36-6 The Periodic Table

For atoms with more than one electron, the Schrödinger equation cannot be solved exactly. However, powerful approximation methods allow us to determine the energy levels of the atoms and wave functions of the electrons to a high degree of accuracy. As a first approximation, the Z electrons in an atom are assumed to be noninteracting. The Schrödinger equation can then be solved, and the resulting wave functions used to calculate the interaction of the electrons, which in turn can be used to better approximate the wave functions. Because the spin of an electron can have two possible components along an axis, there is an additional quantum number m_s, which can have the possible values $+\frac{1}{2}$ or $-\frac{1}{2}$. The state of each electron is thus described by the four quantum numbers n, ℓ, m, and m_s. The energy of the electron is determined mainly by the principal quantum number n (which is related to the radial dependence of the wave function) and by the orbital angular-momentum quantum number ℓ. Generally, the lower the values of n, the lower the energy; and for a given value of n, the lower the value of ℓ, the lower the energy. The dependence of the energy on ℓ is due to the interaction of the electrons in the atom with each other. In hydrogen, of course, there is only one electron, and the energy is independent of ℓ. The specification of n and ℓ for each electron in an atom is called the **electron configuration.** Customarily, ℓ is specified according to the same code used to label the states of the hydrogen atom rather than by its numerical value. The code is

	s	p	d	f	g	h
ℓ value	0	1	2	3	4	5

The n values are sometimes referred to as shells, which are identified by another letter code: $n = 1$ denotes the K shell;† $n = 2$, the L shell; and so on.

The electron configuration of atoms is constrained by the Pauli exclusion principle, which states that no two electrons in an atom can be in the same quantum state; that is, no two electrons can have the same set of values for the quantum numbers n, ℓ, m_ℓ, and m_s. Using the exclusion principle and the restrictions on the quantum numbers discussed in the previous sections (n is a positive integer, ℓ is an integer that ranges from 0 to $n - 1$, m_ℓ can have $2\ell + 1$ values from $-\ell$ to ℓ in integral steps, and m_s can be either $+\frac{1}{2}$ or $-\frac{1}{2}$), we can understand much of the structure of the periodic table.

† The designation of the $n = 1$ shell as K is usually found when dealing with X-ray levels where the final shell in an inner electron transition is labeled as K, L, M, and so on.

We have already discussed the lightest element, hydrogen, which has just one electron. In the ground (lowest energy) state, the electron has $n = 1$ and $\ell = 0$, with $m_\ell = 0$ and $m_s = +\frac{1}{2}$ or $-\frac{1}{2}$. We call this a 1s electron. The 1 signifies that $n = 1$, and the s signifies that $\ell = 0$.

As electrons are added to make the heavier atoms, the electrons go into those states that will give the lowest total energy consistent with the Pauli exclusion principle.

Helium ($Z = 2$)

The next element after hydrogen is helium ($Z = 2$), which has two electrons. In the ground state, both electrons are in the K shell with $n = 1$, $\ell = 0$, and $m_\ell = 0$; one electron has $m_s = +\frac{1}{2}$ and the other has $m_s = -\frac{1}{2}$. This configuration is lower in energy than any other two-electron configuration. The resultant spin of the two electrons is zero. Since the orbital angular momentum is also zero, the total angular momentum is zero. The electron configuration for helium is written $1s^2$. The 1 signifies that $n = 1$, the s signifies that $\ell = 0$, and the superscript 2 signifies that there are two electrons in this state. Since ℓ can be only 0 for $n = 1$, these two electrons fill the K ($n = 1$) shell. The energy required to remove the most loosely bound electron from an atom in the ground state is called the **ionization energy.** This energy is the binding energy of the last electron placed in the atom. For helium, the ionization energy is 24.6 eV, which is relatively large. Helium is therefore basically inert.

Lithium ($Z = 3$)

The next element, lithium, has three electrons. Since the K shell ($n = 1$) is completely filled with two electrons, the third electron must go into a higher energy shell. The next lowest energy shell after $n = 1$ is the $n = 2$ or L shell. The outer electron is much farther from the nucleus than are the two inner $n = 1$ electrons. It is most likely to be found at a radius near that of the second Bohr orbit, which is four times the radius of the first Bohr orbit.

The nuclear charge is partially screened from the outer electron by the two inner electrons. Recall that the electric field outside a spherically symmetric charge density is the same as if all the charge were at the center of the sphere. If the outer electron were completely outside the charge cloud of the two inner electrons, the electric field the outer electron would see would be that of a single charge $+e$ at the center due to the nuclear charge of $+3e$ and the charge $-2e$ of the inner electron cloud. However, the outer electron does not have a well-defined orbit; instead, it is itself a charge cloud that penetrates the charge cloud of the inner electrons to some extent. Because of this penetration, the effective nuclear charge $Z'e$ is somewhat greater than $+1e$. The energy of the outer electron at a distance r from a point charge $+Z'e$ is given by Equation 36-6, with the nuclear charge $+Z$ replaced by $+Z'$.

$$E = -\frac{1}{2}\frac{kZ'e^2}{r} \tag{36-46}$$

The greater the penetration of the inner electron cloud, the greater the effective nuclear charge $Z'e$ and the lower the energy. Because the penetration is greater for ℓ values closer to zero (see Figure 36-12), the energy of the outer electron in lithium is lower for the s state ($\ell = 0$) than for the p state ($\ell = 1$). The electron configuration of lithium in the ground state is therefore $1s^22s$. The ionization energy of lithium is only 5.39 eV. Because its outer electron is so loosely bound to the atom, lithium is very active chemically. It behaves like a one-electron atom, similar to hydrogen.

Beryllium (Z = 4)

The energy of the beryllium atom is a minimum if both outer electrons are in the 2s state. There can be two electrons with $n = 2$, $\ell = 0$, and $m_\ell = 0$ because of the two possible values for the spin quantum number m_s. The configuration of beryllium is thus $1s^2 2s^2$.

Boron to Neon (Z = 5 to Z = 10)

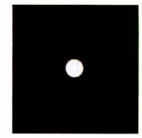
Since the 2s subshell is filled, the fifth electron must go into the next available (lowest energy) subshell, which is the 2p subshell, with $n = 2$ and $\ell = 1$. Since there are three possible values of m (+1, 0, and −1) and two values of m_s for each value of m_ℓ, there can be six electrons in this subshell. The electron configuration for boron is $1s^2 2s^2 2p$. The electron configurations for the elements carbon ($Z = 6$) to neon ($Z = 10$) differ from that for boron only in the number of electrons in the 2p subshell. The ionization energy increases with Z for these elements, reaching the value of 21.6 eV for the last element in the group, neon. Neon has the maximum number of electrons allowed in the $n = 2$ shell. The electron configuration for neon is $1s^2 2s^2 2p^6$. Because of its very high ionization energy, neon, like helium, basically is chemically inert. The element just before neon, fluorine, has a hole in the 2p subshell; that is, it has room for one more electron. It readily combines with elements such as lithium that have one outer electron. Lithium, for example, will donate its single outer electron to the fluorine atom to make an F^- ion and a Li^+ ion. These ions then bond together to form a molecule of lithium fluoride.

Sodium to Argon (Z = 11 to Z = 18)

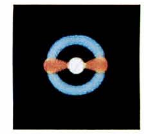
The eleventh electron must go into the $n = 3$ shell. Since this electron is very far from the nucleus and from the inner electrons, it is weakly bound in the sodium ($Z = 11$) atom. The ionization energy of sodium is only 5.14 eV. Sodium therefore combines readily with atoms such as fluorine. With $n = 3$, the value of ℓ can be 0, 1, or 2. Because of the lowering of the energy due to penetration of the electron shield formed by the other ten electrons (similar to that discussed for lithium) the 3s state is lower than the 3p or 3d states. This energy difference between subshells of the same n value becomes greater as the number of electrons increases. The electron configuration of sodium is $1s^2 2s^2 2p^6 3s^1$. As we move to elements with higher values of Z, the 3s subshell and then the 3p subshell fill. These two subshells can accommodate 2 + 6 = 8 electrons. The configuration of argon ($Z = 18$) is $1s^2 2s^2 2p^6 3s^2 3p^6$. One might expect the nineteenth electron to go into the third subshell (the d subshell with $\ell = 2$), but the penetration effect is now so strong that the energy of the next electron is lower in the 4s subshell than in the 3d subshell. There is thus another large energy difference between the eighteenth and nineteenth electrons, and so argon, with its full 3p subshell, is basically stable and inert.

Elements With Z > 18

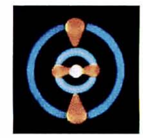
The nineteenth electron in potassium ($Z = 19$) and the twentieth electron in calcium ($Z = 20$) go into the 4s subshell rather than the 3d subshell. The electron configurations of the next ten elements, scandium ($Z = 21$) through zinc ($Z = 30$),



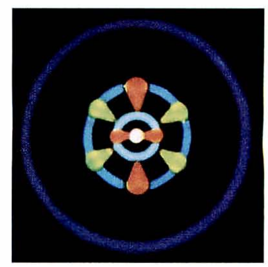
Hydrogen



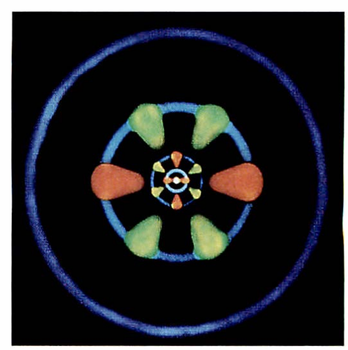
Carbon



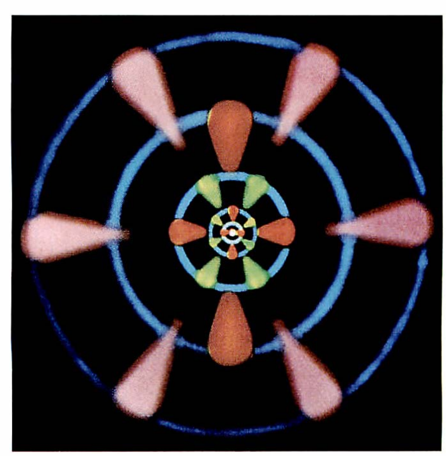
Silicon



Iron



Silver



Europium

A schematic depiction of the electron configurations in atoms. The spherically symmetric s states can contain 2 electrons and are colored white and blue. The dumbbell-shaped p states can contain up to 6 electrons and are colored orange. The d states can contain up to 10 electrons and are colored yellow-green. The f states can contain up to 14 electrons and are colored purple.

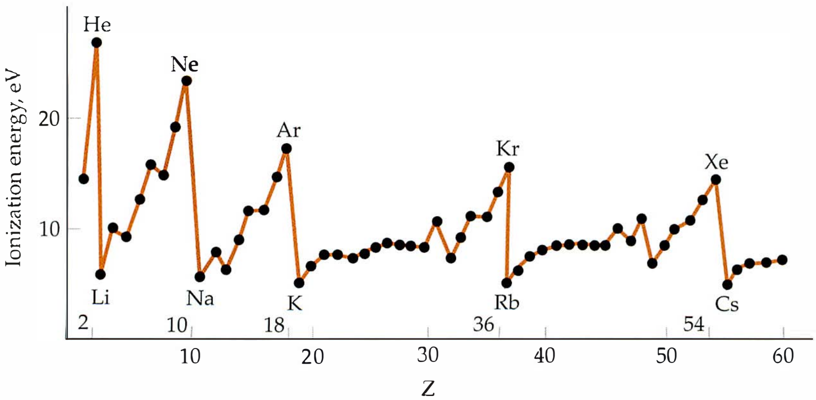


FIGURE 36-17 Ionization energy versus Z for Z = 1 to Z = 60. This energy is the binding energy of the last electron in the atom. The binding energy increases with Z until a shell is closed at Z = 2, 10, 18, 36, and 54. Elements with a closed shell plus one outer electron, such as sodium (Z = 11), have very low binding energies because the outer electron is very far from the nucleus and is shielded by the inner core electrons.

differ only in the number of electrons in the 3d shell, except for chromium (Z = 24) and copper (Z = 29), each of which has only one 4s electron. These ten elements are called **transition elements.**

Figure 36-17 shows a plot of the ionization energy versus Z for Z = 1 to Z = 60. The peaks in ionization energy at Z = 2, 10, 18, 36, and 54 mark the closing of a shell or subshell. Table 36-1 gives the ground-state electron configurations of the elements up to atomic number 109.

TABLE 36-1

Electron Configurations of the Atoms in Their Ground States

For some of the rare-earth elements (*Z* = 57 to 71) and the heavy elements (*Z* > 89) the configurations are not firmly established.

		Shell (*n*):	*K* (1)	*L* (2)		*M* (3)			*N* (4)				*O* (5)				*P* (6)			*Q* (7)
			s	s	p	s	p	d	s	p	d	f	s	p	d	f	s	p	d	s
Z	Element	Subshell (ℓ):	(0)	(0)	(1)	(0)	(1)	(2)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(1)
1	H	hydrogen	1																	
2	He	helium	2																	
3	Li	lithium	2	1																
4	Be	beryllium	2	2																
5	B	boron	2	2	1															
6	C	carbon	2	2	2															
7	N	nitrogen	2	2	3															
8	O	oxygen	2	2	4															
9	F	fluorine	2	2	5															
10	Ne	neon	2	2	6															
11	Na	sodium	2	2	6	1														
12	Mg	magnesium	2	2	6	2														
13	Al	aluminum	2	2	6	2	1													
14	Si	silicon	2	2	6	2	2													
15	P	phosphorus	2	2	6	2	3													
16	S	sulfur	2	2	6	2	4													
17	Cl	chlorine	2	2	6	2	5													
18	Ar	argon	2	2	6	2	6													
19	K	potassium	2	2	6	2	6		1											

TABLE 36-1 (continued)

Electron Configurations of the Atoms in Their Ground States

For some of the rare-earth elements (Z = 57 to 71) and the heavy elements (Z > 89) the configurations are not firmly established.

		Shell (n):	K (1)	L (2)		M (3)			N (4)				O (5)				P (6)			Q (7)
			s	s	p	s	p	d	s	p	d	f	s	p	d	f	s	p	d	s
Z	Element	Subshell (ℓ):	(0)	(0)	(1)	(0)	(1)	(2)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(1)
20	Ca	calcium		2	2	6	2	6	.	2										
21	Sc	scandium		2	2	6	2	6	1	2										
22	Ti	titanium		2	2	6	2	6	2	2										
23	V	vanadium		2	2	6	2	6	3	2										
24	Cr	chromium		2	2	6	2	6	5	1										
25	Mn	manganese		2	2	6	2	6	5	2										
26	Fe	iron		2	2	6	2	6	6	2										
27	Co	cobalt		2	2	6	2	6	7	2										
28	Ni	nickel		2	2	6	2	6	8	2										
29	Cu	copper		2	2	6	2	6	10	1										
30	Zn	zinc		2	2	6	2	6	10	2										
31	Ga	gallium		2	2	6	2	6	10	2	1									
32	Ge	germanium		2	2	6	2	6	10	2	2									
33	As	arsenic		2	2	6	2	6	10	2	3									
34	Se	selenium		2	2	6	2	6	10	2	4									
35	Br	bromine		2	2	6	2	6	10	2	5									
36	Kr	krypton		2	2	6	2	6	10	2	6									
37	Rb	rubidium		2	2	6	2	6	10	2	6	.	.	1						
38	Sr	strontium		2	2	6	2	6	10	2	6	.	.	2						
39	Y	yttrium		2	2	6	2	6	10	2	6	1	.	2						
40	Zr	zirconium		2	2	6	2	6	10	2	6	2	.	2						
41	Nb	niobium		2	2	6	2	6	10	2	6	4	.	1						
42	Mo	molybdenum		2	2	6	2	6	10	2	6	5	.	1						
43	Tc	technetium		2	2	6	2	6	10	2	6	6	.	1						
44	Ru	ruthenium		2	2	6	2	6	10	2	6	7	.	1						
45	Rh	rhodium		2	2	6	2	6	10	2	6	8	.	1						
46	Pd	palladium		2	2	6	2	6	10	2	6	10	.	.						
47	Ag	silver		2	2	6	2	6	10	2	6	10	.	1						
48	Cd	cadmium		2	2	6	2	6	10	2	6	10	.	2						
49	In	indium		2	2	6	2	6	10	2	6	10	.	2	1					
50	Sn	tin		2	2	6	2	6	10	2	6	10	.	2	2					
51	Sb	antimony		2	2	6	2	6	10	2	6	10	.	2	3					
52	Te	tellurium		2	2	6	2	6	10	2	6	10	.	2	4					
53	I	iodine		2	2	6	2	6	10	2	6	10	.	2	5					
54	Xe	xenon		2	2	6	2	6	10	2	6	10	.	2	6					
55	Cs	cesium		2	2	6	2	6	10	2	6	10	.	2	6	.	.	1		
56	Ba	barium		2	2	6	2	6	10	2	6	10	.	2	6	.	.	2		
57	La	lanthanum		2	2	6	2	6	10	2	6	10	.	2	6	1	.	2		

TABLE 36-1 (continued)

Electron Configurations of the Atoms in Their Ground States

For some of the rare-earth elements (Z = 57 to 71) and the heavy elements (Z > 89) the configurations are not firmly established.

		Shell (n):	K (1)	L (2)		M (3)			N (4)				O (5)				P (6)			Q (7)
			s	s	p	s	p	d	s	p	d	f	s	p	d	f	s	p	d	s
Z	Element	Subshell (ℓ):	(0)	(0)	(1)	(0)	(1)	(2)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(1)
58	Ce	cerium	2	2	6	2	6	10	2	6	10	1	2	6	1	.	2			
59	Pr	praseodymium	2	2	6	2	6	10	2	6	10	3	2	6	.	.	2			
60	Nd	neodymium	2	2	6	2	6	10	2	6	10	4	2	6	.	.	2			
61	Pm	promethium	2	2	6	2	6	10	2	6	10	5	2	6	.	.	2			
62	Sm	samarium	2	2	6	2	6	10	2	6	10	6	2	6	.	.	2			
63	Eu	europium	2	2	6	2	6	10	2	6	10	7	2	6	.	.	2			
64	Gd	gadolinium	2	2	6	2	6	10	2	6	10	7	2	6	1	.	2			
65	Tb	terbium	2	2	6	2	6	10	2	6	10	9	2	6	.	.	2			
66	Dy	dysprosium	2	2	6	2	6	10	2	6	10	10	2	6	.	.	2			
67	Ho	holmium	2	2	6	2	6	10	2	6	10	11	2	6	.	.	2			
68	Er	erbium	2	2	6	2	6	10	2	6	10	12	2	6	.	.	2			
69	Tm	thulium	2	2	6	2	6	10	2	6	10	13	2	6	.	.	2			
70	Yb	ytterbium	2	2	6	2	6	10	2	6	10	14	2	6	.	.	2			
71	Lu	lutetium	2	2	6	2	6	10	2	6	10	14	2	6	1	.	2			
72	Hf	hafnium	2	2	6	2	6	10	2	6	10	14	2	6	2	.	2			
73	Ta	tantalum	2	2	6	2	6	10	2	6	10	14	2	6	3	.	2			
74	W	tungsten (wolfram)	2	2	6	2	6	10	2	6	10	14	2	6	4	.	2			
75	Re	rhenium	2	2	6	2	6	10	2	6	10	14	2	6	5	.	2			
76	Os	osmium	2	2	6	2	6	10	2	6	10	14	2	6	6	.	2			
77	Ir	iridium	2	2	6	2	6	10	2	6	10	14	2	6	7	.	2			
78	Pt	platinum	2	2	6	2	6	10	2	6	10	14	2	6	9	.	1			
79	Au	gold	2	2	6	2	6	10	2	6	10	14	2	6	10	.	1			
80	Hg	mercury	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2			
81	Tl	thallium	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	1		
82	Pb	lead	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	2		
83	Bi	bismuth	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	3		
84	Po	polonium	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	4		
85	At	astatine	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	5		
86	Rn	radon	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	6		
87	Fr	francium	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	6	.	1
88	Ra	radium	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	6	.	2
89	Ac	actinium	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	6	1	2
90	Th	thorium	2	2	6	2	6	10	2	6	10	14	2	6	10	.	2	6	2	2
91	Pa	protactinium	2	2	6	2	6	10	2	6	10	14	2	6	10	1	2	6	2	2
92	U	uranium	2	2	6	2	6	10	2	6	10	14	2	6	10	3	2	6	1	2
93	Np	neptunium	2	2	6	2	6	10	2	6	10	14	2	6	10	4	2	6	1	2
94	Pu	plutonium	2	2	6	2	6	10	2	6	10	14	2	6	10	6	2	6	.	2
95	Am	americium	2	2	6	2	6	10	2	6	10	14	2	6	10	7	2	6	.	2

TABLE 36-1 (continued)

Electron Configurations of the Atoms in Their Ground States

For some of the rare-earth elements (Z = 57 to 71) and the heavy elements (Z > 89) the configurations are not firmly established.

		Shell (n):	K(1)	L(2)		M(3)			N(4)				O(5)				P(6)			Q(7)
			s	s	p	s	p	d	s	p	d	f	s	p	d	f	s	p	d	s
Z	Element		(0)	(0)	(1)	(0)	(1)	(2)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(3)	(0)	(1)	(2)	(1)
		Subshell (ℓ):																		
96	Cm	curium	2	2	6	2	6	10	2	6	10	14	2	6	10	7	2	6	1	2
97	Bk	berkelium	2	2	6	2	6	10	2	6	10	14	2	6	10	8	2	6	1	2
98	Cf	californium	2	2	6	2	6	10	2	6	10	14	2	6	10	10	2	6	.	2
99	Es	einsteinium	2	2	6	2	6	10	2	6	10	14	2	6	10	11	2	6	.	2
100	Fm	fermium	2	2	6	2	6	10	2	6	10	14	2	6	10	12	2	6	.	2
101	Md	mendelevium	2	2	6	2	6	10	2	6	10	14	2	6	10	13	2	6	.	2
102	No	nobelium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	.	2
103	Lr	lawrencium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	1	2
104	Rf	rutherfordium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	2	2
105	Db	dubnium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	3	2
106	Sg	seaborgium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	4	2
107	Bh	bohrium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	5	2
108	Hs	hassium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	6	2
109	Mt	meitnerium	2	2	6	2	6	10	2	6	10	14	2	6	10	14	2	6	7	2