	0.010	
HOD	$\nu_1(a')$	2724 [27]	13.5 [27]	0.0061	0.047
	$\nu_2(a')$	1403	54.7	0.094	
	$\nu_3(a')$	3707	30.1	0.0074	
HOCl	$\nu_1(a')$	3609 [28]	56.2 [29]	0.015	0.11 ^d
	$\nu_2(a')$	1240	73.4	0.16	
	$\nu_3(a')$	725	11	0.068	
N ₂ O	$\nu_1(\sigma^+)$	1285 [9]	59.1 [30]	0.12	0.18 ^b
	$\nu_2(\pi)$	589	8.20 [31]	0.080	
	$\nu_3(\sigma^+)$	2224	289. [32]	0.20	
O ₃	$\nu_1(a_1)$	1103 [9]	2.38 [33]	0.0066	0.13
	$\nu_2(a_1)$	701	4.4 [34]	0.030	
	$\nu_3(b_1)$	1042	85.7 [34]	0.27	
OCS	$\nu_1(\sigma^+)$	859 [9]	8.22 [35]	0.038	0.24 ^c
	$\nu_2(\pi)$	521	2.90 [31]	0.036	
	$\nu_3(\sigma^+)$	2062	600. [31]	0.48	
SO ₂	$\nu_1(a_1)$	1151 [9]	23.5 [36]	0.060	0.33
	$\nu_2(a_1)$	518	27.03	0.34	
	$\nu_3(b_1)$	1362	192	0.35	

^aSame result as reference [5].

^bThe estimated error is 5%.

^cThe estimated error is between 5 and 10%.

^dThe estimated error is more than 10%.

MOLECULAR DIPOLE POLARIZABILITIES

Table 3. Four-atomic molecules

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$
BCl ₃	$\nu_2(a_2'')$	455 [9]	1.499[37]	0.024	
	$\nu_3(e')$	956	231.26	0.85	
	$\nu_4(e')$	249	0.7823	0.043	0.41
BF ₃	$\nu_2(a_2'')$	691 [9]	81.7 [38]	0.58	
	$\nu_3(e')$	1454	809.9	1.3	
	$\nu_4(e')$	480	23.	0.34	0.98 ^c
C ₂ H ₂	$\nu_3(\sigma_u^+)$	3282[39]	70.4 [39]	0.022	
	$\nu_5(\pi_u)$	730	177.1	1.1	0.50 ^b
C ₂ HD	$\nu_1(\sigma^+)$	3336[39]	30.1 [39]	0.0091	
	$\nu_2(\sigma^+)$	1854	1.0	0.00098	
	$\nu_3(\sigma^+)$	2582	21.7	0.011	
	$\nu_4(\pi)$	518	20.0	0.25	
	$\nu_5(\pi)$	678	114.8	0.84	0.49 ^b
C ₂ D ₂	$\nu_3(\sigma_u^+)$	2439[39]	37.7 [39]	0.021	
	$\nu_5(\pi_u)$	537	94.3	1.1	0.50 ^b
C ₂ N ₂	$\nu_3(\sigma_u^+)$	2158[40]	4.48 [41]	0.0032	
	$\nu_5(\pi_u)$	233	36.9 [42]	2.3	1.0
COBr ₂	$\nu_1(a_1)$	1828 [9]	231.52 [43]	0.23	
	$\nu_2(a_1)$	425	3.87	0.072	
	$\nu_3(a_1)$	181	0.217	0.022	
	$\nu_4(b_1)$	757	256.34	1.5	
	$\nu_5(b_1)$	350	0.994	0.027	
	$\nu_6(b_2)$	512	1.82	0.023	0.83 ^b
COCl ₂	$\nu_1(a_1)$	1827[43]	245.26 [43]	0.25	
	$\nu_2(a_1)$	567	14.48	0.15	
	$\nu_3(a_1)$	285	0.0698	0.0029	
	$\nu_4(b_1)$	850	376.45	1.8	
	$\nu_5(b_1)$	440	0.176	0.0031	
	$\nu_6(b_2)$	580	4.90	0.049	0.98 ^b
COF ₂	$\nu_1(a_1)$	1928[43]	381.74 [43]	0.35	
	$\nu_2(a_1)$	965	56.44	0.21	
	$\nu_3(a_1)$	626	7.036	0.061	
	$\nu_4(b_1)$	1249	370.79	0.80	
	$\nu_5(b_1)$	584	5.20	0.052	
	$\nu_6(b_2)$	774	30.64	0.17	0.72 ^b
CSCl ₂	$\nu_1(a_1)$	1137[44]	210.80 [44]	0.55	
	$\nu_2(a_1)$	505	13.81	0.18	
	$\nu_3(a_1)$	220	0	0	
	$\nu_4(b_1)$	816	162.93	0.83	
	$\nu_5(b_1)$	294	0.303	0.012	
	$\nu_6(b_2)$	473	2.36	0.036	0.71 ^b
CSF ₂	$\nu_1(a_1)$	1368[44]	390.35 [44]	0.71	
	$\nu_2(a_1)$	787	8.925	0.049	
	$\nu_3(a_1)$	526	6.717	0.082	
	$\nu_4(b_1)$	1189	201.54	0.48	
	$\nu_5(b_1)$	417	0.25	0.0048	
	$\nu_6(b_2)$	622	1.33	0.012	0.59 ^b

Table 3. Four-atomic molecules (continued)

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$
HCOF	$\nu_1(a')$	2981 [45]	17.52 [45]	0.0067	
	$\nu_2(a')$	1837	191.10	0.19	
	$\nu_3(a')$	1343	1.09	0.0020	
	$\nu_4(a')$	1065	132.65	0.39	
	$\nu_5(a')$	663	17.76	0.14	
	$\nu_6(a'')$	1012	0.53	0.0017	0.32 ^b
DCOF	$\nu_1(a')$	2262 [45]	35.12 [45]	0.023	
	$\nu_2(a')$	1797	155.46	0.16	
	$\nu_3(a')$	1073	156.36	0.46	
	$\nu_4(a')$	968	35.81	0.13	
	$\nu_5(a')$	658	17.27	0.13	
	$\nu_6(a'')$	857	0.38	0.0017	0.40 ^b
H ₂ CO	$\nu_1(a_1)$	2783 [9]	52.7 [46]	0.023	
	$\nu_2(a_1)$	1746	58.3	0.065	
	$\nu_3(a_1)$	1500	9.28	0.014	
	$\nu_4(b_1)$	2843	75.1	0.031	
	$\nu_5(b_1)$	1249	6.03	0.013	
	$\nu_6(b_2)$	1167	3.84	0.0095	0.069 ^d
NF ₃	$\nu_1(a_1)$	1032 [9]	29.5 [47]	0.094	
	$\nu_2(a_1)$	647	1.55	0.013	
	$\nu_3(e)$	907	399.	1.6	
	$\nu_4(e)$	492	1.36	0.019	0.78 ^c
NH ₃	$\nu_1(a_1)$	3337 [9]	4.9 [48]	0.0015	
	$\nu_2(a_1)$	950	148.	0.55	
	$\nu_3(e)$	3444	3.2	0.00091	
	$\nu_4(e)$	1627	27.1	0.035	0.26 ^{a,d}
PF ₃	$\nu_1(a_1)$	892 [9]	110.25 [49]	0.47	
	$\nu_2(a_1)$	487	24.14	0.34	
	$\nu_3(e)$	860	416.1	1.9	
	$\nu_4(e)$	344	8.576	0.24	1.3 ^b
PH ₃	$\nu_1(a_1)$	2323 [9]	64.0 [48]	0.040	
	$\nu_2(a_1)$	992	20	0.069	
	$\nu_3(e)$	2328	64.0	0.040	
	$\nu_4(e)$	1118	25.1	0.068	0.096 ^d

^aSame result as reference [5].

^bThe estimated error is 5%.

^cThe estimated error is between 5 and 10%.

^dThe estimated error is more than 10%.

MOLECULAR DIPOLE POLARIZABILITIES

Table 4. Five-atomic molecules

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$	
CCl ₄	v ₃ (t ₂)	793[50]	322	[50]	1.7	0.77 ^d
	v ₄ (t ₂)	310	0.20		0.0070	
CF ₄	v ₃ (t ₂)	1283 [9]	935.3	[51]	1.9	0.89 ^d
	v ₄ (t ₂)	632	12.3		0.10	
CF ₃ Br	v ₁ (a ₁)	1085 [9]	463.6	[52]	1.3	1.2 ^d
	v ₂ (a ₁)	761	29.36		0.17	
	v ₃ (a ₁)	350	0.25		0.0068	
	v ₄ (e)	1209	464.8		1.1	
	v ₅ (e)	550	2.394		0.027	
	v ₆ (e)	305	0.25		0.0089	
CFCl ₃	v ₁ (a ₁)	1085[53]	156.	[54]	0.45	1.0 ^d
	v ₂ (a ₁)	539	1.13	[53]	0.013	
	v ₃ (a ₁)	347	0.29	[53]	0.0083	
	v ₄ (e)	846	378.1	[54]	1.8	
	v ₅ (e)	384	0.05	[53]	0.0011	
	v ₆ (e)	243	0.01	[53]	0.00057	
CF ₂ Cl ₂	v ₁ (a ₁)	1095[55]	298	[55]	0.84	1.2
	v ₂ (a ₁)	665	12.3		0.094	
	v ₃ (a ₁)	442	0.2		0.0038	
	v ₄ (a ₁)	261	2.6 ^b		0.13	
	v ₆ (b ₁)	1152	199		0.51	
	v ₇ (b ₁)	475	0.1		0.0021	
	v ₈ (b ₂)	915	307		1.2	
	v ₉ (b ₂)	432	0.1		0.0024	
CF ₂ Cl	v ₁ (a ₁)	1102[56]	561	[56]	1.6	1.5 ^d
	v ₂ (a ₁)	783	35		0.19	
	v ₃ (a ₁)	470	0		0	
	v ₄ (e)	1210	672		1.6	
	v ₅ (e)	560	3.1		0.033	
	v ₆ (e)	350	0		0	
CF ₃ I	v ₁ (a ₁)	1074[53]	573.3	[53]	1.7	1.3 ^d
	v ₂ (a ₁)	743	43.0		0.26	
	v ₃ (a ₁)	284	0.15		0.0063	
	v ₄ (e)	1185	445.2		1.1	
	v ₅ (e)	539	2.1		0.024	
	v ₆ (e)	260	0.04		0.0020	
CH ₄	v ₃ (t ₂)	3019[57]	65.5	[58]	0.024	0.038 ^d
	v ₄ (t ₂)	1311	31.8		0.062	
CD ₄	v ₃ (t ₂)	2260[57]	28.8	[58]	0.019	0.036 ^d
	v ₄ (t ₂)	998	18.4		0.062	
CH ₃ D	v ₁ (a ₁)	2950[50]	7.2	[50]	0.0028	0.043
	v ₂ (a ₁)	2205	7.2		0.0050	
	v ₃ (a ₁)	1300	12.2		0.024	
	v ₄ (e)	3021	53.0		0.020	
	v ₅ (e)	1477	4.1		0.0063	
	v ₆ (e)	1156	15.7		0.040	
CH ₂ D ₂	v ₁ (a ₁)	2976[50]	13.8	[50]	0.0053	0.043
	v ₂ (a ₁)	2140	5.6		0.0041	
	v ₃ (a ₁)	1436	4.4		0.0072	
	v ₄ (a ₁)	1032	5.2		0.016	
	v ₆ (b ₁)	3020	26.0		0.0096	
	v ₇ (b ₁)	1091	8.1		0.023	
	v ₈ (b ₂)	2255	12.2		0.0081	
	v ₉ (b ₂)	1234	11.1		0.025	
CHD ₃	v ₁ (a ₁)	3000[50]	18.3	[50]	0.0069	0.038
	v ₂ (a ₁)	2141	2.5		0.0018	
	v ₃ (a ₁)	1000	7.0		0.024	
	v ₄ (e)	2260	22.7		0.015	
	v ₅ (e)	1291	7.1		0.014	
	v ₆ (e)	1035	8.1		0.026	

Table 4. Five-atomic molecules (continued)

Molecule	Band	$\omega_{\text{H}}(\text{cm}^{-1})$	$A_{\text{H}}(\text{km/mol})$	$P_{\text{H}}(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$
CH ₃ Br	$\nu_1(a_1)$	2972[59]	16.452[59]	0.0063	
	$\nu_2(a_1)$	1305	15.388	0.031	
	$\nu_3(a_1)$	611	11.186	0.10	
	$\nu_4(e)$	3056	5.196	0.0019	
	$\nu_5(e)$	1445	12.591	0.020	
	$\nu_6(e)$	952	7.237	0.027	0.083 ^d
CD ₃ Br	$\nu_1(a_1)$	2157[59]	8.89 [59]	0.0065	
	$\nu_2(a_1)$	993	12.547	0.043	
	$\nu_3(a_1)$	578	6.730	0.068	
	$\nu_4(e)$	2293	2.200	0.0014	
	$\nu_5(e)$	1056	5.377	0.016	
	$\nu_6(e)$	712	1.951	0.013	0.065 ^d
CH ₂ DBr	$\nu_1(a')$	3001[59]	11.737[59]	0.0044	
	$\nu_2(a')$	1225	12.759	0.029	
	$\nu_3(a')$	594	9.010	0.086	
	$\nu_4(a')$	2244	4.866	0.0033	
	$\nu_5(a')$	1425	8.603	0.014	
	$\nu_6(a')$	769	3.544	0.020	
	$\nu_7(a'')$	3052	2.934	0.0011	
	$\nu_8(a'')$	1240	4.962	0.011	
	$\nu_9(a'')$	930	4.343	0.017	0.082 ^d
CHD ₂ Br	$\nu_1(a')$	2196[59]	9.306[59]	0.0065	
	$\nu_2(a')$	1208	8.297	0.019	
	$\nu_3(a')$	584	7.984	0.079	
	$\nu_4(a')$	3027	7.792	0.0029	
	$\nu_5(a')$	1036	7.686	0.024	
	$\nu_6(a')$	816	6.004	0.030	
	$\nu_7(a'')$	2288	1.772	0.0011	
	$\nu_8(a'')$	1290	8.297	0.017	
	$\nu_9(a'')$	717	0.897	0.0059	0.082 ^d
CHCl ₃	$\nu_1(a_1)$	3034[60]	0.346 [60]	0.00013	
	$\nu_2(a_1)$	681	5.11	0.037	
	$\nu_3(a_1)$	366	0.293	0.0074	
	$\nu_4(e)$	1221	47.6	0.11	
	$\nu_5(e)$	769	267.6	1.5	
	$\nu_6(e)$	258	0.129	0.0065	0.74
CDCl ₃	$\nu_1(a_1)$	2259[60]	0.108 [60]	0.000072	
	$\nu_2(a_1)$	655	4.65	0.037	
	$\nu_3(a_1)$	362	0.434	0.011	
	$\nu_4(e)$	914	69.5	0.28	
	$\nu_5(e)$	744	209.1	1.3	
	$\nu_6(e)$	258	0.155	0.0079	0.71
CH ₂ Cl ₂	$\nu_1(a_1)$	2997 [9]	6.9 [61]	0.0026	
	$\nu_2(a_1)$	1467	0.6	0.00094	
	$\nu_3(a_1)$	717	8.0	0.053	
	$\nu_4(a_1)$	282	0.6	0.025	
	$\nu_6(b_1)$	3055	0	0	
	$\nu_7(b_1)$	898	1.2	0.0050	
	$\nu_8(b_2)$	1268	26.6	0.056	
	$\nu_9(b_2)$	758	95.0	0.56	0.31 ^e
	CHDCl ₂	$\nu_1(a')$	3024 [9]	3.1 [61]	0.0011
$\nu_2(a')$		2249	2.4	0.0016	
$\nu_3(a')$		1282	0.6	0.0012	
$\nu_4(a')$		778	2.8	0.016	
$\nu_5(a')$		692	5.7	0.040	
$\nu_6(a')$		283	0.6	0.025	
$\nu_7(a'')$		1223	17.0	0.038	
$\nu_8(a'')$		890	29.0	0.12	
$\nu_9(a'')$		738	72.0	0.45	0.31 ^d

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Table 4. Five-atomic molecules (continued)

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}_m^2\text{J}^{-1})$
CD ₂ Cl ₂	$\nu_1(a_1)$	2205[61]	4.3 [61]	0.0030	
	$\nu_2(a_1)$	1050	0.2	0.00061	
	$\nu_3(a_1)$	687	8.0	0.057	
	$\nu_4(a_1)$	280	0.6	0.026	
	$\nu_6(b_1)$	2304	0	0	
	$\nu_7(b_1)$	710	0.5	0.0033	
	$\nu_8(b_2)$	960	50.0	0.18	
	$\nu_9(b_2)$	727	67.0	0.43	
CH ₃ Cl	$\nu_1(a_1)$	2930 [9]	17.34 [62]	0.0068	
	$\nu_2(a_1)$	1355	6.799	0.013	
	$\nu_3(a_1)$	732	23.18	0.15	
	$\nu_4(e)$	3006	9.571	0.0036	
	$\nu_5(e)$	1452	12.29	0.020	
	$\nu_6(e)$	1017	4.027	0.013	
					0.089 ^{a,d}
CD ₃ Cl	$\nu_1(a_1)$	2161[62]	11.39 [62]	0.0082	
	$\nu_2(a_1)$	1029	10.76	0.034	
	$\nu_3(a_1)$	695	15.36	0.11	
	$\nu_4(e)$	2286	5.109	0.0033	
	$\nu_5(e)$	1058	6.914	0.021	
	$\nu_6(e)$	775	1.108	0.0062	
					0.079 ^{a,e}
CHF ₃	$\nu_1(a_1)$	3036 [9]	24.6 [63]	0.0090	
	$\nu_2(a_1)$	1117	95.9 ^b	0.26	
	$\nu_3(a_1)$	700	14.3	0.099	
	$\nu_4(e)$	1372	87.6	0.16	
	$\nu_5(e)$	1152	493.6 ^b	1.3	
	$\nu_6(e)$	507	4.9	0.064	
					0.81 ^f
CDF ₃	$\nu_1(a_1)$	2261[64]	24.93 [65]	0.016	
	$\nu_2(a_1)$	1111	85.47	0.23	
	$\nu_3(a_1)$	694	12.39	0.087	
	$\nu_4(e)$	1202	531.74	1.2	
	$\nu_5(e)$	975	43.69	0.16	
	$\nu_6(e)$	502	5.04	0.068	
					0.79 ^d
CH ₂ F ₂	$\nu_1(a_1)$	2948[66]	29.80 [66]	0.012	
	$\nu_2(a_1)$	1508	0	0	
	$\nu_3(a_1)$	1113	54.99	0.15	
	$\nu_4(a_1)$	529	4.70	0.057	
	$\nu_6(b_1)$	3014	41.00	0.015	
	$\nu_7(b_1)$	1178	8.95	0.022	
	$\nu_8(b_2)$	1435	10.34	0.017	
	$\nu_9(b_2)$	1090	243.94	0.69	
CD ₂ F ₂	$\nu_1(a_1)$	2129[66]	15.31 [66]	0.011	
	$\nu_2(a_1)$	1165	172.48	0.43 ^c	
	$\nu_8(b_2)$	1158			
	$\nu_3(a_1)$	1026	113.52	0.37 ^c	
	$\nu_9(b_2)$	1002			
	$\nu_4(a_1)$	522	4.88	0.060	
	$\nu_6(b_1)$	2284	18.20	0.012	
$\nu_7(b_1)$	962	7.80	0.028		
					0.41 ^e
CH ₃ F	$\nu_1(a_1)$	2910[67]	24.73 [68]	0.0099	
	$\nu_2(a_1)$	1460	0.8947	0.0014	
	$\nu_3(a_1)$	1049	94.99	0.29	
	$\nu_4(e)$	3006	61.02	0.023	
	$\nu_5(e)$	1468	8.679	0.014	
	$\nu_6(e)$	1182	2.617	0.0063	
					0.15 ^e
CD ₃ F	$\nu_1(a_1)$	2110[67]	21.533[68]	0.016	
	$\nu_2(a_1)$	1135	41.460	0.11	
	$\nu_3(a_1)$	992	73.343	0.25	
	$\nu_4(e)$	2259	38.374	0.025	
	$\nu_5(e)$	1071	4.736	0.014	
	$\nu_6(e)$	911	0.358	0.0015	
					0.18 ^e
CH ₃ I	$\nu_1(a_1)$	2970 [9]	11.03 [62]	0.0042	
	$\nu_2(a_1)$	1252	20.67	0.045	
	$\nu_3(a_1)$	535	1.931	0.023	
	$\nu_4(e)$	3060	2.15	0.00078	
	$\nu_5(e)$	1436	10.56	0.017	
	$\nu_6(e)$	882	8.929	0.039	
					0.057 ^{a,d}

Table 4. Five-atomic molecules (continued)

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha} (10^{-40} \text{C}^2 \text{m}^2 \text{J}^{-1})$	
CD ₃ I	$\nu_1(a_1)$	2130 [9]	6.034 [62]	0.0045		
	$\nu_2(a_1)$	951	13.782	0.051		
	$\nu_3(a_1)$	501	0.982	0.013		
	$\nu_4(e)$	2298	0.683	0.00044		
	$\nu_5(e)$	1049	6.252	0.019		
	$\nu_6(e)$	656	3.172	0.025		0.050 ^{a,e}
GeH ₄	$\nu_3(t_2)$	2114 [9]	313.1 [69]	0.24		
	$\nu_4(t_2)$	819	281.6	1.4		0.73 ^d
GeD ₄	$\nu_3(t_2)$	1522 [9]	171.4 [69]	0.25		
	$\nu_4(t_2)$	596	137.2	1.3		0.68 ^d
HCBrc1F	ν_1	3026 [70]	3 [71]	0.0011		
	ν_2	1311	34	0.067		
	ν_3	1205	75	0.17		
	ν_4	1078	189	0.55		
	ν_5	788	198	1.1		
	ν_6	664	71	0.54		
	ν_7	427	5	0.093		
	ν_8	315	1	0.034		
	ν_9	226	0	0		1.1 ^f
SiF ₄	$\nu_3(t_2)$	1032 [9]	590.6 [72]	1.9		
	$\nu_4(t_2)$	389	113.7	2.5		1.9 ^e
SiH ₄	$\nu_3(t_2)$	2191 [9]	320.5 [73]	0.23		
	$\nu_4(t_2)$	914	296.3	1.2		0.63 ^e
SiHD ₃	$\nu_1(a_1)$	2182 [9]	65.7 [73]	0.047		
	$\nu_2(a_1)$	1573	} 121.	0.16 ^c		
	$\nu_4(e)$	1598				
	$\nu_3(a_1)$	683	} 96.4	0.70 ^c		
	$\nu_6(e)$	683				
	$\nu_5(e)$	851	80.5	0.38		0.56 ^e
SiD ₄	$\nu_3(t_2)$	1597 [9]	127 [73]	0.17		
	$\nu_4(t_2)$	681	136	0.99		0.51 ^e
SiHCl ₃	$\nu_1(a_1)$	2261 [74]	40.6 [75]	0.027		
	$\nu_2(a_1)$	499	19.9	0.27		
	$\nu_3(a_1)$	254	8.1	0.42		
	$\nu_4(e)$	811	208.2	1.1		
	$\nu_5(e)$	600	224.6	2.1		
	$\nu_6(e)$	176	2.4	0.26		1.8
SnH ₄	$\nu_3(t_2)$	1901 [9]	922.18 [76]	0.86		
	$\nu_4(t_2)$	677	778.35	5.7		2.9 ^d
SnD ₄	$\nu_3(t_2)$	1368 [9]	460.2 [76]	0.83		
	$\nu_4(t_2)$	487	419.1	6.0		3.0 ^e

^aSame result as reference [5].

^bEstimated value.

^cAn average value of the overlap frequencies was used to determine the polarization.

^dThe estimated error is 5%.

^eThe estimated error is between 5 and 10%.

^fThe estimated error is more than 10%.

Table 5. Six-atomic molecules

Molecule	Band	$\omega_{\text{H}}(\text{cm}^{-1})$	$A_{\text{n}}(\text{km}/\text{mol})$	$P_{\text{n}}(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$
C_2H_4	$\nu_7(\text{b}_{1\text{u}})$	949.2 [77]	81.25 [78]	0.30	0.15 ^{a,b}
	$\nu_9(\text{b}_{2\text{u}})$	3105.5	24.9 [77]	0.0087	
	$\nu_{10}(\text{b}_{2\text{u}})$	810.3	20.3 [78]	0.0010	
	$\nu_{11}(\text{b}_{3\text{u}})$	2989.5	13.51 [77]	0.0051	
	$\nu_{12}(\text{b}_{3\text{u}})$	1443.5	9.76 [77]	0.016	
cis- $\text{C}_2\text{D}_2\text{H}_2^{\text{d}}$	$\nu_5(\text{b}_1)$	3056 [77]	6.714 [77]	0.0024	0.16 ^{a,b}
	$\nu_9(\text{a}_1)$	3043	12.74	0.0046	
	$\nu_1(\text{a}_1)$	2349	4.98	0.0030	
	$\nu_{11}(\text{b}_1)$	2254	6.27	0.0042	
	$\nu_2(\text{a}_1)$	1558	0	0	
	$\nu_{12}(\text{b}_1)$	1344	6.87	0.013	
	$\nu_3(\text{a}_1)$	1213	0	0	
	$\nu_6(\text{b}_1)$	1035	0.39	0.0012	
	$\nu_7(\text{b}_2)$	843	71.92	0.34	
	$\nu_{10}(\text{a}_1)$	656	0	0	
trans- $\text{C}_2\text{D}_2\text{H}_2^{\text{d}}$	$\nu_9(\text{b}_{\text{u}})$	3065 [77]	19.64 [77]	0.0071	0.14 ^{a,b}
	$\nu_{11}(\text{b}_{\text{u}})$	2271	9.32	0.0061	
	$\nu_{12}(\text{b}_{\text{u}})$	1300	7.70	0.015	
	$\nu_4(\text{a}_{\text{u}})$	988	36.95	0.13	
	$\nu_7(\text{a}_{\text{u}})$	727	24.76	0.16	
	$\nu_{10}(\text{b}_{\text{u}})$	660	0.043	0.00033	
C_2D_4	$\nu_7(\text{b}_{1\text{u}})$	720 [77]	41.717 [77]	0.27	0.13 ^{a,b}
	$\nu_9(\text{b}_{2\text{u}})$	2345	12.21	0.0075	
	$\nu_{10}(\text{b}_{2\text{u}})$	589	0.043	0.00042	
	$\nu_{11}(\text{b}_{3\text{u}})$	2200	7.621	0.0053	
	$\nu_{12}(\text{b}_{3\text{u}})$	1078	5.189	0.015	
trans- $\text{C}_2\text{F}_2\text{H}_2$	$\nu_6(\text{a}_{\text{u}})$	873 [79]	56.71 [79]	0.25	0.56 ^c
	$\nu_7(\text{a}_{\text{u}})$	325	12.70	0.41	
	$\nu_9(\text{b}_{\text{u}})$	3116	9.47	0.0033	
	$\nu_{10}(\text{b}_{\text{u}})$	1274	14.70	0.031	
	$\nu_{11}(\text{b}_{\text{u}})$	1160	217.76	0.55	
	$\nu_{12}(\text{b}_{\text{u}})$	338	1.44	0.043	

^aSame result as reference [5].

^bThe estimated error is 5%.

^cThe estimated error is between 5 and 10%.

^dThis assignment is according to reference [77].

Table 6. Seven-atomic molecules

Molecule	Band	$\omega_{\text{H}}(\text{cm}^{-1})$	$A_{\text{H}}(\text{km/mol})$	$P_{\text{H}}(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$
C_3H_4 (allene)	$\nu_5(\text{b}_2)$	3007[80]	5.4	[80]	0.0020
	$\nu_6(\text{b}_2)$	1957	48.8		0.043
	$\nu_7(\text{b}_2)$	1398	7.0		0.012
	$\nu_8(\text{e})$	3085	4.3		0.0015
	$\nu_9(\text{e})$	999	8.8		0.030
	$\nu_{10}(\text{e})$	841	91.2		0.44
	$\nu_{11}(\text{e})$	356	14.6		0.39
					0.40 ^b
C_3D_4	$\nu_5(\text{b}_2)$	2230[80]	1.7 ^a	[80]	0.0012
	$\nu_6(\text{b}_2)$	1921	44.0		0.040
	$\nu_7(\text{b}_2)$	1032	2.3		0.0073
	$\nu_8(\text{e})$	2330	3.6 ^a		0.0022
	$\nu_9(\text{e})$	829	5.8		0.029
	$\nu_{10}(\text{e})$	667	50.9		0.39
	$\nu_{11}(\text{e})$	307	11.8		0.42
					0.39 ^b
CH_3CCH (methyl-acetylene)	$\nu_1(\text{a}_1)$	3334[81]	45.1	[81]	0.014
	$\nu_2(\text{a}_1)$	2930	14.9		0.0059
	$\nu_3(\text{a}_1)$	2142	5.3		0.0039
	$\nu_4(\text{a}_1)$	1380	1.5		0.0027
	$\nu_5(\text{a}_1)$	930	1.0		0.0039
	$\nu_6(\text{e})$	2981	17.7		0.0067
	$\nu_7(\text{e})$	1452	17.9		0.029
	$\nu_8(\text{e})$	1052	0.4		0.0012
	$\nu_9(\text{e})$	633	87.3		0.74
	$\nu_{10}(\text{e})$	327	16.7		0.53
					0.59 ^c
CD_3CCH	$\nu_1(\text{a}_1)$	3336[81]	44.8	[81]	0.014
	$\nu_2(\text{a}_1)$	2142	} 12.8		0.0096 ^d
	$\nu_3(\text{a}_1)$	2110			
	$\nu_4(\text{a}_1)$	1115		0.2	0.00054
	$\nu_5(\text{a}_1)$	830	0.4	0.0020	
	$\nu_6(\text{e})$	2233	7.9	0.0054	
	$\nu_7(\text{e})$	1048	10.6	0.033	
	$\nu_8(\text{e})$	838	0.8	0.0038	
	$\nu_9(\text{e})$	639	89.6	0.74	
	$\nu_{10}(\text{e})$	303	13.6	0.50	
					0.58 ^c
CH_3CCD	$\nu_1(\text{a}_1)$	2931[81]	15.1	[81]	0.0059
	$\nu_2(\text{a}_1)$	2616	32.5	[81]	0.016
	$\nu_3(\text{a}_1)$	2008	0.5	[81]	0.00042
	$\nu_4(\text{a}_1)$	1380	0.6 ^a	[82]	0.0011
	$\nu_5(\text{a}_1)$	914	0.3	[81]	0.0012
	$\nu_6(\text{e})$	2980	15.9	[81]	0.0060
	$\nu_7(\text{e})$	1452	16.4 ^a	[82]	0.026
	$\nu_8(\text{e})$	1052	1.0	[81]	0.0031
	$\nu_9(\text{e})$	498	37.1	[81]	0.51
	$\nu_{10}(\text{e})$	315	21.0	[81]	0.71
					0.56 ^c
SF_6	$\nu_3(\text{t}_{1u})$	948[83]	1361	[83]	5.1
	$\nu_4(\text{t}_{1u})$	615	74		0.66
					2.5 ^b

^aEstimated value.

^bThe estimated error is 5%.

^cThe estimated error is between 5 and 10%.

^dAn average value of the overlap frequencies was used to determine the polarization.

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Table 7. Molecules with eight or more atoms

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$	
C ₂ F ₆	$\nu_5(a_{2u})$	1116 [84]	237 [84]	0.64		
	$\nu_6(a_{2u})$	714	32.7	0.22		
	$\nu_7(e_u)$	1250	820	1.8		
	$\nu_8(e_u)$	522	7.9	0.098		
	$\nu_9(e_u)$	219	4.31	0.30		1.3 ^{a,e}
C ₂ H ₆	$\nu_5(a_{2u})$	2915 [85]	47.81 [85]	0.019		
	$\nu_6(a_{2u})$	1379.2	4.00	0.0071		
	$\nu_7(e_u)$	2995.5	123.2	0.046		
	$\nu_8(e_u)$	1472.2	13.4	0.021		
	$\nu_9(e_u)$	821.5	6.099	0.031		0.055 ^{a,c}
C ₂ D ₆	$\nu_5(a_{2u})$	2095 [85]	24.20 [85]	0.019		
	$\nu_6(a_{2u})$	1077	2.91	0.0085		
	$\nu_7(e_u)$	2236	64.40	0.044		
	$\nu_8(e_u)$	1082	9.12	0.026		
	$\nu_9(e_u)$	593.7	3.312	0.032		0.057 ^{a,c}
C ₃ H ₆ (cyclo- propane)	$\nu_6(a_2'')$	3102 [86]	28.13 [86]	0.0099		
	$\nu_7(a_2'')$	854	0.45	0.0021		
	$\nu_8(e_1')$	3024	41.94	0.015		
	$\nu_9(e_1')$	1438	2.04	0.0033		
	$\nu_{10}(e_1')$	1028	21.50	0.069		
	$\nu_{11}(e_1')$	869	33.03	0.15		0.11 ^d
C ₃ D ₆	$\nu_6(a_2'')$	2337 [86]	14.01 [86]	0.0087		
	$\nu_7(a_2'')$	615	0.24	0.0021		
	$\nu_8(e_1')$	2209	15.50	0.011		
	$\nu_9(e_1')$	1072	5.22	0.015		
	$\nu_{10}(e_1')$	887	3.25	0.014		
	$\nu_{11}(e_1')$	717	29.99	0.20		0.11 ^d
CH ₂ CHCHCH ₂	$\nu_{10}(a_u)$	1013 [87]	31.7 ^b [88]	0.10		
	$\nu_{11}(a_u)$	908	67.3	0.28		
	$\nu_{12}(a_u)$	522	11	0.14		
	$\nu_{13}(a_u)$	162	0.94 ^b	0.12		
	$\nu_{17}(b_u)$	3101	34 ^b	0.012		
	$\nu_{18}(b_u)$	3055	2 ^b	0.00072		
	$\nu_{19}(b_u)$	2984	20 ^b	0.0076		
	$\nu_{20}(b_u)$	1596	17	0.023		
	$\nu_{21}(b_u)$	1381	4.4	0.0078		
	$\nu_{22}(b_u)$	1294	3.0	0.0061		
	$\nu_{23}(b_u)$	990	2.4 ^b	0.0083		
	$\nu_{24}(b_u)$	301	3.11 ^b	0.12		0.36 ^d
	C ₆ F ₆	$\nu_4(a_{2u})$	215 [89]	2.60[90]	0.19	
$\nu_{12}(e_{1u})$		1531	546.	0.79		
$\nu_{13}(e_{1u})$		1006	406.	1.4		
$\nu_{14}(e_{1u})$		315	2.50	0.085		1.1
C ₆ H ₆	$\nu_4(a_{2u})$	673 [91]	88.2 [91]	0.66		
	$\nu_{12}(e_{1u})$	3080	60.1	0.021		
	$\nu_{13}(e_{1u})$	1486	13.1	0.020		
	$\nu_{14}(e_{1u})$	1038	8.8	0.028		0.32 ^{a,d}
C ₆ D ₆	$\nu_4(a_{2u})$	496 [92]	49.8 [92]	0.68		
	$\nu_{12}(e_{1u})$	2287	35.3	0.023		
	$\nu_{13}(e_{1u})$	1335	2.90	0.0055		
	$\nu_{14}(e_{1u})$	814	8.02	0.041		0.33 ^c
C ₅ H ₁₀ (cyclo- pentane)	$\nu_6(a_1'')$	2966 [93]	203 ^b [93]	0.078		
	$\nu_7(a_1'')$	545	0.8	0.0091		
	$\nu_8(e_1)$	2878	96 ^b	0.039		
	$\nu_9(e_1)$	1462	12	0.019		
	$\nu_{10}(e_1)$	1312	0.8	0.0016		
	$\nu_{11}(e_1)$	897	4.2	0.018		0.072 ^d

Table 7. Molecules with eight or more atoms (continued)

Molecule	Band	$\omega_n(\text{cm}^{-1})$	$A_n(\text{km/mol})$	$P_n(\text{cm}^3/\text{mol})$	$\bar{\alpha}(10^{-40}\text{C}^2\text{m}^2\text{J}^{-1})$
C_6H_{12} ^f (cyclohexane)	$\nu_{20}(\text{e}_U)$	183 [93]	0.2 ^b [93]	0.020	
	$\nu_{15}(\text{a}_{2U})$	521	0.8	0.010	
	$\nu_{21}(\text{e}_U)$	862	4.	0.018	
	$\nu_{16}(\text{a}_{2U})$	905	2.6	0.011	
	$\nu_{22}(\text{e}_U)$				
	$\nu_{23}(\text{e}_U)$	1262	3.54	0.0075	
	$\nu_{24}(\text{e}_U)$	1342	0.4	0.00075	
	$\nu_{17}(\text{a}_{2U})$	1456	22.5	0.036	
	$\nu_{25}(\text{e}_U)$				
	$\nu_{18}(\text{a}_{2U})$	2862	94.	0.039	
	$\nu_{26}(\text{e}_U)$				
	$\nu_{19}(\text{a}_{2U})$	2932	287.	0.11	0.11 ^d
	$\nu_{27}(\text{e}_U)$				

^aSame result as reference [5].

^bEstimated value.

^cThe estimated error is 5%.

^dThe estimated error is between 5 and 10%.

^eThe estimated error is more than 10%.

^fThis assignment is according to reference [93].

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