

## 7g. Constants of Diatomic Molecules

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### *Explanation of Columns in Table 7g-1*

- (1) Identification of molecule.
- (2) Mass numbers of the constituent atoms to which the data refer. If, in the original paper, the mass numbers are not clearly specified, or, if the data refer to the normal isotopic mixture, the mass numbers for the most abundant isotope are given in parentheses.
- (3) Reduced mass  $\mu$  in unified atomic mass units ( $^{12}\text{C} = 12.0000000$ ). Precise atomic masses were taken from the 1961 nuclidic mass table [L. A. König, J. H. E. Mattauch, and A. H. Wapstra, *Nucl. Phys.* **31**, 18 (1962)].
- (4) Designation of the ground state of the molecule. For multiplet II,  $\Delta$ , . . . states the spin-orbit coupling constant  $A$  has been added.
- (5) (6) (8) (9) Rotational constant  $B_e$ .

Rotation-vibration interaction constant  $\alpha_e$ .  
(from  $B_e = B_e - \alpha_e(v + \frac{1}{2}) + \dots$ ).

Vibrational frequency  $\omega_e$ .

Anharmonic constant  $\omega_e x_e$  (from  $G(v) = \omega_e(v + \frac{1}{2}) - \omega_e x_e(v + \frac{1}{2})^2 + \dots$ ).

All constants in  $\text{cm}^{-1}$ . They are derived from the analyses of molecular spectra in the microwave, infrared, visible, and vacuum uv region. For  ${}^1\Sigma$  states, the constants in these columns correspond to the coefficients  $Y_{01}$ ,  $-Y_{11}$ ,  $Y_{10}$ , and  $-Y_{20}$ , respectively, in the Dunham series expansion for the term values

$$T_{vJ} = \sum_{lm} Y_{lm}(v + \frac{1}{2})^l J^m (J + 1)^m$$

- (7) Equilibrium internuclear distance  $r_e$  in  $\text{\AA}$ , calculated without correction from

$$r_e = \left( \frac{h}{8\pi^2 c \mu B_e} \right)^{\frac{1}{2}}$$

- (10) Dissociation energy  $D_0^\circ$  in electron-volts (eV). Data obtained by a large variety of both spectroscopic and thermochemical methods have been included.

Uncertain quantities are enclosed in parentheses ( ). Quantities in square brackets [ ] in columns (5) and (8) refer to  $B_e$  and  $\Delta G(\frac{1}{2})$  respectively. \* after  $\omega_e$  and  $\omega_e x_e$  indicates that these numbers are for the natural isotopic mixture rather than for the isotope specified in column (2).

The physical constants and conversion factors given in Appendix VII of the following book have been used throughout: G. Herzberg, "Electronic Spectra and Electronic

## CONSTANTS OF DIATOMIC MOLECULES

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Structure of Polyatomic Molecules," D. Van Nostrand Company, Inc., Princeton, N.J., 1966.

The data included in the table are taken from a new compilation of vibrational and rotational constants for the electronic states of all known diatomic molecules. This compilation is presently being prepared by G. Herzberg and K. P. Huber and will provide further details and the literature references. A critical table of dissociation energies has recently been published by A. G. Gaydon in his book "Dissociation Energies and Spectra of Diatomic Molecules," 3d edition, Chapman & Hall, Ltd., London, 1968.

TABLE 7g-1. CONSTANTS OF DIATOMIC MOLECULES

(1)	<i>m</i> (2)	<i>m</i> (2)	$\mu$ (3)	Ground state (4)	<i>B</i> (5)	$\alpha$ (6)	$r_s$ (7)	$\omega_s$ (8)	$\omega_{\infty}$ (9)	$D_0^*$ (10)
$\text{Ar}_2$	107	109	53.91770	12'	0.12790	0.00076	102.4	0.643	1.63	(1.76)
$\text{ArAl}$	107	27	21.544070	12'	0.12790	0.00076	2.4728	256.60	1.13	2.0
$\text{ArAu}$	(107)	107	(69) 20476	12'	0.0848337*	0.0002359*	2.3971	(200)	0.6871	3.0
$\text{ArBr}$	107	79	45.40207*	12'	0.12298380*	0.00059530*	2.2808	250.49	1.17	3.2
$\text{ArCl}$	107	35	26.349782	12'	0.12298380*	0.00059530*	2.2808	543.49	1	1.76
$\text{ArCu}$	(107)	(63)	(39) 61190*	12'	0.0019	0.0019	2.29.5	229.5	2.50	3.6
$\text{ArF}$	107	19	16.131608	12'	0.2657	0.0019	313.45	313.45	184.7	0.65
$\text{ArGa}$	(107)	(60)	(41) 40678*	12'	6.449	0.201	1.6180	159.9	34.00	2.4
$\text{ArH}$	107	1	0.99841288	12'	3.2572	0.0722	1.6180	150.7	17.17	2.4
$\text{ArI}$	107	2	1.9768579*	12'	0.044876	0.0001473	2.5444	206.52	0.445	2.6
$\text{ArIn}$	107	127	58.02466	12'	0.3028	0.0025	55.8	0.42	490.4*	(2.4)
$\text{ArO}$	107	115	55.38014	12'	0.3028	0.0025	2.000	490.4*	3.04	
$\text{AsSe}$	(107)	(80)	(45) 73067*	12'	A = (4.135)		(233)			
$\text{AsSn}$	(107)	(120)	(56) 51557	12'	(410)					1.3
$\text{AsTe}$	(107)	(130)	(58) 64437	12'						0.30
$\text{Al}$	27	27	13.490767*	12'	0.2054	0.0112	195.3	350.01	2.02	1.8
$\text{AlAu}$	27	197	23.730767*	12'*(0*)	0.12991	0.00066*	2.466	333.00	1.16	3.3
$\text{AlBr}$	27	79	20.107087*	12'	0.1501	0.000853	2.3384	378.0	1.28	4.4
$\text{AlCl}$	27	35	15.230144	12'	0.243926	0.01002	2.296	481.30	1.95	5.0
$\text{AlF}$	27	19	11.1484731	12'	0.552468	0.04950	1.6544	301.94	4.74	6.8
$\text{AlH}$	27	1	0.97153601	12'	6.3906*	0.1358*	1.6478	132.56	29.06	2.91
$\text{AlH}^+$	27	2	1.8741981*	12'	3.3186	0.0597	1.6453	1211.95	15.158	2.94
$\text{AlI}$	27	1	2.601	6.763	0.398	1.601*	1.601*			
$\text{AlII}$	27	127	22.250735*	12'	0.0558*	0.0558*	316.1	1.0	3.7	
$\text{AlO}$	27	16	10.0419499	12'	0.6413*	0.0558*	1.6178	979.23	6.97	4.9
$\text{AlP}$	27	31	14.4200738	12'	0.2799	0.0018	2.028*	B17.12	3.33	2.2
$\text{AlS}$	27	32	14.6327874	12'	0.2799	0.0018	467.6	2.08	3.4	
$\text{AlSe}$	27	(80)	(20) 171277.0	12'						3.37
$\text{AlTe}$	27	(130)	(22) 341268*	12'			30.7		0.0096,	
$\text{Al}_3$	40	40	19.9811919	12'					2.64	
$\text{Al}_3^+$	40	40	12*	0.10165	0.0034	2.104*	420.4	1.12	3.94	
$\text{Al}_3^-$	75	75	37.40070*	12'	(22)*		314.8	1.25	2.7	
$\text{Al}_3^{+/-}$	75	75	(23) 341218*	12'	(22)*		443	2	(2.7)	
$\text{AlF}$	75	19	15.155352,	12'	(22)		(≥680)			

A <sub>1</sub> H <sub>1</sub>	1	0.99444817	$\Sigma^+$	[7.199.]	[1.5344]	.....	.....	<3.6
	2	1.9613749,	$\Sigma^-$	[3.669.]	[1.504]	.....	5.38	2.7,
A <sub>3</sub> N <sub>1</sub>	14	11.797903,	$\Sigma^0$	0.5457	1.618	1068.0	4.88	(6.5)
A <sub>3</sub> O <sub>1</sub>	16	13.80933,	$\pi^0$	0.48519	1.6336	966.5*	.....	$\leq 4.980_4$
A <sub>5</sub> O <sup>+</sup>	16	.....	$\Sigma^+$	0.6199	1.568*	[1091.32]	(5)	(7.7)
A <sub>6</sub> I <sub>1</sub>	197	98.483276	$\Sigma^+$	0.028013	2.419	190.9	0.420	2.2,
AuBa	197	(138)	$\Sigma^0$	0.4038	1.536	128.8	0.18	(2.8)
AuBe	9	8.3178757	$\Sigma^-$	0.033320	1.6336	607.68	3.51	(3.2)
AuBi	269	101.39785,	$\pi^0$	0.0000723	2.0405	157.7	0.25	(2.6)
AuCa	40	33.222141,	$\Sigma^+$	0.00400	2.0405	220.0	0.02	(2.4)
AuCl	35	29.5986607,	$\Sigma^0$	0.0000723	2.0405	382.8	1.30	(3.5)
AuCr	197	(52)	$\Sigma^-$	0.0000723	2.0405	250	0.7	2.1*
AuCu	197	(63)	$\Sigma^0$	0.0000723	2.0405	225.62	0.67	(2.0)
AuGa	69	51.05848,	$\pi^0$	0.0000723	2.0405	[251.7]	.....	.....
AuGe	197	(74)	$\Sigma^+$	0.0000723	2.0405	.....	.....	.....
AuH <sub>1</sub>	1	1.00289470	$\Sigma^+$	7.2401	0.2136	1.5238	2305.01	3.2,
	2	1.9937152,	$\Sigma^-$	3.6415	0.07614	1.5238	1634.98	21.655
AuMg <sub>1</sub>	24	21.381386,	$\Sigma^0$	0.13214	0.00073	2.4427	307.9	1.1
AuPh	197	(208)	$\pi^0$	0.00073	0.00073	1.58.6	0.6	(2.6)
AuPd	197	(106)	$\Sigma^+$	0.00073	0.00073	270	.....	(1.4)
AuSe	197	(86)	$\Sigma^-$	0.00073	0.00073	[391.2]	(1.35)	1.4*
AuSi <sub>1</sub>	28	24.497348,	$\Sigma^0$	0.00073	0.00073	190.4	(1.26)	.....
AuSn	197	(120)	$\pi^0$	0.00073	0.00073	153.33	0.19	(2.6)
AuSr	197	(88)	$\Sigma^+$	0.00073	0.00073	212.5	0.50	(2.8)
AuTe	197	(130)	$\Sigma^-$	0.00073	0.00073	1051.3	9.35	3.2,
B <sub>2</sub>	107	107.78430,	$\Sigma^0$	1.212	0.014	193.8	0.42	2.9
BaBr	11	11	$\pi^0$	.....	.....	279.3	0.39	(4.3)
BaCl	79	(50.19401.)	$\Sigma^+$	.....	.....	468.0	1.79	4.5*
BaO	35	27.895369	$\Sigma^-$	.....	.....	[2.162.]	14.50	6.05
BaS	138	(16.698012.)	$\Sigma^0$	[0.2158.]	0.06549	1168.31	<1.95	.....
BBr	11	9.6015017	$\pi^0$	3.38285	2.2317	2.2317	<1.97	.....
BC <sub>1</sub>	12	(5.7416023.)	$\Sigma^+$	1.70712	0.02369	829.89	7.35	.....
BCI	35	8.3731666	$\Sigma^-$	0.3126146	0.0013935	1.3397	669.8,	$\geq 5.74$
BeBr	9	(8.0885079)	$\Sigma^0$	[0.10308]	[2.5102]	377.1	1.22	4.37
BeCl	9	7.1654925	$\pi^0$	0.490	0.0035	684.31	3.52	4.49
						1.38,	.....	4.6*
						1.715,	839.12	5.11
						713.8	3.5	5.5,
						846.4	5.14	(4.3)
						.....	.....	3.9,

TABLE 7g-1. CONSTANTS OF DIATOMIC MOLECULES (Continued)

(1)	$m_1$ (2)	$m_2$ (2)	$\mu$ (3)	Ground state (4)	$R_s$ (5)	$\alpha$ (6)	$\tau_s$ (7)	$\omega_s$ (8)	$\omega_{ex}$ (9)	$D_0^o$ (10)
BeF	9	19	3.1125863	12*	1.4877	0.01685	1.3615	1265.6	9.12	5.8*
BeH	9	1	0.90645690	12*	10.308	0.300	1.3432	2058.6	35.5	(2.1)
BeH <sup>+</sup>	9	2	1.6461989 <sub>b</sub>	12*	5.0807	0.1218	1.3426	2221.7	39.79	(3.2)
BeO	9	1	...	12*	10.7896	0.2835	1.3123	1647.64	21.85	4.6*
BeS	9	16	5.7643286	12*	5.9546	0.1233	1.3114	1487.323	11.8297	(4.1)
BF	11	19	7.0304618	12*	1.6510	0.0190	1.3309	997.94	6.137	7.8
BiH	11	1	8.9701832	12*	0.79059	0.00634	1.7415	1402.1	11.8	3.42
BiH <sup>+</sup>	11	2	0.92330324	12*	1.516 <sub>a</sub>	0.019 <sub>a</sub>	1.2629	2366.9 <sub>a</sub>	41.39 <sub>a</sub>	(28)
Bi <sub>2</sub>	11	1	1.70261630	12*	12.021	0.412	1.2324	1759.	1.230 <sub>a</sub>	3.46
BiBr	209	104	4.902020 <sub>a</sub>	12*	6.54 <sub>a</sub>	0.17 <sub>a</sub>	[1.2147]	...	1.2147	1.95
BiCl	209	79	57.285377	12*	0.022806	0.000050	2.6597	172.71	0.32227	2.04
BiF	209	35	20.956251 <sub>a</sub>	12*	...	...	...	209.50	0.466	2.74
BiH	209	19	17.4151001	12*	(0.115)	...	(2.21)	308.0	0.96	3.08
BiI	209	1	1.00298823	12*	0.231 <sub>a</sub>	0.0015	2.04 <sub>a</sub>	512.6	2.34	(3.4)
BiL	209	2	1.9948766 <sub>a</sub>	12*	5.137	0.148	1.808 <sub>a</sub>	1698.9	31.6	(2.7)
BiO	209	127	78.95721 <sub>a</sub>	12*	2.592	0.054	1.805 <sub>a</sub>	1205.5	16.1	(2.7)
BiPb	209	16	14.8577356	12*	0.3034	0.0022	1.934	163.9	0.31	3.47
BiS	209	(208)	104.238661 <sub>a</sub>	12*	...	...	...	692.4	4.34	3.1
BiSe	209	32	27.729687 <sub>a</sub>	12*	[0.112764]	...	[2.3210]	408.71	1.46	2.89
BiTe	209	80	57.80949 <sub>a</sub>	12*	...	...	...	[264.8]	0.52	2.39
BN	11	14	6.163512 <sub>a</sub>	12*	1.666	0.025	1.281	1514.6	12.3	(5.1)
BO	11	16	6.5209399 <sub>a</sub>	12*	1.7820	0.0166	1.2044	1885.69	11.810	8.2*
Br <sub>2</sub>	79	81	39.93242 <sub>a</sub>	12*	0.081101	0.000321	2.2809	323.33	1.081	1.9704 <sub>a</sub>
Br <sub>2</sub> <sup>+</sup>	79	81	...	12*	...	...	...	(376)	(1.25)	3.25
BrCl	79	35	24.231733	12*	A = -3150	...	...	...	...	...
BrF	79	19	15.312218 <sub>a</sub>	12*	0.152469	0.000775	2.1361	443.5*	1.8*	2.233
BrO	79	16	13.2694297	12*	0.355843	0.002612	1.7589	672.6	4.5	(8.4)
BS	11	32	8.1893677	12*	[0.427789]	...	[1.7213]	778.7*	0.81*	2.39
BS <sup>+</sup>	(11)	(28)	(7.9003922)	12*	0.7948 <sub>a</sub>	0.0060 <sub>a</sub>	1.6092	1180.17	0.31	6.2*
C <sub>2</sub>	12	12	6.0000000	12*	...	...	...	1.2425	1854.71	2.9
C <sub>2</sub> <sup>+</sup>	12	12	(26.5228009)	12*	1.8108 <sub>a</sub>	0.0176 <sub>a</sub>	1.7468 <sub>a</sub>	0.0167	1.2682	11.58 <sub>a</sub>
CaBr	(40)	79	(18.6496680)	12*	...	...	...	285.3	0.86	(3.9)
CaCl	(40)	35	(12.8767408)	12*	0.15195	0.00078 <sub>a</sub>	...	2.4390	369.8	4.0*
CaF	40	19	(0.3510)	12*	...	...	...	(1.931)	587.1	5.4

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$\text{CaH}$	1	(0.98303388)	$\Sigma^+$	4.2778	0.0963	2.0022	1209	19.5
	(40)	2	(1.01746264)	$\Sigma^+$	2.196	0.035	2.001	$\leq 1.70$
	(40)	127	(30.392038)	( $\Sigma^+$ )	.....	.....	242.0	0.64
	(40)	16	(11.4229222)	$\Sigma^+$	0.4444	0.0034	733.4	(3.3)
	(40)	32	17.761768*	$\Sigma^+$	0.17667	0.000837	462.23	5.28
	40	12	(10.4161613)	$\Pi^+$	[0.4872]	[1.8226]	1.78	1.78
				$A = +466$				$\leq 4.11$
$\text{CCl}_2$	12	35	8.03413851	$\pi_{1g}$	-0.6970	0.0067	1.445	[866.1]
				$A_0 = +135$			(0.2)	(3.8)
$\text{Cd}$	(114)	(112)	(56.44717)	.....	.....	.....	230.0	0.08
		(114)	(79)	(46.61856)	(2)	.....	330.5	(1.6)
$\text{CdCl}$	(114)	35	(26.754971)	$\Sigma^+$	.....	.....	1.2	2.1
$\text{CdF}$	(114)	19	(16.2825736)	(2)	.....	.....	(535)	
$\text{CdH}$	(114)	1	(0.99898613)	$\Sigma^+$	5.437	0.218	1.3617	1430.7
	(114)	2	(1.07910066)	$\Sigma^+$	2.788	0.168	1.748	46.3
$\text{CdH}^+$	(114)	1	.....	$\Sigma^+$	0.071	0.189	1.6072	0.678
	(114)	2	.....	$\Sigma^+$	3.075	0.0682	1.664	0.704
$\text{CdI}$	(114)	127	(60.02651)	$\Sigma^+$	.....	.....	1262.5	(2.0)
$\text{CdO}$	(114)	18	(14.025397)	.....	.....	.....	178.5	0.325
$\text{CdS}$	(114)	32	(24.064643)	.....	.....	.....		(1.4)
$\text{CaO}$	(140)	16	(14.3538823)	( $\Phi$ )	[0.35687]	[1.4141]	[830]	$\leq 3.8$
					(constants for $\Omega = 3$ component)			$\leq 2.0$
$\text{CaS}$	(140)	(32)	(26.024731)	.....	.....	.....		8.1*
$\text{CF}$	12	19	7.3545396	$\pi_{1g}$	1.4172 <sub>0</sub>	0.0184 <sub>0</sub>	1.2717	1308.1
				$A_0 = +77$				5.9*
$\text{CH}$	12	1	0.92974056	$\pi_{1g}$	14.457	0.534	1.1100	11.10
				$A = +28$			2850.1	5.4;
$\text{CH}^+$	12	2	1.72463608	$\pi_{1g}$	7.808	0.212	1.1189	63.3
$\text{Cl}_2$	12	1	.....	$\Sigma^+$	14.177*	0.4917	1.1309	3.47
	35	35	17.484427	$\Sigma^+$	0.24407	0.00153	1.9375	3.52
$\text{Cl}^+$	35	35	.....	$\Pi_{1g}$	0.2696	0.00166	1.801	4.09
$\text{ClF}$	35	19	12.3102870	$\Sigma^+$	0.5164802	0.004358,	1.6233	2.4795,
$\text{ClO}$	35	16	10.9749310	$\pi_{1g}$	[0.620525]	.....	786.34	4.01
				$A = -282$	.....	[1.5733]	6.23	2.56
$\text{CN}$	12	14	6.46219328	$\Sigma^+$	1.8992	0.01701	1.1720	7.5
$\text{CN}^+$	12	14	.....	$\Sigma^+$	1.8964	0.0188	2068.745	13.134
				12	.....	1.1728	2033.05	16.14
$\text{CO}$	12	16	6.85620870	$\Sigma^+$	1.931271	(constants for lowest observed 12 state)	1.1983	4.9*
$\text{CO}^+$	12	16	.....	$\Sigma^+$	1.93720	0.017513	2169.8233	11.209,
$\text{Co}$	50	50	20.466504*	.....	0.01896	1.1151	2214.24	15.164
$\text{CoBr}$	59	(71)	(33.738542)	.....	.....	.....	(320)	8.34
$\text{CoCl}$	59	(35)	(2.946552)	.....	.....	.....	(420)	1.6,
$\text{CoII}$	59	1	0.99088003	(44)	[7.151]	.....	[1.524]	
	59	2	1.0475429	(44)	[3.722]	.....	[1.525]	

TABLE 7g-1. CONSTANTS OF DIATOMIC MOLECULES (*Continued*)

(1)		$m_1$ (2)	$m_2$ (2)	$\mu$ (3)	Ground state (4)	$B_s$ (5)	$\alpha_s$ (6)	$r_s$ (7)	$\omega_s$ (8)	$D_0^*$ (10)
CoO...		.59	16	12.5804778	$\Sigma^+$	0.7986	0.00597	1.5022	(850)	(6)
CP...		12	31	8.64911824	$\Sigma^+$	.....	.....	1239.67	6.86	3.7 <sub>s</sub>
Cr <sub>3</sub> ...		(52)	(52)	(2.5, 970256, <sub>s</sub> )	$\Sigma^+$	.....	.....	.....	.....	(6, 9)
CrBr...		(52)	(79)	(31, 32; 1279)	$\Sigma^+$	.....	.....	.....	.....	1.6
CrCl...		(52)	(35)	(26, 898785, <sub>s</sub> )	$(\Sigma^+)$	.....	.....	.....	.....	3.3 <sub>s</sub>
CrF...		(52)	19	(13, 910374.1)	$(\Sigma^+)$	.....	.....	.....	.....	3.7 <sub>s</sub>
CrH...		(52)	1	(6, 98864215)	$\Sigma^+$	6.220	0.179	1.6557	(292)	4.5 <sub>s</sub>
CrI...		(52)	2	(1, 9389166, <sub>s</sub> )	$\Sigma^+$	[3, 142]	.....	[1, 6633]	(536)	.....
CrO...		(52)	127	(36, 855, 837)	$\Sigma^+$	.....	.....	.....	[15811]	.....
CS...		(52)	16	(12, 2200256)	$\eta$	0.5286	0.0050	1.614 <sub>s</sub>	898.8	2.9 <sub>s</sub>
Cs <sub>3</sub> ...		12	32	8.72519425	$\Sigma^+$	0.82005	0.00592	1.5349	1285.08	6.46
Cs <sub>5</sub> ...		133	133	66.45255	$\Sigma^+_o$	(0.0127)	0.000026, <sub>s</sub>	(4, 17)	42.0164	7.8 <sub>s</sub>
CsBr...		133	79	49.51600,	$\Sigma^+_o$	0.03606939	0.00012410, <sub>s</sub>	3.0722	149.5	0.45 <sub>s</sub>
CsCl...		133	35	27.684694	$\Sigma^+_o$	0.07209140	0.000333753	2.9063	209*	0.36
Cs <sub>6</sub> ...		12	(80)	(10, 413; 3609.)	$\Sigma^+_o$	0.58 <sub>s</sub>	0.004	1.67	0.75	4.1 <sub>s</sub>
CsF...		133	19	16.622294,	$\Sigma^+_o$	0.18436909	0.00117371	1035.9	4.8 <sub>s</sub>	4.5 <sub>s</sub>
CsH...		133	1	1.00024035	$\Sigma^+_o$	2.708 <sub>s</sub>	0.057 <sub>s</sub>	2.1453	353	6.8
CsI...		133	(202)	(80, 15787)	$(\Sigma^+)$	.....	.....	2.494 <sub>s</sub>	1.7	5.1 <sub>s</sub>
Cs <sub>2</sub> Hg...		133	127	64.91771	$\Sigma^+_o$	0.02362732	0.00006325, <sub>s</sub>	891.2 <sub>s</sub>	12.79	(1, 9)
CsI...		133	(85)	(51, 81051)	$\Sigma^+_o$	.....	.....	119.2	0.25	3.4 <sub>s</sub>
CaRb...		63	63	31.464797	$\Sigma^+_o$	0.10874	0.000614	49.4	.....	.....
CaBr...		63	81	35.399211	$\Sigma^+_o$	0.1008	0.0004, <sub>s</sub>	2.2197	266.1	1.025
CaCl...		63	35	22.478148 <sub>s</sub>	$\Sigma^+_o$	0.17818 <sub>s</sub>	0.00101	2.7 <sub>s</sub>	313.4	3.4 <sub>s</sub>
CaF...		63	19	14.5928365	$\Sigma^+_o$	0.3784029	0.0032298	2.0515	417.74	3.8 <sub>s</sub>
CaH...		63	1	0.99193919	$\Sigma^+_o$	7.938	0.249	1.7449	622.6 <sub>s</sub>	4.4 <sub>s</sub>
CaI...		63	2	1.9516387,	$\Sigma^+_o$	4.0375	0.09140	1.4632	1940.4	2.73
CaO...		63	127	42.068553	$\Sigma^+_o$	0.0735	0.0003	1.4627	1384.38	2.76
		63	16	12.7533705	$\Sigma^+_o$	(0, 4429)	.....	2.33 <sub>s</sub>	264.50	<3.27
							[(1, 7276)]	633*	0.60	.....
									4.4*	2.7 <sub>s</sub>
CuS...		(63)	(32)	(21, 2007824)	$A = (+)272$	.....	.....	414.2	1.70	2.9 <sub>s</sub>
CuSe...		(63)	(80)	(35, 206516)	$A = (433)$	.....	.....	300.0	0.50	.....
					$A = (1590)$	.....	.....	254.0	1.01	1.8 <sub>s</sub>
						.....	.....	.....	.....	6.5 <sub>s</sub>
						.....	.....	.....	.....	6.5 <sub>s</sub>

## CONSTANTS OF DIATOMIC MOLECULES

TABLE 7g-1. CONSTANTS OF DIATOMIC MOLECULES (Continued)

(1)	$m_1$ (2)	$m_2$ (2)	$\mu$ (3)	Ground state (4)	$B_s$ (5)	$\alpha_s$ (6)	$r_s$ (7)	$\omega_s$ (8)	$\omega_{ex}$ (9)	$D_0^o$ (10)
HBr.....	1	81	0.90542703	12 <sup>+</sup>	8.46488	0.25328	1.4114	2648.975	45.217 <sub>s</sub>	3.759
	2	81	1.9651864 <sub>1</sub>	12 <sup>+</sup>	4.287 <sub>s</sub>	0.083 <sub>s</sub>	1.4114	1684.75	22.71 <sub>s</sub>	3.806
	3	81	2.9076698 <sub>4</sub>	12 <sup>+</sup>	2.8974	0.0550	1.4116	[1130.26]	...	3.828
HBr <sup>+</sup> .....	1	...	...	1H <sub>1</sub>	8.072 <sub>0</sub>	0.236 <sub>1</sub>	1.4184	[2248.24]	(45.4)	3.934
HCl.....	1	35	0.97959272	12 <sup>+</sup>	10.59341 <sub>4</sub>	0.30718 <sub>1</sub>	1.2745	2690.946 <sub>s</sub>	52.8186	4.4333
	2	35	1.3044136 <sub>1</sub>	12 <sup>+</sup>	5.448794	0.13294 <sub>1</sub>	1.2746	2445.163	27.1825	4.4849
	3	35	2.7765712 <sub>4</sub>	12 <sup>+</sup>	3.7458	0.0611	1.2731	[1135.51]	...	4.509 <sub>s</sub>
HCl <sup>+</sup> .....	1	35	...	1H <sub>1</sub>	9.9463	0.383	1.3154	2675.4	53.5	4.70 <sub>s</sub>
	2	35	...	1H <sub>1</sub>	5.1158	0.1170	1.3154	[11863.96]	...	4.75 <sub>s</sub>
He <sub>2</sub> .....	4	4	2.00130180 <sub>4</sub>	12 <sup>+</sup>	...	0.224	1.080 <sub>s</sub>	...	35.2	...
He <sub>2</sub> <sup>+</sup> .....	4	4	...	12 <sup>+</sup>	7.211	0.798 <sub>s</sub>	4.138.32	80.88	2.2 <sub>s</sub>	5.85 <sub>s</sub>
HF.....	1	19	0.95705545	12 <sup>+</sup>	20.9557	0.798 <sub>s</sub>	0.01980	0.0174	2018.10 <sub>s</sub>	5.92 <sub>s</sub>
	2	19	1.32104538	12 <sup>+</sup>	11.000	0.2907	0.9176	2408.54	45.76 <sub>s</sub>	5.95 <sub>s</sub>
HF <sup>+</sup> .....	3	19	2.0028411 <sub>4</sub>	12 <sup>+</sup>	7.692	0.1557	...	3.40	32.54	3.40
	1	19	...	1H <sub>1</sub>	...	...	...	90	...	...
HIO.....	(180)	16	(14.689234 <sub>4</sub> )	12 <sup>+</sup>	[0.3860]	...	[1.724]	(968)	...	7.9
	(200)	(202)	(100.482250)	12 <sub>s</sub> <sup>+</sup>	...	...	3.3	(36)	...	0.07 <sub>s</sub>
HgBr.....	(202)	79	(56.74551 <sub>1</sub> )	(12 <sup>+</sup> )	...	...	...	88.13	0.0665	0.71
HgCl.....	(202)	35	(20.807955 <sub>1</sub> )	(12 <sup>+</sup> )	...	...	[2.23]	292.61	1.6025	1.0 <sub>s</sub>
HgF.....	(202)	19	(17.364959 <sub>1</sub> )	(12 <sup>+</sup> )	...	...	...	490	3.8	(1.9)
HgH.....	(202)	1	(1.00222118 <sub>1</sub> )	12 <sup>+</sup>	5.549 <sub>s</sub>	0.312	1.7405	1387.09	83.01	0.376
	(202)	2	(1.9942153 <sub>1</sub> )	12 <sup>+</sup>	2.7989	0.1133	1.7339	695.15	49.93	0.398
HgH <sup>+</sup> .....	(202)	1	...	12 <sup>+</sup>	6.613	0.206	1.594 <sub>s</sub>	2033.87	46.16	(2.3)
	(202)	2	...	12 <sup>+</sup>	3.328	0.0736	1.595 <sub>s</sub>	1442.15	23.24	(2.4)
HgI.....	(202)	127	(77.93524 <sub>4</sub> )	(12 <sup>+</sup> )	...	...	...	125.0	1.0	0.35
HgS.....	(202)	(32)	(27.002570 <sub>1</sub> )	...	...	...	...	...	...	≤2.1 <sub>s</sub>
HgTl.....	(202)	(205)	(101.73073 <sub>1</sub> )	12 <sup>+</sup>	6.5108 <sub>s</sub>	0.1686 <sub>s</sub>	1.6032	26.9	0.69	(0.031)
	1	127	0.99988452	12 <sup>+</sup>	6.108 <sub>s</sub>	0.06129	1.66C90	2:08.09	38.98 <sub>s</sub>	3.056 <sub>s</sub>
	2	127	1.9826357 <sub>4</sub>	12 <sup>+</sup>	3.28414	[2.19326]	[1.6132]	1139.939	20.087	3.097 <sub>s</sub>
Hf <sup>+</sup> .....	3	127	2.9460330 <sub>4</sub>	12 <sup>+</sup>	1H <sub>1</sub>	...	...	(270)	...	...
	1	127	...	1H <sub>1</sub>	A = -13470	...	...	...	...	3.13
HeO.....	165	16	14.580864 <sub>4</sub>	12 <sub>s</sub> <sup>+</sup>	0.037389	0.0001210	2.666 <sub>s</sub>	214.51886	0.60738	6.6 <sub>s</sub>
I <sub>2</sub> .....	127	127	63.45217 <sub>4</sub>	12 <sub>s</sub> <sup>+</sup>	...	...	...	...	...	1.5424 <sub>s</sub>

## CONSTANTS OF DIATOMIC MOLECULES

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		$\pi \Pi_u \}$	$A = -5080$	$0.000199$	$2.4699$	$268.71$	$0.83$	$1.817$
I <sub>2</sub> <sup>+</sup>	127	127	48.65878, 27.414065,	0.050788 0.1141556	0.0005357 0.001887	2.3200 1.9086	384.293 608.14	1.50, 2.4,
IBr	127	70	16.5245694	0.2799, 0.12*	0.0548943 0.1090580,	2.5322 2.4012	221.0 317.4	0.65 1.01
ICl	127	35	(115)	0.5745204	0.0605177, 0.0018*	0.0605177, 0.0018*	335.33 1.837	3.9, 1.01
IP	127	19	16.490327,	0.27*	0.0624, 0.1004,	0.142,* 0.051	1.76.04 1048	4.44 12.4
InBr	115	81	47.490327,	0.27*	0.1004, 0.2523	0.142,* 0.051	177.1 177.1	2.64 0.4
InCl	115	35	26.806804	0.27*	0.036857, (12)	0.0001040	2.7540 703.09	5.24 3.71
InF	115	19	16.302865,	0.27*	0.0001040	0.0001040	703.09	≤3.25 3.71
InH	115	1	0.909004243	0.27*	0.0001040	0.0001040	703.09	2.9, 1.62
InI	115	2	1.9794006,	0.27*	0.0001040	0.0001040	703.09	2.52 ≤3.25
InL	115	127	60.30322	0.27*	0.0001040	0.0001040	703.09	2.52 ≤3.25
InO	115	16	14.040451,	0.27*	0.0001040	0.0001040	703.09	2.9, 1.54
InS	115	32	(25.012376)	0.27*	0.0001040	0.0001040	703.09	2.56 2.50
InSb	115	121	(58.91379)	0.27*	0.0001040	0.0001040	703.09	2.1, 1.9
InSe	115	80	(47.134364)	0.27*	0.0001040	0.0001040	703.09	6.44 (3.6,)
InTe	115	130	(60.97284)	0.27*	0.0001040	0.0001040	703.09	0.514 0.514
IO	127	16	14.2045817	0.34026	0.00269,	1.8676	681.47	4.2,
IrC	127	12	(11.2974351,)	0.34026	0.00269,	1.8676	681.47	4.2,
IrO	193	16	(14.7705681)	0.56713	0.00165	3.9050	92.021	0.2629
K <sub>2</sub>	39	39	19.481857,	0.27*	0.08122108	0.00040481	2.8208	213*
KBr	39	79	26.084986	0.27*	0.1286347	0.0007899	2.6656	281*
KCl	39	35	18.129177,	0.27*	0.1286347	0.0007899	2.1714	1.36
KF	39	19	12.7712448	0.27*	0.299373,	0.0233349,	126	2.4
KH	39	1	0.8241435	0.27*	0.412,	0.081,	2.242,	14.34
KI	39	2	1.9151069,	0.27*	1.753,	0.0318	2.240,	7.74
KI <sub>2</sub>	39	202	(32.062532,)	(22)	0.00087472	0.00020776	3.0478	187
KI <sub>3</sub>	39	127	29.810831	0.27*	0.00087472	0.00020776	3.0478	0.57
Kr <sub>2</sub>	94	84	(41.955752,)	0.27*	0.00087472	0.00020776	3.0478	0.046, (0.015)
Kr <sub>2</sub> <sup>+</sup>	84	139	69.45303	0.27*	[0.2458]	[2.026]	[550]	≥0.995 2.56
La <sub>2</sub>	139	19	16.712596,	0.27*	0.0014	1.826	811.6	2.23
LaF	139	16	14.243296,	0.27*	0.3526	0.0014	811.6	8.2, 5.9,
LaO	139	32	(25.389954)	0.27*	0.6727,	0.00704	2.6727	2.592 1.117
LaS	139	7	3.5080027	0.27*	0.555394,	0.005640,	563.2*	3.5,* 4.3,
La <sub>2</sub>	7	7	6.443102,	0.27*	0.706525	0.008012	2.0207	4.2,* 4.8,
LaBr	7	79	5.8435748	0.27*	1.33	0.004204,	(167)	7.929
LaCl	7	35	6.304204,	0.27*	5.1238105	0.020300	1.5639	910.34
LaCs	7	133	1.33	0.27*	1.345261	0.020300	1.5957	1405.649
LaF	7	19	0.38123834	0.27*	7.5131	0.2132	1.5957	1055.12
LaH	7	1	1.5618708,	0.27*	4.233107	0.011550	1.5957	13.228
LaI	7	2	6.348441,	0.27*	0.443181,	0.0404090	2.3919	498.16
LaK	7	127	(5.3454392)	0.27*	7II	(1.62)	(207)	3.5,
LaO	7	16	4.8768327	0.27*	7II	(1.62)	(745)	.....

TABLE 7g-1. CONSTANTS OF DIATOMIC MOLECULES (Continued)

(1)	$m_1$ (2)	$m_2$ (2)	$\mu$ (3)	Ground state (4)	$B_e$ (5)	$a_e$ (6)	$r_e$ (7)	$\omega_e$ (8)	$\omega_{eX}$ (9)	$D_0^*$ (10)
LiRb.....	(7) (175)	(85) (14.6550027)	12 <sup>+</sup>	.....	.....	.....	.....	.....	.....	7.2, 0.0495
LiO.....	16	11.9925223	12 <sup>+</sup>	0.0028;	0.00378	3.89	51.12	1.64,	1.34	≤3.35
Mg <sub>2</sub> .....	24	18.3945354,	(12 <sup>+</sup> )	.....	.....	.....	373.8	.....	.....	3.24
MgBr.....	24	35	14.126871,	0.24502	0.0015,	2.1991	[162.12]	(2.05)	(2.05)	4.75
MgCl.....	24	19	10.6012335	0.51922	0.00470	1.7500	[711.69]	(4.94)	(4.94)	≤2.49
MgF.....	24	1	(0.06718516)	5.818	0.1668	1.7304	1497.0	32.4	.....	.....
MgH.....	(24)	2	(1.35807370)	3.0307	0.0454	1.7302	1077.76	16.00	.....	(2.1)
MgH <sup>+</sup> .....	(24)	1	.....	6.411	0.296	1.6484	1395.3	30.2	.....	.....
MgI.....	(24)	2	(20.1724356)	3.321	0.064	1.6524	1226.6	16.30	.....	(2.4)
MgI <sub>2</sub> .....	(24)	16	9.3957763	0.5743	0.0850	1.7490	[312]	5.4	.....	3.5,
Ni <sub>2</sub> O.....	24	55	(13.5042728)	0.5743	0.0850	1.7490	785.0,	5.4	.....	<2.4
NiS.....	(24)	55	27.469026,	(12 <sup>+</sup> )	.....	.....	525.2	2.93	.....	0.33
Mn.....	55	55	.....	.....	.....	.....	.....	.....	.....	.....
MnBr.....	55	(79)	(32.390087)	(12 <sup>+</sup> )	.....	.....	288	(0.9)	3.2,	3.2,
MnCl.....	55	(35)	(21.367888)	(12 <sup>+</sup> )	.....	.....	383	(0.7)	3.7,	3.7,
MnF.....	55	19	14.166538	(12 <sup>+</sup> )	.....	.....	618.5	2.6	4.3,	4.3,
NiH.....	55	1	0.989669997	5.6841	0.1570	1.7311	1548.0	28.8	.....	(2.5)
NiI.....	55	2	1.9428734,	2.8956	0.0514	1.7310	1102.5	13.9	.....	.....
NiI <sub>2</sub> .....	55	127	38.340221	(12 <sup>+</sup> )	.....	.....	[240]	(1.5)	2.8,	2.8,
NiO.....	55	16	12.3881675	.....	.....	.....	839.5	4.7	3.7,	3.7,
NiS.....	55	(32)	(20.210343)	.....	.....	.....	.....	.....	.....	2.0,
MoO.....	(98)	16	(13.748766)	12 <sup>+</sup>	1.9987	0.01781	1.0976	2358.07	14.18	5.0
N <sub>i</sub> .....	14	14	7.90153719	12 <sup>+</sup>	1.932	0.020	1.116	2207.19	16.14	9.780
N <sub>i</sub> <sup>+</sup> .....	14	14	.....	1.88011	.....	.....	[1.1316]	(1960)	8.72	.....
N <sub>i</sub> <sup>++</sup> .....	14	14	Data for lowest 12 <sup>+</sup>	0.15471	0.00070	3.0788	159.23	0.726	0.726	0.726
N <sub>2</sub> .....	23	23	11.4948863	12 <sup>+</sup>	0.1512532,	0.0009409,	2.5020	302*	1.5,*	3.80
NaBr.....	23	23	17.303437,	12 <sup>+</sup>	0.2180630,	0.016248	2.3608	366*	2.0,*	4.25
NaCl.....	23	35	13.370687,	12 <sup>+</sup>	19.589477	.....	2.6	(98)	.....	0.69
NaCs.....	23	133	10.4621901	12 <sup>+</sup>	0.4389005,	0.0045571	1.9259	536	3.4	4.9,
NaF.....	23	19	0.06349966	12 <sup>+</sup>	4.9012	0.1353	1.8874	1172.2	19.72	2.0,
NaH.....	23	1	1.8518630,	12 <sup>+</sup>	2.5575	0.0520	1.8866	[826.16]	1.0,	3.0,
NaI.....	23	2	19.463752,	12 <sup>+</sup>	0.1178055,	0.0006477,	2.7114	258	1.0,	0.62,
NaK.....	23	127	(14.458700)	12 <sup>+</sup>	.....	.....	123.29	0.400	0.455	0.455
NaRb.....	23	(85)	(18.091511)	12 <sup>+</sup>	.....	.....	106.64	0.455	0.57	0.57

NbO	0.3	16	13.645648 <sub>6</sub>	$ A  \approx 1.5$	0.4321	0.3021	1.690*	989.0 <sub>4</sub>	3.6 <sub>4</sub>	7.8 <sub>1</sub>		
NBr	14	79	11.89282888	$\Sigma^-$	0.444	0.3040	1.73 <sub>7</sub>	691.75	4.720	2.9 <sub>6</sub>		
NCl	14	35	9.9990236	$\Sigma^-$	[0.63468 <sub>3</sub> ]	.....	[1.6.44]	827.0	5.1	(4.1)		
NdF	(142)	19	(16.755233 <sub>4</sub> )	.....	.....	.....	.....	.....	.....	5.8 <sub>7</sub>		
NaO	(142)	16	(14.3748606)	.....	.....	.....	.....	.....	.....	7.4 <sub>4</sub>		
NF	14	19	8.0613378 <sub>8</sub>	$\Sigma^-$	1.2036 <sub>8</sub>	0.01492	1.3.70	1141.37	8.40	(4.1)		
NH	14	1	0.94010028	$\Sigma^-$	10.067 <sub>6</sub>	0.145 <sub>7</sub>	1.0372	[3125.54]	(70)	3.5 <sub>6</sub>		
NH <sub>2</sub>	14	2	1.76038610	$\Sigma^-$	8.9074	0.2530	1.0367	(2418)	(45)	3.6 <sub>4</sub>		
NH <sup>+</sup>	14	1	.....	$\Sigma_1^+$	[15.35]	.....	[1.0811]	[2922]	.....	4.1		
				$A = +78$	.....	.....	.....	.....	.....			
		14	2	.....	[8.244]	.....	[1.0776]	[2143.04]	.....			
Ni <sub>2</sub>	(58)	(58)	(28.967671)	.....	.....	.....	.....	.....	.....	2.3 <sub>4</sub>		
NiBr	(58)	(79)	(33.400121)	.....	.....	.....	.....	.....	.....	3.6 <sub>9</sub>		
NiCl	(58)	(35)	(21.804685 <sub>0</sub> )	.....	.....	.....	.....	.....	.....	3.8 <sub>2</sub>		
NiF	(58)	19	(14.3068434)	$\Sigma^-$	7.815	0.231	1.476	2000	40	2.6		
NiH	58	1	0.99059317	$\Sigma_1^+$	4.037	0.090	1.465	430	20			
		58	2	1.946350 <sub>3</sub>	$\Delta_1^+$	.....	.....	.....	.....	.....		
NiI	(58)	127	(30.776343)	.....	1.7048 <sub>3</sub>	0.0176 <sub>3</sub>	1.1508	1904.12	14.088	2.0 <sub>9</sub>		
NiO	(58)	16	(12.5343926)	$\Pi_1^+$	.....	.....	.....	.....	.....	3.7 <sub>5</sub>		
NO	.....	14	16	7.4066332 <sub>0</sub>	$A = -490$	.....	.....	.....	.....	6.507		
NO <sup>+</sup>	14	16	.....	$\Sigma^+$	2.002	0.0202	1.062 <sub>0</sub>	2377.1	16.35	10.858		
NS	.....	14	32	9.7380290 <sub>2</sub>	$\Pi_1^+$	0.7754 <sub>4</sub>	0.0061	1.4941	1219.6	7.6	(6.0)	
NS <sup>+</sup>	14	32	.....	$\Sigma_1^+$	(1.08)	.....	(1.20)	.....	.....			
NSE	14	(80)	(11.19132661)	$\Pi_1^+$	1.44567	0.01579	1.2075	>944	5.4	(5.1)		
O <sub>2</sub>	16	16	7.99745747	$\Sigma_1^+$	1.6920	0.01984	1.1161	1580.361 <sub>1</sub>	12.0730	5.115 <sub>8</sub>		
O <sub>2</sub> <sup>+</sup>	16	16	.....	$\Sigma_1^+$	.....	.....	.....	1903.85	16.13	6.67 <sub>4</sub>		
O <sub>2</sub> <sup>-</sup>	16	16	.....	$\Sigma_1^+$	.....	.....	.....	.....	.....			
OF	16	16	8.3828822 <sub>3</sub>	$\Pi_1^+$	.....	.....	(1.36)	1108	9	4.1 <sub>6</sub>		
OH	.....	16	1	0.34808710	$\Pi_1^+$	18.807	0.408	0.9707 <sub>4</sub>	[1028.5] in Ar matrix			
OH <sup>+</sup>	16	2	1.78884794	$\Sigma_1^+$	9.991	0.258	0.9712	2716.1	42.15	4.45 <sub>7</sub>		
O <sub>2</sub> <sup>-</sup>	16	1	.....	$\Sigma_1^+$	16.781	0.724	1.0294	[2955]	(85)	4.8 <sub>1</sub>		
O <sub>2</sub> <sup>-</sup>	16	2	.....	$\Sigma_1^+$	8.900	0.274 <sub>6</sub>	1.0290	[2187]	(51)	4.8 <sub>1</sub>		
O <sub>2</sub> <sup>-</sup>	16	1	.....	$\Sigma_1^+$	.....	.....	.....	.....	.....	4.76		
P <sub>2</sub>	16	1	15.1808817	$\Sigma_1^+$	0.30348	0.01143	1.8939	780.89	2.80	5.031		
P <sub>2</sub> <sup>+</sup>	31	31	.....	$\Sigma_1^+$	0.3038	0.0021	<1.892 <sub>0</sub>	[>733.7]	.....	(3.7)		
Pb <sub>2</sub>	(208)	(208)	(103.988322)	$\Pi_1^+$	.....	.....	.....	256.5	2.9 <sub>6</sub>	1.0 <sub>6</sub>		
Pb <sub>2</sub> Br	(208)	79	(57.20968 <sub>8</sub> )	$\Pi_1^+$	.....	.....	.....	207.5	0.50	2.5		

(not certain that this

is the ground state)

TABLE 7R-1. CONSTANTS OF DIATOMIC MOLECULES (Continued)

(1)	$n_1$ (2)	$n_2$ (2)	$\mu$ (3)	Ground state (4)	$B_s$ (5)	$\alpha_s$ (6)	$r_s$ (7)	$\omega_s$ (8)	$\omega_{\text{eff}}$ (9)	$D_0^*$ (10)
PbCl	(208) (208)	35 10	(29.035541) (17.4081885)	$\text{H}_1^1(1)$ $\text{H}_1^1(1)$	0.2414 $A = +8266$	0.0018 0.144	2.00, 1.888,	303.8 1564.1	0.88 2.30	3.1 3.6,
PbF										$\leq 1.59$
PbH	(208)	1	(1.00206499)	$A = +8200$	4.971					
PbI	(208)	127	(78.81349)	$\text{H}_1^1(1)$ $\Sigma^+(0^+)$	0.3073056 0.1163195	0.0019148 0.0004365	1.9218 2.2868	160.5 429.40	0.25 3.70	(2.0) 3.83
PbO	208	16	14.85263391	$\Sigma^+(0^+)$	0.05058952	0.00012093	2.40/22	277.6*	1.30	3.4,
PbS	208	32	27.711940*	$0^+$				211.96	0.51*	2.9,
PbSe	208	80	57.732418	$0^+$					0.43	2.63
PbTe	(208)	(130)	(79.96121)	$0^+$						$\leq 1.4$ ,
Pd <sup>+</sup>	(108)	(108)	(53.44710)							$\leq 4.77$
PdC	(106)	12	(10.778659)							
PdH	(106)	2	(1.9765122)							
PdO	(106)	16	(13.896135)							
PF	31	19	11.7755965	$\Sigma^-$	0.5665	0.00456	1.530,	846.75	4.48	2.9
PF <sup>+</sup>	31	19		$\Pi_L$	0.6380	0.0048	1.500,	1053.25	5.047	(4.9) (6.7)
PH	31	1	0.97800596	$\Sigma^-$	$[8.412]$					(3.0)
PH <sup>+</sup>	31	2	1.89112947	$\Sigma^-$	[4.363]					
PH <sup>+</sup>	31	1		$\Pi_L$	8.505,	0.240,				3.0,
PN	31	2	9.0433616*	$\Sigma^+(0^+)$	$[4.350]$	0.00557	[1.4114]	1337.24	6.083	
PO	31	14	10.5479381	$\Sigma^+(0^+)$	0.7802,	0.0056	1.4759	1233.3,	6.47	$\leq 6.15$
PO <sup>+</sup>	31	16	14.3643633	$\Sigma^+(0^+)$	0.7337					
PO <sup>+</sup>	141	16	15.7325010	$\Sigma^+(0^+)$						
PS	31	32								
PS <sup>+</sup>	31	32		$A = +321$						
PbB	(195)	(11)	(10.4208884)	$\Sigma^+$						
PbC	195	12	11.3042295	$\Sigma$	0.5303	0.0032	1.676,	1051.18	4.87	
PbH	(195)	1	(1.00262229)	$\Sigma_L$	7.198	0.198	1.5283	[2293.50]		
PbO	(195)	16	(14.7821844)	$\Sigma^+$						
RaCl	(226)	(35)	(30.283614)	$\Sigma^+$						
Rb <sup>+</sup>	(85)	(85)	(42.455855)	$\Sigma^+$						
RbBr	85	79	40.90270,	$\Sigma^+$						
RbCl	85	35	24.768529	$\Sigma^+$						
RbF	85	19	15.524831	$\Sigma^+$						

## CONSTANTS OF DIATOMIC MOLECULES

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RbH.....	(85)	1	(0.90800356)	$\Sigma^+$	3.020	0.072	2.367	936.94	14.21
RbI.....	85	127	50.87275.	$\Sigma^+$	0.03283203	0.00010946	3.1769	139	0.34
RhC.....	103	12	10.746788.	$\Sigma^-$	0.6027	0.00396	1.614	1049.87	4.94
RhO.....	103	16	13.843208	$\Sigma^-$	.....	.....	.....	.....	6.01
RuC.....	(102)	12	(10.735774.)	$\Sigma^-$	.....	.....	.....	.....	4.3
RuO.....	(102)	16	(13.824938)	$\Sigma^-$	.....	.....	.....	.....	6.54
Si.....	32	32	15.9880369	$\Sigma^+$	0.2954,	0.06570	1.8802	880.8	13.1
Sb.....	(121)	(123)	(60.94787)	$\Sigma^-$	.....	.....	725.64,	2.84	5.3
SbBi.....	(121)	209	(76.592008)	$\Sigma^-$	.....	.....	269.85	0.50	3.06
SbBr.....	(121)	(70)	(47.75009.)	$\Sigma^-$	.....	.....	220.0	0.50	(3.0)
SbCl.....	(121)	35	(27.123863)	$\Sigma^-$	.....	.....	(242.1)	(0.56)	(3.2)
SbF.....	(121)	19	(16.418463)	$\Sigma^-$	.....	.....	(369.0)	(0.92)	(4.6)
SbH.....	(121)	1	(0.9949368)	$\Sigma^-$	[5.87]	[1.69]	942.0	5.6	(4.8)
SbN.....	(121)	2	(1.0810906.)	$\Sigma^-$	[2.94]	[1.70]	817	5.0	(4.1)
SbO.....	(121)	14	(12.540581.)	$\Sigma^-$	.....	.....	.....	.....	(4.2)
SbSe.....	(121)	16	(14.126107.)	$\Pi_B$	.....	.....	.....	.....	.....
SbTe.....	(121)	(80)	(48.11370.)	$\Pi_B$	.....	.....	326.1	1.04	(3.1)
Sc.....	(130)	(62.62182)	(2H)	$\Pi_B$	.....	.....	(284)	(0.2)	2.78
ScF.....	45	45	22.477959.	$\Sigma^+$	0.3950	0.00266	1.787	735.6	1.64
ScO.....	45	19	13.3546098	$\Sigma^+$	[0.51349]	.....	[1.6683]	971.55	0.04
ScS.....	45	16	11.3974776	$\Sigma^+$	0.08992	0.000288	2.1680	385.3028	6.94
Se.....	45	(32)	(18.784147.)	$\Sigma^+$	[0.363]	.....	[1.73]	0.94363	4.9
SeF.....	80	80	39.558256	$\Pi_B$	.....	.....	.....	.....	3.410
SeII.....	(80)	19	(15.349416.)	$A = -580$	[7.08]	.....	[1.457]	(2400)	.....
SeIII.....	(80)	1	(0.40527385)	$A_0 = -1600$	0.4704	0.0032,	1.639	915.43	4.52
SeO.....	80	16	13.3274820	$\Sigma^-$	[9.461]	(constants for F <sub>1</sub> levels)	[1.3504]	(2702)	4.34
SeS.....	(80)	(32)	(22.836079.)	$\Pi_B$	[0.306]	.....	[1.3504]	(60)	(3.9)
SiI.....	32	1	0.9702732	$A_0 = -377$	[4.900.]	(0.11.)	[1.3474]	(1940)	3.53
SiII.....	32	2	1.8947416.	$\Pi_B$	[9.134.]	.....	[1.3714]	(31)	3.57
SiI.....	32	1	13.988463c	$\Sigma^-$	0.2390	0.0013	2.245	510.98	2.02
SiBr.....	28	28	(20.654728)	$\Sigma^-$	.....	.....	125.4	1.5	(3.7)
SiBr <sup>+</sup> .....	(28)	(79)	.....	$A = +418$	.....	.....	535.8	1.6	(5.5)
SiC.....	(28)	12	(8.3979222.)	$\Sigma^-$	.....	.....	535.89	2.29	4.6
SiCl.....	28	35	15.542282.	$\Pi_B$	0.25619	0.00163	2.0576	535.89	(4.5)
SiF.....	28	19	11.3148106	$\Pi_B$	0.5813,	0.00490	1.6008	857.26	5.57
				$A = +162$					

TABLE 7g-1. CONSTANTS OF DIATOMIC MOLECULES (Continued)

(1)	$m_1$ (2)	$m_2$ (3)	$\mu$ (4)	Ground state (5)	$B_e$ (5)	$a_e$ (6)	$r_e$ (7)	$\omega_e$ (8)	$\omega_{ex}$ (9)	$D_0^o$ (10)
SII.....	(28)	1	(0.97278225)	$A = -1$ $\text{II}_r$ $\text{III}_r$	7.4979	0.2140	1.5203	2045	36	3.06
SII.....	(28)	2	(1.8788414)	$A = +1$ $\text{II}_r$ $\text{III}_r$	2.8840	0.0801	1.5197	1471	19	3.09
SI.....	28	127	22.923324 <sub>4</sub>	$A = +$ (757)	12 <sup>+</sup>	0.7310	0.00567	1151.68 <sub>6</sub>	1.0 <sub>1</sub>	
SIN.....	28	14	9.3321338		12 <sup>+</sup>	0.7267514	0.005038 <sub>6</sub>	1.5097	1241.4 <sub>4</sub>	6.26
SiO.....	28	16	10.1767074		12 <sup>+</sup>	Spectrum previously attributed to SiO <sup>+</sup> now known to be due to SiN.			5.92	(6.2)
SiO <sup>+</sup>	..	..	..		12 <sup>+</sup>	0.3035290	0.0014736	1.9293	2.58	8.26
SiS.....	28	32	14.920688 <sub>7</sub>		12 <sup>+</sup>	0.1920116	0.0007767	2.0583	580.0*	6.37
SiSe.....	28	80	20.722468 <sub>0</sub>		12 <sup>+</sup>				481.2	5.4 <sub>4</sub>
SiTe.....	28	(130)	(23.019425)		12 <sup>+</sup>				1.30	4.60
SmO.....	(152)	16	(14.471297 <sub>4</sub> )		12 <sup>+</sup>					6.1 <sub>4</sub>
Sn <sub>2</sub> .....	(120)	(118)	(59.446777)		12 <sup>+</sup>					1.9 <sub>8</sub>
SnBr.....	(120)	(79)	(47.593074 <sub>7</sub> )	$A = +$ 2467	12 <sup>+</sup>				247.7	0.62
SnCl.....	(120)	35	(27.073116)	$A = +$ 2361	12 <sup>+</sup>				354.0	1.1
SnF.....	118	19	16.361890	$A = +$ 2317	12 <sup>+</sup>	0.2733	0.0011	1.942	586.1*	≤ 4.25
SnH <sub>2</sub> .....	(120)	1	(0.99942466)	$A = -$ 2178	12 <sup>+</sup>	5.383	0.137	1.770 <sub>1</sub>	1715	0.62
SnI.....	(120)	2	(1.98062844)	$A = -$ 2178	12 <sup>+</sup>	2.7195	0.040	1.7390	1218	2.6 <sub>6</sub>
SnO.....	(120)	127	(61.65195)		12 <sup>+</sup>	0.3557190	0.002142 <sub>6</sub>	1.8325	199.0	0.5 <sub>6</sub>
SnS.....	120	16	14.112333 <sub>1</sub>		12 <sup>+</sup>	0.1308861 <sub>1</sub>	0.000506 <sub>6</sub>	2.2090	822.1	0.49
SnSe.....	120	32	25.241415		12 <sup>+</sup>	0.0649977 <sub>4</sub>	0.0001704 <sub>4</sub>	2.3236	487.26	4.7 <sub>7</sub>
SnTe.....	120	80	47.95128 <sub>0</sub>		12 <sup>+</sup>				331.2*	0.736*
SO.....	(130)	(62.352094)			12 <sup>+</sup>				259.5	0.50
SO.....	32	16	10.3613020 <sub>0</sub>		12 <sup>+</sup>	0.720817	0.00573 <sub>4</sub>	1.4311	1148.10	3.05
SiBr.....	(88)	70	(41.58494 <sub>7</sub> )		12 <sup>+</sup>				216.5	5.35 <sub>8</sub>
SiCl.....	(88)	35	(25.017065)		12 <sup>+</sup>				302.3	3.9
SiF.....	(88)	19	(15.622111)		12 <sup>+</sup>	0.25045	0.00148	2.0757	500.1	4.2 <sub>4</sub>
SiH.....	(88)	1	(0.99640162)		12 <sup>+</sup>	3.6751	0.0814	2.1456	2.21	5.5 <sub>4</sub>
SiL.....	(88)	2	(1.0680885 <sub>4</sub> )		12 <sup>+</sup>	1.8600	0.0292	2.1449	1206.2	≤ 1.68
SrO.....	(88)	127	(51.03244)		12 <sup>+</sup>	0.33798	0.00219	1.9198	173.9	≤ 1.70
SrS.....	(88)	88	16	13.535985 <sub>7</sub>	12 <sup>+</sup>	0.33798	0.00219	1.9198	653.2*	3.92*
SrS.....	(88)	(32)	(23.444936)		12 <sup>+</sup>					3.4 <sub>7</sub>

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S <sub>2</sub> Se	(88)	(41.86045 <sub>b</sub> )	(80)	16	14.6956719	$A_{\infty} + 1753$	$\Sigma_{\Delta}$	0.40288	0.00182	1.6874	1028.69	3.51	2.8 <sub>e</sub>
TaO	181	16	14.532117 <sub>b</sub>	16	14.44807 <sub>b</sub>	$A_{\infty} + 1753$	$\Sigma_{\Delta}$	0.40288	0.00182	1.6874	1028.69	3.51	8.4
TbO	159	16	(64.44807 <sub>b</sub> )	16	(64.44807 <sub>b</sub> )	$A_{\infty} + 1753$	$\Sigma_{\Delta}$	0.40288	0.00182	1.6874	1028.69	3.51	7.5 <sub>e</sub>
Te <sub>2</sub>	(130)	(128)	(1.00006663)	(130)	(1.00006663)	$A_0 = -2250$	$\Sigma_{\Delta}$	[5.56]	[2.59]	[1.741]	251	0.55	2.65
TeO	128	16	14.217027 <sub>b</sub>	16	14.217027 <sub>b</sub>	$O^*$	$\Sigma_{\Delta}$	0.3560	0.00237 <sub>b</sub>	1.8256	797.69	4.00	3.9 <sub>e</sub>
TeS	(130)	(32)	(25.657389)	(130)	(80)	(O <sup>+</sup> )	$\Sigma_{\Delta}$	0.3560	0.00237 <sub>b</sub>	1.8256	470.0	1.4	(3.4 <sub>e</sub> )
TeSe	(130)	(32)	(49.476277)	(130)	(80)	(O <sup>+</sup> )	$\Sigma_{\Delta}$	0.3560	0.00237 <sub>b</sub>	1.8256	318.6	1.0	2.8 <sub>e</sub>
ThN	232	14	13.2061101 <sub>b</sub>	16	14.9034507	$\Sigma^+$	$\Sigma_{\Delta}$	0.332644	0.001302	1.8403	895.77	2.39	5.6
ThO	232	16	14.9034507	16	14.9034507	$\Sigma^+$	$\Sigma_{\Delta}$	0.332644	0.001302	1.8403	895.77	2.39	8.5
ThP	232	31	27.326119 <sub>b</sub>	31	27.326119 <sub>b</sub>	$\Sigma^+$	$\Sigma_{\Delta}$	.....	.....	.....	.....	.....	4.0
Tl <sub>2</sub>	(48)	(48)	(23.973973 <sub>b</sub> )	(48)	(48)	(9.5979161 <sub>b</sub> )	$\Sigma^+$	.....	.....	.....	.....	.....	1.3 <sub>e</sub>
TlC	(48)	(48)	(20.22129 <sub>b</sub> )	(48)	(35)	(20.22129 <sub>b</sub> )	$\Sigma^+$	.....	.....	.....	.....	.....	$\leq 5.5$
TlCl	(48)	(48)	(11.9938851)	(48)	(16)	(11.9938851)	$\Sigma_{\Delta}$	0.5355	0.0030	1.6200	379.7	3.41	6.9 <sub>e</sub>
TlO	(48)	(48)	(19.181616 <sub>b</sub> )	(32)	(32)	(19.181616 <sub>b</sub> )	$\Delta = + (50)$	.....	.....	.....	1008.26	4.13	4.0
TlS	(48)	(48)	(102.48723)	(205)	(205)	(58.01440 <sub>a</sub> )	$\Sigma^+$	0.0423896	0.0001278	2.6182	192.10	0.39	(0.6)
Tl <sub>3</sub>	(205)	81	29.87256 <sub>b</sub>	(205)	35	17.386879 <sub>b</sub>	$\Sigma^+$	0.09139701 <sub>b</sub>	0.000039793 <sub>b</sub>	2.4848	287.47	1.24	3.42 <sub>e</sub>
TlBr	(205)	35	0.00289416 <sub>b</sub>	(205)	19	0.00289416 <sub>b</sub>	$\Sigma^+$	0.2231501 <sub>b</sub>	0.0015033 <sub>b</sub>	2.0844	477.3	2.3	3.82 <sub>e</sub>
TlCl	(205)	19	(1.9945039 <sub>b</sub> )	(205)	1	(1.9945039 <sub>b</sub> )	$\Sigma^+$	4.806	0.154	1.870 <sub>b</sub>	1390.7	22.7	4.57 <sub>e</sub>
TlF	(205)	127	78.37846 <sub>b</sub>	(205)	2	78.37846 <sub>b</sub>	$\Sigma^+$	2.419	0.057	1.869	987.7	12.04	2.00 <sub>e</sub>
TlH	(205)	169	14.61148 <sub>b</sub>	(238)	14	13.225122	$\Sigma^+$	0.0271674 <sub>b</sub>	0.0000663 <sub>b</sub>	2.8137	(150)	.....	2.77 <sub>e</sub>
TlI	(205)	169	14.9878026	(238)	16	(28.186418 <sub>b</sub> )	$\Sigma^+$	.....	.....	.....	.....	.....	6.0
TmO	(238)	16	12.1729619	(238)	16	12.1729619	$\Sigma^+$	0.5480	0.0034	1.589 <sub>b</sub>	1011.58	4.97	5.4 <sub>e</sub>
UN	(238)	16	(14.7153823)	(129)	(129)	(65.193613)	$\Sigma^+$	.....	.....	.....	[(1055)]	.....	5.8 <sub>e</sub>
UO	(238)	16	(129)	(129)	89	14.452715	$\Sigma^+$	.....	.....	.....	.....	.....	6.4 <sub>e</sub>
US	(238)	16	(28.186418 <sub>b</sub> )	(238)	16	(28.186418 <sub>b</sub> )	$\Sigma^+$	.....	.....	.....	.....	.....	6.7
VO	51	16	1.00201939	(184)	16	(1.00201939)	$\Sigma^+$	3.995	0.0986	2.052 <sub>b</sub>	203.6	1.23	1.6 <sub>e</sub>
WO	(184)	16	(1.9910471 <sub>b</sub> )	(132)	(129)	(4.647934 <sub>b</sub> )	$\Sigma^+$	2.0121	0.0352	2.0513	1249.54	21.055	(2.1)
Xe <sub>2</sub> <sup>+</sup>	(132)	(129)	(25.097289)	(132)	89	1.00201939	$\Sigma^+$	0.1162	0.0003	2.404	886.38	10.475	1.6 <sub>e</sub>
Y <sub>2</sub>	89	89	1.00201939	(174)	(35)	(29.115457)	$\Sigma^+$	.....	.....	.....	380.7	1.3	$\leq (3.8)$
YbCl	(174)	(35)	(1.00201939)	(174)	(174)	(1.00201939)	$\Sigma^+$	.....	.....	.....	.....	.....	$> 0.0467$
YbH	(174)	1	(1.9910471 <sub>b</sub> )	(174)	2	(4.647934 <sub>b</sub> )	$\Sigma^+$	.....	.....	.....	.....	.....	1.6 <sub>e</sub>
YbO	(174)	16	(4.647934 <sub>b</sub> )	(174)	35	25.097289	$\Sigma^+$	.....	.....	.....	.....	.....	1.6 <sub>e</sub>
YCl	(174)	35	.....	.....	.....	.....	.....	.....	.....	.....	.....	.....	$\leq (3.8)$

(constants for lowest observed  $\Sigma$  state)(constants for lowest observed  $\Sigma$  state)

TABLE 7g-1. CONSTANTS OF DIATOMIC MOLECULES (Continued)

$m_1$	$m_2$	$\mu$	Ground state	$B_s$	$\alpha_s$	$r_s$	$\omega_s$	$\omega_{\text{ext}}$	$D_0^\circ$
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)
YF	89	19	$15.653395$	$[\Sigma^+]$	0.29041	0.00163	1.3257	636.3	2.50
YL <sub>a</sub>	89	139	54.20931	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
YO	89	16	13.556054	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
YS	89	(32)	(23.515467)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZnCl	(64)	36	(22.604390)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZnF	(64)	19	(14.6459382)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZaH	(64)	1	(0.99218372)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZaH <sup>+</sup>	(64)	2	(1.9525855)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZaH <sup>+</sup>	(64)	1	[0.3881]	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZnI	(64)	2	[0.3881]	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZnO	(64)	16	(12.793910)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZnS	(64)	(32)	(21.313048)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZnSe	(64)	(80)	(35.517195)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZrN	(64)	14	(12.115950)	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45
ZrO	90	16	13.579058	$[\Sigma^+]$	[0.3881]	(0.0016)	[1.790]	882.5	2.45