7h. Constants of Polyatomic Molecules

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7h-1. Introduction. The following tables present some of the more important data on simple polyatomic molecules derived from infrared, Raman, and microwave spectra. Tables 7h-1 through 7h-4 give the fundamental vibrational frequencies (in cm^{-1}) of most triatomic and four-atomic molecules for which these quantities are available and for a few important five- and six-atomic molecules. The point groups to which the molecules belong are indicated in the last column. The numbering of the vibrations is in accordance with the practice followed by many authors in recent years[1] and now established by international agreement.[2]

For most molecules listed the fundamentals are active in both the infrared and the Raman spectrum. However, for molecules of high symmetry, certain vibrations cannot occur in the Raman spectrum, others cannot occur in the infrared spectrum, and a few in neither one: for triatomic linear symmetric molecules ($D_{\infty h}$), ν_1 is Raman active and ν_2 and ν_3 infrared active; for four-atomic linear symmetric molecules ($D_{\infty h}$), ν_1, ν_2, and ν_4 are Raman active and ν_3 and ν_5 infrared active; for four-atomic planar molecules with a threefold axis (D_{3h}), ν_1 is Raman active, ν_2 infrared active, and ν_3 and ν_4 are both Raman and infrared active; for five-atomic tetrahedral molecules (T_d) all vibrations are Raman active but only ν_3 and ν_4 are infrared active; for linear symmetric six-atomic molecules, the vibrations ν_1, ν_2, ν_3, ν_6, ν_7 are Raman active and the remaining ones are infrared active; for six-atomic molecules with three mutually perpendicular planes of symmetry (V_h), the vibrations ν_7, ν_9, ν_{10}, ν_{11}, ν_{12} are infrared active and all others, except ν_4, are Raman active; for six-atomic molecules of C_{2h} symmetry, ν_1, ν_2, ν_3, ν_4, ν_5, and ν_8 are Raman active, and the others are infrared active.

Tables 7h-5 through 7h-15 give the rotational constants $A_{[0]}$, $B_{[0]}$, $C_{[0]}$ of selected triatomic, four-atomic, five-atomic, and six-atomic molecules. These rotational constants are, apart from the factor $h/8\pi^2c$, the reciprocal moments of inertia, and therefore from them the geometrical parameters of the molecule can be determined if a sufficient number of isotopes have been investigated. The geometrical parameters thus obtained are also listed in Tables 7h-5 through 7h-15.

The constants $A_{[0]}$, $B_{[0]}$, $C_{[0]}$ refer to the lowest vibrational level which still includes the zero-point vibration. In a few cases in which these constants have been determined for the true equilibrium positions, the equilibrium contants A_e, B_e, C_e are also listed.

Microwave spectra give the constants in megahertz while infrared and Raman

[1] G. Herzberg. "Molecular Spectra and Molecular Structure. II. Infrared and Raman Spectra of Polyatomic Molecules," D. Van Nostrand Company, Inc., Princeton, N.J., 1945.
[2] R. S. Mulliken, *JCP* **23**, 1997 (1955).

spectra give them in cm^{-1}. Here all microwave values have been converted to cm^{-1} by dividing by $c = 2.997925 \times 10^{10}$ cm/sec.

In the alphabetical order used, D is counted as an H in order to have the deuterated molecules appear with the corresponding nondeuterated ones. Element symbols without mass numbers refer to the most abundant isotope.

Many of the data have been taken from the books by Herzberg[1]; by Gordy, Smith, and Trambarulo[2]; by Townes and Schawlow[3]; and the more recent compilations of Shimanouchi[4] and Starck[5]. In addition, some of the literature up to 1968 has been included. For detailed tables of microwave data reference should be made to the Microwave Spectral Tables prepared by Cord, Petersen, Lojko, and Haas.[6]

7h-2. Fundamental Vibrations

TABLE 7h-1. TRIATOMIC MOLECULES

Molecule	ν_1 cm^{-1}	ν_2 cm^{-1}	ν_3 cm^{-1}	Point group	Molecule	ν_1 cm^{-1}	ν_2 cm^{-1}	ν_3 cm^{-1}	Point group
BO_2	1070	464	1322	$D_{\infty h}$	HIO	.....	1187	985	C_s
BO_2^-	1070‡	610‡	1970‡	$D_{\infty h}$	H_2S	2614.6	1182.7	2627	C_{2v}
BrCN	575	341.5	2198.3	$C_{\infty v}$	HDS	.....	1090	(2684)	C_s
C_3	(1230)‡	63.1	2040	$D_{\infty h}$	D_2S	1896.4	855.5	1910	C_{2v}
CF_2	1102	667	(1222)	C_{2v}	H_2Se	2344.5	1034.2	2357.8	C_{2v}
ClCN	714	378.4	2215.6	$C_{\infty v}$	HDSe	1691	912	2352	C_s
Cl_2O	640	(300)	686	C_{2v}	D_2Se	1686.7	741.4	1697.4	C_{2v}
ClO_2	945.5	447.4	1110.5	C_{2v}	HSiBr	1547.8	771.4	408.6	C_s
CNC	.....	321	.....	$D_{\infty h}$	HSiCl	.....	805.5	522.4	C_s
CO_2	1388.2 1285.5†	667.4	2349.2	$D_{\infty h}$	ICN	470*	321*	2158*	$C_{\infty v}$
CO_2^+	1280	.....	(1469)	$D_{\infty h}$	KrF_2	449	232.6	588	$D_{\infty h}$
CS_2	658.0	396.7	1533	$D_{\infty h}$	N_3^-	1350*	630*	2080*	$D_{\infty h}$
FCN	(2294)	451.3	1076.5	$C_{\infty v}$	NF_2	1074.3	(573)‡	(931)‡	C_{2v}
F_2O	928	461	831	C_{2v}	NH_2	.....	1497.2	.....	C_{2v}
HCF	.....	1403	.....	C_s	N_2O	1284.9	588.8	2223.8	$C_{\infty v}$
HCN	2096.9	712.0	3311.5	$C_{\infty v}$	N_2O^+	1736.6	461.2	1126.4	$C_{\infty v}$
DCN	1925.3	569.0	2630.3	$C_{\infty v}$	NO_2	1318	749.8	1617.8	C_{2v}
HCO	(2700)	1820.2	1083.0	C_s	NO_2^-	1345*	816*	1236*	C_{2v}
HCP	3216.9	674.3	1278.2	$C_{\infty v}$	NO_2^+	1400*	538*	2358*	$(D_{\infty h})$
HF_2^-	(595)‡	1240‡	1500‡	$C_{\infty v}$(?)	NOCl	1799	596	332	C_s
$HgBr_2$	225	41	293	$D_{\infty h}$	NOF	1844.0	765.9	521	C_s
$HgCl_2$	360	70	413	$D_{\infty h}$	O_3	1110	705	1042.2	C_{2v}
HgI_2	156	33	(235)	$D_{\infty h}$	OCN^-	2180*	870*	.....	$C_{\infty v}$
HNO	3596	1562	1110	C_s	OCS	2062.2	520.4	859.0	$C_{\infty v}$
H_2O	3656.7	1594.8	3755.8	C_{2v}	SCN^-	2066*	483*	750*	$C_{\infty v}$
HDO	2726.7	1402.2	3707.5	C_s	$SeCN^-$	2051.5*	575*	.....	$C_{\infty v}$
D_2O	2671.5	1178.3	2788.0	C_{2v}	SiCC	1742	.....	591	$C_{\infty v}$
HOCl	3609.2	1242	739	C_s	SO_2	1151.4	517.7	1361.8	C_{2v}
DOCl	2666.0	911	739	C_s	UO_2^{++}	860‡	(252)‡	930‡	C_{2v}
					XeF_2	515	213.2	558	$D_{\infty h}$

( ) Values in parentheses are uncertain or have been obtained indirectly.
* Observed in liquid.
† Fermi resonance between ν_1 and $2\nu_2$.
‡ Observed in crystal or solid matrix.

[1] G. Herzberg, "Molecular Spectra and Molecular Structure," vol. II, "Infrared and Raman Spectra of Polyatomic Molecules," 1945, vol. III, "Electronic Spectra and Electronic Structure of Polyatomic Molecules," D. Van Nostrand Company, Inc., Princeton, N.J., 1945, 1966.

[2] W. Gordy, W. V. Smith, and R. F. Trambarulo, "Microwave Spectroscopy," John Wiley & Sons, Inc., New York, 1953.

[3] C. H. Townes and A. L. Schawlow, "Microwave Spectroscopy," McGraw-Hill Book Company, New York, 1955.

[4] T. Shimanouchi, Tables of Molecular Vibrational Frequencies, parts 1–3, *Nat'l. Standard Ref. Data Ser. NBS* 6, pp. 11, 17, 1967–1968.

[5] B. Starck, in Landolt-Börnstein New Series Group II, vol. 4, 1967.

[6] M. S. Cord, J. D. Petersen, M. S. Lojko, and R. H. Haas, Microwave Spectral Tables, *NBS Monograph* 70, vols. 3, 4, and 5, 1968.

TABLE 7h-2. FOUR-ATOMIC MOLECULES

Molecule	ν_1 cm^{-1}	ν_2 cm^{-1}	ν_3 cm^{-1}	ν_4 cm^{-1}	ν_5 cm^{-1}	ν_6 cm^{-1}	Point group
$AsCl_3$	410	193	370	159	.....	.....	C_{3v}
AsF_3	740.3	336.5	702.2	262.3	.....	.....	C_{3v}
AsH_3	2116.1	906	2123	1003	.....	.....	C_{3v}
AsD_3	1523.1	660.0	1529.3	714	.....	.....	C_{3v}
BBr_3	279	372	802	151	.....	.....	D_{3h}
BCl_3	471	460	956	243	.....	.....	D_{3h}
BI_3	189*	305*	692*	.....	.....	.....	D_{3h}
BF_3	888	691.4	1453.7	480.4	.....	.....	D_{3h}
$BiCl_3$	288	130	242	96	.....	.....	C_{3v}
BrO_3^-	803*	428*	828*	350*	.....	.....	C_{3v}
CH_3	.....	611‡	.....	.....	.....	.....	D_{3h}
CD_3	.....	463‡	.....	.....	.....	.....	D_{3h}
C_2H_2	3372.7	1973.7	3294.9	611.7	729.2	.....	$D_{\infty h}$
C_2HD	3335.6	1853.8	2583.6	518.4	677.8	.....	$C_{\infty v}$
C_2D_2	2703.8	1763.8	2439.2	510.7	536.4	.....	$D_{\infty h}$
C_2I_2	2113	191	718	307	(115)	.....	$D_{\infty h}$
C_2N_2	2329.9	854.2	2157.8	507.2	233.1	.....	$D_{\infty h}$
Cl_2CO	1827	567	285	580	849	440	C_{2v}
Cl_2CS	1139	503	288	471	818	292	C_{2v}
ClF_3	752	527	326	703	434	364	C_s
ClO_3^-	940*	617*	988*	479*	.....	.....	C_{3v}
CO_3^{--}	1063*	878*	1415*	680*	.....	.....	D_{3h}
F_2BO	1369	856.0	491.0	.....	.....	.....	C_{2v}
FClCO	1868	1095	776	501	415	667	C_s
F_2CO	1942	965	584	774	1249	626	C_{2v}
HC_2Br	3325	2085	618	618	295	.....	$C_{\infty v}$
HC_2Cl	3340	2110	756	604	326	.....	$C_{\infty v}$
DC_2Cl	2612	1980	742	472	(312)	.....	$C_{\infty v}$
HC_2F	3355	2255	1055	578	367	.....	$C_{\infty v}$
HCO_2^-	2825*	1584*	1386*	1352*	773*	1069*	C_{2v}
H_2CO	2766.4	1746.1	1500.6	2843.4	1251.2	1167	C_{2v}
HDCO	2845	2120.5	1723.3	1399	1041	1074	C_s
D_2CO	2055.8	1700	1105.7	2159.7	990	938	C_{2v}
HFCO	2981.0	1836.9	1342.5	1064.8	662.5	(1175)	C_s
HN_3	3335.6	2139.8	1263.7	1150.5	534.2	607.0	C_s
HNCO	3531	2274	1527	777.1	659.8	577.5	C_s
HNCS	3537.9	1973	999	615	467	834	C_s
cis-HNO_2	3426	1639	(1370)	856	620	638	C_s
trans-HNO_2	3590	1698	1264	793	598	544	C_s
cis-DNO_2	2530	.....	.....	816	(591)	508	C_s
trans-DNO_2	2650	1690	1018	739	591	416	C_s
H_2O_2	3599	(1380)	880	309	3608	1266	C_2
D_2O_2	2510*	1009*	878*	229	2482*	1004*	C_2
H_2S_2	2513*	882*	510*	416	2577	886	C_2
IO_3^-	779*	390‡	826*	330*	.....	.....	C_{3v}
NCl_3	535*	347*	637*	254*	.....	.....	C_{3v}
NF_3	1032	647	905	493	.....	.....	C_{3v}
trans-N_2F_2	(1636)	(1010)	(592)	360	989	421	C_{2h}
NH_3	3336.7	950.4	3443.8	1626.8	.....	.....	C_{3v}
NH_2D	.....	.....	1592	884	.....	.....	C_s
NHD_2	.....	2418	1234	813	2556	1464	C_s
ND_3	2420.4	747.5	2564.0	1191.2	.....	.....	C_{3v}
N_2H_2	.....	1481*	.....	3120.1	1286*	.....	C_{2h}
NO_3^-	1048*	824*	1357*	720*	.....	.....	D_{3h}
P_4	606	363	465	.....	.....	.....	T_d
PBr_3	380	162	400	116	.....	.....	C_{3v}
PCl_3	507	260	493	189	.....	.....	C_{3v}

TABLE 7h-2. FOUR-ATOMIC MOLECULES (*Continued*)

Molecule	ν_1 cm^{-1}	ν_2 cm^{-1}	ν_3 cm^{-1}	ν_4 cm^{-1}	ν_5 cm^{-1}	ν_6 cm^{-1}	Point group
PF_3	892	487	860	344	.....	.....	C_{3v}
$PFBr_2$	817	421	.....	.....	393	.....	C_s
$PFCl_2$	827	524	.....	.....	496	.....	C_s
PF_2Cl	860	527	.....	.....	833	.....	C_s
$PFClBr$	822	503	415	.....	.....	.....	C_1
PH_3	2322.9	992.0	2327.7	1118.3	.....	.....	C_{3v}
PH_2D	.....	1700	1097	892	.....	.....	C_s
PHD_2	2320	.....	906	.....	.....	980	C_s
PD_3	1694	730	1700	806	.....	.....	C_{3v}
$SbCl_3$	360	165	320	134	.....	.....	C_{3v}
SbH_3	1890.9	781.5	1894.2	830.0	.....	.....	C_{3v}
SbD_3	1358.8	561.1	1362.0	592.5	.....	.....	C_{3v}
S_2Cl_2	448	438	206	102	538	242	(C_2)
SO_3	1067	498	1391.2	531	.....	.....	D_{3h}
$SOBr_2$	1121	405	267	120	379	223	C_s
$SOCl_2$	1230	490	344	194	445	284	C_s
SOF_2	1333	808	530	(410)	748	390	C_s

( ) Values in parentheses are uncertain or have been obtained indirectly.
* Observed in liquid or solution.
‡ Observed in crystal or solid matrix.

TABLE 7h-3. SOME FIVE-ATOMIC MOLECULES

Molecule	ν_1 cm^{-1}	ν_2 cm^{-1}	ν_3 cm^{-1}	ν_4 cm^{-1}	ν_5 cm^{-1}	ν_6 cm^{-1}	Point group
CH_4	2916.7	1533.6	3018.9	1306.2	.....	.....	T_d
CD_4	2108.9	1091.9	2259.3	995.6	.....	.....	T_d
CH_3D	2973, 2914 †	2200.0	1300	3016.9	1471	1155	C_{3v}
CHD_3	2993	2142	1003	2263	1291	1036	C_{3v}
CF_4	908.5	435.0	1283.0	631.7	.....	.....	T_d
CCl_4	459.0	221	794.3, 756 †	310.0	.....	.....	T_d
CBr_4	267*	122*	671*	182*	.....	.....	T_d
CI_4	178‡	90‡	555‡	123‡	.....	.....	(T_d)
SiH_4	2187.0	974.6	2190.6	914.2	.....	.....	T_d
SiF_4	800	268	1031.8	389.4	.....	.....	T_d
$SiCl_4$	425	149	619.0	221.3	.....	.....	T_d
$SiBr_4$	249*	90*	487*	137*	.....	.....	T_d
SiI_4	168	63	405	94	.....	.....	T_d
GeH_4	2106	930.9	2113.6	819.3	.....	.....	T_d
GeF_4	(740)	(200)	800	260	.....	.....	T_d
$GeCl_4$	396*	134*	453*	172*	.....	.....	T_d
$GeBr_4$	235*	79*	327*	112*	.....	.....	T_d
GeI_4	159	60	264	80	.....	.....	T_d
SnH_4	.....	758	1901.1	677	.....	.....	T_d
$SnCl_4$	366	104	403	134	.....	.....	T_d
$SnBr_4$	220	64	279	88	.....	.....	T_d
CH_3F	2964.5	1460.5	1048.6	3005.8	1466.5	1182.4	C_{3v}
CH_3Cl	2966.7	1354.9	732.1	3042.4	1452.1	1017.3	C_{3v}
CH_3Br	2972	1305.9	611.1	3056.6	1442.7	954.7	C_{3v}
CH_3I	2953.2	1250.8	533.2	3060.3	1437.4	882.4	C_{3v}
CHF_3	3034.5	1139.5	697.0	1377.5	1152	508	C_{3v}
$CHCl_3$	3032.0	671.1	364.8	1218	768	256	C_{3v}
$CHBr_3$	3042	541	222	1149	669	155	C_{3v}
CHI_3	(3040)*	385*	145*	1064*	581*	92*	C_{3v}
CF_3Cl	1104	782	475	1217	559	351	C_{3v}
CF_3Br	1083	762	350	1208	549	305	C_{3v}
CF_3I	1073	741	285	1185	540	267*	C_{3v}
SiH_3F	2206	990	872	2196	(956)	728.1	C_{3v}
SiH_3Cl	2201	949	551	2195	954.4	664.0	C_{3v}
SiH_3Br	2200	930	430	2196	950.4	632.6	C_{3v}
SiH_3I	2191.8	903	(355)	2205.6	941.0	592.4	C_{3v}
$SiHCl_3$	2274	497	250*	810	600	179*	C_{3v}
$SiHBr_3$	2232*	358*	169*	769*	473*	111*	C_{3v}
GeH_3F	2120.6	859.0	689.1	2131.8	874.2	642.5	C_{3v}
GeH_3Cl	2121	848	423	2129.1	874.7	603.9	C_{3v}
GeH_3Br	2116	833	305	2127.0	871.4	578.1	C_{3v}
GeH_3I	2112	812	248	2120.6	853.0	558.7	C_{3v}

( ) Values in parentheses are uncertain or have been obtained indirectly.
* Observed in liquid or solution.
† Fermi resonance.
‡ Observed in crystal or solid matrix.

TABLE 7h-4. SOME SIX-ATOMIC MOLECULES

Molecule	ν_1 cm^{-1}	ν_2 cm^{-1}	ν_3 cm^{-1}	ν_4 cm^{-1}	ν_5 cm^{-1}	ν_6 cm^{-1}	ν_7 cm^{-1}	ν_8 cm^{-1}	ν_9 cm^{-1}	ν_{10} cm^{-1}	ν_{11} cm^{-1}	ν_{12} cm^{-1}	Point group
$HC\equiv C-C\equiv CH$	(3293)*	2184	874	3329	2020	627	482	630	(220)	.....	.....	.....	$D_{\infty h}$
C_2H_4	3026.4	1622.6	1342.2	1023	3102.5	1222	949.3	943	3105.5	826.0	2988.7	1443.5	V_h
C_2D_4	2251*	1515*	981*	(726)	2305	(1009)	720.0	780	2345	(586)	2201.0	1077.9	V_h
C_2F_4	1872	778	394	(190)	1340	551	407	510	1337	218	1186	558	V_h
C_2Cl_4	1571*	447*	237*	(110)	1000*	347*	288*	512*	908*	176*	777*	310*	V_h
C_2Br_4	1546*	266*	144*	(66)	886*	211*	245*	463*	766*	119*	635*	188*	V_h
C_2I_4	1448*	181*	106*	.....	780*	146*	225‡	(418)	638*	94‡	525*	129‡	V_h
$H_2C:CF_2$	3058.3	1728.5	1410	925.3	550	590	3099.8	1302	955	438	801	613	C_{2v}
cis-$C_2H_2F_2$	3135	1715	1266	1014	(255)	(866)	(482)	3135	1376	1127	768	756	C_{2v}
trans-$C_2H_2F_2$	.....	.....	.....	.....	.....	874	325	774	3115	1274	1159	(410)	C_{2h}
$H_2C:CCl_2$	3035*	1627	1400	603	299	686*	3130*	1095	800	372	875	460	C_{2v}
cis-$C_2H_2Cl_2$	3086	1591	1179*	711*	173*	876*	406*	3072	1303	857	571	697	C_{2v}
trans-$C_2H_2Cl_2$	3071*	1576*	1270*	844*	349*	898	(192)	758*	3090	1200	827	265*	C_{2h}
$H_2C:CBr_2$	3023*	1593*	1379*	467*	184*	668*	3108*	1065*	696*	322*	886*	405*	C_{2v}
cis-$C_2H_2Br_2$	3084	1584*	1150*	580*	109*	866	372*	3059*	1264	757	466	670	C_{2v}
trans-$C_2H_2Br_2$	3089*	1581*	1250*	745*	217*	899	.....	736*	3099	1163	688	(192)	C_{2h}
N_2O_4	1360	813	283	.....	1724*	500*	680	.....	1749	380	1265	752	V_h
N_2H_4	3325	3261*	1493	1098	873*	780	377	3350	3314	1628	1275	950	C_2
CH_3CN	2965.3	2267.3	1400.0	919.9	3009.0	1454.0	1041.0	361.0	.....	.....	.....	.....	C_{3v}
CH_3NC	2965.8	2166.0	1410.0	944.6	3014.3	1466.9	1129.3	263	.....	.....	.....	.....	C_{3v}
CH_3OH	3682	2977	2844	1477	1455	1340	1056	1034	(2977)	1477	1171*	270	C_s
CH_3SH	2946	2869	2607	1475	1335	1070	803	704	2999	1430	955	(600)	C_s

( ) Values in parentheses are uncertain or have been obtained indirectly.
* Observed in liquid only.
‡ Observed in crystal or solid matrix.

7h-3. Rotational Constants and Geometrical Parameters

TABLE 7h-5. TRIATOMIC LINEAR MOLECULES

Molecule	$B_{[0]}$, cm^{-1}	Point group	Geometrical parameters
$Br^{79}C^{12}N^{14}$	0.1374348	$C_{\infty v}$	$r_0(CBr) = 1.790$ Å $r_0(CN) = 1.159$ Å
$Br^{79}C^{13}N^{14}$	0.1358729		
$Br^{79}C^{12}N^{15}$	0.1315857		
$Br^{81}C^{12}N^{14}$	0.1366539		
$Br^{81}C^{13}N^{14}$	0.1350802		
$Br^{81}C^{12}N^{15}$	0.1308165		
$Cl^{35}C^{12}N$	0.1991648	$C_{\infty v}$	$r_0(CCl) = 1.631$ Å $r_0(CN) = 1.159$ Å
$Cl^{35}C^{13}N$	0.1981294		
$Cl^{36}C^{12}N$	0.19707		
$Cl^{37}C^{12}N$	0.1950433		
$Cl^{37}C^{13}N$	0.1939576		
$C^{12}O_2$	B_0 = 0.3902 $B_e = 0.3916_3$	$D_{\infty h}$	$r_0(CO) = 1.1621$ Å; $r_e(CO) = 1.1601$ Å
$C^{13}O_2$	0.30025	$D_{\infty h}$	$r_0(CO) = 1.1618$ Å
CO_2^+	0.3804	$D_{\infty h}$	$r_0(CO) = 1.177$ Å
CS_2	0.1092	$D_{\infty h}$	$r_0(CS) = 1.554$ Å
$FC^{12}N^{14}$	0.3520502	$C_{\infty v}$	$r_0(CF) = 1.262$ Å $r_0(CN) = 1.159$ Å
$FC^{13}N^{14}$	0.3518367		
$FC^{12}N^{15}$	0.3397823		
$HC^{12}N$	B_0 = 1.47822 $B_e = 1.4849$	$C_{\infty v}$	$r_0(CH) = 1.064$ Å; $r_e(CH) = 1.0657$ Å $r_0(CN) = 1.156$ Å; $r_e(CN) = 1.1530$ Å
$HC^{13}N$	1.43999		
$DC^{12}N$	B_0 = 1.20775 $B_e = 1.2118$		
$DC^{13}N$	1.18707		
$HC^{12}P$	0.6663292	$C_{\infty v}$	$r_0(CH) = 1.0667$ Å $r_0(CP) = 1.542$ Å
$HC^{13}P$	0.6384179		
$DC^{12}P$	0.5665385		
$DC^{13}P$	0.5479633		
$I^{127}C^{12}N$	0.1075931	$C_{\infty v}$	$r_0(CI) = 1.995$ Å $r_0(CN) = 1.159$ Å
$I^{127}C^{13}N$	0.105974		
$N_2{}^{14}O$	B_0 = 0.4190113 $B_e = 0.42118_1$	$C_{\infty v}$	$r_0(NN) = 1.126$ Å; $r_e(NN) = 1.126$ Å $r_0(NO) = 1.191$ Å; $r_e(NO) = 1.186$ Å
$N^{14}N^{15}O$	0.4189825		
$N^{15}N^{14}O$	B_0 = 0.4048567 $B_e = 0.40693_5$		
$N_2{}^{15}O$	0.4048592		
$O^{16}C^{12}S^{32}$	0.202857	$C_{\infty v}$	$r_0(CO) = 1.1637$ Å $r_0(CS) = 1.5584$ Å
$O^{16}C^{13}S^{32}$	0.2022025		
$O^{16}C^{12}S^{33}$	0.2003016		
$O^{16}C^{12}S^{34}$	0.1978974		
$O^{16}C^{12}S^{35}$	0.19504		
$O^{16}C^{12}S^{36}$	0.193456		
$O^{16}C^{13}S^{34}$	0.197194		
$O^{16}C^{14}S^{32}$	0.201581		
$O^{17}C^{12}S^{32}$	0.190258		
$O^{18}C^{12}S^{32}$	0.190292		
$O^{18}C^{12}S^{34}$	0.185458		
$O^{18}C^{13}S^{32}$	0.189829		
$O^{16}C^{12}Se^{74}$	0.1366207	$C_{\infty v}$	$r_0(CO) = 1.1588$ Å $r_0(CSe) = 1.7090$ Å
$O^{16}C^{12}Se^{76}$	0.1357085		
$O^{16}C^{12}Se^{77}$	0.1352681		
$O^{16}C^{12}Se^{78}$	0.1348404		
$O^{16}C^{12}Se^{79}$	0.1344213		
$O^{16}C^{12}Se^{80}$	0.1340143		
$O^{16}C^{12}Se^{82}$	0.1332276		
$O^{16}C^{13}Se^{78}$	0.1335960		
$O^{16}C^{13}Se^{80}$	0.1327598		
$Te^{122}C^{12}S^{32}$	0.05284063	$C_{\infty v}$	$r_0(TeC) = 1.904$ Å $r_0(CS) = 1.557$ Å
$Te^{123}C^{12}S^{32}$	0.05273401		
$Te^{124}C^{12}S^{32}$	0.05262940		
$Te^{125}C^{12}S^{32}$	0.05252608		
$Te^{126}C^{12}S^{32}$	0.05242467		
$Te^{128}C^{12}S^{32}$	0.05222620		
$Te^{130}C^{12}S^{32}$	0.05203367		

TABLE 7h-6. TRIATOMIC, ASYMMETRIC TOP MOLECULES

Molecule	$A_{[0]}$ (cm^{-1})	$B_{[0]}$ (cm^{-1})	$C_{[0]}$ (cm^{-1})	Point group	Geometrical parameters
H_2O.....	27.8778	14.5092	9.2869	C_{2v}	r_0(OH) = 0.9568 Å; $\measuredangle_0$(HOH) = 105.05°
HDO.....	23.3786	9.1020	6.4173	C_s	r_e(OH) = 0.9572 Å; $\measuredangle_e$(HOH) = 104.52°
D_2O.....	15.3846	7.2716	4.8458	C_{2v}	
H_2S^{32}.....	10.3599	9.0156	4.7315	C_{2v}	r_e(HS) = 1.335$_6$ Å; $\measuredangle_e$HSH = 92.1°
HDS.....	9.683	4.843	3.140	C_s	
H_2Se^{80}....	8.1703	7.7272	3.9013	C_{2v}	r_e(HSe) = 1.460$_5$ Å; $\measuredangle_e$HSeH = 90.9°
D_2Se^{80}....	4.1905$_5$	3.8662$_1$	1.9861$_4$		
H_2Te.....	6.248$_6$	6.097$_0$	3.036$_1$	C_{2v}	r_0(HTe) = 1.653 Å; $\measuredangle$HTeH = 90.2$_5$°
BH_2.....	41.64	7.24$_8$	6.00$_8$	C_{2v}	r_0(BH) = 1.18 Å; $\measuredangle$HBH = 131°
NH_2.....	23.72$_8$	12.94$_2$	8.16$_9$	C_{2v}	r_0(NH) = 1.024 Å; $\measuredangle$HNH = 103.4°
HCO.....	22.36$_5$	1.494$_4$	1.400$_3$	C_s	r_0(CH) = 1.08 Å(assumed); $\measuredangle$HCO = 119.5°; r_0(CO) = 1.19$_8$ Å
DCO.....	13.64$_1$	1.281$_2$	1.171$_3$		
HNO.....	18.4792	1.4115	1.3071	C_s	r_0(NH) = 1.063 Å; r_0(NO) = 1.212 Å; $\measuredangle$HNO = 108.6°
DNO.....	10.5222	1.2920	1.1462		
HPO.....	8.855	0.7024	0.6488	C_s	
HCF.....	15.5$_5$	1.221	1.126	C_s	
HCCl....	15.75	0.6054	0.5882	C_s	
NO_2.....	8.00251	0.433665	0.410493	C_{2v}	r_0(NO) = 1.193 Å; $\measuredangle$ONO = 134.1°
CF_2.....	2.94736	0.41719	0.36469	C_{2v}	r_0(CF) = 1.300 Å; $\measuredangle$FCF = 104.94°
SiF_2.....	1.02076	0.29433	0.22784	C_{2v}	r_0(SiF) = 1.591 Å; $\measuredangle$FSiF = 101.0°
O_3.....	3.55345	0.445276	0.394749	C_{2v}	r_0(O'O) = 1.278 Å; $\measuredangle$OO'O = 116.8°
SO_2.....	2.02736	0.34417	0.293535	C_{2v}	r_0(SO) = 1.432 Å; $\measuredangle$OSO = 119.5$_5$°
S_2O.....	1.39811	0.16875$_3$	0.15034$_2$	C_s	r_0(SO) = 1.46$_5$ Å; r(SS) = 1.88$_4$; $\measuredangle$SSO = 118.0°
NOF.....	3.175189	0.395077	0.350519	C_s	r_0(NO) = 1.13 Å; r_0(NF) = 1.52 Å; $\measuredangle$ONF = 110°
$NOCl^{35}$...	2.8493	0.191383	0.179343	C_s	r_0(NCl) = 1.975 Å; r_0(NO) = 1.139 Å; $\measuredangle$ClNO = 113.3°
$NOCl^{37}$...	2.8486	0.186825	0.175327		
$NOBr^{79}$...	2.7799	0.12499	0.11962	C_s	r_0(NBr) = 2.14 Å; r_0(NO) = 1.15 Å; $\measuredangle$BrNO = 114°
$NOBr^{81}$...	2.7799	0.12417	0.11886		
$NS^{32}F$....	1.65841	0.290615	0.246607	C_s	r_0(SF) = 1.646 Å; r_0(SN) = 1.446 Å; $\measuredangle$NSF = 116.9°
$NS^{34}F$....	1.61101	0.290245	0.245262		
$Cl^{35}O_2$....	1.73718	0.331971	0.277992	C_{2v}	r_0(ClO) = 1.473 Å; $\measuredangle$OClO = 117.6°
F_2O.....	1.960777	0.363466	0.305792	C_{2v}	r_0(OF) = 1.409 Å; $\measuredangle$FOF = 103.3°

TABLE 7h-7. FOUR-ATOMIC LINEAR MOLECULES

Molecule	$B_{[0]}$ cm^{-1}	Point group	Geometrical parameters
C_2H_2	1.1766	$D_{\infty h}$	r_0(CC) = 1.208 Å; r_e(CC) = 1.204 Å
	B_e = 1.1817		r_0(CH) = 1.057 Å; r_e(CH) = 1.059 Å
C_2HD	0.9910	$C_{\infty v}$	
	B_e = 0.9948		
C_2D_2	0.84787	$D_{\infty h}$	
	B_e = 0.85075		
$C_2N_2^{14}$	0.15712	$D_{\infty h}$	r_0(C—C) = 1.389 Å; r_0(C≡N) = 1.154 Å (assumed)
$C_2N_2^{15}$	0.14774		
$HC_2^{12}Cl^{35}$	0.189606	$C_{\infty v}$	r_0(CH) = 1.052 Å; r_0(CC) = 1.211 Å; r_0(CCl) = 1.632 Å
$HC_2^{12}Cl^{37}$	0.185874		
$DC_2^{12}Cl^{35}$	0.173020		
$DC_2^{12}Cl^{37}$	0.169592		
FCCH	0.323764	$C_{\infty v}$	r_0(CH) = 1.053 Å; r_0(CC) = 1.198 Å; r_0(CF) = 1.279 Å
$FC^{13}CH$	0.323579		
$FCC^{13}H$	0.312681		
FCCD	0.291403		
$FC^{13}CD$	0.291332		
$FCC^{13}D$	0.283071		

TABLE 7h-8. FOUR-ATOMIC SYMMETRIC TOP MOLECULES

Molecule	$A_{[0]}$ or $C_{[0]}$ cm^{-1}	$B_{[0]}$ cm^{-1}	Point group	Geometrical parameters
$AsCl_3^{35}$	.....	0.071623	C_{3v}	r_0(AsCl) = 2.161 Å; ∢ClAsCl = 98.4°
$AsCl_3^{37}$	.....	0.068204		
AsF_3	.....	0.1961013	C_{3v}	r_0(AsF) = 1.712 Å; ∢FAsF = 102° (assumed)
AsH_3	.....	3.75154	C_{3v}	r_0(AsH) = 1.517 Å; ∢HAsH = 91.7°
AsD_3	.....	1.91723		
BF_3	0.17635	0.3527	D_{3h}	r_0(BF) = 1.295 Å
$N^{14}F_3$	.....	0.356261	C_{3v}	r_0(NF) = 1.371 Å; ∢FNF = 102.1°
$N^{15}F_3$	.....	0.354557		
NH_3	6.196	9.9443	C_{3v}	r_0(NH) = 1.017 Å; ∢HNH = 107.8°
ND_3	3.117	5.1423		
PCl_3^{35}	.....	0.087305	C_{3v}	r_0(PCl) = 2.043 Å; ∢ClPCl = 100.1°
PCl_3^{37}	.....	0.082974		
PF_3	.....	0.260847	C_{3v}	r_0(PF) = 1.535 Å; ∢FPF = 100.1° (assumed)
PH_3	.....	4.45236	C_{3v}	r_0(PH) = 1.419 Å; ∢HPH = 93.3°
PD_3	.....	2.31728		
$Sb^{121}Cl_3$	.....	0.05850	C_{3v}	r_0(SbCl) = 2.325 Å; ∢ClSbCl = 99.5°
$Sb^{123}Cl_3$	.....	0.05840		
$Sb^{121}H_3$	.....	2.93643	C_{3v}	r_0(SbH) = 1.704 Å; ∢HSbH = 91.1°
$Sb^{123}H_3$	.....	2.93588		
$Sb^{121}D_3$	.....	1.49081		
$Sb^{123}D_3$	.....	1.49027		

TABLE 7h-9. FOUR-ATOMIC ASYMMETRIC TOP MOLECULES

Molecule	$A_{[0]}$ cm^{-1}	$B_{[0]}$ cm^{-1}	$C_{[0]}$ cm^{-1}	Point group	Geometrical parameters
$CCl_2^{35}O$	0.264141	0.115913	0.0804639	C_{2v}	$r_0(CO) = 1.166$ Å; $r_0(CCl) = 1.746$ Å; $\measuredangle ClCCl = 111.3°$
$CCl^{35}Cl^{37}O$	0.262440	0.112743	0.0787704	C_s	
$C^{13}F_2O^{16}$	0.394034	0.392037	0.196166	C_{2v}	$r_0(CF) = 1.312$ Å; $r_0(CO) = 1.174$ Å; $\measuredangle FCF = 108.0°$
$C^{12}F_2O^{18}$	0.394095	0.391847	0.196129		
$C^{13}F_2O^{18}$	0.394055	0.362869	0.188574		
CH_2O	9.4053	1.29536	1.13428	C_{2v}	$r_0(CH) = 1.102$ Å; $r_0(CO) = 1.210$ Å; $\measuredangle HCH = 121.1°$
$C^{13}HFO^{16}$	3.04056	0.39227	0.34680	C_s	$r_0(CF) = 1.338$ Å; $r_0(CO) = 1.181$ Å; $r_0(CH) = 1.095$ Å; $\measuredangle FCO = 122.8°$; $\measuredangle HCO = 127.3°$
$C^{12}HFO^{18}$	2.95221	0.39211	0.34548		
$C^{13}DFO^{16}$	2.17117	0.39233	0.33162		
$C^{13}HFO^{18}$	2.99439	0.37035	0.32901		
$Cl^{35}F_3$	0.458573	0.153830	0.115039	C_s	ClF_2F': $r_0(ClF) = 1.698$ Å; $\measuredangle FClF = 175.0°$; $r_0(ClF') = 1.598$ Å; $\measuredangle F'ClF = 87.5°$
$Cl^{37}F_3$	0.455421	0.153836	0.114840		
HN_3^{14}	20.34	0.401416	0.392988	C_s	HN′N″N‴: $r_0(N'H) = 1.00$ Å; $\measuredangle N'N''N''' = (180°)$ (assumed); $r_0(N'N'') = 1.237$ Å; $r_0(N''N''') = 1.133$ Å; $\measuredangle HN'N'' = 114.1°$
$HN^{15}N_2^{14}$	(20.58)	0.389187	0.381192		
$HN_2^{14}N^{15}$	(20.58)	0.388327	0.380432		
DN_3^{14}	11.47	0.378603	0.365769		
HNCO	30.59	0.369289	0.363938	C_s	$r_0(HN) = 0.987$ Å; $\measuredangle HNC = 128.1°$; $r_0(NC) = 1.207$ Å; $r_0(CO) = 1.171$ Å; $\measuredangle NCO = (180°)$ (assumed)
DNCO	17.34	0.344025	0.336221		
$HNC^{32}S^{32}$	44.90	0.196250	0.194989	C_s	$r_0(NH) = 0.989$ Å; $r_0(NC) = 1.210$ Å; $r_0(CS) = 1.561$ Å; $\measuredangle HNC = 135.0°$; $\measuredangle NCS = 180°$ (assumed)
$HNC^{32}S^{34}$	.....	0.191626	0.190423		
$DNC^{32}S^{32}$	23.58	0.183477	0.181634		
H_2O_4	10.068	0.8740	0.8384	C_2	$r_0(OH) = 0.950$ Å; $r_0(OO) = 1.475$ Å; $\measuredangle OOH = 94.8°$; dihedral angle $= 119.8°$
cis N_2F_2	0.656682	0.265075	0.188510	C_{2v}	$r_0(NF) = 1.384$ Å; $r_0(NN) = 1.214$ Å; $\measuredangle FNN = 114.5°$
cis $N^{14}N^{15}F_2$	0.643874	0.263556	0.186677		

TABLE 7h-10. FIVE-ATOMIC LINEAR MOLECULES

Molecule	$B_{[0]}$, cm^{-1}	Point group	Geometrical parameters
$HC^{12}C^{12}C^{12}N^{14}$	0.151740	$C_{\infty v}$	$r_0(CH) = 1.057$ Å; $r_0(C\equiv C) = 1.203$ Å; $r_0(C—C) = 1.382$ Å; $r_0(CN) = 1.157$ Å
$HC^{12}C^{12}C^{13}N^{14}$	0.151112		
$HC^{12}C^{13}C^{12}N^{14}$	0.151099		
$HC^{13}C^{12}C^{12}N^{14}$	0.147050		
$HC^{12}C^{12}C^{12}N^{15}$	0.147332		
$DC^{12}C^{12}C^{12}N^{14}$	0.140817		
$DC^{12}C^{12}C^{13}N^{14}$	0.140181		
$DC^{12}C^{13}C^{12}N^{14}$	0.140350		
$DC^{13}C^{12}C^{12}N^{14}$	0.137002		
$DC^{12}C^{12}C^{12}N^{15}$	0.136775		
C_3O_2	0.07321	$D_{\infty h}$	$r_0(CO) = 1.160$ Å (assumed); $r_0(CC) = 1.280$ Å

TABLE 7h-11. FIVE-ATOMIC SYMMETRIC AND SPHERICAL TOP MOLECULES

Molecule	$A_{[0]}$ or $C_{[0]}$, cm^{-1}	$B_{[0]}$, cm^{-1}	Point group	Geometrical parameters
CF_3Br^{79}	.....	0.069984	C_{3v}	$r_0(CF) = 1.33$ Å; $\angle(FCF) = 108°$ (assumed)
CF_3Br^{81}	.....	0.069331	C_{3v}	$r_0(CBr) = 1.908$ Å
CF_3Cl^{35}	.....	0.111262	C_{3v}	$r_0(CF) = 1.328$ Å; $\angle(FCF) = 108°$ (assumed)
CF_3Cl^{37}	.....	0.108458	C_{3v}	$r_0(CCl) = 1.740$ Å
CF_3I	0.1910	0.050809	C_{3v}	$r_0(CF) = 1.33$ Å (assumed); $\angle FCF = 108°$ (assumed); $r_0(CI) = 2.134$ Å
CH_4	.....	5.2412	T_d	$r_0(CH) = 1.0940$ Å; $r_e(CH) = 1.085$ Å; $r_0(CD) = 1.091_8$ Å
CH_3D	5.243	3.878	C_{3v}	
CHD_3	.....	3.2795	C_{3v}	
CD_4	.....	2.6329	T_d	
$CHBr_3^{79}$	.....	0.041616	C_{3v}	$r_0(CH) = 1.06_3$ Å; $\angle(BrCBr) = 110°48'$; $r_0(CBr) = 1.930$ Å
$CHBr_2^{81}$	.....	0.040605		
$CDBr_3^{79}$	.....	0.041344		
$CDBr_3^{81}$	.....	0.040345		
$C^{12}H_3Br^{79}$	5.129	0.319160	C_{3v}	$r_0(CBr) = 1.939$ Å; $\angle(HCH) = 110°58'$; $r_0(CH) = 1.096$ Å
$C^{12}H_3Br^{81}$	5.129	0.317947	C_{3v}	
$C^{13}H_3Br^{79}$	.....	0.304194	C_{3v}	
$C^{13}H_3Br^{81}$	.....	0.302971	C_{3v}	
$C^{12}D_3Br^{79}$	2.591	0.257332	C_{3v}	$r_0(CBr) = 1.9391$ Å; $\angle(DCD) = 111°26'$; $r_0(CD) = 1.104$ Å
$C^{12}D_3Br^{81}$	2.591	0.256218	C_{3v}	
$CHCl_3^{35}$	.....	0.110146	C_{3v}	$r_0(CH) = 1.073$ Å; $\angle(ClCCl) = 110°24'$; $r_0(CCl) = 1.767$ Å
$CHCl_3^{37}$	.....	0.104389	C_{3v}	
$CDCl_3^{35}$	.....	0.108414	C_{3v}	
$C^{12}H_3Cl^{35}$	(5.14)	0.443402	C_{3v}	$r_0(CCl) = 1.7810$ Å; $\angle(HCH) = 110°31'$; $r_0(CH) = 1.113$ Å
$C^{12}H_3Cl^{37}$	.....	0.436574	C_{3v}	
$C^{13}H_3Cl^{35}$	5.124	0.426835	C_{3v}	
$C^{13}H_3Cl^{37}$	.....	0.419957	C_{3v}	
$C^{12}D_3Cl^{35}$	.....	0.361647	C_{3v}	$r_0(CCl) = 1.7810$ Å; $\angle(DCD) = 110°43'$; $r_0(CD) = 1.104$ Å
$C^{12}D_3Cl^{37}$	.....	0.355528	C_{3v}	
$C^{13}H_3Cl^{35}$	.....	0.439892	C_{3v}	
$C^{12}HF_3$	.....	0.345196	C_{3v}	$r_0(CH) = 1.098$ Å; $\angle(FCF) = 108°48'$; $r_0(CF) = 1.332$ Å
$C^{12}DF_3$	.....	0.330940	C_{3v}	
$C^{13}HF_3$	.....	0.347640	C_{3v}	
$C^{12}H_3F$	5.08$_1$	0.851794	C_{3v}	$r_0(CH) = 1.10_9$ Å; $\angle(HCN) = 110°0'$; $r_0(CF) = 1.385$ Å
$C^{13}H_3F$	.....	0.829318	C_{3v}	
$C^{12}D_3F$	.....	0.682132	C_{3v}	
$C^{12}H_3I$	5.134	0.250215	C_{3v}	$r_0(CH) = 1.106$ Å; $\angle(HCH) = 111°10'$; $r_0(CI) = 2.1396$ Å
$C^{13}H_3I$	..	0.237465	C_{3v}	
$C^{12}D_3I$	.....	0.201482	C_{3v}	$r_0(CI) = 2.1392$ Å; $r_0(CD) = 1.104$; $\angle(DCD) = 111°37'$
$Ge^{70}F_3^{19}Cl^{35}$	.....	0.072334	C_{3v}	$r_0(GeF) = 1.688$ Å; $\angle(FGeF) = 107°42'$; $r_0(GeCl) = 2.067$ Å
$Ge^{70}F_3^{19}Cl^{37}$	.....	0.070320	C_{3v}	
$Ge^{72}F_3^{19}Cl^{35}$	.....	0.072301	C_{3v}	
$Ge^{72}F_3^{19}Cl^{37}$	.....	0.070283	C_{3v}	
$Ge^{74}F_3^{19}Cl^{35}$	.....	0.072270	C_{3v}	
$Ge^{74}F_3^{19}Cl^{37}$	.....	0.070248	C_{3v}	
GeH_4	.....	2.70$_4$	T_d	$r_0(GeH) = 1.524$ Å
GeD_4	.....	1.3512	T_d	
$GeHD_3$	.....	1.669	C_{3v}	
GeH_3D	.....	1.969	C_{3v}	
$Ge^{70}H_3Br^{79}$	.....	0.081342	C_{3v}	$r_0(GeH) = 1.55$ Å; $\angle(HGeH) = 112°0'$; $r_0(GeBr) = 2.297$ Å
$Ge^{70}H_3Br^{81}$	.....	0.080395	C_{3v}	
$Ge^{72}H_3Br^{79}$	.....	0.080269	C_{3v}	
$Ge^{72}H_3Br^{81}$	.....	0.079322	C_{3v}	
$Ge^{74}H_3Br^{79}$	.....	0.079251	C_{3v}	
$Ge^{74}H_3Br^{81}$	.....	0.078303	C_{3v}	
$Ge^{76}H_3Br^{79}$	.....	0.078282	C_{3v}	
$Ge^{76}H_3Br^{81}$	.....	0.077332	C_{3v}	
$Ge^{70}HCl_3^{35}$	.....	0.072475	C_{3v}	$r_0(GeCl) = 2.1139$ Å; $\angle(ClGeCl) = 108°17'$; $r_0(GeH) = 1.55$ Å
$Ge^{72}HCl_3^{35}$	.....	0.0723586	C_{3v}	
$Ge^{74}HCl_3^{35}$	.....	0.0722445	C_{3v}	
$Ge^{70}HCl_3^{37}$	.....	0.0688389	C_{3v}	
$Ge^{72}HCl_3^{37}$	.....	0.0687284	C_{3v}	
$Ge^{74}HCl_3^{37}$	.....	0.0686207	C_{3v}	

TABLE 7h-11. FIVE-ATOMIC SYMMETRIC AND SPHERICAL TOP MOLECULES
(Continued)

Molecule	$A_{[0]}$ or $C_{[0]}$, cm^{-1}	$B_{[0]}$, cm^{-1}	Point group	Geometrical parameters
$Ge^{73}H_3Cl^{35}$	.....	0.146825		
$Ge^{74}H_3Cl^{35}$	2.603	0.144563	C_{3v}	$r_0(GeH) = 1.52$ Å; $\sphericalangle(HGeH) = 111°4'$; $r_0(GeCl) = 2.147$ Å
$Ge^{74}H_3Cl^{37}$	.....	0.139359		
$Ge^{76}H_3Cl^{37}$	.....	0.13831		
$Ge^{70}H_3F$	.....	0.33699	C_{3v}	
MnO_3F	.....	0.137732	C_{3v}	
$POCl_3^{35}$	.....	0.067220	C_{3v}	$r_0(PCl) = 1.99$ Å; $\sphericalangle(ClPCl) = 103°36'$; $r_0(PO) = 1.45$ Å
$POCl_2^{37}$	.....	0.064457		
$PO^{16}F_3$	.....	0.153248	C_{3v}	$r_0(PF) = 1.52$ Å; $\sphericalangle(FPF) = 102°30'$; $r_0(PO) = 1.45$ Å
$PO^{18}F_3$	.....	0.146610		
$PS^{32}Cl_3^{35}$	.....	0.046787	C_{3v}	$r_0(PCl) = 2.02$ Å; $\sphericalangle(ClPCl) = 100°30'$; $r_0(PS) = 1.85$ Å
$PS^{32}Cl_2^{37}$	.....	0.045222		
$PS^{34}Cl_3^{35}$	.....	0.045702		
$PS^{32}F_3$	.....	0.088650	C_{3v}	$r_0(PF) = 1.53$ Å; $\sphericalangle(FPF) = 100°18'$; $r_0(PS) = 1.87$ Å
$PS^{33}F_3$	.....	0.087218		
$PS^{34}F_3$	.....	0.086052		
$Re^{185}O_3Cl^{35}$	.....	0.069856		
$Re^{185}O_3Cl^{37}$	.....	0.067547	C_{3v}	$r_0(ReO) = 1.761$ Å; $\sphericalangle(OReO) = 108°20'$; $r_0(ReCl) = 2.230$ Å
$Re^{187}O_3Cl^{35}$	.....	0.069834		
$Re^{187}O_3Cl^{37}$	.....	0.067525		
SiF_3Br^{79}	.....	0.051702	C_{3v}	$r_0(SiF) = 1.560$ Å; $r_0(SiBr) = 2.153$ Å; $\sphericalangle(FSiF) = 108°30'$ (assumed)
SiF_3Br^{81}	.....	0.051173		
SF_3Cl^{35}	.....	0.082650	C_{3v}	$r_0(SiF) = 1.560$ Å; $r_0(SiCl) = 1.989$ Å; $\sphericalangle(FSiF) = 108°30'$ (assumed)
SiF_3Cl^{37}	.....	0.080491		
$Si^{28}H_4$	.....	2.864	T_d	$r_0(SiH) = 1.480$ Å
$SiHD_3$	.....	1.7755	C_{3v}	
$Si^{28}H_3Br^{79}$	.....	0.144159		
$Si^{28}H_3Br^{81}$	.....	0.143187		
$Si^{29}H_3Br^{79}$	.....	0.141196	C_{3v}	$r_0(SiH) = 1.57$ Å; $\sphericalangle(HSiH) = 111°20'$; $r_0(SiBr) = 2.209$ Å
$Si^{29}H_3Br^{81}$	.....	0.140220		
$Si^{30}H_3Br^{79}$	.....	0.138409		
$Si^{30}H_3Br^{81}$	.....	0.137431		
$SiHCl_3^{35}$	.....	0.0824732	C_{3v}	$r_0(SiH) = 1.47$ Å; $\sphericalangle(ClSiCl) = 109°22'$; $r_0(SiCl) = 2.021$ Å
$SiHCl_3^{37}$	.....	0.0782564		
$Si^{28}H_3Cl^{35}$	.....	0.22261		
$Si^{30}H_3Cl^{35}$	.....	0.21634		
$Si^{28}H_3Cl^{37}$	.....	0.21723	C_{3v}	$r_0(SiCl) = 2.048$ Å; $\sphericalangle(HSiH) = 110°57'$; $r_0(SiH) = 1.50$ Å
$Si^{28}D_3Cl^{35}$	.....	0.19739		
$Si^{29}D_3Cl^{35}$	.....	0.19515		
$Si^{30}D_3Cl^{35}$	.....	0.19303		
$Si^{28}D_3Cl^{37}$	.....	0.19256		
$Si^{28}HF_3$	.....	0.240435	C_{3v}	$r_0(SiF) = 1.565$ Å; $\sphericalangle(FSiF) = 108°17'$; $r_0(SiH) = 1.455$ Å (assumed)
$Si^{29}HF_3$	.....	0.240021		
$Si^{30}HF_3$	.....	0.239622		
$Si^{28}H_3F$	.....	0.477927		
$Si^{29}H_3F$	.....	0.473550		
$Si^{30}H_3F$	.....	0.469411	C_{3v}	$r_0(SiH) = 1.503$ Å; $r_0(SiF) = 1.593$ Å; $\sphericalangle(HSiH) = (111°)$ (assumed)
$Si^{28}D_3F$	.....	0.408732		
$Si^{29}D_3F$	.....	0.406120		
$Si^{30}D_3F$	.....	0.403678		
SiH_3I	.....	0.10726	C_{3v}	
SnH_4	.....	2.16,	T_d	$r_0(SnH) = 1.701$ Å
$HnSD_3$	.....	1.3573	C_{3v}	

TABLE 7h-12. FIVE-ATOMIC ASYMMETRIC TOP MOLECULES

Molecule	$A_{[0]}$, cm^{-1}	$B_{[0]}$, cm^{-1}	$C_{[0]}$, cm^{-1}	Point group	Geometrical parameters
CH_2Br_2	$\left[A-\frac{B+C}{2}\right]=0.821$			C_{2v}	r_0(CBr) = 1.907 Å; ∢(HCH) = 112° (elec. diffr.)
CH_2CO	9.37	0.343347	0.330758	C_{2v}	r_0(CH) = 1.075 Å; ∢(HCH) = 122.0° r_0(CO) = 1.16 Å (assumed); r_0(CC) = 1.31$_4$ Å
CHDCO	.....	0.321790	0.306032	C_s	
CD_2CO	.....	0.304237	0.285286	C_{2v}	
$CH_2Cl^{35}_2$	1.06746	0.11076	0.10224	C_{2v}	
$CH_2Cl^{35}Cl^{37}$	1.063344	0.10779	0.099677	C_s	
$CH_2Cl^{37}_2$	1.0592	0.1048	0.09713	C_{2v}	r_0(CCl) = 1.7724 Å; ∢(ClCCl) = 111°47′ r_0(CH) = 1.068 Å; ∢(HCH) = 112°0′
$CHDCl^{35}_2$	0.9072	0.1102	0.1010	C_s	
$CHDCl^{35}Cl^{37}$	0.90364	0.10732	0.09845	C_1	
$CD_2Cl^{35}_2$	0.78976	0.1095	0.09985	C_{2v}	
$CD_2Cl^{35}Cl^{37}$	0.78661	0.10666	0.09740	C_s	
CH_2ClBr	$\left[A-\frac{B+C}{2}\right]=0.897_5$			C_s	r_0(CBr) = 1.911 Å; r_0(CCl) = 1.766 Å (assumed) ∢(HCH) = 112° (elec. diffr.)
CH_2F_2	1.6391	0.3537	0.3085	C_{2v}	r_0(CH) = 1.09 Å; ∢(HCH) = 112° r_0(CF) = 1.36 Å; ∢(FCF) = 108°
CH_2N_2	9.112	0.377109	0.361759	C_{2v}	r_0(NN) = 1.12 Å; r_0(CN) = 1.32 Å; r_0(CH) = 1.08 Å; ∢HCH = 127°
CD_2N_2	.....	0.334984	0.311764		
HCO_2H	2.58548	0.402112	0.347447	C_s	r_0(CH) = 1.097 Å; r_0(CO) = 1.202, 1.343 Å r_0(OH) = 0.972 Å; ∢OCO = 124.9°; ∢HCO = 124.1°; ∢COH = 106.3°
DCO_2H	1.9250	0.402138	0.332087		
HCO_2D	2.2052	0.392356	0.332565		
HNO_3	0.434005	0.403610	0.208831	C_s	r_0(NO) = 1.199, 1.211, 1.406 Å; r_0(OH) = 0.964 Å; ∢ONO = 130.3°, 113.8$_5$°; ∢NOH = 102.1$_4$°
DNO_3	0.432656	0.377355	0.201301		
$S^{32}O_2F_2$	0.171261	0.169218	0.168685	C_{2v}	r_0(SO) = 1.405 Å; ∢OSO = 124.0° r_0(SF) = 1.530 Å; ∢FSF = 96.1°
$S^{34}O_2F_2$	0.171243	0.169117	0.168556		
$Si^{28}H_2F_2$	0.82359$_3$	0.26024	0.21272	C_{2v}	r_0(SiH) = 1.470 Å; r_0(SiF) = 1.577 Å; ∢FSiF = 107.9°
$Si^{28}D_2F_2$	0.62992$_5$	0.24842	0.20435		

TABLE 7h-13. SIX-ATOMIC LINEAR MOLECULES

Molecule	$B_{[2]}$, cm^{-1}	Point group	Geometrical parameters
C_4H_2	0.14689	$D_{\infty h}$	$r_0(C—C) = 1.376$ Å, assuming $r_0(C\equiv C) = 1.205$ Å; $r_0(CH) = 1.046$ Å
C_4D_2	0.12767	$D_{\infty h}$	
$C_4H_2^+$	0.14013	$D_{\infty h}$	

TABLE 7h-14. SIX-ATOMIC SYMMETRIC TOP MOLECULES

Molecule	$B_{[2]}$, cm^{-1}	Point group	Geometrical parameters
$B^{10}H_3CO$	0.299544	C_{3v}	$r_0(BH) = 1.194$ Å; $r_0(BC) = 1.540$ Å; $\sphericalangle(HBH) = 113°52'$; $r_0(CO) = 1.131$ Å
$B^{11}H_3CO$	0.288773	C_{3v}	
$B^{10}D_3CO$	0.251185	C_{3v}	
$B^{11}D_3CO$	0.241721	C_{3v}	
CF_3CN^{14}	0.0982523	C_{3v}	$r_0(CF) = 1.335$ Å; $r_0(CN) = 1.158$ Å (assumed); $\sphericalangle(FCF) = 108°$ (assumed); $r_0(CC) = 1.464$ Å
CF_3CN^{15}	0.0952611	C_{3v}	
$C^{12}H_3C^{12}N^{14}$	0.306842	C_{3v}	$r_0(CH) = 1.092$ Å; $r_0(CC) = 1.460$ Å; $\sphericalangle(HCH) = 109°8'$; $r_0(CN) = 1.158$ Å
$C^{12}H_3C^{12}N^{15}$	0.297599	C_{3v}	
$C^{12}H_3C^{13}N^{14}$	0.306686	C_{3v}	
$C^{13}H_3C^{12}N^{14}$	0.297977	C_{3v}	
$C^{12}D_3C^{12}N^{14}$	0.262119	C_{3v}	
$C^{13}D_3C^{13}N^{14}$	0.261798	C_{3v}	
$CH_3Hg^{198}Br^{81}$	0.03754	C_{3v}	$r_0(HgBr) = 2.406$ Å; $r_0(CH) = 1.092$ Å (assumed); $\sphericalangle(HCH) = 109°7'$ (assumed); $r_0(CHg) = 2.07$ Å
$CH_3Hg^{202}Br^{79}$	0.03802	C_{3v}	
$CH_3Hg^{202}Br^{81}$	0.03743	C_{3v}	
$CH_3Hg^{198}Cl^{35}$	0.069296	C_{3v}	$r_0(CH) = 1.092$ Å (assumed); $\sphericalangle(HCH) = 109°7'$; $r_0(CHg) = 2.059$ Å; $r_0(HgCl) = 2.282$ Å
$CH_3Hg^{198}Cl^{37}$	0.066918	C_{3v}	
$CH_3Hg^{199}Cl^{35}$	0.069286	C_{3v}	
$CH_3Hg^{199}Cl^{37}$	0.066906	C_{3v}	
$CH_3Hg^{200}Cl^{35}$	0.069275	C_{3v}	
$CH_3Hg^{200}Cl^{37}$	0.066895	C_{3v}	
$CH_3Hg^{202}Cl^{35}$	0.069255	C_{3v}	
$CH_3Hg^{202}Cl^{37}$	0.066872	C_{3v}	
$CH_3Hg^{204}Cl^{35}$	0.069234	C_{3v}	
$CH_3Hg^{204}Cl^{37}$	0.066849	C_{3v}	
CH_3NC^{12}	0.335328	C_{3v}	$r_0(CH) = 1.094$ Å; $r_0(C—N) = 1.427$ Å; $\sphericalangle(HCH) = 109°46'$; $r_0(N=C) = 1.167$ Å
CH_3NC^{13}	0.323420	C_{3v}	
CD_3NC^{12}	0.286266	C_{3v}	
CD_3NC^{13}	0.276150	C_{3v}	
SiH_3CN	0.16587	C_{3v}	$r_0(SiH) = 1.47$ Å (assumed); $\sphericalangle HSiC = 108°$ (assumed); $r_0(SiC) = 1.848$, $r_0(CN) = 1.156$ Å
SiD_3CN	0.15127	C_{3v}	

TABLE 7h-15. SIX-ATOMIC ASYMMETRIC TOP MOLECULES

Molecule	$A_{[0]}$ cm^{-1}	$B_{[0]}$ cm^{-1}	$C_{[0]}$ cm^{-1}	Point group	Geometrical parameters
C_2H_4	4.828	1.0012	0.8282	V_h	r_0(CH) = 1.086 Å; ∢HCH = 117.6° r_0(C=C) = 1.339 Å
C_2D_4	2.432	0.7369	0.5630		
CH_2CF_2	0.367003	0.347873	0.17830$_3$	C_{2v}	r_0(CH) = (1.080 Å); ∢HCH = 121.8° r_0(CF) = (1.325 Å); ∢FCF = 108.9° r_0(CC) = (1.313 Å)
CD_2CF_2	0.35324	0.29998	0.16199		
CH_2CFCl^{35}	0.35630	0.17019	0.11503	C_s	
CH_2CFCl^{37}	0.35629	0.16528	0.11276		
CH_2CHBr^{79}	.....	0.13886	0.12885	C_s	
CH_2CHBr^{81}	.....	0.13804	0.12816		
CH_2CHCl^{35}	.....	0.201136	0.181635	C_s	r_0(CH) = 1.07$_9$ Å; r_0(CH') = 1.090 Å; r_0(CC) = 1.33$_2$ Å r_0(CCl) = 1.72$_6$ Å; ∢CCH = 119.5°, 123.8°, 121.0°; ∢CCCl = 122.3°
CH_2CHCl^{37}	.....	0.196922	0.178165		
CH_2CHI	.....	0.10870	0.10229	C_s	
CH_3OH	.....	0.82299	0.79263	C_s	r_0(C—O) = 1.425 Å; ∢COH = 108.5° r_0(CH) = 1.094 Å; ∢HCH = 108.6° r_0(OH) = 0.945 Å methyl tilt 3.3°
CD_3OH	.....	0.66186	0.64272		
CH_3OD	.....	0.78273	0.73309		
CH_3SH	(5.68)	0.4305$_4$	0.4130$_8$	C_s	r_0(CH) = 1.104 Å; r_0(SH) = 1.329 Å r_0(CS) = 1.818 Å; ∢HCH = 110.3° ∢CSH = 100.3°
CH_3SD	(3.04)	0.4222$_7$	0.3911$_9$		
CD_3SH	(4.03)	0.3516$_3$	0.3398$_9$		
HC_2CHO	2.26912	0.160985	0.150091	C_s	r_0(C=C) = 1.215 Å; r_0(C≡C) = 1.209 Å r_0(C—C) = 1.445 Å; r_0(CH) = 1.106 Å, 1.055 Å ∢CCO = 123.7°, ∢CCC = 178.4°
DC_2CHO	2.22715	0.148895	0.139359		
HC_2CDO	1.72668	0.159825	0.146060		
DC_2CDO	1.70368	0.147739	0.135747		
N_2H_4	3.981$_4$	$B_0 + C_0$ = 1.60633		C_2	r_0(NH) = 1.02 Å (assumed); r_0(NN) = 1.45 Å (assumed) ∢HNH = 106°; ∢HNN = 112° Dihedral angle = 90.0°
NH_2CHO	2.42555	0.37939	0.32802	C_1	r_0(NH') = 1.014 Å; r_0(NH'') = 1.002 Å; r_0(CN) = 1.376 Å; r_0(CH) = 1.102 Å r_0(CO) = 1.193 Å; ∢H'NH'' = 118.9°; ∢H''NC = 120.6° ∢H'NC = 117.1$_5$°; ∢NCO = 123.8°; ∢NCH = 113.2° ∢OCH = 123.0°; ∢H'NC − NCO = 7°; ∢H''NC − NCH = 12°
NH_2CDO	1.83288	0.37936	0.31421		
ND_2CHO	1.99191	0.34002	0.29055		