GLOBAL
EDITION

Chemistry

A Molecular Approach

FIFTH EDITION

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List of Elements with Their Symbols and Atomic Masses

Element	Symbol	Atomic Number	Atomic Mass
Actinium	Ac	89	227.03[a]
Aluminum	Al	13	26.98
Americium	Am	95	243.06[a]
Antimony	Sb	51	121.76
Argon	Ar	18	39.95
Arsenic	As	33	74.92
Astatine	At	85	209.99[a]
Barium	Ba	56	137.33
Berkelium	Bk	97	247.07[a]
Beryllium	Be	4	9.012
Bismuth	Bi	83	208.98
Bohrium	Bh	107	264.12[a]
Boron	B	5	10.81
Bromine	Br	35	79.90
Cadmium	Cd	48	112.41
Calcium	Ca	20	40.08
Californium	Cf	98	251.08[a]
Carbon	C	6	12.01
Cerium	Ce	58	140.12
Cesium	Cs	55	132.91
Chlorine	Cl	17	35.45
Chromium	Cr	24	52.00
Cobalt	Co	27	58.93
Copernicium	Cn	112	285[a]
Copper	Cu	29	63.55
Curium	Cm	96	247.07[a]
Darmstadtium	Ds	110	271[a]
Dubnium	Db	105	262.11[a]
Dysprosium	Dy	66	162.50
Einsteinium	Es	99	252.08[a]
Erbium	Er	68	167.26
Europium	Eu	63	151.96
Fermium	Fm	100	257.10[a]
Flerovium	Fl	114	289[a]
Fluorine	F	9	19.00
Francium	Fr	87	223.02[a]
Gadolinium	Gd	64	157.25
Gallium	Ga	31	69.72
Germanium	Ge	32	72.63
Gold	Au	79	196.97
Hafnium	Hf	72	178.49
Hassium	Hs	108	269.13[a]
Helium	He	2	4.003
Holmium	Ho	67	164.93
Hydrogen	H	1	1.008
Indium	In	49	114.82
Iodine	I	53	126.90
Iridium	Ir	77	192.22
Iron	Fe	26	55.85
Krypton	Kr	36	83.80
Lanthanum	La	57	138.91
Lawrencium	Lr	103	262.11[a]
Lead	Pb	82	207.2
Lithium	Li	3	6.94
Livermorium	Lv	116	292[a]
Lutetium	Lu	71	174.97
Magnesium	Mg	12	24.31
Manganese	Mn	25	54.94
Meitnerium	Mt	109	268.14[a]
Mendelevium	Md	101	258.10[a]
Mercury	Hg	80	200.59
Molybdenum	Mo	42	95.95
Moscovium	Mc	115	289[a]
Neodymium	Nd	60	144.24
Neon	Ne	10	20.18
Neptunium	Np	93	237.05[a]
Nickel	Ni	28	58.69
Nihonium	Nh	113	284[a]
Niobium	Nb	41	92.91
Nitrogen	N	7	14.01
Nobelium	No	102	259.10[a]
Oganesson	Og	118	294[a]
Osmium	Os	76	190.23
Oxygen	O	8	16.00
Palladium	Pd	46	106.42
Phosphorus	P	15	30.97
Platinum	Pt	78	195.08
Plutonium	Pu	94	244.06[a]
Polonium	Po	84	208.98[a]
Potassium	K	19	39.10
Praseodymium	Pr	59	140.91
Promethium	Pm	61	145[a]
Protactinium	Pa	91	231.04
Radium	Ra	88	226.03[a]
Radon	Rn	86	222.02[a]
Rhenium	Re	75	186.21
Rhodium	Rh	45	102.91
Roentgenium	Rg	111	272[a]
Rubidium	Rb	37	85.47
Ruthenium	Ru	44	101.07
Rutherfordium	Rf	104	261.11[a]
Samarium	Sm	62	150.36
Scandium	Sc	21	44.96
Seaborgium	Sg	106	266.12[a]
Selenium	Se	34	78.97
Silicon	Si	14	28.09
Silver	Ag	47	107.87
Sodium	Na	11	22.99
Strontium	Sr	38	87.62
Sulfur	S	16	32.06
Tantalum	Ta	73	180.95
Technetium	Tc	43	98[a]
Tellurium	Te	52	127.60
Tennessine	Ts	117	294[a]
Terbium	Tb	65	158.93
Thallium	Tl	81	204.38
Thorium	Th	90	232.04
Thulium	Tm	69	168.93
Tin	Sn	50	118.71
Titanium	Ti	22	47.87
Tungsten	W	74	183.84
Uranium	U	92	238.03
Vanadium	V	23	50.94
Xenon	Xe	54	131.293
Ytterbium	Yb	70	173.05
Yttrium	Y	39	88.91
Zinc	Zn	30	65.38
Zirconium	Zr	40	91.22

[a] Mass of longest-lived or most important isotope.

Gallium (eka-aluminum)

	Mendeleev's predicted properties	Actual properties
Atomic mass	About 68 amu	69.72 amu
Melting point	Low	29.8 °C
Density	5.9 g/cm^3	5.90 g/cm^3
Formula of oxide	X_2O_3	Ga_2O_3
Formula of chloride	XCl_3	$GaCl_3$

Germanium (eka-silicon)

	Mendeleev's predicted properties	Actual properties
Atomic mass	About 72 amu	72.64 amu
Density	5.5 g/cm^3	5.35 g/cm^3
Formula of oxide	XO_2	GeO_2
Formula of chloride	XCl_4	$GeCl_4$

▲ **FIGURE 9.1 Eka-aluminum and Eka-silicon** Mendeleev's arrangement of elements in the periodic table allowed him to predict the existence of these elements, now known as gallium and germanium, and anticipate their properties.

Mendeleev's arrangement was a huge success, allowing him to predict the existence and properties of yet undiscovered elements such as eka-aluminum (later discovered and named gallium) and eka-silicon (later discovered and named germanium). The properties of these two elements are summarized in Figure 9.1▲. (As noted in Chapter 2, *eka* means "the one beyond" or "the next one" in a family of elements.) However, Mendeleev did encounter some difficulties. For example, according to accepted values of atomic masses, tellurium (with higher mass) should come *after* iodine. But based on their properties, Mendeleev placed tellurium *before* iodine and suggested that the mass of tellurium was erroneous. The mass was correct; later work by the English physicist Henry Moseley (1887–1915) showed that listing elements according to *atomic number*, rather than atomic mass, resolves this problem and results in even better correlation with elemental properties.

Notice the scientific approach in practice in the history of the periodic table. A number of related observations led to a scientific law—the periodic law. Mendeleev's table, an expression of the periodic law, had predictive power as laws usually do. However, it did not explain *why* the properties of elements recurred or *why* certain elements had similar properties. Recall from Chapter 1 that laws *summarize* behavior while theories *explain* behavior. The theory that explains the reasons behind the periodic law is quantum-mechanical theory. In this chapter, we explore the connection between the periodic table and quantum-mechanical theory.

9.3 Electron Configurations: How Electrons Occupy Orbitals

WATCH **NOW!**

KEY CONCEPT VIDEO 9.3
Electron Configurations

Quantum-mechanical theory describes the behavior of electrons in atoms. Since chemical bonding involves the transfer or sharing of electrons, quantum-mechanical theory helps us understand and describe chemical behavior. As we saw in Chapter 8, electrons in atoms exist within orbitals. An **electron configuration** for an atom shows the particular orbitals that electrons occupy for that atom. For example, consider the **ground state**—or lowest energy state—electron configuration for a hydrogen atom:

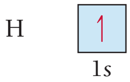
$$\text{H} \qquad \underset{\text{Orbital}}{1s}{}^{1} \longleftarrow \text{Number of electrons in orbital}$$

The electron configuration indicates that hydrogen's one electron is in the 1*s* orbital. Electrons generally occupy the lowest energy orbitals available. Since the 1*s* orbital is the lowest energy orbital in hydrogen (see Section 8.5), hydrogen's electron occupies that orbital. If we could write electron configurations for all the elements, we could see how the arrangements of the electrons within their atoms correlate with the element's chemical properties. However, the Schrödinger equation solutions (the atomic orbitals and their energies) that we described in Chapter 8 are for the hydrogen atom. What do the atomic orbitals of *other atoms* look like? What are their relative energies?

The Schrödinger equation for multielectron atoms has terms to account for the interactions of the electrons with one another that make it too complicated to solve exactly. However, approximate solutions indicate that the orbitals in multielectron atoms are hydrogen-like—they are similar to the *s*, *p*, *d*, and *f* orbitals that we examined in Chapter 8. In order to see how the electrons in multielectron atoms occupy these hydrogen-like orbitals, we must examine two additional concepts: *the effects of electron spin*, a fundamental property of all electrons that affects the number of electrons allowed in any one orbital; and *sublevel energy splitting*, which determines the order of orbital filling within a level.

Electron Spin and the Pauli Exclusion Principle

We can represent the electron configuration of hydrogen ($1s^1$) in a slightly different way with an **orbital diagram**, which gives similar information but symbolizes the electron as an arrow and the orbital as a box. The orbital diagram for a hydrogen atom is:



In an orbital diagram, the direction of the arrow (pointing up or pointing down) represents the orientation of the *electron's spin*. Recall from Section 8.5 that the orientation of the electron's spin is quantized, with only two possibilities—spin up ($m_s = +\frac{1}{2}$) and spin down ($m_s = -\frac{1}{2}$). In an orbital diagram, $m_s = +\frac{1}{2}$ is represented with a half-arrow pointing up (↿) and $m_s = -\frac{1}{2}$ is represented with a half-arrow pointing down (⇂). In a collection of hydrogen atoms, the electrons in about half of the atoms are spin up and the electrons in the other half are spin down. Since no additional electrons are present within the hydrogen atom, we conventionally represent the hydrogen atom electron configuration with its one electron as spin up.

Helium is the first element on the periodic table that contains two electrons. Its two electrons occupy the 1*s* orbital:

He $1s^2$

How do the spins of the two electrons in helium align relative to each other? The answer to this question is addressed by the **Pauli exclusion principle**, formulated by Wolfgang Pauli (1900–1958) in 1925:

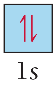
> **Pauli exclusion principle: no two electrons in an atom can have the same four quantum numbers.**

Since two electrons occupying the same orbital have three identical quantum numbers (n, l, and m_l), they must have different spin quantum numbers. Because there are only two possible spin quantum numbers ($+\frac{1}{2}$ and $-\frac{1}{2}$), the Pauli exclusion principle implies that *each orbital can have a maximum of only two electrons, with opposing spins*.

By applying the exclusion principle, we write an electron configuration and orbital diagram for helium as follows:

Electron configuration Orbital diagram

He $1s^2$



The following table shows the four quantum numbers for each of the two electrons in helium:

n	l	m_l	m_s
1	0	0	$+\frac{1}{2}$
1	0	0	$-\frac{1}{2}$

The two electrons have three quantum numbers in common (because they are in the same orbital) but have different spin quantum numbers (as indicated by the opposing half-arrows in the orbital diagram).

Sublevel Energy Splitting in Multielectron Atoms

Understanding the underlying reasons for sublevel energy splitting routinely causes my students confusion. This section of text, beginning here and extending to p. 409, is generally well-written and clear, but I have a few suggestions for improvement.

A major difference in the (approximate) solutions to the Schrödinger equation for multielectron atoms compared to the solutions for the hydrogen atom is the energy ordering of the orbitals. In the hydrogen atom, the energy of an orbital depends only on n, the principal quantum number. For example, the $3s$, $3p$, and $3d$ orbitals (which are empty for hydrogen in its lowest energy state) all have the same energy—they are **degenerate**. The orbitals within a principal level of a *multielectron atom*, in contrast, are not degenerate—their energy depends on the value of l. We say that the energies of the sublevels are *split*. In general, the lower the value of *l within a principal level*, the lower the energy (E) of the corresponding orbital. Thus, for a given value of n:

$$E(s \text{ orbital}) < E(p \text{ orbital}) < E(d \text{ orbital}) < E(f \text{ orbital})$$

In order to understand why the sublevels split in this way, we must examine three key concepts associated with the energy of an electron in the vicinity of a nucleus: (1) Coulomb's law, which describes the interactions between charged particles; (2) shielding, which describes how one electron can shield another electron from the full charge of the nucleus; and (3) penetration, which describes how one atomic orbital can overlap spatially with another, thus penetrating into a region that is close to the nucleus (and therefore less shielded from nuclear charge). We then discuss how these concepts, together with the spatial distributions of electron probability for each orbital, result in the energy ordering that we just saw.

Coulomb's Law

The attractions and repulsions between charged particles, first introduced in Section 2.4, are described by **Coulomb's law**, which states that the potential energy (E) of two charged particles depends on their charges (q_1 and q_2) and on their separation (r):

$$E = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r} \qquad [9.1]$$

In this equation, ε_0 is a constant ($\varepsilon_0 = 8.85 \times 10^{-12}\ \mathrm{C^2/J \cdot m}$). The potential energy is positive for charges of the same sign (plus × plus, or minus × minus) and negative for charges of opposite sign (plus × minus, or minus × plus). The *magnitude* of the potential energy depends inversely on the separation between the charged particles. We can draw three important conclusions from Coulomb's law:

- For like charges, the potential energy (E) is positive and decreases as the particles get *farther apart* (as r increases). Since systems tend toward lower potential energy, like charges repel each other (in much the same way that like poles of two magnets repel each other).
- For opposite charges, the potential energy is negative and becomes more negative as the particles get *closer together* (as r decreases). Therefore, opposite charges (like opposite poles on a magnet) *attract each other.*
- The *magnitude* of the interaction between charged particles increases as the charges of the particles increase. Consequently, an electron with a charge of 1− is more strongly attracted to a nucleus with a charge of 2+ than it is to a nucleus with a charge of 1+.

ANSWER **NOW!**

9.1 Cc Conceptual Connection

COULOMB'S LAW According to Coulomb's law, what happens to the potential energy of two oppositely charged particles as they get closer together?

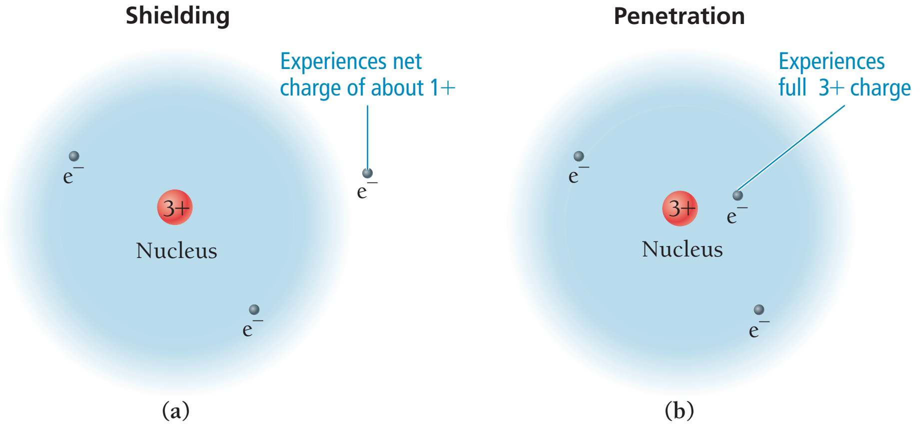
(a) Their potential energy decreases.
(b) Their potential energy increases.
(c) Their potential energy does not change.

Shielding

In multielectron atoms, any one electron experiences both the positive charge of the nucleus (which is attractive) and the negative charges of the other electrons (which are repulsive). We can think of the repulsion of one electron by other electrons as *screening* or **shielding** that electron from the full effects of the nuclear charge. For example, consider a lithium ion (Li^+). The lithium ion contains two electrons, so its electron configuration is identical to that of helium:

$$Li^+ \qquad 1s^2$$

Imagine bringing a third electron toward the lithium ion. When the third electron is far from the nucleus, it experiences the 3+ charge of the nucleus through the *screen* or *shield* of the 2− charge of the two 1*s* electrons, as shown in Figure 9.2(a)▼. We can think of the third electron as experiencing an **effective nuclear charge (Z_{eff})** of approximately 1+ (3+ from the nucleus and 2− from the electrons, for a net charge of 1+). The inner electrons in effect *shield* the outer electron from the full nuclear charge.



▲ **FIGURE 9.2 Shielding and Penetration** **(a)** An electron far from the nucleus is partly shielded by the electrons in the 1*s* orbital, reducing the effective net nuclear charge that it experiences. **(b)** An electron that penetrates the electron cloud of the 1*s* orbital experiences more of the nuclear charge.

Penetration

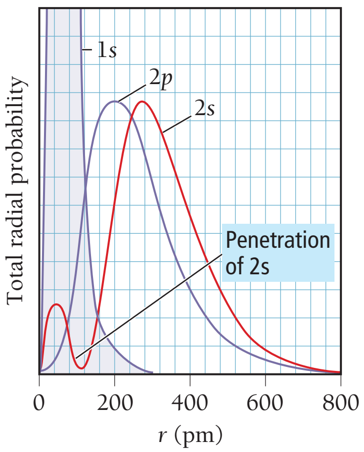
Now imagine allowing this third electron to come closer to the nucleus. As the third electron *penetrates* the electron cloud of the 1*s* electrons, it begins to experience the 3+ charge of the nucleus more fully because it is less shielded by the intervening electrons. If the electron could somehow get closer to the nucleus than the 1*s* electrons, it would experience the full 3+ charge, as shown in Figure 9.2(b)▲. In other words, as the outer electron undergoes **penetration** into the region occupied by the inner electrons, it experiences a greater nuclear charge and therefore (according to Coulomb's law) a lower energy.

The probability of an electron penetrating into the region occupied by inner electrons is described by its radial distribution function (which reflects the wave nature of the electron).

Electron Spatial Distributions and Sublevel Splitting

We now have examined the concepts we need to understand the energy splitting of the sublevels within a principal level. The splitting is a result of the spatial distributions of electrons within a sublevel. Recall from Section 8.6 that the radial distribution function for an atomic orbital shows the total probability of finding the electron within a thin spherical shell at a distance *r* from the nucleus.

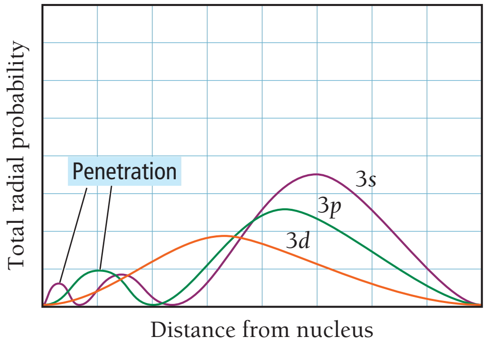
Figure 9.3▶ shows the radial distribution functions of the 2*s* and 2*p* orbitals superimposed on one another (the radial distribution function of the 1*s* orbital is also shown). Notice that, in general, an electron in a 2*p* orbital has a greater probability of being found closer to the nucleus than an electron in a 2*s* orbital. We might initially expect, therefore, that the 2*p* orbital would be lower in energy. However, exactly the opposite is true—the 2*s* orbital is actually lower in energy, *but only when the 1s orbital is occupied*. (When the 1*s* orbital is empty, the 2*s* and 2*p* orbitals are degenerate.) Why? The reason is the bump near $r = 0$ (near the nucleus) for the 2*s* orbital. This bump represents a significant probability of the electron being found very close to the nucleus. Even more importantly, this area of the probability penetrates into the 1*s* orbital—it gets into the region where shielding by the 1*s* electrons is less effective. In contrast, most of the probability in the radial distribution function of the 2*p* orbital lies *outside* the radial distribution function of the 1*s* orbital. Consequently, almost all of the 2*p* orbital is shielded from nuclear charge by the 1*s* orbital. The end result is that the 2*s* orbital—since it experiences more of the nuclear charge due to its greater *penetration*—is lower in energy than the 2*p* orbital. The results are similar when we compare the 3*s*, 3*p*, and 3*d* orbitals. The *s* orbitals penetrate more fully than the *p* orbitals, which in turn penetrate more fully than the *d* orbitals, as shown in Figure 9.4▶.



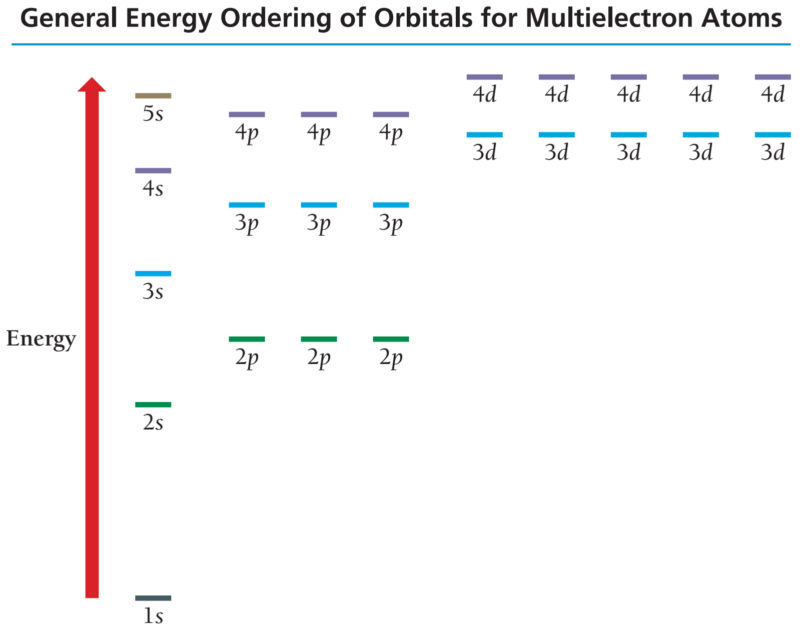
▲ **FIGURE 9.3 Radial Distribution Functions for the 1*s*, 2*s*, and 2*p* Orbitals**

Figure 9.5▼ shows the energy ordering of a number of orbitals in multielectron atoms. Notice these features of Figure 9.5:

- Because of penetration, the sublevels of each principal level are *not* degenerate for multielectron atoms.
- In the fourth and fifth principal levels, the effects of penetration become so important that the 4*s* orbital lies lower in energy than the 3*d* orbitals and the 5*s* orbital lies lower in energy than the 4*d* orbitals.
- The energy separations between one set of orbitals and the next become smaller for 4*s* orbitals and beyond, and the relative energy ordering of these orbitals can actually vary among elements. These variations result in irregularities in the electron configurations of the transition metals and their ions (as we shall see later).



▲ **FIGURE 9.4 Radial Distribution Functions for the 3*s*, 3*p*, 3*d* Orbitals** The 3*s* electrons penetrate most deeply into the inner orbitals, are least shielded, and experience the "greatest" effective nuclear charge. The 3*d* electrons penetrate least. This accounts for the energy ordering of the sublevels: *s* < *p* < *d*.



▲ **FIGURE 9.5 General Energy Ordering of Orbitals for Multielectron Atoms**

ANSWER **NOW!**

9.2 Cc Conceptual Connection

PENETRATION AND SHIELDING

Which statement is true?

(a) An orbital that penetrates into the region occupied by core electrons is more shielded from nuclear charge than an orbital that does not penetrate and therefore has a higher energy.
(b) An orbital that penetrates into the region occupied by core electrons is less shielded from nuclear charge than an orbital that does not penetrate and therefore has a higher energy.
(c) An orbital that penetrates into the region occupied by core electrons is less shielded from nuclear charge than an orbital that does not penetrate and therefore has a lower energy.
(d) An orbital that penetrates into the region occupied by core electrons is more shielded from nuclear charge than an orbital that does not penetrate and therefore has a lower energy.

Electron Configurations for Multielectron Atoms

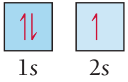
Unless otherwise specified, we use the term *electron configuration* to mean the ground state (or lowest energy) configuration.

Now that we know the energy ordering of orbitals in multielectron atoms, we can determine ground state electron configurations for the rest of the elements. Since we know that electrons occupy the lowest energy orbitals available when the atom is in its ground state and that only two electrons (with opposing spins) are allowed in each orbital, we can systematically build up the electron configurations for the elements. This pattern of orbital filling is known as the **aufbau principle** (the German word *aufbau* means "build up"). For lithium, with three electrons, the electron configuration and orbital diagram are:

Remember that the number of electrons in a neutral atom is equal to its atomic number.

Electron configuration Orbital diagram

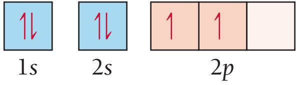
Li $1s^2 2s^1$



For carbon, which has six electrons, the electron configuration and orbital diagram are:

Electron configuration Orbital diagram

C $1s^2 2s^2 2p^2$



Electrons with parallel spins have correlated motion that minimizes their mutual repulsion.

Notice that the $2p$ electrons occupy the p orbitals (of equal energy) singly, rather than pairing in one orbital. This way of filling orbitals is known as **Hund's rule**, which states that *when filling degenerate orbitals, electrons fill them singly first, with parallel spins*. Hund's rule is a result of an atom's tendency to find the lowest energy state possible. When two electrons occupy separate orbitals of equal energy, the repulsive interaction between them is lower than when they occupy the same orbital because the electrons are spread out over different regions of space. By convention, we denote these parallel spins with half-arrows pointing up.

Summarizing Orbital Filling

- Electrons occupy orbitals so as to minimize the energy of the atom; therefore, lower energy orbitals fill before higher energy orbitals. Orbitals fill in the following order: $1s\ 2s\ 2p\ 3s\ 3p\ 4s\ 3d\ 4p\ 5s\ 4d\ 5p\ 6s$.
- Orbitals can hold no more than two electrons each. When two electrons occupy the same orbital, their spins are opposite. This is another way of expressing the Pauli exclusion principle (no two electrons in one atom can have the same four quantum numbers).
- When orbitals of identical energy are available, electrons first occupy these orbitals singly with parallel spins rather than in pairs. Once the orbitals of equal energy are half full, the electrons start to pair (Hund's rule).