Multielectron Atoms and the Periodic Table

Multielectron Atoms

The independent particle approximation knits together the potentials of the innermost electron ($-Zke^2/r$) and the outermost ($-ke^2/r$) with

$$U_{Multielectron}(r) = -Z_{eff}\frac{ke^2}{r}$$

For the orbital energies, replace ke^2 in the hydrogen equations with $Z_{eff}ke^2$:

$$E_{Multielectron}(r) = -Z_{eff}^2\frac{E_R}{n^2} \qquad (17)$$

For the outermost electron, $E_{Ionization} = -Z_{eff}^2 E_R / n^2$, allowing estimation of Z_{eff} from lab measurements of E_I.

This expression, with the variation in Z_{eff} due to the shielding of the nucleus by inner electrons, is what makes the energy levels slightly different for the s, p, d, and f levels as shown in Figure 10.3.

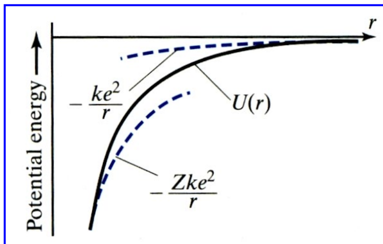


FIGURE 10.1
The IPA potential energy $U(r)$ of an atomic electron in the field of the nucleus plus the average distribution of the other $Z-1$ electrons. As $r \to \infty$, U approaches $-ke^2/r$; as $r \to 0$, U approaches $-Zke^2/r$ as in Eq. (10.5).

In hydrogen, the electrons in all the levels see the same nuclear charge but those with n > 1 are at lower energies because they are farther away from the nucleus. In multielecton (and multiproton) atoms, there is more nuclear charge for each additional electon, but most of that charge (not all of it … mostly $Z_{eff} > 1$) is shielded by inner electrons and they are farther away from the nucleus. For instance, the p electrons are fairly well shielded by the inner s electrons. But they are not very well shielded by the other p electrons.

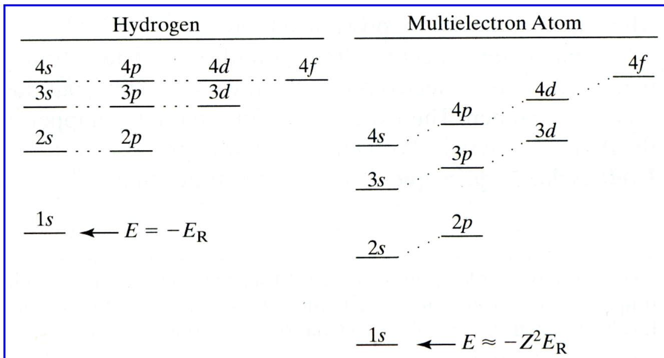
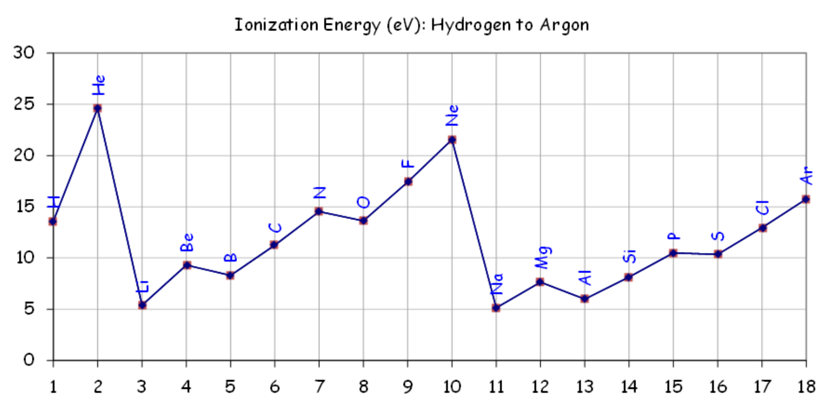


FIGURE 10.3
Schematic energy-level diagrams for a hydrogen atom and for one of the electrons in a multielectron atom. In hydrogen, all states with the same n are degenerate. In multielectron atoms states with lower l are more tightly bound because they penetrate closer to the nucleus. In many atoms this effect results in the $4s$ level being lower than the $3d$, as shown here.

Ionization Energy: Energy input to remove the outer electron
Electron Affinity: Energy released by adding an electron

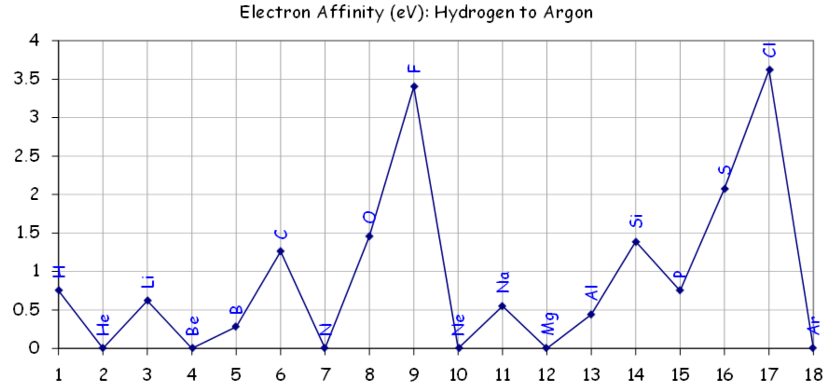


Z	Symbol	Electron Affinity (eV)	Ionization Energy (eV)	Radius (pm)
1	H	0.75	13.6	53
2	He	0	24.59	31
3	Li	0.62	5.39	167
4	Be	0	9.32	112
5	B	0.28	8.3	87
6	C	1.26	11.26	67
7	N	0	14.53	56
8	O	1.46	13.62	48
9	F	3.4	17.42	42
10	Ne	0	21.56	38
11	Na	0.55	5.14	190
12	Mg	0	7.65	145
13	Al	0.44	5.99	118
14	Si	1.39	8.15	111
15	P	0.75	10.49	98
16	S	2.08	10.36	88
17	Cl	3.62	12.97	79
18	Ar	0	15.76	71
19	K	0.5	4.34	243
20	Ca	0	6.11	194
21	Sc	0.19	6.54	184
22	Ti	0.08	6.82	176
23	V	0.53	6.74	171
24	Cr	0.67	6.77	166
25	Mn	0	7.44	161
26	Fe	0.16	7.87	156
27	Co	0.66	7.86	152
28	Ni	1.16	7.64	149
29	Cu	1.23	7.73	145
30	Zn	0	9.39	142

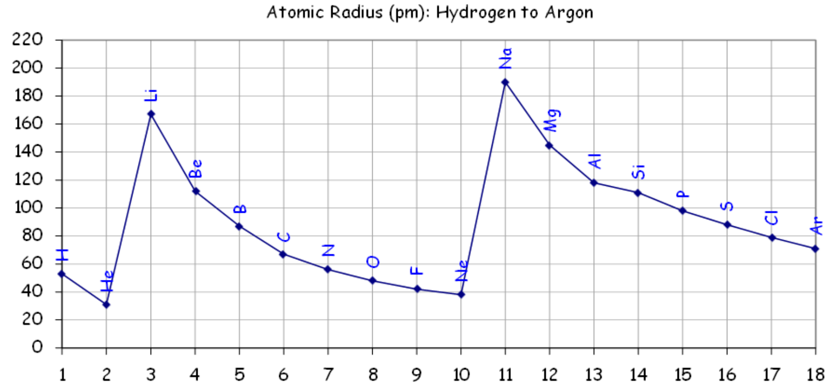
Z	Symbol	Electron Affinity (eV)	Ionization Energy (eV)	Radius (pm)
31	Ga	0.3	6	136
32	Ge	1.2	7.9	125
33	As	0.81	9.81	114
34	Se	2.02	9.75	103
35	Br	3.37	11.81	94
36	Kr	0	14	88
37	Rb	0.49	4.18	265
38	Sr	0	5.7	219
39	Y	0.3	6.38	212
40	Zr	0.43	6.84	206
41	Nb	0.89	6.88	198
42	Mo	0.75	7.1	190
43	Tc	0.55	7.28	183
44	Ru	1.05	7.37	178
45	Rh	1.14	7.46	173
46	Pd	0.56	8.34	169
47	Ag	1.3	7.58	165
48	Cd	0	8.99	161
49	In	0.3	5.79	156
50	Sn	1.2	7.34	145
51	Sb	1.07	8.64	133
52	Te	1.97	9	123
53	I	3.06	10.45	115
54	Xe	0	12.13	108
55	Cs	0.47	3.89	298
56	Ba	0	5.21	253

Z	Symbol	Electron Affinity (eV)	Ionization Energy (eV)	Radius (pm)
57	La	0.5	5.58	N/A
58	Ce	0.5	5.47	N/A
59	Pr	0	5.42	247
60	Nd	0	5.49	206
61	Pm	0	5.55	205
62	Sm	0.3	5.63	238
63	Eu	0	5.67	231
64	Gd	0.5	6.14	233
65	Tb	0.5	5.85	225
66	Dy	0	5.93	228
67	Ho	0	6.02	226
68	Er	0	6.1	226
69	Tm	0.3	6.18	222
70	Yb	0	6.25	222
71	Lu	0.5	5.43	217
72	Hf	0	6.65	208
73	Ta	0.32	7.89	200
74	W	0.82	7.98	193
75	Re	0.15	7.88	188
76	Os	1.1	8.7	185
77	Ir	1.57	9.1	180
78	Pt	2.13	9	177
79	Au	2.31	9.23	174
80	Hg	0	10.44	171
81	Tl	0.2	6.11	156
82	Pb	0.36	7.42	154
83	Bi	0.95	7.29	143
84	Po	1.9	8.42	135
85	At	2.8	9.2	127
86	Rn	0	10.75	120

Electron Affinity (eV): Hydrogen to Argon



Atomic Radius (pm): Hydrogen to Argon



The Quantum Periodic Table

Alkali Metals: Filled Shell + 1
Low Ionozation Energy, large radius
Closed S-Shell
Halogens: Filled Shell - 1
High electron affinity
Filled Shell: Noble Gases

n	s -shell		d and f shells filling										p-shell filling					
1	H																	He
2	Li	Be											B	C	N	O	F	Ne
3	Na	Mg											Al	Si	P	S	Cl	Ar
4/3	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
5/4	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
6/5/4	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
7/6/5	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og

Some tables have all f-shell elee-ments in lower box

	f2	f3	f4	f5	f6	f7	f8	f9	f10	f11	f12	f13	f14	d1	
4	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Lanthanides: Rare Earths
5	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr	Actinides

Filled Shells have high ionization energy, low electron affinity, minimal radii

Noble Gases
Filled outer s- or p-shell, non-reactive

Halogens
Filled p-shell – 1
High electron affinity
Bind by borrowing e$^-$: e.g. NaCl

Alkalai Metals
Filled p-shell + 1
Low Ionization Energy
Largest atoms (outer e$^-$ not tightly bound)
Bind by sharing outer e$^-$: e.g. H_2O, NaCl

Transition Elements
Those with an outer d-shell electron

Inner Transition Elements
Those with an outer f-shell electron

"Rats! I thought lanthanoids and actanoids were gonna be giant robots or something."