7b. The Electronic Structure of Atoms

Explanation of Table 7b-1. COLUMN (3): Electronic structure of the ground state. Rare-gas shells and similar closed shells are indicated by appropriate symbols and only the electrons outside them given explicitly. All structures are based on spectroscopic evidence except in a few cases (e.g., Fr, At) where there is no reasonable doubt about predictions.

The electron printed in boldface when removed produces the ground state of the ion. Where the other electrons are rearranged in the ion this is indicated in a footnote.

COLUMN (4): Ground state of atom.

COLUMN (5): First ionization potential of atom (in electron volts).[1]

COLUMN (6): Ground state of ion. For electron configuration of ion, see column (3).

COLUMN (7): Second ionization potential (ionization potential of singly ionized atom) in electron volts.

COLUMN (8): Resonance potentials (see below).

COLUMN (9): Resonance lines (see below).

RESONANCE POTENTIALS AND RESONANCE LINES: The resonance potential is the energy (in electron volts) required to raise an atom from the ground state to the lowest excited state. The resonance line is the spectrum line absorbed or emitted in this or the reverse transition. There is a clear and unambiguous situation with regard to resonance lines and potentials for atoms with simple structure such as the alkalies. For more complicated atoms the matter needs further amplification.

A line is not considered a resonance line if the excited state has the same parity as the ground state and thus the transition is forbidden as a dipole transition. If the line is allowed as a dipole transition but very weak, i.e., if it violates an approximate dipole-selection rule (usually the spin-selection rule $\Delta S = 0$), it is called subresonance line r. The resonance line R proper is the first line allowed by all the selection rules. Both R and r then are given in such cases. For the heavy elements r may be very strong.

The resonance potentials are in general those corresponding to the lines, with one exception. If there is a lower state than that of the first resonance line for which transitions to the ground state are forbidden by the J-selection rule (but allowed by the parity rule) this state is metastable. It may, however, often be excited by direct electron collisions, and the excitation potential for this state is given as first resonance potential followed by a letter m. There is no observed resonance line corresponding to this transition. An asterisk on the second resonance potential indicates that the corresponding line is that also marked with an asterisk.

A C preceding column (8) means that there are states of the same parity as the ground state between it and the first resonance state. These often belong to the electron configuration of the ground state. A C is *not* listed if these states are merely additional levels of the ground-state multiplet.

[1] For conversion from wave numbers into electron volts or vice versa, see Table 7a-2.

TABLE 7b-1. ELECTRONIC STRUCTURE OF ATOMS[a]

Z	El.	Ground state	Ground state	IP	Ion ground state	IP	Resonance potentials		Resonance lines	
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)		(9)	
1	H	$1s$	^2S	13.599	.....	.....	10.15		1,215.67(^2P)	
2	He	$1s^2$	^1S	24.588	^2S	54.418	20.96m	21.13	591.43($^3P_1$)	584.35(^1P)
3	Li	[He]2s	^2S	5.392	^1S	75.641	1.84		6,707.85($^2P_{\frac{1}{2}}$)	
4	Be	$-2s^2$	^1S	9.323	^2S	18.211	2.71	5.25	4,548.3($^3P_1$)	2,348.61($^1P_1$)
5	B	$-2s^22p$	$^2P_{\frac{1}{2}}$	8.298	^1S	25.156	3.57	4.94	3,470.6($^4P_{\frac{1}{2}}$)	2,497.72(^2S)
6	C	$-2s^22p^2$	$^3P_0$	11.260	$^2P_{\frac{1}{2}}$	24.383	C, 4.16	7.46	2,967.22(^3S)	1,656.998(^3P)
7	N	$-2s^22p^3$	^4S	14.53	$^3P_0$	29.602	C, 10.28		1,200.71(^4P)	
8	O	$-2s^22p^4$	$^3P_2$	13.618	^4S	35.118	C, 9.11	9.48	1,355.60(^5S)	1,302.17(^3S)
9	F	$-2s^22p^5$	$^2P_{\frac{3}{2}}$	17.423	$^3P_2$	34.98	12.69	12.98	976.50(^4P)	954.82(^2P)
10	Ne	$-2s^22p^6$	^1S	21.565	$^2P_{\frac{3}{2}}$	40.964	16.62m	16.84	743.71($^3P_1$)	735.89($^1P_1$)
11	Na	[Ne]3s	^2S	5.139	^1S	47.29	2.10		5,889.95($^2P_{\frac{1}{2}}$)	
12	Mg	$-3s^2$	^1S	7.646	^2S	15.035	2.71m	4.33	4,571.10($^3P_1$)	2,852.12($^1P_1$)
13	Al	$-3s^23p$	$^2P_{\frac{1}{2}}$	5.986	^1S	18.828	3.13		3,961.52(^2S)	
14	Si	$-3s^23p^2$	$^3P_0$	8.152	$^2P_{\frac{1}{2}}$	16.346	C,	4.93		2,516.11($^3P_1$)
15	P	$-3s^23p^3$	^4S	10.487	$^3P_0$	19.72	C, 6.93		1,787.65($^4P_{\frac{1}{2}}$)	1,774.94($^4P_{\frac{3}{2}}$)
16	S	$-3s^23p^4$	$^3P_2$	10.360	^4S	23.4	C, 6.50	6.83	1,900.27(^5S)	1,807.31(^3S)
17	Cl	$-3s^23p^5$	$^2P_{\frac{3}{2}}$	12.967	$^3P_2$	23.80	8.88	9.16	1,389.78($^4P_{\frac{3}{2}}$)	1,347.32($^2P_{\frac{3}{2}}$)
18	A	$-3s^23p^6$	^1S	15.760	$^2P_{\frac{3}{2}}$	27.62	11.55m	11.83	1,066.66($^3P_1$)	1,049.22($^1P_1$)
19	K	[A]4s	^2S	4.341	^1S	31.81	1.61		7,664.91($^2P_{\frac{1}{2}}$)	
20	Ca	$-4s^2$	^1S	6.113	^2S	11.872	1.88	2.92	6,572.78($^3P_1$)	4,226.73($^1P_1$)
21	Sc	$-3d4s^2$	$^2D_{\frac{3}{2}}$	6.54	$^3D_1$	12.80	1.94m	1.98	6,378.82($^4F_{\frac{3}{2}}$)	6,305.67($^2D_{\frac{3}{2}}$)
22	Ti	$-3d^24s^2$	$^3F_2$	6.82	$^2F_{\frac{3}{2}}$	13.57	C, 1.96	2.39	6,296.65($^5G_2$)	5,173.74($^3D_1$)
23	V	$-3d^34s^2$	$^4F_{\frac{3}{2}}$	6.74[b]	$^5D_0$	14.65	C, 2.23	2.54	5,537.72($^5G_{\frac{1}{2}}$)	4,851.48($^4D_{\frac{1}{2}}$)
24	Cr	$-3d^54s$	^7S	6.765	^6S	16.49	C, 2.90		4,289.72($^7P_2$)	
25	Mn	$-3d^54s^2$	^6S	7.435	^7S	15.640	C, 2.27	3.06	5,432.55($^6P_{\frac{3}{2}}$)	4,034.49($^6P_{\frac{5}{2}}$)
26	Fe	$-3d^64s^2$	$^5D_4$	7.87	$^6D_{\frac{1}{2}}$	16.18	C, 2.39	3.20	5,166.29($^7D_5$)	3,859.91($^5D_4$)
27	Co	$-3d^74s^2$	$^4F_{\frac{9}{2}}$	7.864[c]	$^3F_4$	17.05	C, 2.91	3.50	4,233.99($^5F_{\frac{5}{2}}$)	3,526.85($^4F_{\frac{9}{2}}$)
28	Ni	$-3d^84s^2$	$^3F_4$	7.635[d]	$^2D_{\frac{5}{2}}$	18.15	C, 3.18	3.64	3,884.58($^5D_4$)	3,670.43($^3P_2$)
29	Cu	$-3d^{10}4s$	^2S	7.726	^1S	20.292	C, 3.79		3,273.96($^2P_{\frac{1}{2}}$)	
30	Zn	$-3d^{10}4s^2$	^1S	9.394	^2S	17.964	4.01m	5.77	3,075.90($^3P_1$)	2,138.56($^1P_1$)
31	Ga	$-3d^{10}4s^24p$	$^2P_{\frac{1}{2}}$	5.999	^1S	20.51	3.06		4,032.98(^2S)	
32	Ge	$-3d^{10}4s^24p^2$	$^3P_0$	7.900	$^2P_{\frac{1}{2}}$	15.935	C, 4.64m		2,651.58($^3P_1$)	
33	As	$-3d^{10}4s^24p^3$	^4S	9.81	$^3P_0$	18.63	C, 6.26		1,972.62($^4P_{\frac{1}{2}}$)	
34	Se	$-3d^{10}4s^24p^4$	$^3P_2$	9.75	^4S	21.5	C, 5.95	6.30	2,074.79(^5S)	1,960.90($^3S_4$)
35	Br	$-3d^{10}4s^24p^5$	$^2P_{\frac{3}{2}}$	11.814	$^3P_2$	21.6	7.83	8.29	1,576.5($^4P_{\frac{3}{2}}$)	1,488.6($^2P_{\frac{3}{2}}$)
36	Kr	$-3d^{10}4s^24p^6$	^1S	14.000	$^2P_{\frac{3}{2}}$	24.56	9.91m	9.99*	1,235.82*($^3P_1$)	1,164.86(^1P)
37	Rb	[Kr]5s	^2S	4.177	^1S	27.5	1.56		7,947.64($^2P_{\frac{1}{2}}$)	
38	Sr	$-5s^2$	^1S	5.696	^2S	11.030	1.78m	2.68*	6,892.58($^3P_1$)	4,607.33*(^1P)
39	Y	$-4d5s^2$	$^2D_{\frac{3}{2}}$	6.370	^1S	12.236	1.31		9,404.81($^2P_{\frac{1}{2}}$)	
40	Zr	$-4d^25s^2$	$^3F_2$	6.837	$^4F_{\frac{3}{2}}$	13.13	C, 1.83	2.71	6,762.38($^5G_2$)	4,575.52($^3G_2$)
41	Nb	$-4d^45s$	$^6D_{\frac{1}{2}}$	6.883	$^5D_0$	14.32	C, 2.07m	2.97*	5,320.21($^6F_{\frac{1}{2}}$)	4,168.12*($^6F_{\frac{1}{2}}$)
42	Mo	$-4d^55s$	^7S	7.10	^6S	16.15	C, 3.18		3,902.96($^7P_{\frac{1}{2}}$)	
43	Tc	$-4d^55s^2$	^6S	7.28	^7S	15.26	2.09	2.88	5,924.57($^6P_{\frac{7}{2}}$)	4,297.06($^6P_{\frac{5}{2}}$)
44	Ru	$-4d^75s$	$^5F_5$	7.366	$^4F_{\frac{9}{2}}$	16.76	C, 3.13	3.26*	3,964.90($^7D_5$)	3,799.35*($^5D_4$)
45	Rh	$-4d^85s$	$^4F_{\frac{9}{2}}$	7.464	$^3F_4$	18.07	C, 3.36		3,692.36($^4D_{\frac{7}{2}}$)	
46	Pd	$-4d^{10}$	^1S	8.33	$^2D_{\frac{5}{2}}$	19.42	C, 4.22m	5.01*	2,763.09($^3P_1$)	2,447.91*($^1P_1$)
47	Ag	$-4d^{10}5s$	^2S	7.576	^1S	21.48	3.66		3,382.89($^2P_{\frac{1}{2}}$)	
48	Cd	$-4d^{10}5s^2$	^1S	8.994	^2S	16.908	3.73m	5.29	3,261.04($^3P_1$)	2,288.02($^1P_1$)
49	In	$-4d^{10}5s^25p$	$^2P_{\frac{1}{2}}$	5.786	^1S	18.833	3.02		4,101.76(^2S)	
50	Sn	$-4d^{10}5s^25p^2$	$^3P_0$	7.344	$^2P_{\frac{1}{2}}$	14.632	C, 4.29m	4.33*	2,863.32*($^3P_1$)	
51	Sb	$-4d^{10}5s^25p^3$	^4S	8.642	$^3P_0$	16.5	C, 5.36		2,311.47($^4P_{\frac{1}{2}}$)	
52	Te	$-4d^{10}5s^25p^4$	$^3P_2$	9.01	^4S	18.6	C, 5.49	5.78	2,259.02($^5S_2$)	2,142.75($^3S_1$)
53	I	$-4d^{10}5s^25p^5$	$^2P_{\frac{3}{2}}$	10.451	$^3P_2$	19.135	6.77	7.66	2,062.1($^4P_{\frac{5}{2}}$)	1,617.7($^2P_{\frac{3}{2}}$)
54	Xe	$-4d^{10}5s^25p^6$	^1S	12.130	$^2P_{\frac{3}{2}}$	21.21	8.31m	8.44*	1,469.62*($^3P_1$)	1,295.56($^1P_1$)
55	Cs	[Xe]6s	^2S	3.894	^1S	25.1	1.38		8,943.46($^2P_{\frac{1}{2}}$)	8,521.10($^2P_{\frac{3}{2}}$)

TABLE 7b-1. ELECTRONIC STRUCTURE OF ATOMS (*Continued*)

Z	El.	Ground state	Ground state	IP	Ion ground state	IP	Resonance potentials	Resonance lines	
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	
56	Ba	$-6s^2$	^1S	5.212	^2S	10.004	*C*, 1.52*m* 2.24[a]	7,911.36($^3P_1$)	5,535.53[a](^1P)
57	La	$-5d6s^2$	$^2D_{\frac{3}{2}}$	5.61[e]	$^3F_2$	11.06	*C*, 1.64 1.84[a]	7,539.24($^4F_{\frac{3}{2}}$)	6,753.05($^2D_{\frac{5}{2}}$)
58	Ce	$-4f5d6s^2$	$^1G_4$	5.65[f]	$^4H_{\frac{7}{2}}$	10.85			
59	Pr	$-4f^36s^2$	$^4I_{\frac{9}{2}}$	5.42	$^5I_4$	10.55			
60	Nd	$-4f^46s^2$	$^5I_4$	5.49	$^6I_{\frac{7}{2}}$	10.73			
61	Pm	$-4f^56s^2$	$^6H_{\frac{5}{2}}$	5.55	$^7H_2$	10.90			
62	Sm	$-4f^66s^2$	$^7F_0$	5.63	$^8F_{\frac{1}{2}}$	11.07	*C*, 1.71*m* 1.74[a]	7,141.13[a]($^9F_1$)	6,725.88($^9G_1$)
63	Eu	$-4f^76s^2$	^8S	5.68	^9S	11.25	*C*, 1.74 2.66[a]	7,106.48($^{10}P_{\frac{7}{2}}$)	4,661.88[a]($^8P_{\frac{5}{2}}$)
64	Gd	$-4f^75d6s^2$	$^9D_2$	6.16	$^{10}D_{\frac{5}{2}}$	12.1	.....		4,225.85
65	Tb	$-4f^96s^2$	$^6H^{\circ}_{15/2}$	5.98					
66	Dy	$-4f^{10}6s^2$	I_8	5.93	.....	11.67			
67	Ho	$-4f^{11}6s^2$	$^4I^{\circ}_{15/2}$	6.02	.....	11.80			
68	Er	$-4f^{12}6s^2$	$^3H_6$	6.10	$^4H^{\circ}_{15/2}$	11.93			
69	Tm	$-4f^{13}6s^2$	$^2F^{\circ}_{\frac{7}{2}}$	6.18	$^3F_4$	12.05	.....		5,675.83
70	Yb	$-4f^{14}6s^2$	^1S	6.25	^2S	12.17	.....		3,987.99
71	Lu	$-4f^{14}5d6s^2$	$^2D_{\frac{3}{2}}$	6.15	^1S	13.9			
72	Hf	$-4f^{14}5d^26s^2$	$^3F_2$	7.0	$^2D_{\frac{3}{2}}$	14.9	*C*, 2.19		
73	Ta	$-4f^{14}5d^36s^2$	$^4F_{\frac{3}{2}}$	7.88	$^5F_1$	16.2	*C*, 2.90	4,280.47	
74	W	$-4f^{14}5d^46s^2$	$^5D_0$	7.98	$^6D_{\frac{1}{2}}$	17.7	*C*, 2.40*m*	4,082.16($^7P_1$)	
75	Re	$-4f^{14}5d^56s^2$	^6S	7.87	^7S	16.6	*C*, 2.35 3.58	5,275.53($^5P_{\frac{3}{2}}$)	4,008.75($^6P_{\frac{3}{2}}$)
76	Os	$-4f^{14}5d^66s^2$	$^5D_4$	8.7	$^6D_{\frac{9}{2}}$	17	*C*, 2.80	4,420.67($^7D_4$)	3,464.72
77	Ir	$-4f^{14}5d^76s^2$	$^4F_{\frac{9}{2}}$	9.2	.....	.....	*C*, 3.26	3,800.12($^6D_{\frac{9}{2}}$)	
78	Pt	$-4f^{14}5d^96s$	$^3D_3$	9.0	$^2D_{\frac{5}{2}}$	18.56	*C*, 3.74 4.04	3,315.05($^5D_4$)	3,064.71($^3P_2$)
79	Au	[o]6s	^2S	9.22	^1S	20.5	*C*, 4.63	2,675.95($^3P_{\frac{1}{2}}$)	2,427.95($^3P_{\frac{2}{2}}$)
80	Hg	$-6s^2$	^1S	10.437	^2S	18.757	4.67*m* 6.70	2,536.52($^3P_1$)	1,849.57($^1P_1$)
81	Tl	$-6s^26p$	$^2P^{\circ}_{\frac{1}{2}}$	6.108	^1S	20.42	3.29	3,775.72(^3S)	
82	Pb	$-6s^26p^2$	$^3P_0$	7.415	$^2P^{\circ}_{\frac{1}{2}}$	15.032	*C*, 4.33*m* 4.37	2,833.07[a]($^3P_1$)	
83	Bi	$-6s^26p^3$	$^4S^{\circ}$	7.287	$^3P_0$	16.68	*C*, 4.04	3,067.72($^4P_{\frac{1}{2}}$)	
84	Po	$-6s^26p^4$	$^3P_2$	8.43	.....	.....	.....		2,449.99
85	At	$-6s^26p^5$	$^2P^{\circ}_{\frac{3}{2}}$[o]						
86	Rn	$-6s^26p^6$	^1S	10.745	$^2P^{\circ}_{\frac{1}{2}}$[o]		6.77*m* 6.94[a]	1,786.07[a]($^3P_1$)	1,451.56($^1P_1$)
87	Fr	[Rn]7s	^2S[a]	.....	^1S[a]				
88	Ra	$-7s^2$	^1S	5.277	^2S	10.14	1.62*m* 2.57[a]	7,141.21	4,825.91[a]
89	Ac	$-6d7s^2$	$^2D_{\frac{3}{2}}$	6.9	^1S	12.1			
90	Th	$-6d^27s^2$	$^3F_2$	.....	$^4F_{\frac{3}{2}}$	11.5			
91	Pa	$-5f^26d7s^2$	$^4K^{\circ}_{11/2}$						
92	U	$-5f^36d7s^2$	$^5L_6$	6.08	$^4I_{\frac{9}{2}}$				5,915.40
93	Np	$-5f^46d7s^2$	$^6L^{\circ}_{11/2}$	5.8					
94	Pu	$-5f^67s^2$	$^7F_0$	5.8	$^8P_{\frac{1}{2}}$				
95	Am	$-5f^77s^2$	^8S	6.05	^9S				
96	Cm	$-5f^76d7s^2$	$^9D_2$						

[a] Data taken from current literature. Use has been made of Moore, "Atomic Energy Levels," vols. I-III, and "Smithsonian Physical Tables," 9th ed.

[b] Normal state of ion $-3d^4$.

[c] Normal state of ion $-3d^5$.

[d] Normal state of ion $-3d^9$.

[e] Normal state of ion $-5d^2$.

[f] Normal state of ion $-4f5d^2$.

[g] Structure of closed shells [Xe]$4f^{14}5d^{10}$.