SPECTROSCOPIC CONSTANTS OF DIATOMIC MOLECULES

This table lists the leading spectroscopic constants and equilibrium internuclear distance r_e in the ground electronic state for selected diatomic molecules. The constants are those describing the vibrational and rotational energy through the expressions:

$$E_{vib}/hc = \omega_e(v + 1/2) - \omega_e x_e(v + 1/2)^2 + \ldots$$

$$E_{rot}/hc = B_v J(J + 1) - D_v[J(J + 1)]^2 + \ldots$$

where

$$B_v = B_e - \alpha_e(v+1/2) + \ldots$$

$$D_v = D_e + \ldots$$

Here v and J are the vibrational and rotational quantum numbers, respectively, h is Planck's constant, and c is the speed of light. In this customary formulation the constants ω_e, B_e, etc. have dimensions of inverse length; in this table they are given in units of cm^{-1}.

Users should note that higher order terms in the above energy expressions are required for very precise calculations; constants for many of these terms can be found in the references. Also, if the ground electronic state is not $^1\Sigma$, additional terms are needed to account for the interaction between electronic and pure rotational angular momentum. For some molecules in the table the data have been analyzed in terms of the Dunham series expansion:

$$E/hc = \Sigma_{lm}\, Y_{lm}(v+1/2)^l J^m(J+1)^m$$

In such cases it has been assumed that $Y_{10} = \omega_e$, $Y_{01} = B_e$, etc., although in the highest approximations these identities are not precisely correct. Some of the values of r_e in the table have been corrected for breakdown of the Born-Oppenheimer approximation, which can affect the last decimal place. Because of differences in the method of data analysis and limitations in the model, care should be taken in comparing r_e values for different molecules to a precision beyond 0.001 Å.

Molecules are listed in alphabetical order by formula as written in the most common form. In most cases this form places the more electropositive element first, but there are exceptions such as OH, NH, CH, etc.

* Indicates a value for the interval between $v = 0$ and $v = 1$ states instead of a value of ω_e.

References

1. Huber, K. P., and Herzberg, G., *Molecular Spectra and Molecular Structure IV. Constants of Diatomic Molecules*, Van Nostrand Reinhold, New York, 1979.
2. Lovas, F. J., and Tiemann, E., *J. Phys. Chem. Ref. Data*, 3, 609, 1974.
3. *Landolt-Börnstein, Numerical Data and Functional Relationships in Science and Technology, New Series*, II/6 (1974), II/14a (1982), II/14b (1983), II/19a (1992), II/19d-1 (1995), *Molecular Constants*, Springer-Verlag, Heidelberg.

Molecule	State	ω_e cm^{-1}	$\omega_e x_e$ cm^{-1}	B_e cm^{-1}	α_e cm^{-1}	D_e $10^{-6}cm^{-1}$	r_e Å
$^{107}Ag^{79}Br$	$^1\Sigma^+$	249.57	0.63	0.064833	0.0002361	0.0175	2.39311
$^{107}Ag^{35}Cl$	$^1\Sigma^+$	343.49	1.17	0.12298388	0.00059541	0.06305	2.28079
$^{107}Ag^{19}F$	$^1\Sigma^+$	513.45	2.59	0.2657020	0.0019206	0.284	1.98318
$^{107}Ag^{1}H$	$^1\Sigma^+$	1759.9	34.06	6.449	0.201	344	1.618
$^{107}Ag^{2}H$	$^1\Sigma^+$	1250.70	17.17	3.2572	0.0722	85.9	1.6180
$^{107}Ag^{127}I$	$^1\Sigma^+$	206.50	0.46	0.04486821	0.0001414	0.00847	2.54463
$^{107}Ag^{16}O$	$^2\Pi_{1/2}$	490.2	3.1	0.3020	0.0025	0.45	2.003
$^{27}Al_2$	$^3\Sigma_g^-$	350.01	2.02	0.2054	0.0012	0.31	2.466
$^{27}Al^{79}Br$	$^1\Sigma^+$	378.0	1.28	0.15919713	0.00086045	0.11285	2.29481
$^{27}Al^{35}Cl$	$^1\Sigma^+$	481.30	1.95	0.24393012	0.00161113	0.2503	2.13011
$^{27}Al^{19}F$	$^1\Sigma^+$	802.3	4.77	0.5524798	0.0049841	1.0464	1.65437
$^{27}Al^{1}H$	$^1\Sigma^+$	1682.56	29.09	6.3907	0.1858	356.5	1.6478
$^{27}Al^{2}H$	$^1\Sigma^+$	1211.95	15.14	3.3186	0.0697	97	1.6463
$^{27}Al^{127}I$	$^1\Sigma^+$	316.1	1.0	0.11769985	0.00055859		2.53710
$^{27}Al^{16}O$	$^2\Sigma^+$	979.23	6.97	0.6414	0.0058	1.08	1.6179
$^{27}Al^{32}S$	$^2\Sigma^+$	617.1	3.33	0.2799	0.0018	0.22	2.029
$^{75}As_2$	$^1\Sigma_g^+$	429.55	1.12	0.10179	0.000333		2.1026
$^{75}As^{1}H$	$^3\Sigma^-$	2130*		7.3067	0.2117	327	1.52315
$^{75}As^{2}H$	$^3\Sigma^-$	1484*		3.6688		90	1.5306
$^{75}As^{14}N$	$^1\Sigma^+$	1068.54	5.41	0.54551	0.003366	0.53	1.6184
$^{75}As^{16}O$	$^2\Pi_{1/2}$	967.08	4.85	0.48482	0.003299	0.49	1.6236
$^{197}Au_2$	$^1\Sigma_g^+$	190.9	0.42	0.028013	0.0000723	0.00250	2.4719
$^{197}Au^{1}H$	$^1\Sigma^+$	2305.01	43.12	7.2401	0.2136	279	1.5239
$^{197}Au^{2}H$	$^1\Sigma^+$	1634.98	21.65	3.6415	0.07614	70.9	1.5238
$^{11}B_2$	$^3\Sigma_g^-$	1051.3	9.35	1.212	0.014		1.590
$^{11}B^{79}Br$	$^1\Sigma^+$	684.31	3.52	0.4894	0.0035	1.00	1.888
$^{11}B^{35}Cl$	$^1\Sigma^+$	840.29	5.49	0.684282	0.006812	1.84	1.71528
$^{11}B^{19}F$	$^1\Sigma^+$	1402.1	11.8	1.516950	0.019056	7.105	1.26267
$^{11}B^{1}H$	$^1\Sigma^+$	2366.9	49.40	12.021	0.412	1242	1.2324
$^{11}B^{2}H$	$^1\Sigma^+$	1703.3	28	6.54	0.17	400	1.2324
$^{11}B^{14}N$	$^3\Pi$	1514.6	12.3	1.666	0.025	8.1	1.281
$^{11}B^{16}O$	$^2\Sigma^+$	1885.69	11.81	1.7820	0.0166	6.32	1.2045

Molecule	State	ω_e cm^{-1}	$\omega_e x_e$ cm^{-1}	B_e cm^{-1}	α_e cm^{-1}	D_e 10^{-6}cm^{-1}	r_e Å
$^{11}B^{32}S$	$^2\Sigma^+$	1180.17	6.31	0.7949	0.0061	1.40	1.6092
$^{138}Ba^{79}Br$	$^2\Sigma^+$	193.77	0.41	0.0415082	0.0001219	0.00762	2.84449
$^{138}Ba^{35}Cl$	$^2\Sigma^+$	279.92	0.82	0.08396717	0.00033429	0.03022	2.68276
$^{138}Ba^{19}F$	$^2\Sigma^+$	468.9	1.79	0.2159	0.0012	0.175	2.163
$^{138}Ba^{1}H$	$^2\Sigma^+$	1168.31	14.50	3.38285	0.06599	112.67	2.23175
$^{138}Ba^{2}H$	$^2\Sigma^+$	829.77	7.32	1.7071	0.02363	28.77	2.2304
$^{138}Ba^{127}I$	$^2\Sigma^+$	152.14	0.27	0.02680587	0.00006634	0.00333	3.08476
$^{138}Ba^{16}O$	$^1\Sigma^+$	669.76	2.03	0.3126140	0.0013921	0.2724	1.93969
$^{138}Ba^{32}S$	$^1\Sigma^+$	379.42	0.88	0.10331	0.0003188	0.0306	2.5074
$^{9}Be^{19}F$	$^2\Sigma^+$	1247.36	9.12	1.4889	0.0176	8.28	1.3610
$^{9}Be^{1}H$	$^2\Sigma^+$	2060.78	36.31	10.3164	0.3030	1022.1	1.3426
$^{9}Be^{2}H$	$^2\Sigma^+$	1530.32	20.71	5.6872	0.1225	313.8	1.3419
$^{9}Be^{16}O$	$^1\Sigma^+$	1487.32	11.83	1.6510	0.0190	8.20	1.3309
$^{9}Be^{32}S$	$^1\Sigma^+$	997.94	6.14	0.79059	0.00664	2.00	1.7415
$^{209}Bi_2$	$^1\Sigma_g^+$	172.71	0.34	0.022781	0.000055	0.00150	2.6596
$^{209}Bi^{1}H$	$^3\Sigma^-$	1635.73	31.6	5.137	0.148	183	1.805
$^{209}Bi^{2}H$	$^3\Sigma^-$	1173.32	16.1	2.592	0.054	50.6	1.804
$^{79}Br_2$	$^1\Sigma_g^+$	325.32	1.08	0.082107	0.0003187	0.02092	2.2811
$^{79}Br^{35}Cl$	$^1\Sigma^+$	444.28	1.84	0.152470	0.000770	0.07183	2.13607
$^{79}Br^{19}F$	$^1\Sigma^+$	670.75	4.05	0.35584	0.00261	0.401	1.75894
$^{79}Br^{16}O$	$^2\Pi_{3/2}$	779	6.8	0.429598	0.003639	0.523	1.717
$^{12}C_2$	$^1\Sigma_g^+$	1854.71	13.34	1.8198	0.0177	6.92	1.2425
$^{12}C^{35}Cl$	$^2\Pi_{1/2}$	866.72*	6.2	0.6936	0.00672	1.9	1.6450
$^{12}C^{19}F$	$^2\Pi_{1/2}$	1308.1	11.10	1.4172	0.0184	6.5	1.2718
$^{12}C^{1}H$	$^2\Pi_{1/2}$	2858.5	63.0	14.457	0.534	1450	1.1199
$^{12}C^{2}H$	$^2\Pi_{1/2}$	2099.8	34.02	7.806	0.208	420	1.1190
$^{12}C^{14}N$	$^2\Sigma^+$	2068.59	13.09	1.8997830	0.0173717	6.4034	1.17181
$^{12}C^{16}O$	$^1\Sigma^+$	2169.81	13.29	1.93128075	0.01750390	6.1216	1.12823
$^{12}C^{31}P$	$^2\Sigma^+$	1239.67	6.86	0.7986	0.00597	1.33	1.562
$^{12}C^{32}S$	$^1\Sigma^+$	1285.15	6.50	0.8200434	0.0059182	1.336	1.53482
$^{12}C^{80}Se$	$^1\Sigma^+$	1035.36	4.86	0.5750	0.00379	0.71	1.67609
$^{40}Ca^{35}Cl$	$^2\Sigma^+$	367.53	1.31	0.1522302	0.0007990	0.1029	2.43676
$^{40}Ca^{19}F$	$^2\Sigma^+$	581.1	2.74	0.339	0.0026	0.45	1.967
$^{40}Ca^{1}H$	$^2\Sigma^+$	1298.34	19.10	4.2766	0.0970	183.7	2.0025
$^{40}Ca^{2}H$	$^2\Sigma^+$	910*		2.1769	0.035	47.9	2.002
$^{40}Ca^{127}I$	$^2\Sigma^+$	238.70	0.63	0.0693263	0.0002634	0.0234	2.82859
$^{40}Ca^{16}O$	$^1\Sigma^+$	732.03	4.83	0.444441	0.003282	0.6541	1.8221
$^{40}Ca^{32}S$	$^1\Sigma^+$	462.23	1.78	0.1766757	0.0008270	0.1032	2.31775
$^{114}Cd^{1}H$	$^2\Sigma^+$	1337.1*		5.323		314	1.781
$^{114}Cd^{2}H$	$^2\Sigma^+$			2.704		76	1.775
$^{35}Cl_2$	$^1\Sigma_g^+$	559.7	2.68	0.2440	0.0015	0.186	1.988
$^{35}Cl^{19}F$	$^1\Sigma^+$	786.15	6.16	0.516479	0.004358	0.88	1.62831
$^{35}Cl^{16}O$	$^2\Pi_{3/2}$	853.8	5.5	0.62345	0.0058	1.33	1.56963
$^{52}Cr^{1}H$	$^6\Sigma^+$	1581*	32	6.220	0.179	347	1.656
$^{52}Cr^{2}H$	$^6\Sigma^+$	1182*		3.14		88.8	1.664
$^{52}Cr^{16}O$	$^5\Pi$	898.4	6.8	0.5231	0.0070		1.615
$^{133}Cs_2$	$^1\Sigma_g^+$	42.02	0.08	0.0127	0.0000264	0.00464	4.47
$^{133}Cs^{79}Br$	$^1\Sigma^+$	149.66	0.37	0.03606925	0.00012401	0.00838	3.07225
$^{133}Cs^{35}Cl$	$^1\Sigma^+$	214.17	0.73	0.07209149	0.00033756	0.03268	2.90627
$^{133}Cs^{19}F$	$^1\Sigma^+$	352.56	1.62	0.18436969	0.0011756	0.20168	1.34535
$^{133}Cs^{1}H$	$^1\Sigma^+$	891.0	12.9	2.7099	0.0579	113	2.4938
$^{133}Cs^{2}H$	$^1\Sigma^+$	619.1*		1.354		20	2.505
$^{133}Cs^{127}I$	$^1\Sigma^+$	119.18	0.25	0.02362736	0.00006826	0.00371	3.31519
$^{133}Cs^{16}O$	$^2\Sigma^+$	357.5*		0.223073	0.001303	0.348	2.3007
$^{63}Cu_2$	$^1\Sigma_g^+$	264.55	1.02	0.10874	0.000614	0.0716	2.2197
$^{63}Cu^{79}Br$	$^1\Sigma^+$	314.8	0.96	0.10192625	0.00045214	0.04274	2.17344
$^{65}Cu^{35}Cl$	$^1\Sigma^+$	415.29	1.58	0.17628802	0.00099647	0.12706	2.05118
$^{63}Cu^{19}F$	$^1\Sigma^+$	622.7	3.95	0.3794029	0.0032298	0.563	1.74493
$^{63}Cu^{1}H$	$^1\Sigma^+$	1941.26	37.51	7.9441	0.2563	520	1.46263
$^{63}Cu^{2}H$	$^1\Sigma^+$	1384.14	18.97	4.0381	0.0917	136.2	1.4626

Molecule	State	ω_e cm^{-1}	$\omega_e x_e$ cm^{-1}	B_e cm^{-1}	α_e cm^{-1}	D_e 10^{-6}cm^{-1}	r_e Å
$^{63}Cu^{127}I$	$^1\Sigma^+$	264.5	0.60	0.07328742	0.00028390	0.02244	2.33832
$^{63}Cu^{16}O$	$^2\Pi_{3/2}$	640.17	4.43	0.44454	0.00456	0.85	1.7244
$^{63}Cu^{32}S$	$^2\Pi_{3/2}$	415.0	1.75	0.1891		0.18	2.051
$^{19}F_2$	$^1\Sigma_g^+$	916.64	11.24	0.89019	0.013847	3.3	1.41193
$^{56}Fe^{16}O$	$^5\Delta$	965*		0.650		0.72	1.444
$^{69}Ga^{81}Br$	$^1\Sigma^+$	263.0	0.81	0.081839	0.0003207	0.032	2.35248
$^{69}Ga^{35}Cl$	$^1\Sigma^+$	365.67	1.25	0.1499046	0.0007936	0.1008	2.20169
$^{69}Ga^{19}F$	$^1\Sigma^+$	622.2	3.2	0.3595161	0.0028642	0.50	1.77437
$^{69}Ga^{1}H$	$^1\Sigma^+$	1604.52	28.77	6.137	0.181	342	1.663
$^{69}Ga^{2}H$	$^1\Sigma^+$			3.083	0.06	84	1.663
$^{69}Ga^{127}I$	$^1\Sigma^+$	216.38	0.47	0.0569359	0.0001897	0.015770	2.57464
$^{69}Ga^{16}O$	$^2\Sigma$	767.5	6.24	0.4271		0.37	1.744
$^{74}Ge^{79}Br$	$^2\Pi_{1/2}$	295	0.7				
$^{74}Ge^{35}Cl$	$^2\Pi_{1/2}$	407.6	1.36				
$^{72}Ge^{1}H$	$^2\Pi_{1/2}$	1833.77	37	6.726	0.192	326	1.5880
$^{72}Ge^{2}H$	$^2\Pi_{1/2}$	1320.09	19	3.415	0.070	83.2	1.5874
$^{74}Ge^{16}O$	$^1\Sigma^+$	986.49	4.47	0.4856981	0.0030787	0.4709	1.62464
$^{74}Ge^{32}S$	$^1\Sigma^+$	575.8	1.80	0.18656576	0.00074910	0.07883	2.01209
$^{74}Ge^{80}Se$	$^1\Sigma^+$	408.7	1.36	0.09634051	0.00028904	0.02207	2.13463
$^{74}Ge^{130}Te$	$^1\Sigma^+$	323.9	0.75	0.06533821	0.00017246	0.012	2.34017
$^{1}H_2$	$^1\Sigma_g^+$	4401.21	121.34	60.853	3.062	47100	0.74144
$^{2}H_2$	$^1\Sigma_g^+$	3115.50	61.82	30.444	1.0786	11410	0.74152
$^{3}H_2$	$^1\Sigma_g^+$	2546.5	41.23	20.335	0.5887		0.74142
$^{1}H^{81}Br$	$^1\Sigma^+$	2648.97	45.22	8.46488	0.23328	345.8	1.41444
$^{2}H^{81}Br$	$^1\Sigma^+$	1884.75	22.72	4.245596	0.084	88.32	1.4145
$^{1}H^{35}Cl$	$^1\Sigma^+$	2990.95	52.82	10.59342	0.30718	531.94	1.27455
$^{2}H^{35}Cl$	$^1\Sigma^+$	2145.16	27.18	5.448796	0.113292	140	1.27458
$^{1}H^{19}F$	$^1\Sigma^+$	4138.32	89.88	20.9557	0.798	2151	0.91681
$^{2}H^{19}F$	$^1\Sigma^+$	2998.19	45.76	11.0102	0.3017	594	0.91694
$^{1}H^{127}I$	$^1\Sigma^+$	2309.01	39.64	6.4263650	0.1689	206.9	1.60916
$^{202}Hg^{1}H$	$^2\Sigma^+$	1203.24*		5.3888		395.3	1.7662
$^{202}Hg^{2}H$	$^2\Sigma^+$	896.12*		2.739		91	1.757
$^{127}I_2$	$^1\Sigma_g^+$	214.50	0.61	0.03737	0.000114	0.0043	2.666
$^{127}I^{79}Br$	$^1\Sigma^+$	268.64	0.81	0.0568325	0.0001969	0.0102	2.46899
$^{127}I^{35}Cl$	$^1\Sigma^+$	384.29	1.50	0.1141587	0.0005354	0.0403	2.32088
$^{127}I^{19}F$	$^1\Sigma^+$	610.24	3.12	0.2797111	0.0018738	0.2356	1.90976
$^{127}I^{16}O$	$^2\Pi_{3/2}$	681.5	4.3	0.34026	0.00270	0.36	1.8676
$^{115}In^{81}Br$	$^1\Sigma^+$	221.0	0.65	0.05489468	0.00018672	0.01350	2.54315
$^{115}In^{35}Cl$	$^1\Sigma^+$	317.39	1.03	0.1090583	0.0005177	0.0515	2.40117
$^{115}In^{19}F$	$^1\Sigma^+$	535.4	2.6	0.2623241	0.0018798	0.252	1.98540
$^{115}In^{1}H$	$^1\Sigma^+$	1476.0	25.61	4.995	0.143	223	1.8380
$^{115}In^{2}H$	$^1\Sigma^+$	1048.2	12.4	2.523	0.051	58	1.837
$^{115}In^{127}I$	$^1\Sigma^+$	177.08	0.34	0.03686702	0.00010411	0.00639	2.75364
$^{39}K_2$	$^1\Sigma_g^+$	92.02	0.28	0.056743	0.000165	0.0863	3.9051
$^{39}K^{79}Br$	$^1\Sigma^+$	213	0.80	0.08122109	0.00040481	0.04462	2.82078
$^{39}K^{35}Cl$	$^1\Sigma^+$	281	1.30	0.1286348	0.0007899	0.1087	2.66665
$^{39}K^{19}F$	$^1\Sigma^+$	426.26	2.45	0.27993741	0.00233492	0.4829	2.17146
$^{39}K^{1}H$	$^1\Sigma^+$	983.6	14.3	3.416400	0.085313	163.55	2.243
$^{39}K^{2}H$	$^1\Sigma^+$	707	7.7	1.754	0.0318	50	2.240
$^{39}K^{127}I$	$^1\Sigma^+$	186.53	0.57	0.06087473	0.00026776	0.02593	3.04784
$^{139}La^{16}O$	$^2\Sigma^+$	812.8	2.22	0.35252001	0.00142365	0.2626	1.82591
$^{7}Li_2$	$^1\Sigma_g^+$	351.43	2.61	0.67264	0.00704	9.87	2.6729
$^{7}Li^{79}Br$	$^1\Sigma^+$	563.2	3.5	0.555399	0.005644	2.159	2.17043
$^{7}Li^{35}Cl$	$^1\Sigma^+$	642.95	4.47	0.7065225	0.0080102	3.409	2.02067
$^{7}Li^{19}F$	$^1\Sigma^+$	910.57	8.21	1.3452583	0.0202887	11.745	1.56386
$^{7}Li^{1}H$	$^1\Sigma^+$	1405.65	23.20	7.51373	0.21665	862	1.59490
$^{7}Li^{2}H$	$^1\Sigma^+$	1054.80	12.94	4.23310	0.09155	276	1.5941
$^{7}Li^{127}I$	$^1\Sigma^+$	496.85	2.85	0.4431766	0.0040862	1.4104	2.39192
$^{7}Li^{16}O$	$^2\Pi$	814.62	7.78	1.212830	0.017899	0.1079	1.68822
$^{24}Mg_2$	$^1\Sigma_g^+$	51.12	1.64	0.09287	0.00378	1.22	3.891

Molecule	State	ω_e cm^{-1}	$\omega_e x_e$ cm^{-1}	B_e cm^{-1}	α_e cm^{-1}	D_e 10^{-6}cm^{-1}	r_e Å
$^{24}Mg^{35}Cl$	$^2\Sigma^+$	462.12*	2.1	0.2456154	0.0016204	0.2723	2.19639
$^{24}Mg^{19}F$	$^2\Sigma^+$	711.69*	4.9	0.51922	0.00470	1.080	1.7500
$^{24}Mg^{1}H$	$^2\Sigma^+$	1495.20	31.89	5.8257	0.1859	344	1.7297
$^{24}Mg^{2}H$	$^2\Sigma^+$	1077.9	16.1	3.0306	0.06289	92	1.7302
$^{24}Mg^{16}O$	$^1\Sigma^+$	784.78	5.26	0.57470436	0.00532377	1.2328	1.74838
$^{55}Mn^{1}H$	$^7\Sigma$	1548.0	28.8	5.6841	0.1570	303.9	1.7311
$^{55}Mn^{2}H$	$^7\Sigma$	1103	13.9	2.8957	0.051	79.5	1.7310
$^{14}N_2$	$^1\Sigma_g^+$	2358.57	14.32	1.99824	0.017318	5.76	1.09769
$^{14}N^{79}Br$	$^3\Sigma^-$	691.75	4.72	0.444	0.0040		1.79
$^{14}N^{35}Cl$	$^3\Sigma^-$	827.96	5.30	0.649770	0.006414	1.598	1.61071
$^{14}N^{19}F$	$^3\Sigma^-$	1141.37	8.99	1.2057	0.01492	5.39	1.3170
$^{14}N^{1}H$	$^3\Sigma^-$	3282.3	78.4	16.6993	0.6490	1709.7	1.0362
$^{14}N^{2}H$	$^3\Sigma^-$	2398	42	8.7913	0.2531	490.4	1.0361
$^{14}N^{16}O$	$^2\Pi_{1/2}$	1904.20	14.07	1.67195	0.0171	0.5	1.15077
$^{14}N^{32}S$	$^2\Pi_{1/2}$	1218.7	7.28	0.769602	0.0064	1.2	1.4940
$^{23}Na_2$	$^1\Sigma_g^+$	159.13	0.72	0.154707	0.008736	0.581	3.0789
$^{23}Na^{79}Br$	$^1\Sigma^+$	302	1.5	0.1512533	0.0009410	0.1554	2.50204
$^{23}Na^{35}Cl$	$^1\Sigma^+$	366	2.05	0.2180631	0.0016248	0.3120	2.36080
$^{23}Na^{19}F$	$^1\Sigma^+$	535.66	3.57	0.4369011	0.0045580	1.163	1.92595
$^{23}Na^{1}H$	$^1\Sigma^+$	1172.2	19.72	4.9033634	0.1370919	343.40	1.88654
$^{23}Na^{2}H$	$^1\Sigma^+$	826.1*		2.557089	0.051600	93.46	1.88654
$^{23}Na^{127}I$	$^1\Sigma^+$	258	1.1	0.1178056	0.0006478	0.0973	2.71145
$^{23}Na^{16}O$	$^2\Pi$	492.3		0.424630	0.004506	1.2638	2.05155
$^{93}Nb^{16}O$	$^4\Sigma^-$	989.0	3.8	0.4321	0.0021	0.22	1.691
$^{58}Ni^{1}H$	$^2\Delta_{5/2}$	1926.6	38	7.700	0.23	481	1.476
$^{58}Ni^{2}H$	$^2\Delta_{5/2}$	1390.1	19	3.992	0.092	130	1.465
$^{16}O_2$	$^3\Sigma_g^-$	1580.19	11.98	1.44563	0.0159	4.839	1.20752
$^{16}O^{1}H$	$^2\Pi_{3/2}$	3737.76	84.88	18.911	0.7242	1938	0.96966
$^{16}O^{2}H$	$^2\Pi_{3/2}$	2720.24	44.05	10.021	0.276	537.4	0.9698
$^{31}P_2$	$^1\Sigma_g^+$	780.77	2.84	0.30362	0.00149	0.188	1.8934
$^{31}P^{35}Cl$	$^3\Sigma^-$	551.38	2.23	0.2528748	0.0015119	0.2124	2.01461
$^{31}P^{19}F$	$^3\Sigma^-$	846.75	4.49	0.5665	0.00456		1.58938
$^{31}P^{1}H$	$^3\Sigma^-$	2365.2	44.5	8.5371	0.2514	436	1.42140
$^{31}P^{2}H$	$^3\Sigma^-$	1699.2	23.0	4.4081	0.0928	116	1.4220
$^{31}P^{14}N$	$^1\Sigma^+$	1337.24	6.98	0.7864854	0.0055364	1.091	1.49087
$^{31}P^{16}O$	$^2\Pi_{1/2}$	1233.34	6.56	0.7337	0.0055	1.3	1.4759
$^{208}Pb_2$		110.5	0.35				
$^{208}Pb^{79}Br$	$^2\Pi_{1/2}$	207.5	0.50				
$^{208}Pb^{35}Cl$	$^2\Pi_{1/2}$	303.9	0.88				
$^{208}Pb^{19}F$	$^2\Pi_{1/2}$	502.73	2.28	0.22875	0.001473	0.183	2.0575
$^{208}Pb^{1}H$	$^2\Pi_{1/2}$	1564.1	29.75	4.971	0.144	201	1.839
$^{208}Pb^{16}O$	$^1\Sigma^+$	720.96	3.52	0.30730373	0.00190977	0.2138	1.92181
$^{208}Pb^{32}S$	$^1\Sigma^+$	429.17	1.26	0.11632307	0.00043510	0.03418	2.28678
$^{208}Pb^{80}Se$	$^1\Sigma^+$	277.6	0.51	0.05059953	0.00012993	0.0070	2.40218
$^{208}Pb^{130}Te$	$^1\Sigma^+$	212.0	0.43	0.03130774	0.00006743	0.0027	2.59492
$^{195}Pt^{12}C$	$^1\Sigma^+$	1051.13	4.86	0.53044	0.003273	0.546	1.6767
$^{195}Pt^{1}H$	$^2\Delta_{5/2}$	2294.68*	46	7.1963	0.1996	261	1.52852
$^{195}Pt^{2}H$	$^2\Delta_{5/2}$	1644.3*	23	3.640	0.071	66	1.524
$^{85}Rb^{79}Br$	$^1\Sigma^+$	169.46	0.46	0.04752798	0.00018596	0.01496	2.94474
$^{85}Rb^{35}Cl$	$^1\Sigma^+$	228	0.92	0.0876404	0.0004537	0.04947	2.78673
$^{85}Rb^{19}F$	$^1\Sigma^+$	376	1.9	0.2106640	0.0015228	0.2684	2.27033
$^{85}Rb^{1}H$	$^1\Sigma^+$	936.9	14.21	3.020	0.072	123	2.367
$^{85}Rb^{127}I$	$^1\Sigma^+$	138.51	0.33	0.03283293	0.00010946	0.00738	3.17688
$^{85}Rb^{16}O$	$^2\Sigma^+$	388.4*		0.246481	0.002174	0.397	2.25420
$^{32}S_2$	$^3\Sigma_g^-$	725.65	2.84	0.2955	0.001570	0.19	1.8892
$^{32}S^{19}F$	$^2\Pi_{3/2}$			0.552174			1.60058
$^{32}S^{1}H$	$^2\Pi_{3/2}$	2711.6	59.9	9.5995	0.2785	480.6	1.34066
$^{32}S^{2}H$	$^2\Pi_{3/2}$	1885	31	4.95130	0.10308	130	1.34049
$^{32}S^{16}O$	$^3\Sigma^-$	1149.2	5.6	0.7208171	0.005737	1.134	1.48109
$^{121}Sb^{35}Cl$	$^3\Sigma^-$	374.7	0.6				

Molecule	State	ω_e cm^{-1}	$\omega_e x_e$ cm^{-1}	B_e cm^{-1}	α_e cm^{-1}	D_e 10^{-6}cm^{-1}	r_e Å
$^{121}Sb^{19}F$	$^3\Sigma^-$	605.0	2.6	0.2792	0.0020	0.23	1.918
$^{121}Sb^{1}H$	$^3\Sigma^-$			5.684		240	1.723
$^{121}Sb^{2}H$	$^3\Sigma^-$			2.8782		45	1.7194
$^{121}Sb^{14}N$	$^1\Sigma^+$	942.0	5.6				
$^{121}Sb^{16}O$	$^2\Pi_{1/2}$	816	4.2	0.3580	0.0022	0.270	1.826
$^{45}Sc^{19}F$	$^1\Sigma^+$	735.6	3.8	0.3950	0.00266		1.788
$^{80}Se_2$	$^3\Sigma_g^-$	385.30	0.96	0.08992	0.000288	0.024	2.166
$^{80}Se^{1}H$	$^2\Pi_{3/2}$	2400*		8.02	0.23	330	1.48
$^{80}Se^{2}H$	$^2\Pi_{3/2}$	1708*		3.94			1.48
$^{80}Se^{16}O$	$^3\Sigma^-$	914.69	4.52	0.4655	0.00323	0.5	1.648
$^{28}Si_2$	$^3\Sigma_g^-$	510.98	2.02	0.2390	0.0014	0.21	2.246
$^{28}Si^{35}Cl$	$^2\Pi_{1/2}$	535.60	2.17	0.2561	0.0016	0.25	2.058
$^{28}Si^{19}F$	$^2\Pi_{1/2}$	857.19	4.73	0.5812	0.00494	1.07	1.6011
$^{28}Si^{1}H$	$^2\Pi_{1/2}$	2041.80	35.51	7.4996	0.2190	397	1.5201
$^{28}Si^{2}H$	$^2\Pi_{1/2}$	1469.32	18.23	3.8840	0.0781	105.4	1.5199
$^{28}Si^{14}N$	$^2\Sigma^+$	1151.4	6.47	0.7311	0.00565	1.2	1.572
$^{28}Si^{16}O$	$^1\Sigma^+$	1241.54	5.97	0.7267521	0.0050379	0.9923	1.50975
$^{28}Si^{32}S$	$^1\Sigma^+$	749.64	2.58	0.30352788	0.00147308	0.201	1.92926
$^{28}Si^{80}Se$	$^1\Sigma^+$	580.0	1.78	0.1920117	0.0007767	0.0842	2.05832
$^{120}Sn^{79}Br$	$^2\Pi_{1/2}$	247.2	0.6				
$^{120}Sn^{35}Cl$	$^2\Pi_{1/2}$	351.1	1.06	0.1117	0.0004		2.361
$^{118}Sn^{19}F$	$^2\Pi_{1/2}$	577.6	2.69	0.2727	0.0014	0.26	1.944
$^{120}Sn^{1}H$	$^2\Pi_{1/2}$			5.31488		207.5	1.78146
$^{120}Sn^{2}H$	$^2\Pi_{1/2}$	1188.0*		2.6950	0.049	53.4	1.7770
$^{120}Sn^{127}I$	$^2\Pi_{1/2}$	199.0	0.6				
$^{120}Sn^{16}O$	$^1\Sigma^+$	822.13	3.72	0.35571998	0.00214432	0.26638	1.83251
$^{120}Sn^{32}S$	$^1\Sigma^+$	487.26	1.36	0.13686139	0.00050563	0.0424	2.20898
$^{120}Sn^{80}Se$	$^1\Sigma^+$	331.2	0.74	0.0649978	0.0001705	0.011	2.32557
$^{120}Sn^{130}Te$	$^1\Sigma^+$	259.5	0.50	0.04247917	0.00009543	0.0055	2.52280
$^{88}Sr^{79}Br$	$^2\Sigma^+$	216.60	0.52	0.0541847	0.0001827	0.01356	2.73522
$^{88}Sr^{35}Cl$	$^2\Sigma^+$	302.3	0.95				
$^{88}Sr^{19}F$	$^2\Sigma^+$	502.4	2.3	0.2505346	0.0015513	0.2498	2.07537
$^{88}Sr^{1}H$	$^2\Sigma^+$	1206.2	17.0	3.6751	0.0814	135	2.1456
$^{88}Sr^{2}H$	$^2\Sigma^+$	841	8.6	1.8609	0.0292	34.7	2.1449
$^{88}Sr^{127}I$	$^2\Sigma^+$	173.77	0.35	0.0367097	0.0001060	0.00655	2.94364
$^{88}Sr^{16}O$	$^1\Sigma^+$	653.5	3.96	0.33798	0.00219	0.36	1.91983
$^{181}Ta^{16}O$	$^2\Delta_{3/2}$	1028.69	3.51	0.40284	0.00182	0.2450	1.68746
$^{130}Te_2$	$^3\Sigma_g^-$	247.07	0.51	0.039681	0.000106	0.0044	2.5574
$^{130}Te^{1}H$	$^2\Pi_{3/2}$			5.56			1.74
$^{130}Te^{16}O$	0^+	797.11	4.00	0.3554	0.00237	0.27	1.825
$^{232}Th^{16}O$	$^1\Sigma^+$	895.77	2.39	0.332644	0.001302	0.1833	1.84032
$^{48}Ti^{16}O$	$^3\Delta_1$	1009.02	4.50	0.53541	0.00301	0.603	1.6202
$^{205}Tl^{81}Br$	$^1\Sigma^+$	192.10	0.39	0.0423899	0.0001276	0.0083	1.61817
$^{205}Tl^{35}Cl$	$^1\Sigma^+$	284.71	0.86	0.09139702	0.00039784	0.0377	2.48483
$^{205}Tl^{19}F$	$^1\Sigma^+$	476.86	2.24	0.22315014	0.00150380	0.1955	2.08439
$^{205}Tl^{1}H$	$^1\Sigma^+$	1390.7	22.7	4.806	0.154	254	1.870
$^{205}Tl^{2}H$	$^1\Sigma^+$	987.7	12.04	2.419	0.057	60	1.869
$^{205}Tl^{127}I$	$^1\Sigma^+$	150*		0.0271676	0.0000664	0.0036	2.81361
$^{51}V^{16}O$	$^4\Sigma^-$	1011.3	4.86	0.54825	0.00352	0.6	1.5893
$^{89}Y^{35}Cl$	$^1\Sigma$	380.7	1.3	0.1160	0.0003	0.09	2.41
$^{89}Y^{19}F$	$^1\Sigma^+$	631.29	2.50	0.29042	0.00163	0.237	1.9257
$^{89}Y^{16}O$	$^2\Sigma^+$	861.0	2.9	0.3881	0.0018	0.32	1.790
$^{174}Yb^{1}H$	$^2\Sigma^+$	1249.54	21.06	3.9931	0.0957	161.8	2.0526
$^{174}Yb^{2}H$	$^2\Sigma^+$	886.6	10.57	2.01162	0.03425	41.60	2.0516
$^{64}Zn^{35}Cl$	$^2\Sigma$	390.5	1.6				
$^{64}Zn^{19}F$	$^2\Sigma$	628	3.5				
$^{64}Zn^{1}H$	$^2\Sigma^+$	1607.6	55.14	6.6794	0.2500	466	1.5949
$^{64}Zn^{2}H$	$^2\Sigma^+$	1072	28	3.350		124	1.6054
$^{64}Zn^{127}I$	$^2\Sigma$	223.4	0.6				
$^{90}Zr^{16}O$	$^1\Sigma^+$	969.8	4.9	0.42263	0.0023	0.319	1.7116