FIGURE 2.1. *Two rocks.*

FIGURE 2.2. *The rock from Figure 2.1 in a hand.*

FIGURE 2.3. *The other rock from Figure 2.1, but now in a context from which its size can be judged.*

FIGURE 2.4. *The light bulb illuminates the rose. The light that bounces off the rose enters the eye, enabling us to see the rose.*
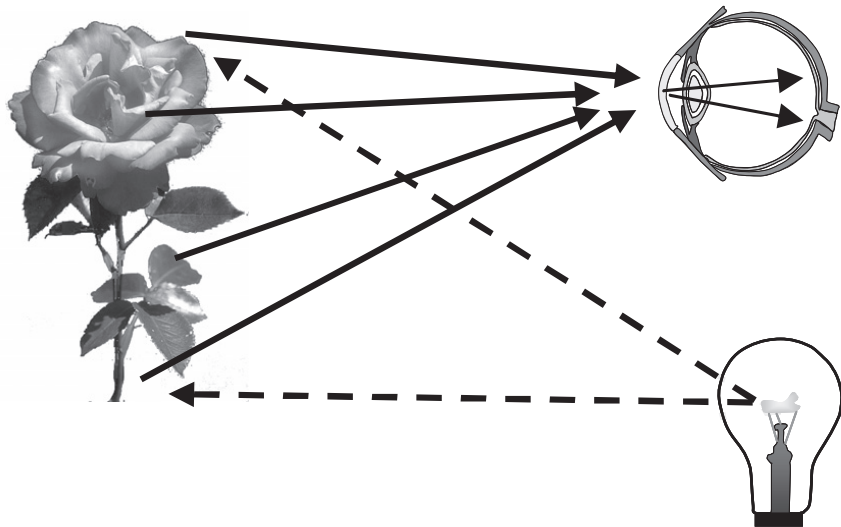
FIGURE 2.5. *A free particle in the form of a rock is shown moving along a trajectory.*
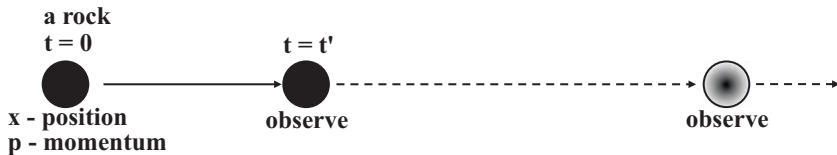
FIGURE 2.6. *A free particle in the form of a rock is moving along a trajectory. At time t = 0, it has position x and momentum p. At a later time, t = t', it has moved to a new position where it is observed, and its future position is predicted. However, some time later, a bird flies into the rock. The prediction made at t' is no longer valid.*
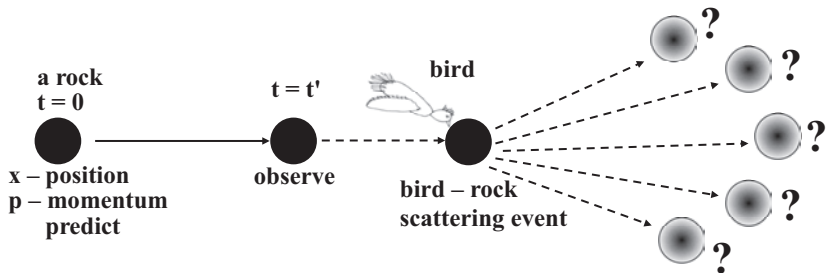
Figure 2.7. *At time, $t = 0$, an electron is moving along some trajectory. At time, $t = t'$, we observe it in a minimally invasive manner by letting it interact with a single particle of light, a photon. (Photons are discussed in detail later.) The electron-photon interaction causes a nonnegligible disturbance. It is not possible to make a causal prediction of what happens after the observation.*
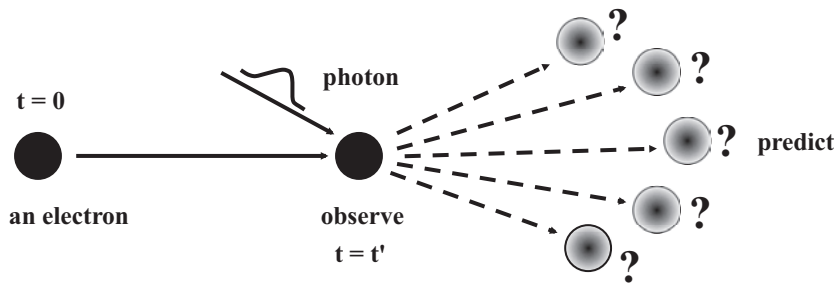
FIGURE 3.1. *A wave traveling in the x direction. The black line represents zero amplitude of the wave. The wave undergoes positive and negative oscillations about zero. The distance between the peaks is the wavelength. The wave is traveling along x with a velocity V.*
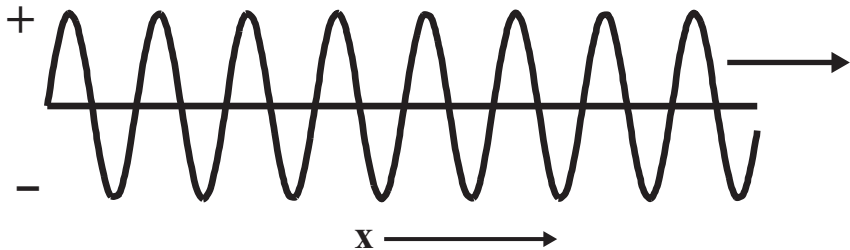
FIGURE 3.2. *Two identical waves that are in phase. The waves undergo positive and negative oscillations about zero (horizontal line). The positive peaks line up, and the negative peaks line up. They undergo constructive interference (are added together) to form a wave with twice the amplitude.*
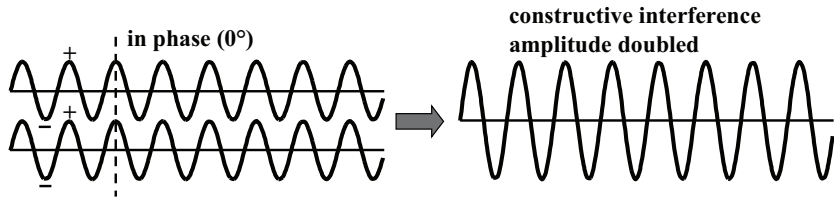
Figure 3.3. *Two identical waves that are 180° out of phase. The waves undergo positive and negative oscillations about zero (horizontal line). The positive peaks of the top wave line up exactly with the negative peaks of the bottom wave, and the negative peaks of the top wave line up exactly with the positive peaks of the bottom wave. The two waves undergo destructive interference when they are added together to produce zero amplitude.*
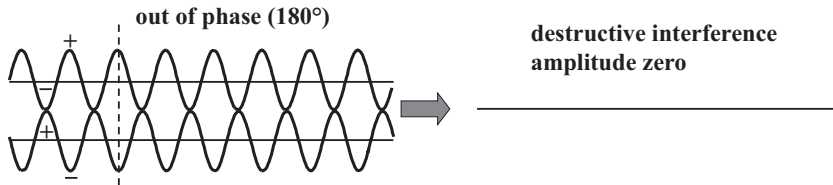
FIGURE 3.4. *The incoming light wave hits a 50% reflecting mirror. Half of the light goes through the mirror and half reflects from it. The light in each leg of the interferometer reflects from the end mirrors. Part of each beam crosses in the overlap region at a small angle. To the right of the circled overlap region is a blowup of what is seen along the x direction when two beams cross. An interference pattern is formed in which the intensity varies along x from a maximum value to zero periodically.*
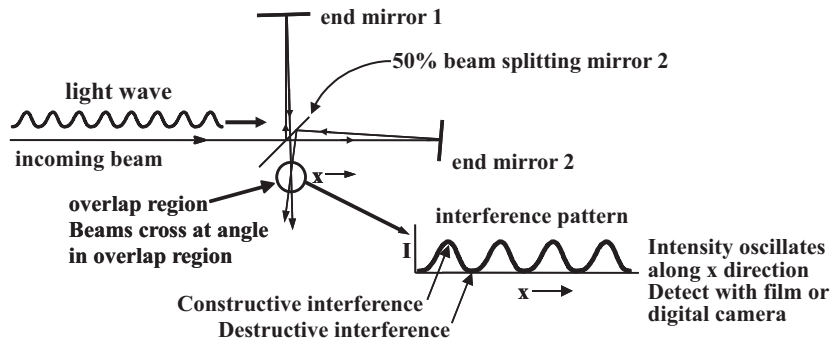
FIGURE 4.1. *The photoelectric effect. Light impinges on a metal, and electrons (negatively charged particles) are ejected. In the classical picture, light is a wave, and the interaction of the wave with the electrons in the metal causes them to fly out.*
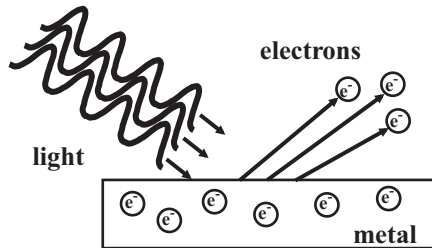
FIGURE 4.2. *A wave picture of the intensity dependence of the photoelectric effect. Low-intensity light has a small wave amplitude. Therefore, the wave should "hit" the electrons gently, and they will come out of the metal with a low speed. High-intensity light has a large wave amplitude. The large wave should hit the electrons hard, and the electrons will come out of the metal with a high speed.*
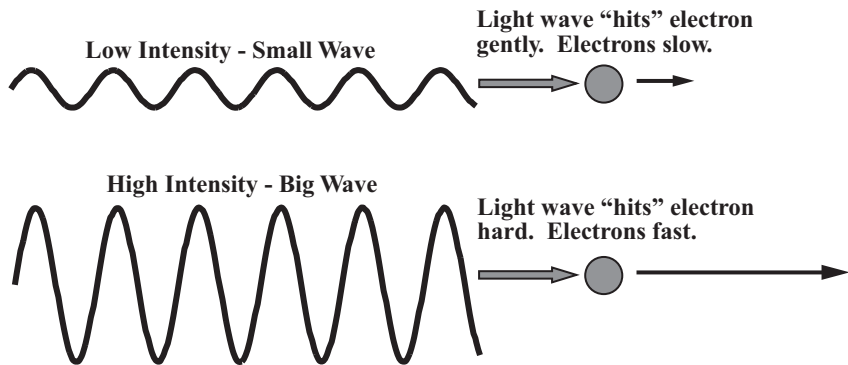
FIGURE 4.3. *Einstein described light as composed of discreet quanta of light "particles" called photons. In the photoelectric effect, one photon hits one electron and knocks it out of the metal.*
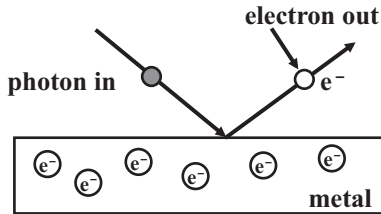
FIGURE 4.4. *An increase in the intensity of a light beam corresponds to the beam being composed of more photons. More photons can hit and eject more electrons, so an increase in intensity results in more electrons flying out of the metal.*
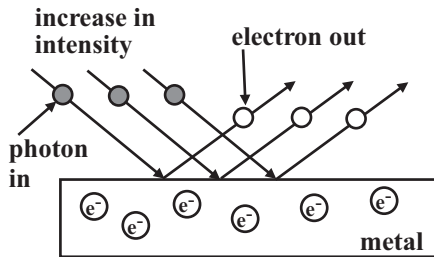
FIGURE 5.1. *The beam of light is composed of photons that hit a 50% reflecting mirror. In the initial incorrect description of the interference effect in terms of photons, it was thought that half of the photons go into each leg of the interferometer. The photons from each leg cross in the overlap region, and it was believed that the photons from one leg interfere with photons from the other leg to produce the interference pattern. The idea that photons from one leg interfere with photons from the other leg is not correct.*
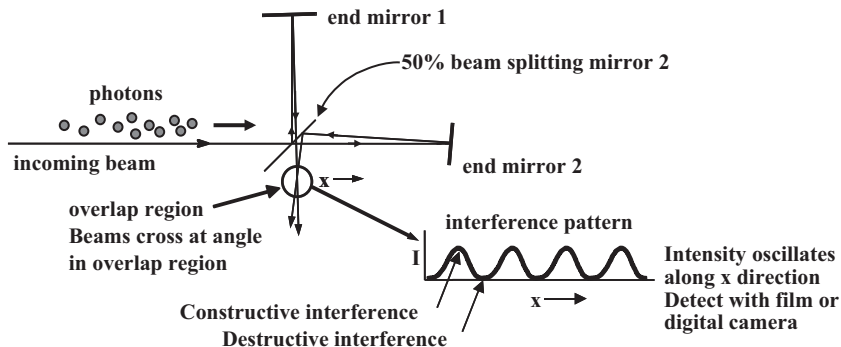
FIGURE 6.1. *The wavefunction for a free particle with momentum p, which has wavelength, λ = h/p. A quantum mechanical wavefunction can have two parts, called real and imaginary. Both waves have the same wavelength. They are just shifted by one-fourth of a wavelength, which is the same as a 90° shift in the phase. These two components are separate from each other. They do not interfere either constructively or destructively. For a free particle with the well-defined value of the momentum, p, the wave function extends from positive infinity to negative infinity, +∞ to −∞.*
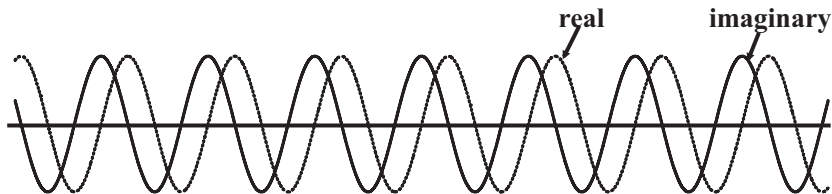

real   imaginary

Figure 6.2. *Five waves are shown that have different wavelengths. The wavelengths are λ = 1.2, 1.1, 1.0, 0.9, and 0.8. The phases are adjusted so all of the peaks of the waves match at 0 on the horizontal axis. However, because the waves have different wavelengths, they do not match up at other positions, in contrast to Figure 3.2. Note that at a position of approximately 10 or − 10, the dark gray wave has a positive peak, but the dashed light gray wave has a negative peak.*
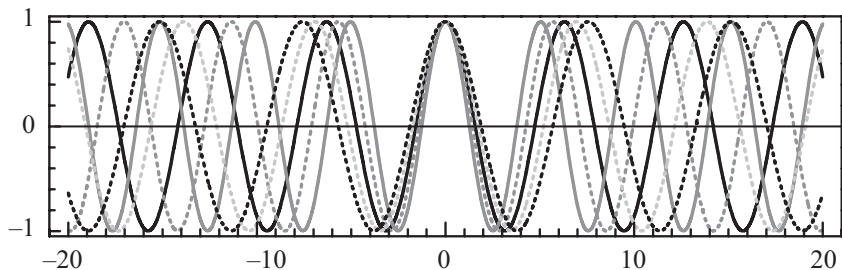
FIGURE 6.3. *The superposition of the five waves shown in Figure 6.2. At $x = 0$ (horizontal axis), all of the waves in figure 6.2 are in phase, so they add constructively. Near $x = 0$, the waves are still pretty much in phase, but the next set of maxima at about $x = 6$ and -6 are not as large as the maximum at $x = 0$. In the regions between 10 and 20 and -10 and -20, the difference in wavelengths makes some of the waves positive, where others are negative. There is significant cancellation.*
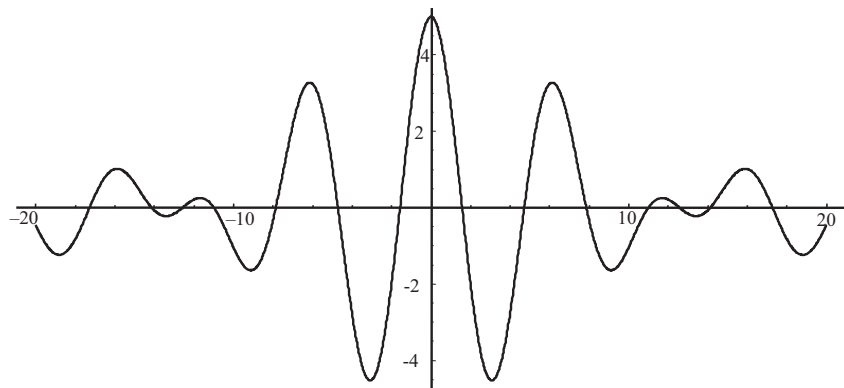
Figure 6.4. *The superimposition of 250 waves with equally spaced wavelengths spanning the wavelength range 0 to 4. Compared to Figure 6.3, which is the superposition of five waves, this superposition has a much larger peak at $x = 0$, the region of maximum constructive interference, and destructive interference reduces the other regions more. The amplitude of the superposition is dying out going toward $+ 20$.*
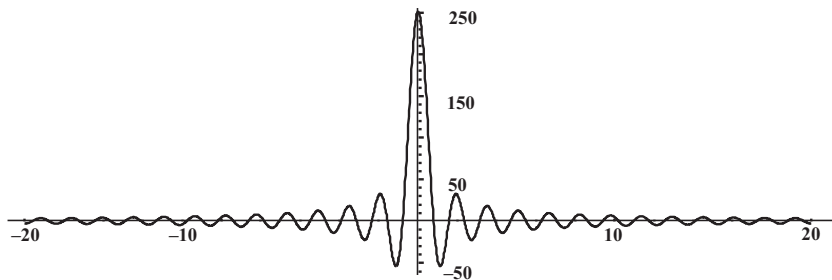
FIGURE 6.5. *A plot of the probability of finding a particle in a particular momentum eigenstate with momentum p given that it is in a superposition of momentum probability amplitude waves. p_0 is the middle wave with the biggest amplitude in the distribution. Δp is a measure of the width of the distribution of eigenstates.*
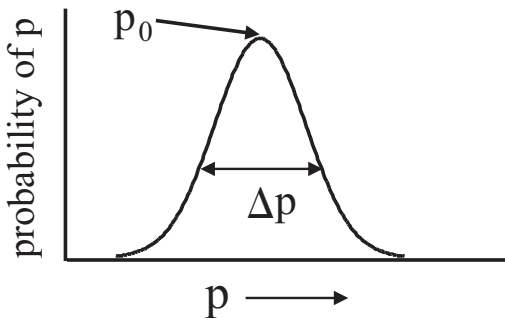
FIGURE 6.6. *A plot of the probability of finding the particle at a location x given that it is in the superposition of momentum eigenstates shown in Figure 6.5. x_0 is the middle position with the greatest probability. Δx is a measure of the width of the spatial distribution.*
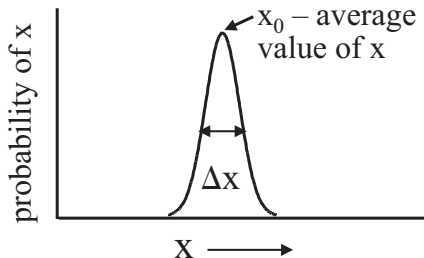
FIGURE 6.7. *The momentum (p) probability distributions and position (x) probability distributions for two wave packets. At the top, there is a large spread p (large Δp), which produces a small spread in x (small Δx). At the bottom, there is a small spread in p (small Δp), which gives rise to a large spread in x (large Δx).*
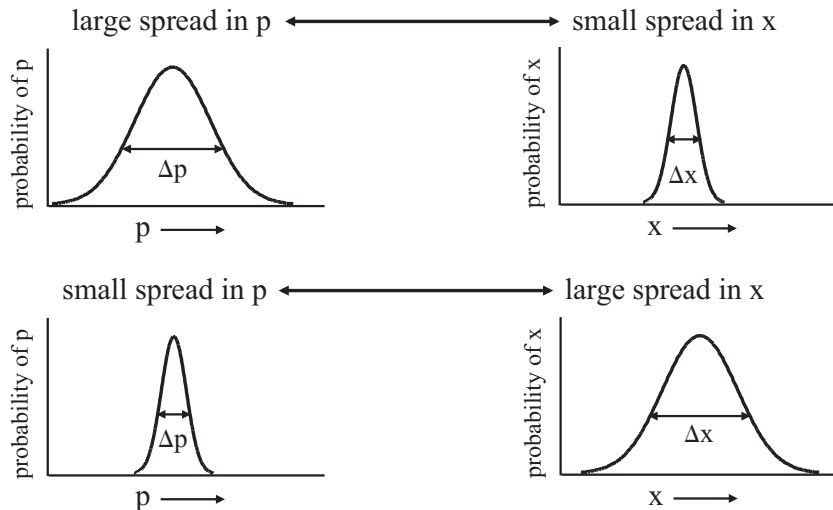
Figure 7.1. *Geometry of light diffraction from a grating. The grating is composed of a reflective surface, usually silver or gold, with very fine parallel grooves in it. The grating is shown here from the side. The grooves run into the page. The grooves have a very uniform spacing, d; α is the angle of the incoming light. The outgoing angles β depend on the color. Therefore, the colors are separated by diffraction.*
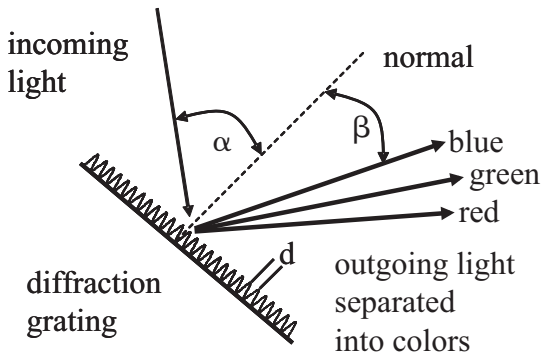
Figure 7.2. *Incoming photon wave packets are diffracted from a grating. The different colors reflect off of the grooves. For a particular color, there is a direction in which the waves corresponding to that color constructively interfere. They add to make a large amplitude wave, so the color looks very bright in that particular direction.*
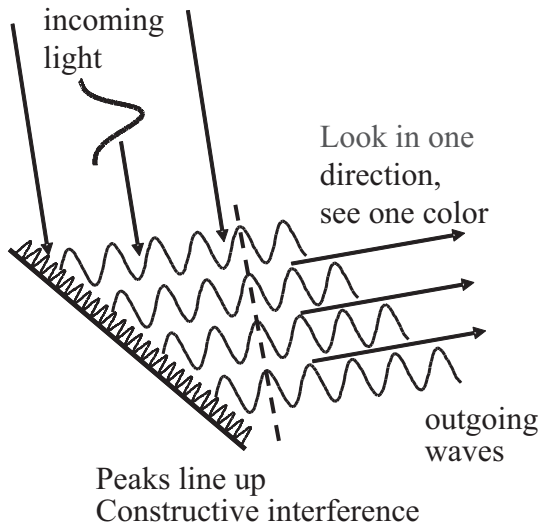
FIGURE 7.3. *A schematic of a cathode ray tube (CRT). The hot filament heats the cathode, which "boils" off electrons. The positively charged acceleration grid accelerates the negatively charged electrons. Voltages applied to the control grids steer the electrons to particular points on the screen. The screen is covered with tiny adjacent red, green, and blue spots that glow with their particular color when hit with electrons. By rapidly scanning the electron beam to hit the appropriate colors in a given spot on the screen the image is made.*
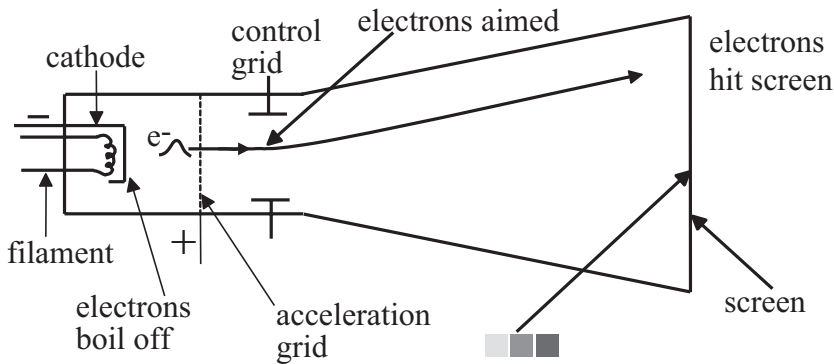
Figure 7.4. *A schematic of low-energy electron diffraction (LEED) from the surface of a crystal. An incoming beam of electrons, with low enough energy not to penetrate the crystal, strikes the surface. The lines of atoms act like the grooves of the diffraction grating in Figure 7.1. They diffract the incoming electron waves.*
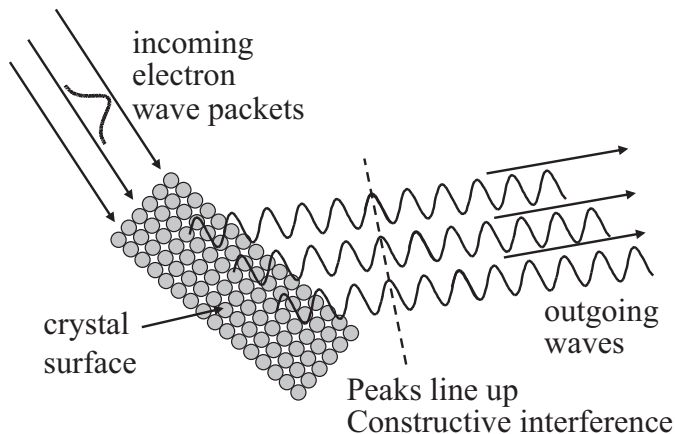
incoming electron wave packets

crystal surface

outgoing waves

Peaks line up
Constructive interference

FIGURE 7.5. *The lattice from Figure 7.4, with examples of different rows of atoms shown by the lines. For each line passing through the centers of atoms in a row, it is possible to draw more lines that are parallel to the initial line and that also pass through the centers of atoms. The spacings between these distinct parallel rows are different. Each set of rows causes diffraction in a different direction.*
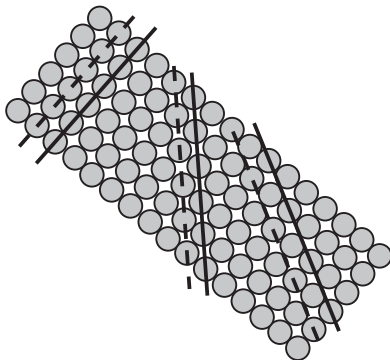
FIGURE 7.6. *Experimental data showing diffraction of electrons from the surface of a crystal. The various light spots are the electron diffraction spots. There are many spots because the diffraction occurs from the many different parallel rows of atoms (see Figure 7.5).*
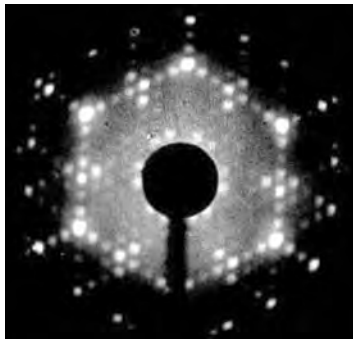
FIGURE 8.1. *A perfect one-dimensional box. The walls are infinitely high, infinitely thick, infinitely massive, and completely impenetrable. There is no air resistance in the box. In the box, Q, the potential energy is zero, and outside the box, it is infinite. The box has length, L.*
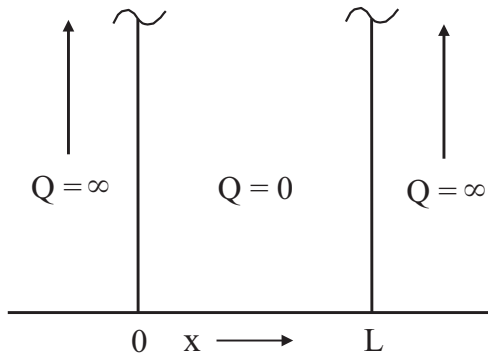

$Q = \infty$ $Q = 0$ $Q = \infty$

0   x ⟶   L

Figure 8.2. *A ball in a perfect one-dimensional racquetball court. There is no air resistance, and the ball is perfect. When the ball strikes the wall at L, it bounces off, hits the wall at 0, and keeps bouncing back and forth. Because the court is perfect, the ball is perfect, and there is no air resistance; once the ball starts bouncing, it keeps bouncing back and forth indefinitely.*
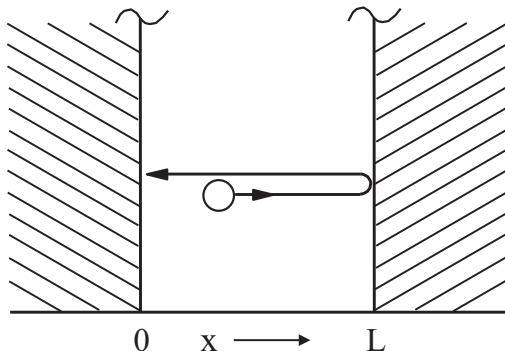
FIGURE 8.3. *A wavefunction inside the box that is discontinuous. The wavefunction is called φ. The vertical axis is the amplitude of the wavefunction. The dashed line shows where the wavefunction is zero, which must be outside the box. The wavefunction has a nonzero value at the walls and then must drop discontinuously (not smoothly) to zero outside the box.*
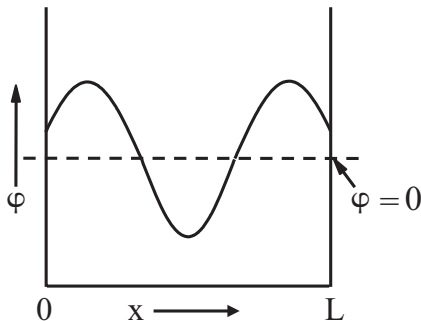
FIGURE 8.4. *Three examples of wavefunctions, φ, inside the box that are continuous. They have been shifted upward for clarity of presentation. The vertical axis is the amplitude of the wavefunction. The dashed line shows where the wave function is zero, which it must be outside the box. The wavefunctions, which have zero values at the walls, are continuous across the walls.*
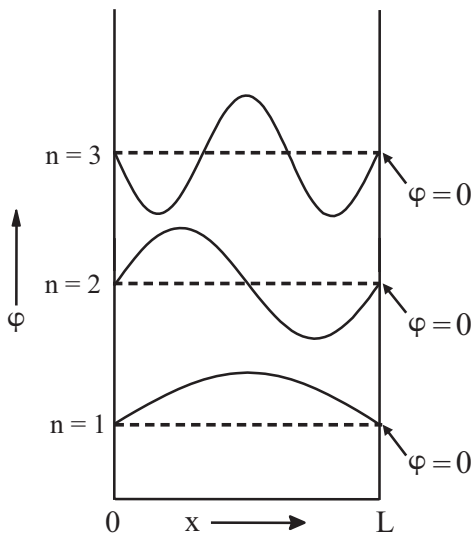
FIGURE 8.5. *The squares of the first three wavefunctions, φ^2, for the particle in a box. They have been shifted upward for clarity of presentation. The vertical axis is the amplitude of the wavefunction squared. The dashed line shows where the wavefunction is zero. The square of the wavefunctions are always positive because they represent probabilities. The wavefunctions shown in Figure 8.4 can be positive or negative.*
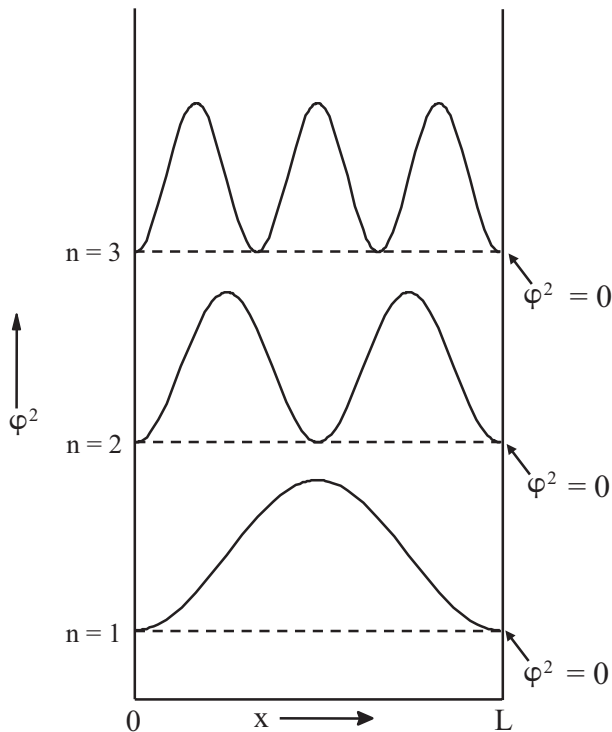
FIGURE 8.6. *Particle in a box energy levels. The quantum number is n. E is the energy, which increases as the square of the quantum number. The energy is plotted in units of $h^2/8mL^2$, so that it is easy to see how the energy increases. The dashed line is zero energy. The lowest energy level does not have E = 0, in contrast to a classical particle in a box.*
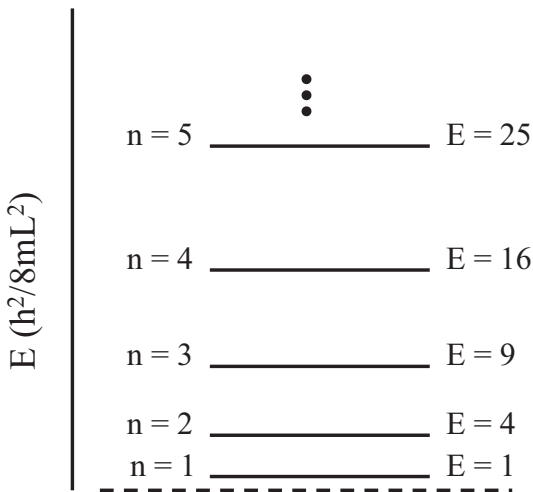
FIGURE 8.7. *Particle in a box energy levels. The quantum number is n. E is the energy plotted in units of $h^2/8mL^2$. The arrows indicate absorption of photons that can take an electron from the lowest energy level, n = 1, to higher energy levels, n = 2, n = 3, etc. For a photon to be absorbed, its energy must match the difference in energy between two energy levels.*
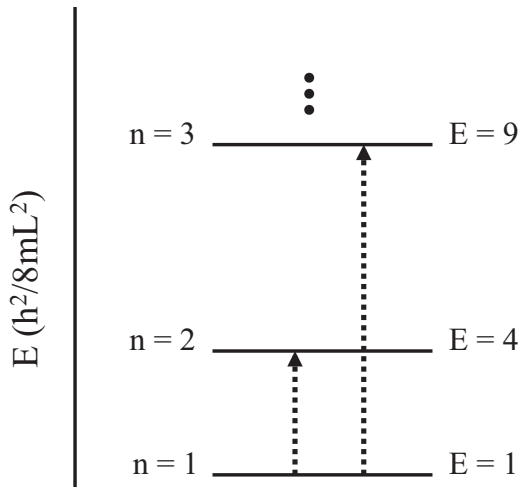
Figure 9.1. *The black body spectrum of the sun calculated using the Planck formula for black body radiation from a hot object. The curve is a good representation of the solar spectrum without some of the fine details. The lower axis is the frequency in wave numbers (see text). The top axis is the wave length in nanometers. The green light is 500 nm. Very blue is 400 nm; very red is 666 nm. The vertical axis is the amount of light (see text).*
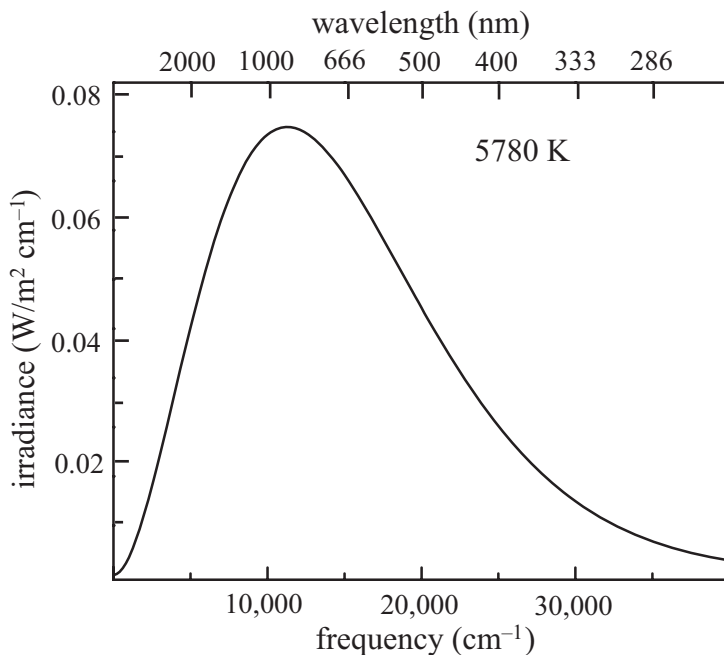
FIGURE 9.2. *The visible portion of the solar spectrum. The continuous range of colors is the black body spectrum. The dark lines or bands are colors that do not reach Earth, so they appear as colors missing from the solar spectrum. The wavelengths of the lines and the spectrum are given in nm, nanometers, which are billionths (10^{-9}) meters.*
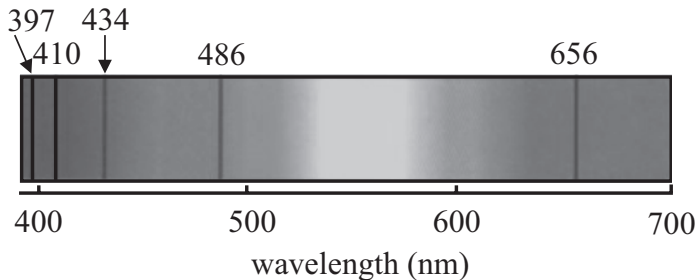
FIGURE 9.3. *Schematic of some of the energy levels that give rise to the Lyman and Balmer series of hydrogen atom emission lines. The down arrows indicate that light is being emitted from a hydrogen arc lamp, for example. For absorption, shown by the black lines in Figure 9.2, the arrows would point up. The level spacings are indicative but not to the true scale.*
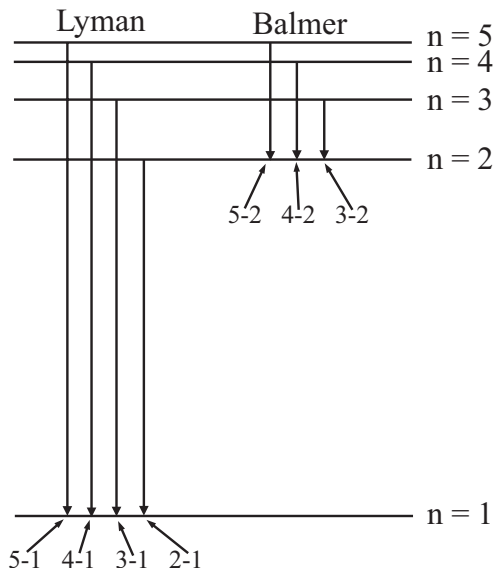
TABLE 10.1. *Quantum Numbers.*

$$n \implies 1, 2, 3, 4, 5, \cdots$$

$$l \implies 0 \text{ to } n-1 \text{ (integer steps)} \longrightarrow \begin{bmatrix} l = 0 & s & \text{called} \\ l = 1 & p & \text{orbital} \\ & & \text{or state} \\ l = 2 & d & \\ l = 3 & f & \end{bmatrix}$$

$$m \implies +l \text{ to } -l \text{ (integer steps)}$$

$$s \implies +1/2 \text{ or } -1/2 \longrightarrow \text{s only if more than one electron}$$

Figure 10.1. *Hydrogen energy level diagram. The spacings between the levels are not to scale. The first five energy levels are shown. The energy only depends on the principal quantum number, n. The orbitals and the number of each type are also shown. For n = 4, there is a single s orbital, three different p orbitals, five different d orbitals, and seven different f orbitals. The diagram would continue with the n = 6 level. The different levels are sometimes referred to as shells.*
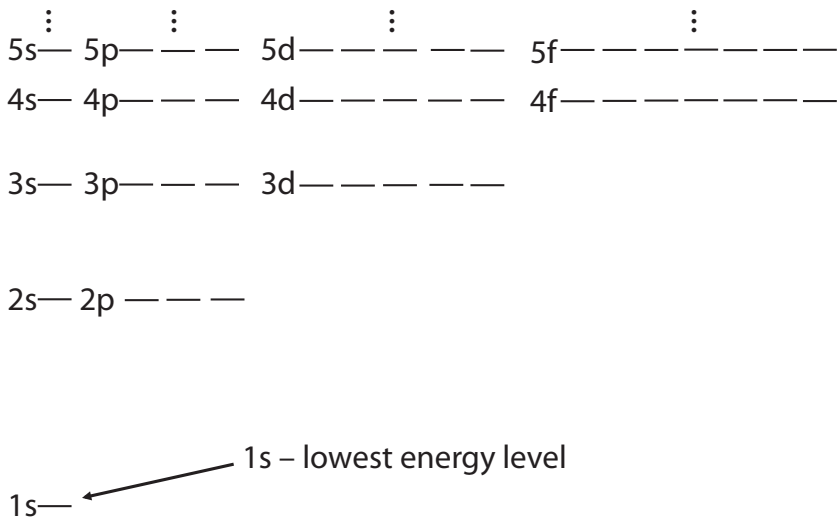
FIGURE 10.2. *The 1s, 2s, and 3s orbitals shown in two-dimensional representations. These are actually spherical. Darker represents a greater probability of finding the electron. Solid circles are distances with peaks in the probability. Dashed circles are nodes where the probability goes to zero. The way the orbitals are represented, they have a fairly sharp outer edge. The orbitals are waves that become very small at large distances, but only decay to zero as the distance from the center goes to infinity.*
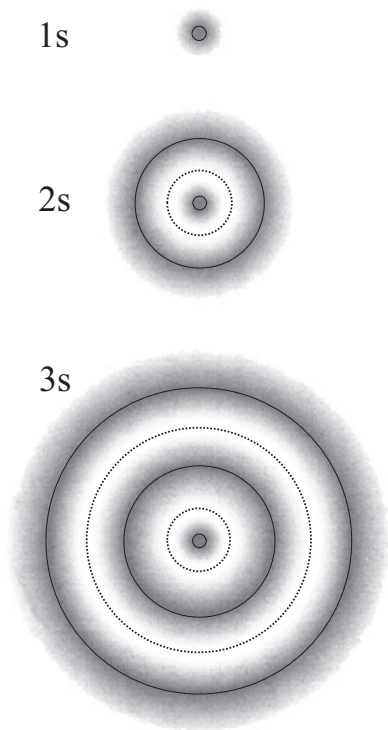
1s

2s

3s

Figure 10.3. *A plot of the 1s wavefunction* $\Psi(r)$ *as a function of r, the distance from the proton.* $\Psi(r)$ *is proportional to the probability of finding the electron along a line radially outward from the center of the atom. The distance r is in Å, which is* 10^{-10} *m.*
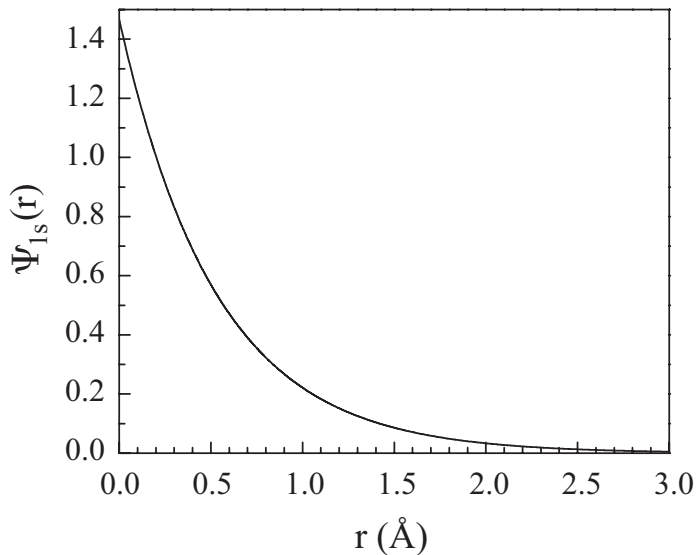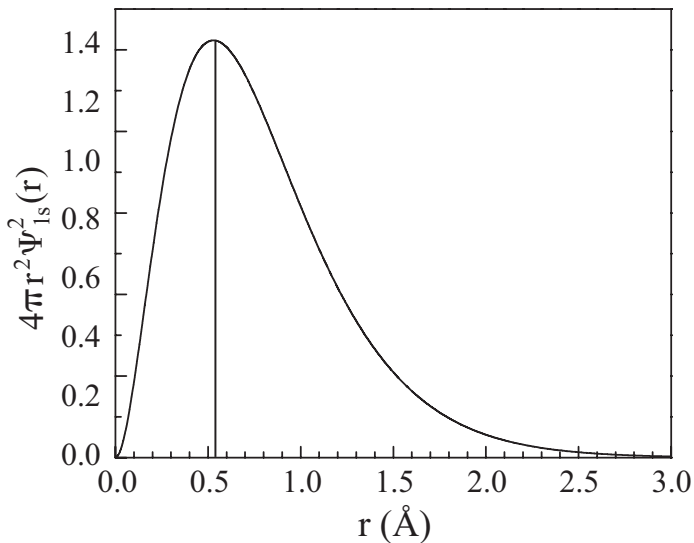
FIGURE 10.4. *A plot of the radial distribution function for the 1s orbital as a function of r, the distance from the proton. The radial distribution function is the probability of finding the electron in a thin spherical shell a distance r from the proton. The radial distribution function takes into account that the electron can be found in any direction radially outward from the proton. The distance r is in Å, which is 10^{-10} m.*

$$a_0 = \frac{\epsilon_o\, h^2}{\pi \mu e^2}$$

FIGURE 10.5. *A plot of the 2s hydrogen atom wavefunction (top panel) and the radial distribution function (bottom panel), as functions of r, the distance from the proton. The wavefunction begins positive, goes through a node at slightly more than 1 Å ($2a_0$), and then decays to zero. The radial distribution function shows that the maximum probability of finding the electron peaks at about 2.8 Å, with most of the probability between 2 and 4 Å (see Figure 10.2). The distance r is in Å, which is 10^{-10} m.*
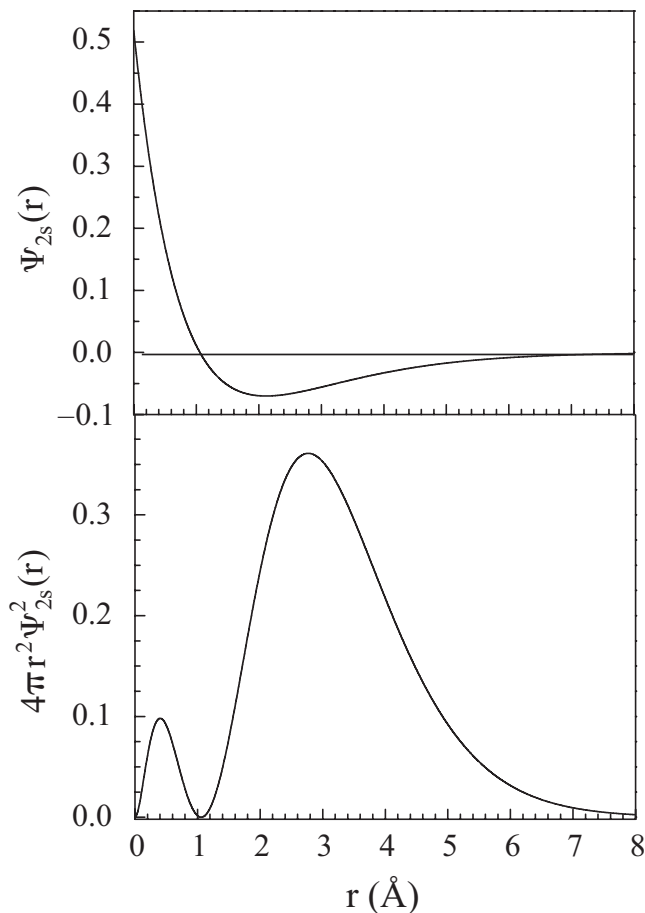
FIGURE 10.6. *A plot of the 3s hydrogen atom wavefunction (top panel) and the radial distribution function (bottom panel), as functions of r, the distance from the proton. The wavefunction begins positive, goes through a node, becomes negative, goes through a second node, and becomes positive again. It then decays to zero. The radial distribution function shows that the maximum probability of finding the electron peaks at about 7 Å, with most of the probability between 5 and 11 Å (see Figure 10.2). The distance r is in Å, which is 10^{-10} m.*
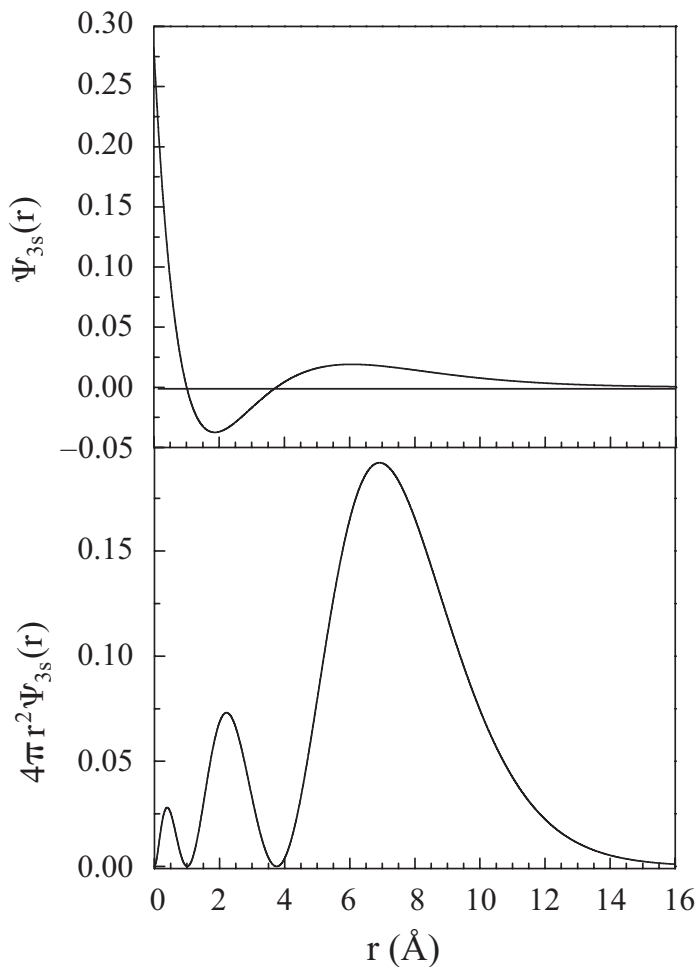
Figure 10.7. *Schematic of the three hydrogen atom 2p orbitals, $2p_z$, $2p_y$, and $2p_x$. Each orbital has two lobes, one positive and one negative. Each has an angular nodal plane, that is, a plane where the probability of finding the electron is zero. The $2p_z$ orbital has its lobes along the z axis, and the nodal plane is the xy plane, which is shaded. The $2p_y$ orbital has its lobes along the y axis, and the nodal plane is the xz plane. The $2p_x$ orbital has its lobes along the x axis, and the nodal plane is the yz plane. The lobes in each diagram show where most of the electron probability amplitude is located. These probability amplitude waves delay smoothly to zero away from the nucleus (the proton) and do not stop abruptly as in the diagrams.*
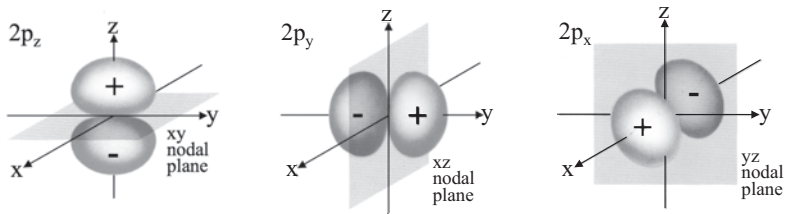
FIGURE 10.8. *Schematics of the five hydrogen atom 3d orbitals, which are named in relation to their shapes. Each orbital has two angular nodes, as well as positive and negative lobes. The angular nodes are the planes in four of the diagrams and the cones and disk in the fifth diagram. When a nodal plane is crossed, the wavefunction changes sign. The lobes in each diagram show where most of the electron probability amplitude is located. Four of the orbitals consist of four lobes. The d_z2 orbital has a different shape. It sill has two nodal surfaces, the xy plane and the conical surfaces. These probability amplitude waves decay smoothly to zero away from the nucleus (the proton) and do not stop abruptly as in the diagrams.*
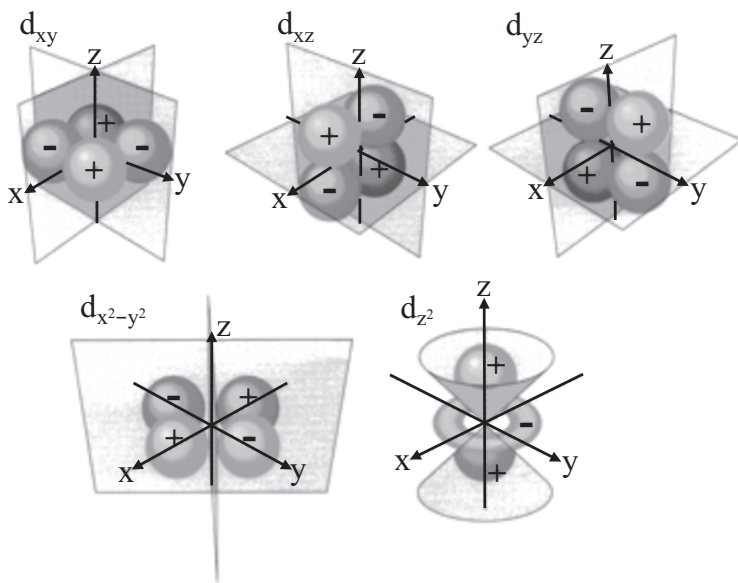
FIGURE 11.1. *Energy level diagram for atoms with many electrons. The spacings between the levels are not to scale. The energy depends on the principal quantum number, n, and the angular momentum quantum number, l, in contrast to the hydrogen atom (Figure 10.1), where the energy only depends on n. For n = 4, there is a single s orbital (l = 0), three different p orbitals (l = 1), five different d orbitals (l = 2), and seven different f orbitals (l = 3).*
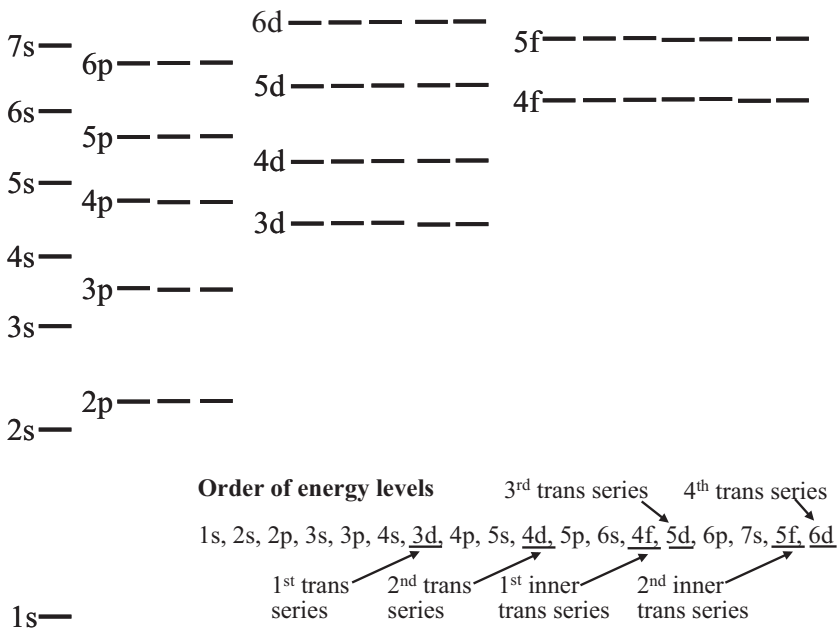
FIGURE 11.2. *Left-hand side: an electron represented by an arrow in an orbital. Right-hand side: two electrons in the same orbital. The s quantum numbers must be + 1/2 and − 1/2, represented by an up arrow and a down arrow, to obey the Pauli Exclusion principle. The spins are said to be paired.*
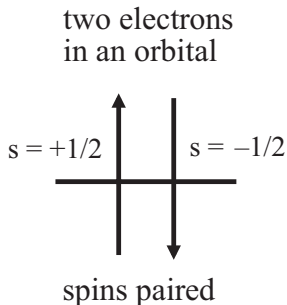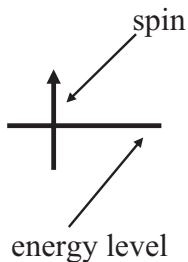
FIGURE 11.3. *Illustration of Hund's Rule. When filling the 2p orbitals, electron 1 is placed in 2p_x, electron 2 in 2p_y, and electron 3 in 2p_z. These are all spin up. Electron 4 will have to have its spin down, that is, pair, to avoid violating the Pauli Principle.*
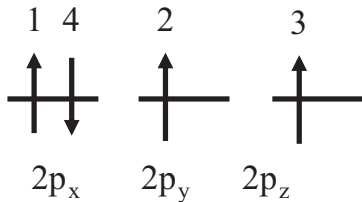
FIGURE 11.4. *The Periodic Table of Elements.*

TABLE 11.1. *List of the Elements—Alphabetical by Element*

Element	Symbol	Atomic Number	Element	Symbol	Atomic Number
Actinium	Ac	89	Mercury	Hg	80
Aluminum	Al	13	Meitnerium	Mt	109
Americium	Am	95	Molybdenum	Mo	42
Antimony	Sb	51	Neodymium	Nd	60
Argon	Ar	18	Neon	Ne	10
Arsenic	As	33	Neptunium	Np	93
Astatine	At	85	Nickel	Ni	28
Barium	Ba	56	Niobium	Nb	41
Berkelium	Bk	97	Nitrogen	N	7
Beryllium	Be	4	Nobelium	No	102
Bismuth	Bi	83	Osmium	Os	76
Bohrium	Bh	107	Oxygen	O	8
Boron	B	5	Palladium	Pd	46
Bromine	Br	35	Phosphorus	P	15
Cadmium	Cd	48	Platinum	Pt	78
Calcium	Ca	20	Plutonium	Pu	94
Californium	Cf	98	Polonium	Po	84
Carbon	C	6	Potassium	K	19
Cerium	Ce	58	Praseodymium	Pr	59
Cesium	Cs	55	Promethium	Pm	61
Chlorine	Cl	17	Protactinium	Pa	91
Chromium	Cr	24	Radium	Ra	88
Cobalt	Co	27	Radon	Rn	86
Copper	Cu	29	Rhenium	Re	75
Curium	Cm	96	Rhodium	Rh	45
Dubnium	Db	105	Rubidium	Rb	37
Dysprosium	Dy	66	Ruthenium	Ru	44
Einsteinium	Es	99	Rutherfordium	Rf	104
Erbium	Er	68	Samarium	Sm	62
Euorpium	Eu	63	Scandium	Sc	21
Fermium	Fm	100	Seaborgium	Sg	106
Fluorine	F	9	Selenium	Se	34
Francium	Fr	87	Silicon	Si	14
Gadolinium	Gd	64	Silver	Ag	47
Gallium	Ga	31	Sodium	Na	11
Germanium	Ge	32	Strontium	Sr	38
Gold	Au	79	Sulfur	S	16
Hafnium	Hf	72	Tantalum	Ta	73
Hassium	Hs	108	Technetium	Tc	43
Helium	He	2	Tellurium	Te	52
Holmium	Ho	67	Terbium	Tb	65
Htdrogen	H	1	Thallium	Tl	81
Indium	In	49	Thorium	Th	90
Iodine	I	53	Thulium	Tm	69
Iridium	Ir	77	Tin	Sn	50
Iron	Fe	26	Titanium	Ti	22
Krypton	Kr	36	Tungsten	W	74
Lanthanum	La	57	Uranium	U	92
Lawrencium	Lr	103	Vanadium	V	23
Lead	Pb	82	Xenon	Xe	54
Lithium	Li	5	Ytterbium	Yb	70
Lutetium	Lu	71	Yttrium	Y	39
Magnesium	Mg	12	Zinc	Zn	30
Manganese	Mn	25	Zirconium	Zr	40
Mendelevium	Md	101			

FIGURE 11.5. *The electron configuration for neon (Ne, 10). The second shell is complete.*
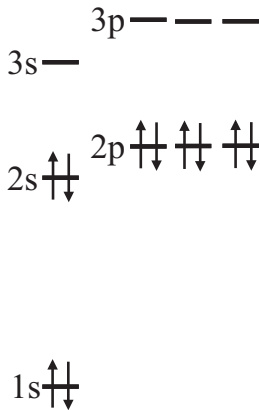
FIGURE 11.6. *The electron configuration for argon (Ar, 18). The third row is complete.*
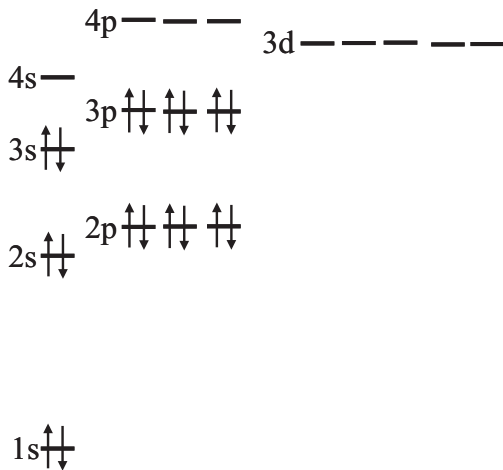
Figure 12.1. *A plot of the energy of two hydrogen atoms as they are brought close together. When the H atoms are very far apart, the energy of the system is the sum of the 1s orbital energies of two H atoms. This is taken to be the zero of energy, the dashed line. As the atoms come together, the energy decreases to a minimum. If they are brought even closer together, the energy increases rapidly.*
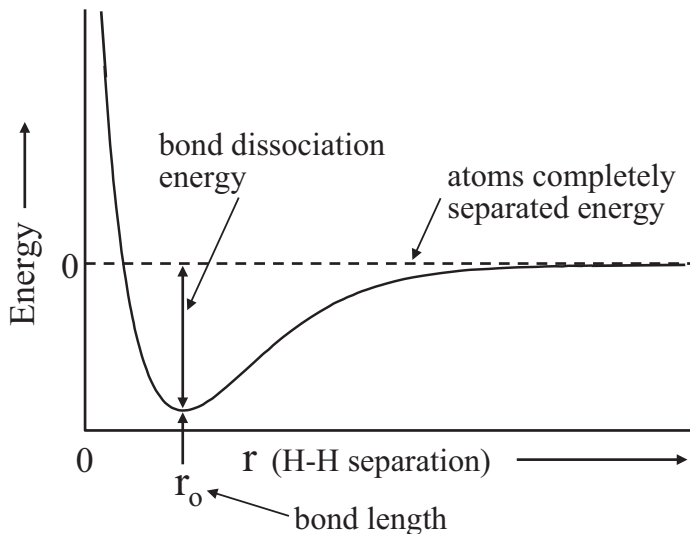
Figure 12.2. *The upper portion is a schematic of two hydrogen atom 1s orbitals. These are actually delocalized electron probability amplitude waves, represented here simply as circles. The lower proportion shows what happens when the two atoms are brought together to form the H_2 molecule. The two atomic orbitals combine to make a molecular orbital.*
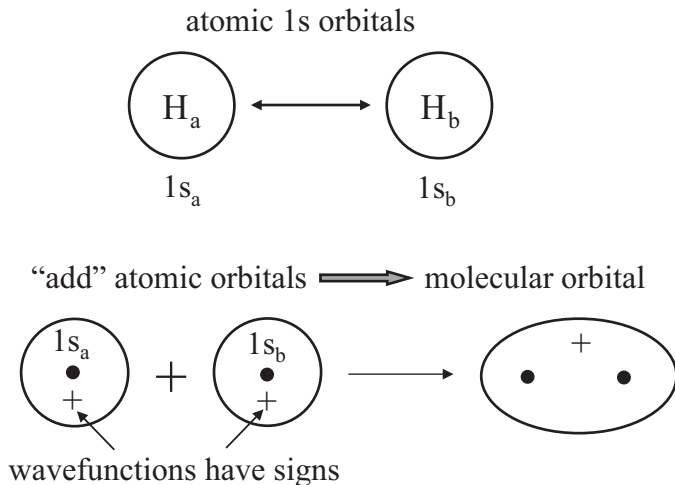
atomic 1s orbitals

Figure 12.3. *A one-dimensional plot of the square of the two 1s orbitals that belonged to H atoms a and b (solid curves), and the square of the sum of the atomic orbitals, which is the square of the molecular orbital. The electron density is concentrated between the two nuclei.*
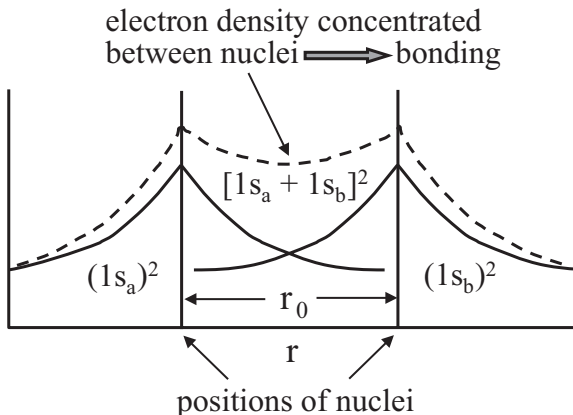
Figure 12.4. *The left side is a schematic of two hydrogen atom 1s orbitals that are being added together. Note that the probability amplitude waves have opposite signs. The two atomic orbitals combine to make a molecular orbital. Because of the opposite signs, there is destructive interference, in contrast to Figure 12.2.*

destructive interference   molecular orbital

$1s_a$ + $1s_b$ $\longrightarrow$

note signs   node – no electron density
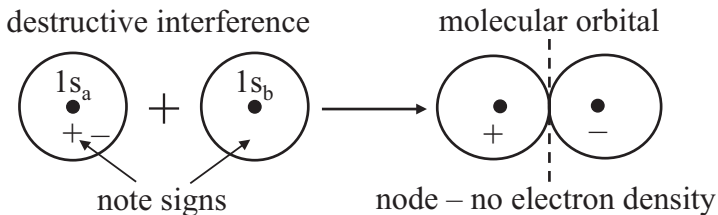
Figure 12.5. *A schematic plot of the energy curves of the bonding and antibonding molecular orbitals for two hydrogen atoms as they are brought closer together. In contrast to the bonding MO, the energy of the antibonding MO increases as the atomic separation is decreased.*
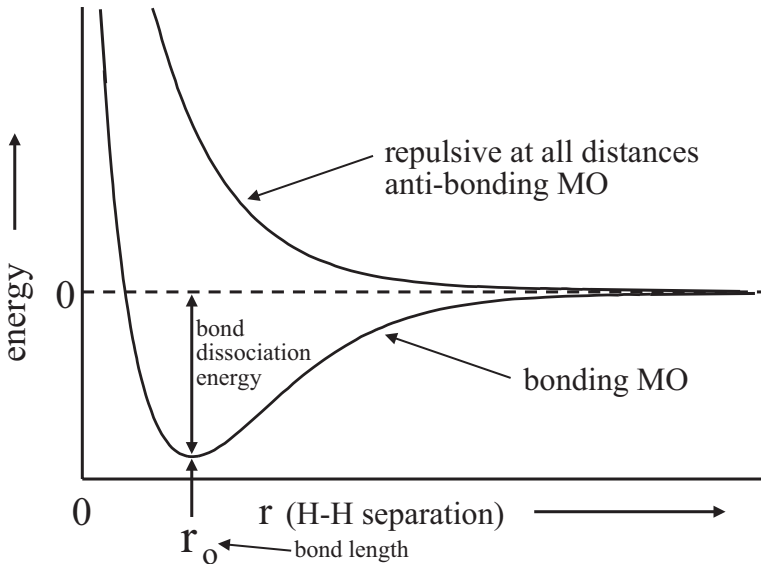
Figure 12.6. *An energy level diagram that represents the combination of the two atomic 1s orbitals to form the bonding and antibonding MOs at the bond length separation r_0, which is the distance of the energy minimum of the bonding MO. The bonding MO is lower in energy and the antibonding MO is higher in energy than the atomic orbitals by the same amount. The bonding MO is called σ^b, and the antibonding MO is called σ^*.*
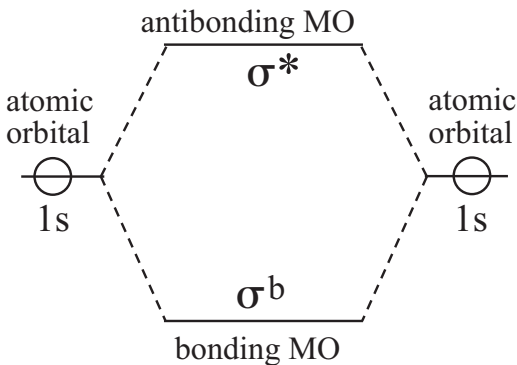
FIGURE 12.7. *The MO diagram for the hydrogen molecule. The two electrons (arrows), one from each hydrogen atom, go into the lowest energy level with their spins paired. The energy is lower than the separated atoms. An electron pair sharing bond is formed.*
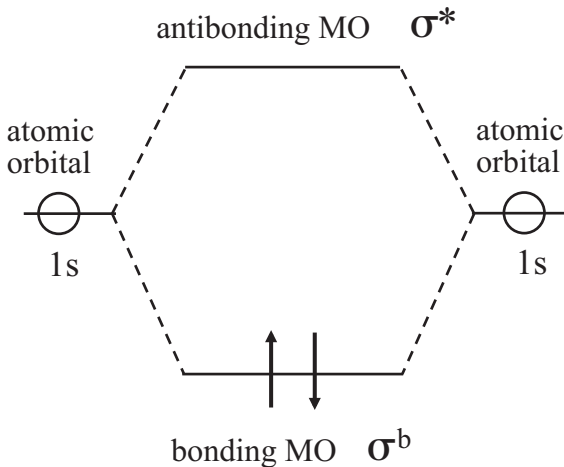
FIGURE 12.8. *The MO diagram for the hypothetical helium molecule. There are four electrons (arrows), two from each helium atom. Two go into the bonding MO. Because of the Pauli Principle, the other two go into the antibonding MO. There is no net reduction in energy and, therefore, no bond.*
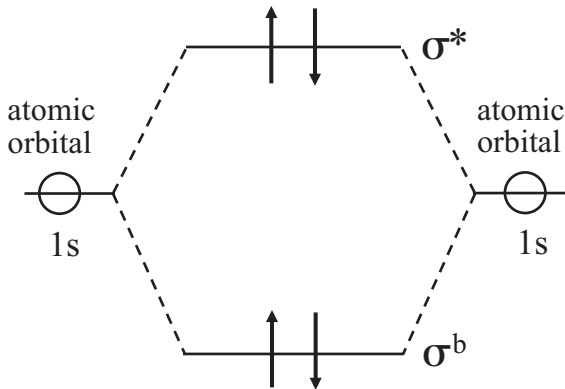
FIGURE 12.9. *The MO energy level diagrams for four molecules, the hydrogen molecule ion H_2^+, the hydrogen molecule H_2, the helium molecule ion He_2^+, and the helium molecule He_2.*
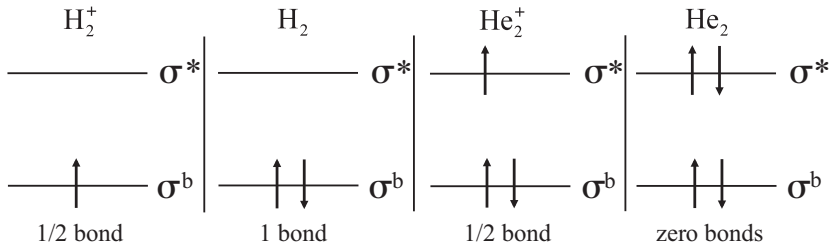
TABLE 12.1. *Properties of the hydrogen molecule ion H_2^+, the hydrogen molecule H_2, the helium molecule ion He_2^+, and the helium molecule He_2.*

	Bonding electrons	Antibonding electrons	Net	Bond order	Bond length	Bond energy
H_2^+	1	0	1	½	1.06	4.2
H_2	2	0	2	1	0.74	7.2
He_2^+	2	1	1	½	1.08	5.4
He_2	2	2	0	0	none	none
					(Å)	(10^{-19} J)

FIGURE 13.1. *A pair of p orbitals brought close to each other. Upper portion: the orbitals are brought together end to end. There is electron density along the line connecting the nuclei. Bottom portion: the orbitals are brought together side to side. There is no electron density along the line connecting the nuclei.*

Lobes of p orbitals point at each other.

Electron density along line connecting nucleus.
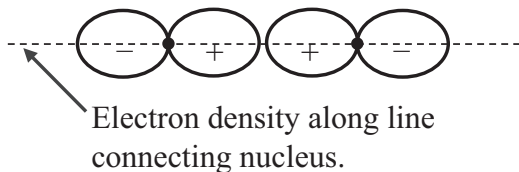
Lobes of p orbitals are side to side.

No electron density along line connecting nuclei.
Nodal plane contains nuclei.
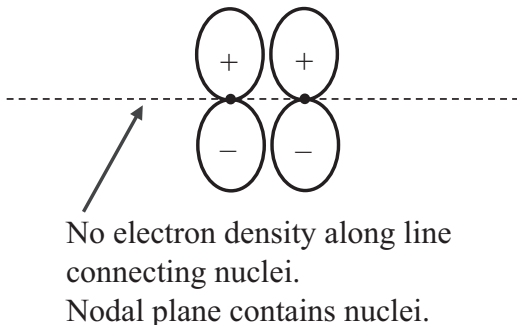
FIGURE 13.2. *Upper portion: a pair of s orbitals are overlapped in two ways to give σ bonding (constructive interference) and σ antibonding (destructive interference) molecular orbitals. Lower portion: a pair of p orbitals are overlapped in two ways to give σ bonding (constructive interference) and σ antibonding (destructive interference) molecular orbitals. In all cases, there is electron density along the line through the nuclei.*
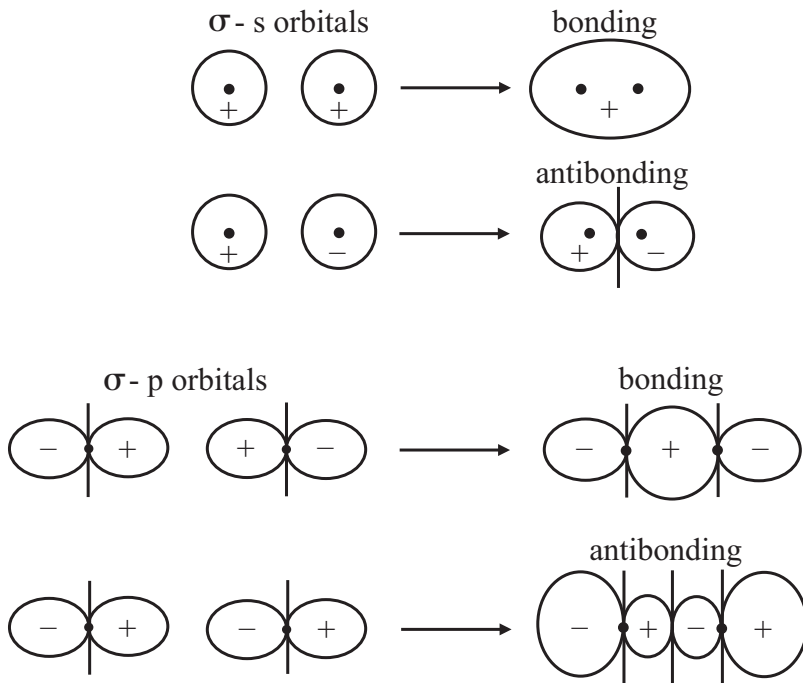
FIGURE 13.3. *Upper potion: a pair of p orbitals are overlapped side to side to give a π bonding molecular orbital (constructive interference). There is no electron density along the line connecting the nuclei. Lower portion: a pair of p orbitals are overlapped side to side to give a π antibonding molecular orbital (destructive interference). Note the signs of the lobes of the p atomic orbitals. The antibonding MO has a node between the nuclei.*

π - p orbitals

bonding

Node along internuclear axis, but not between nuclei.

Node along internuclear axis.

antibonding

Node between nuclei.
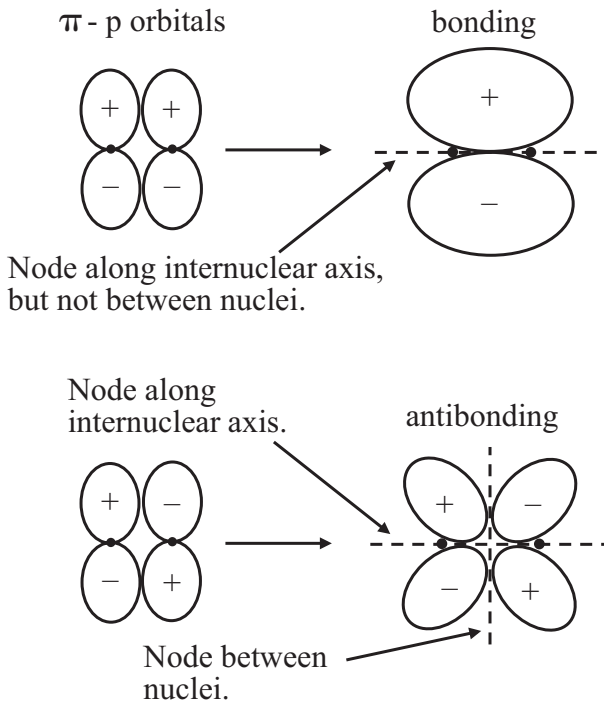
Figure 13.4. *Two atoms are brought together along the z axis. P_z orbitals will approach end to end; p_x and p_y orbitals will approach side to side.*
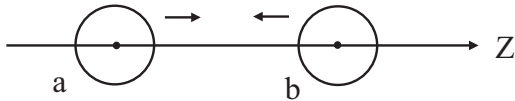
FIGURE 13.5. *The energy level diagram for two fluorine atoms, a and b, brought together to form molecular orbitals. The atomic orbital energies are on the right and left sides. The bonding (b) and antibonding (*) MO energy levels are in the center. There are σ and π MOs. The three atomic p orbitals have the same energies. These are shown as three closely spaced lines. The spacings between the levels are not to scale.*
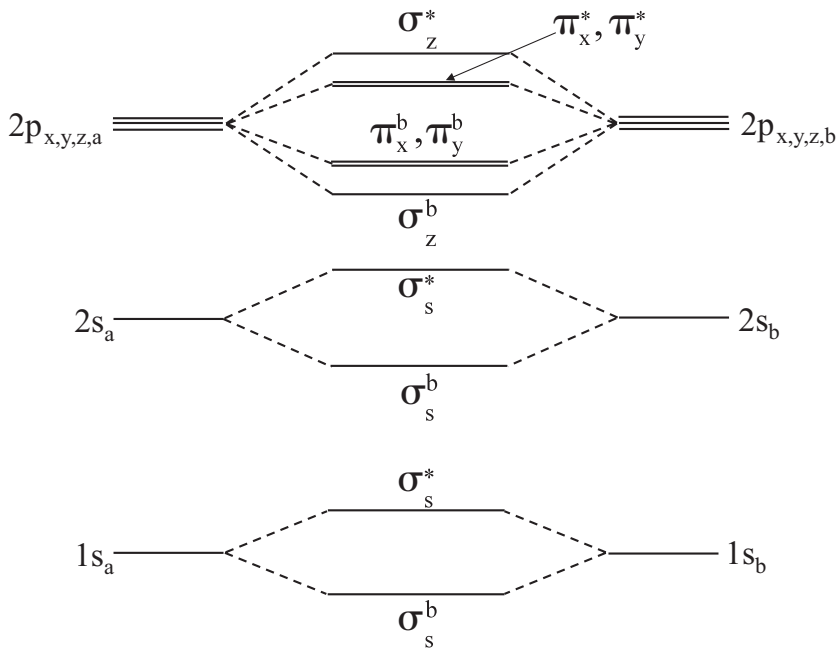
FIGURE 13.6. *The molecular orbital energy level diagram for the F_2, fluorine diatomic molecule. The atomic orbital energies are not shown. Two fluorine atoms have 18 electrons. These have been placed in the orbitals following the rules discussed for atomic orbitals in Chapter 11. There is one more filled bonding MO than antibonding MO. F_2 has a single bond.*
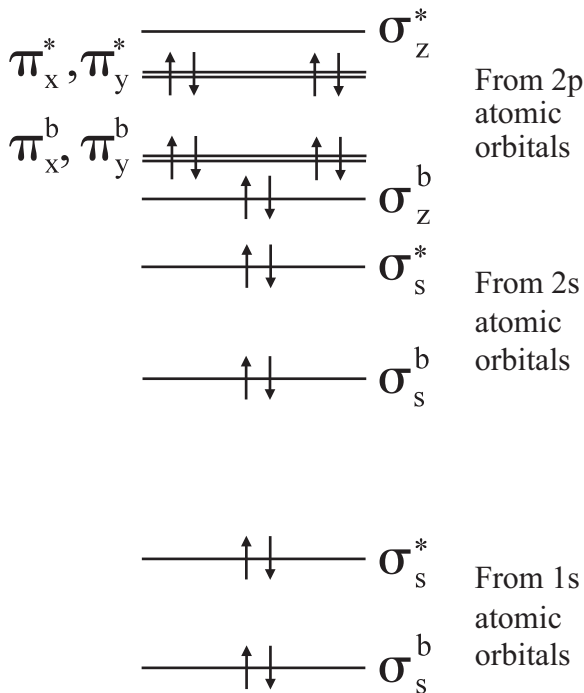
Figure 13.7. *The MO energy level diagram for the hypothetical molecule, Ne_2. Two neon atoms have 20 electrons. There are the same number of bonding and antibonding electrons, so there is no bond. Ne_2 does not exist.*
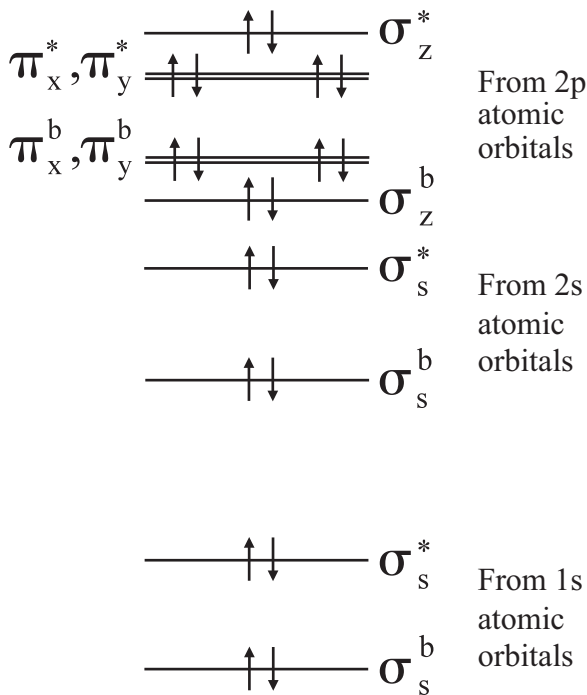
FIGURE 13.8. *The MO energy level diagram for oxygen, O_2. There is one extra pair of σ bonding electrons and one extra pair of π bonding electrons. O_2 has a double bond. Note the unpaired electrons in the π anti-bonding MOs.*
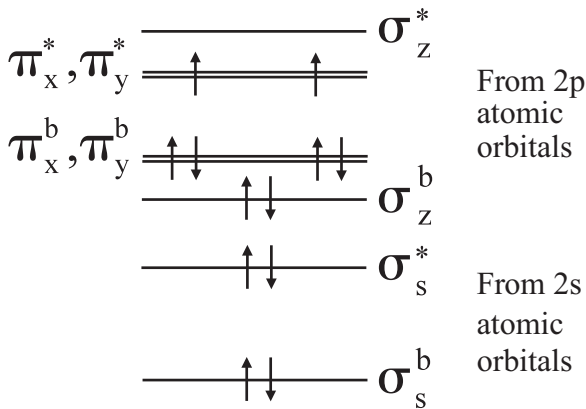
FIGURE 13.9. *The MO energy level diagram for nitrogen, N_2. There is one extra pair of σ bonding electrons and two extra pairs of p bonding electrons. N_2 has a triple bond.*
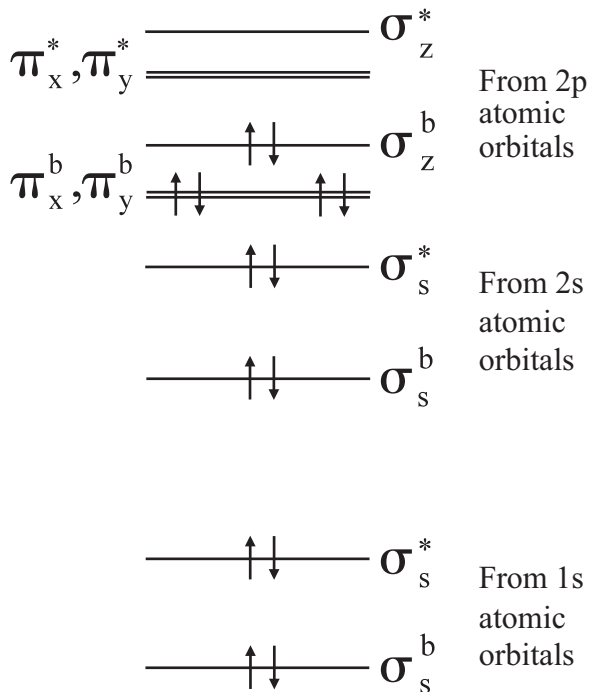
TABLE 13.1. *The Effect of Bond Order on Bond Properties.*

	F_2	O_2	N_2
bond order	single (1)	double (2)	triple (3)
bond length (Å)	1.42	1.21	1.10
bond energy (10^{-19} J)	2.6	8.3	15.6

FIGURE 13.10. *Top: H and F atoms brought together along the z axis. Circles show the relative size of the atoms. Middle: overlap of the H 1s and F $2p_y$ orbitals. There is equal constructive (+) and destructive (−) interference in the overlap region. No MO formation. Bottom: overlap of the H 1s and the F $2p_z$ orbitals. There is constructive interference in the overlap region.*
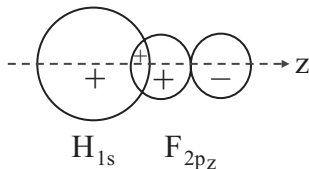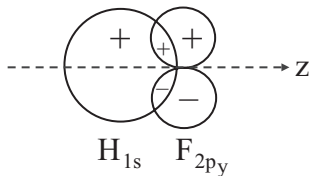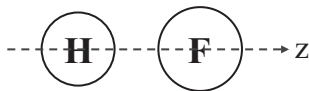
Figure 13.11. *Molecular orbital energy level diagram for HF. The atomic orbitals of the valence electrons are shown at the right and left. The F $2p_z$ atomic orbital combines with the H 1s atomic orbital to give a bonding (σ^b) and antibonding (σ^*) MO. σ^b is filled with one H electron and one F electron. σ^* is unfilled. The net is one bond. The other F electrons do not participate in the bonding. They are lone pairs of electrons.*
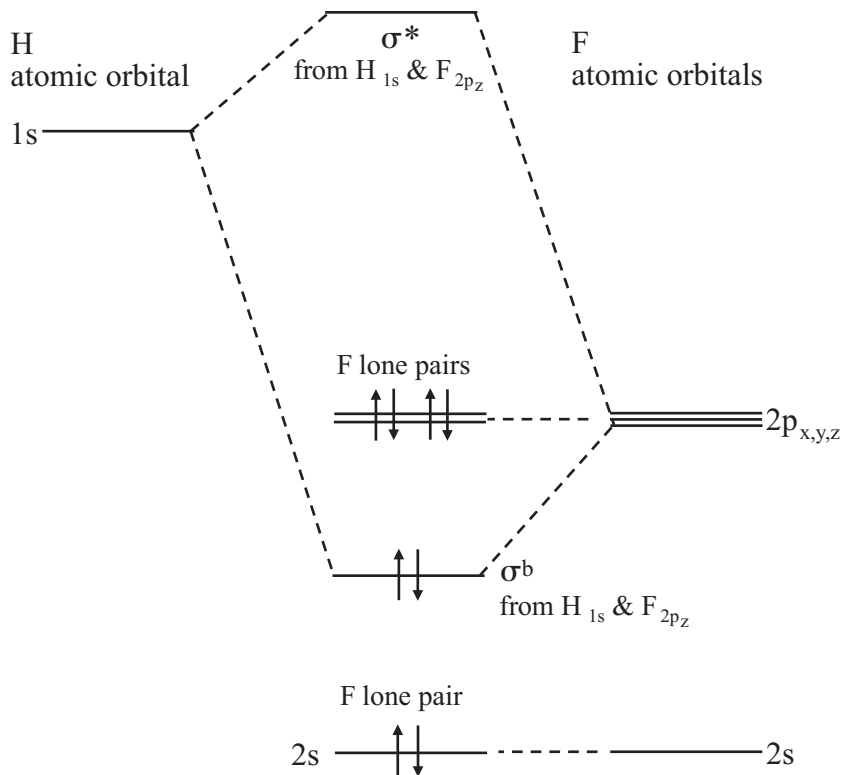
FIGURE 13.12. *Representations of the HF molecule. H: light; F: dark. Top: a ball-and-stick version that shows how the atoms are bonded and the relative sizes of the atoms. Bottom: a space-filling version that is more realistic.*
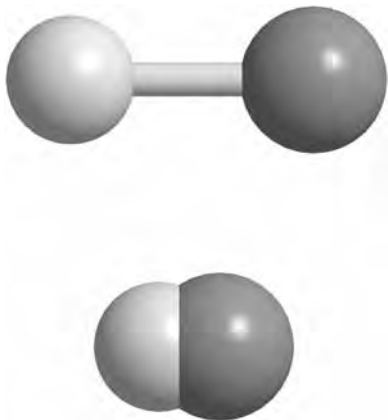
Figure 14.1. *Left: diagram showing the bond connectivity of methane, but not its three-dimensional shape. Right: a three-dimensional ball-and-stick model of methane that shows the tetrahedral shape of the molecule.*
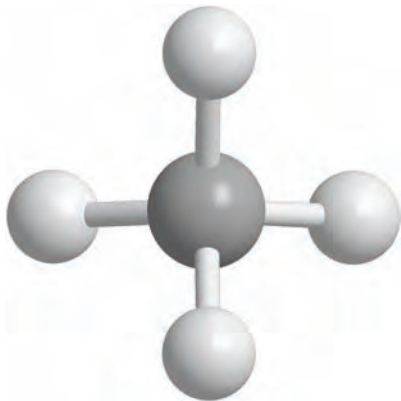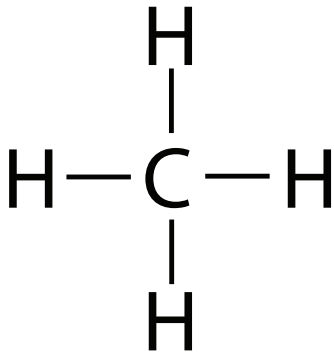
FIGURE 14.2. *Methane (left), ammonia (center), and water (right). Lone pair electrons repel the bond pair electrons, pushing the bonds closer together, which reduces the angle between bonds to H atoms from the central atom.*
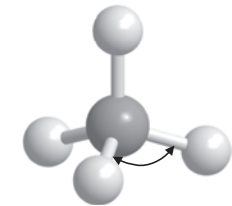
< HCH = 109.5°
perfect tetrahedron
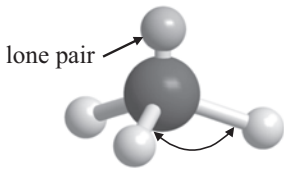
< HNH = 107.3°
1 lone pair repulsion
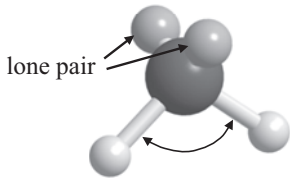
< HOH = 104.5°
2 lone pair repulsions

FIGURE 14.3. *Left: BH₃. The atoms lie in a plane. The HB bonds are single, and the hydrogens form a perfect equilateral triangle. Each HBH bond angle is 120. Right: H₂CO (formaldehyde). The atoms lie in a plane. The CO bond is a double bond. The angles are unequal.*
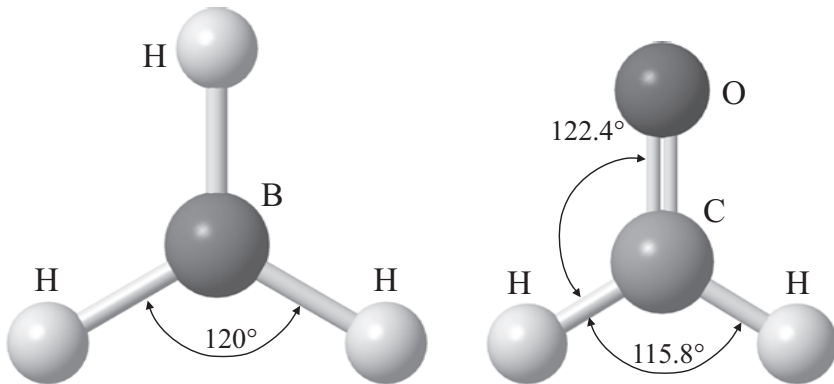
Figure 14.4. *Top: Atomic carbon valence orbitals with the four valence electrons. Bottom: When bonding, a carbon atom "promotes" a 2s to a 2p electron to give four unpaired electrons used to form four bonds to other atoms.*

$2s$ ⇅   ↑ ↑ — $2p$

carbon atomic configuration

$2s$ ↑   ↑ ↑ ↑ $2p$

with bonding –
promote 2s electron to 2p

FIGURE 14.5. *Top: Be valence electrons with one promoted to the $2p_z$ orbital. Next: The 2s and $2p_z$ orbitals of Be shown separated. Next: The sum of 2s and $2p_z$ to form the hybrid atomic orbital sp_{z+}. Next: $2s - 2p_z$ to form the hybrid orbital sp_{z-}. Bottom: The two hybrid orbitals of Be point in opposite directions along z.*
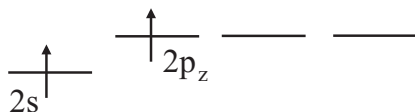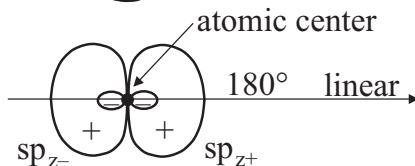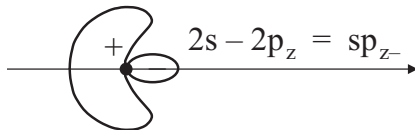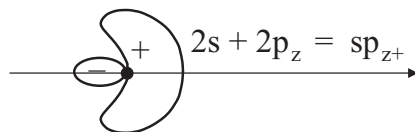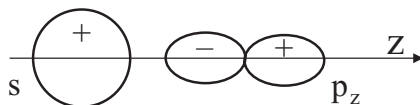
FIGURE 14.6. *Top: Two H atoms approach a Be. Middle: The H 1s orbitals form electron pair bonds with the two Be sp hybrid orbitals to produce the linear BeH₂ molecular shown as a ball and stick model at the bottom.*

H_a $1s_a$ sp_{z-} Be sp_{z+} H_b $1s_b$

BeH_2
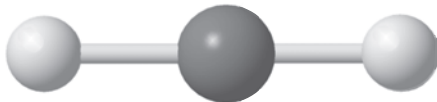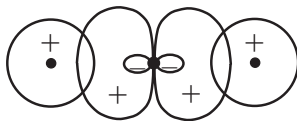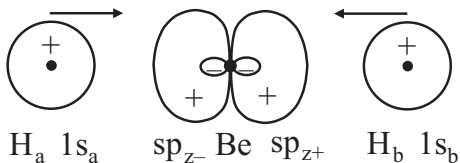
FIGURE 14.7. *Top: B valence electrons with one promoted to a 2p orbital. Middle: the 2s, $2p_x$, and $2p_y$ orbitals of B combine in three combinations to form three hybrid atomic orbitals, sp_a^2, sp_b^2 and sp_c^2. The angle between the lobes is 120. Bottom: The three B hybrid orbitals forming bonds with the three H atom 1s orbitals.*
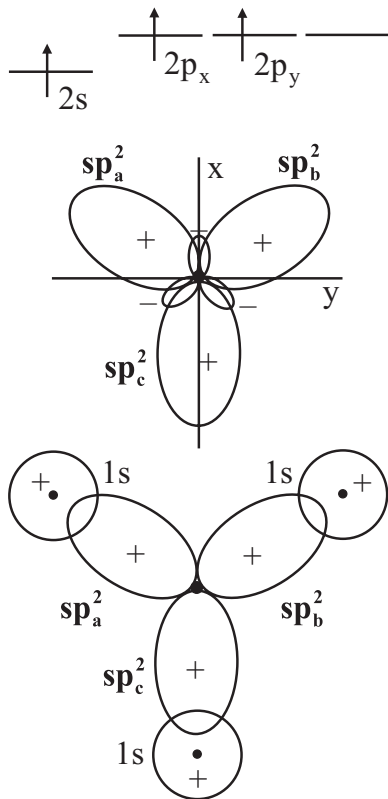
FIGURE 14.8. *Four carbon sp³ hybrid atomic orbitals and four hydrogen 1s orbitals for carbon bonding to four hydrogens in methane. Dashed orbitals in the plane of the page. Solid orbitals out of the plane. Dot-dash orbitals into the plane. Only the positive lobes of the sp³ hybrids are shown. The four sp³ hybrids form a perfect tetrahedron.*
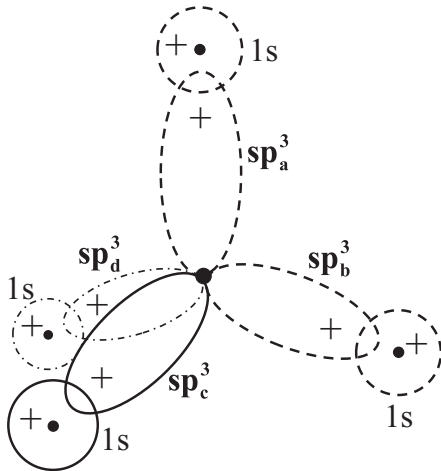
FIGURE 14.9. *Three diagrams of ethane, C_2H_6. Top: The bonds be-*
tween atoms. Middle: Each carbon has four sp^3 hybrid atomic orbit-
als, three bond to hydrogens and the fourth to the other carbon.
Solid lines: in the plane of the page; dashed lines: out of the plane;
dotted lines: into the plane. Bottom: Method for showing spatial ar-
rangement. Lines: in the plane of the page; filled triangles stick out of
the page; open triangles stick into the page. Each carbon's bonds are
tetrahedral, with bond angles 109.5°. The C-C bond is longer than the
C-H bonds.
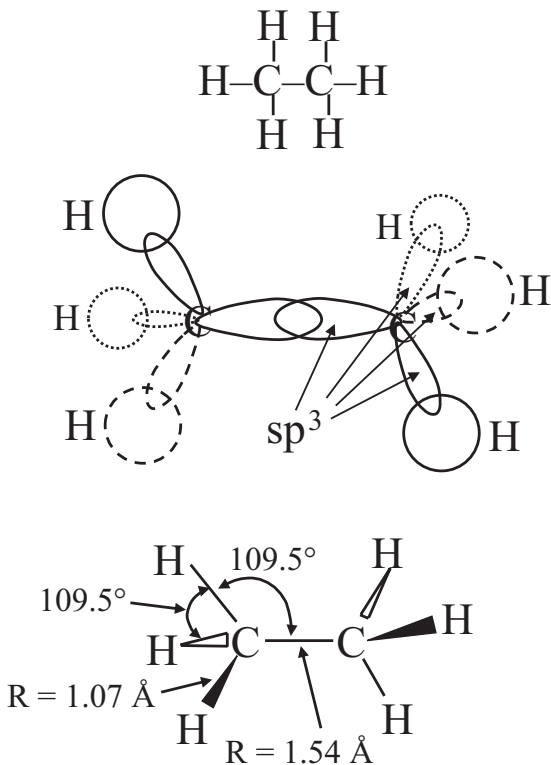
FIGURE 14.10. *Ethane ball-and-stick model (top), space-filling model (bottom). The atoms are the same size in the two models.*
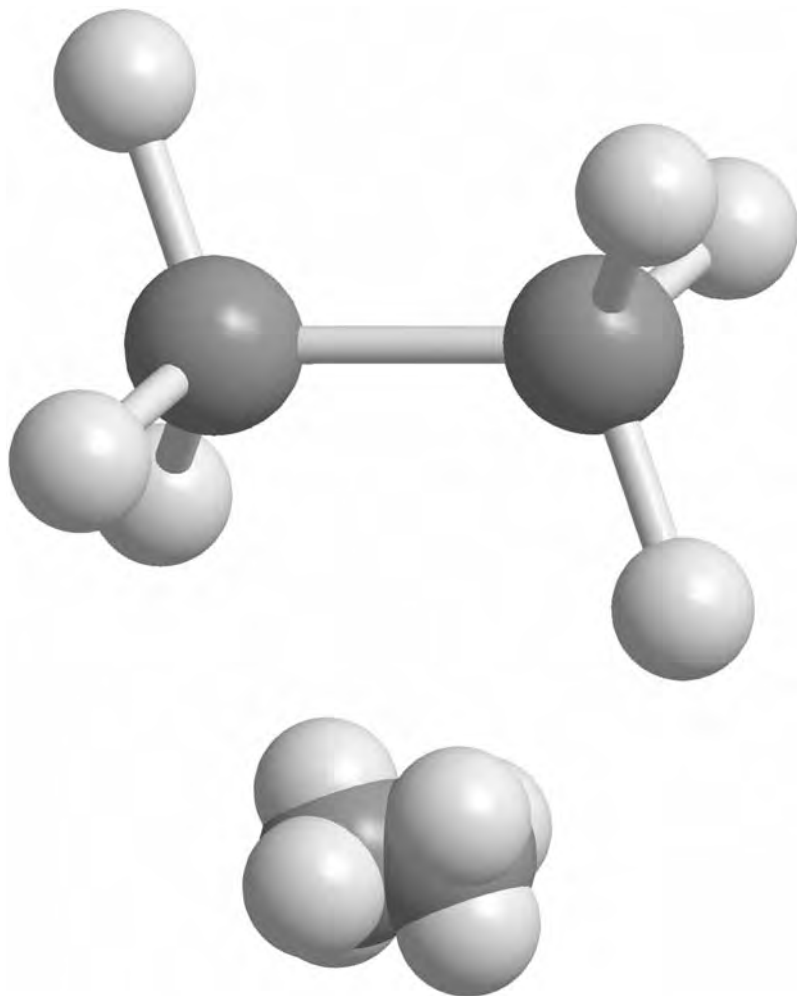
Figure 14.11. *A diagram and a ball-and-stick model of propane, C_3H_8. The carbon centers are tetrahedral.*
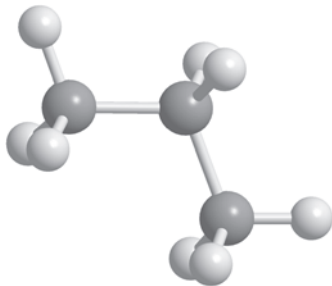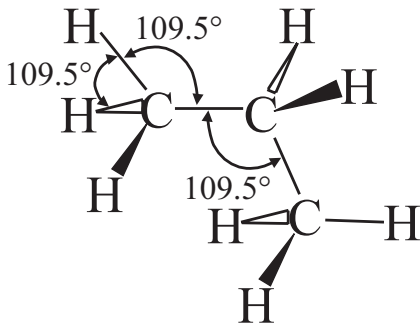
Figure 14.12. *Two structural isomers of butane, C_4H_{10}. In the diagram at the top, CH_3 represents a carbon bonded to three hydrogens. N-butane is a linear chain in the sense that each carbon is bonded to at most two other carbons. Isobutane is branched. The central carbon is bonded to three other carbons.*
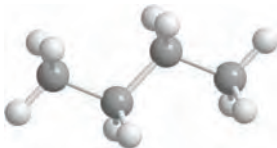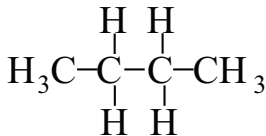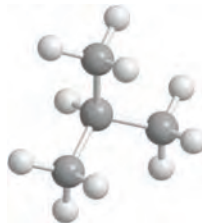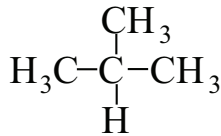
FIGURE 14.13. *Two conformers of n-butane. The gauche form is obtained from the trans form by a 120° rotation about the center C-C bond.*

n-butane
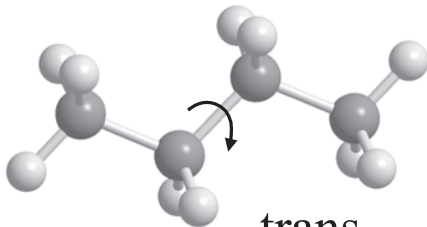
trans
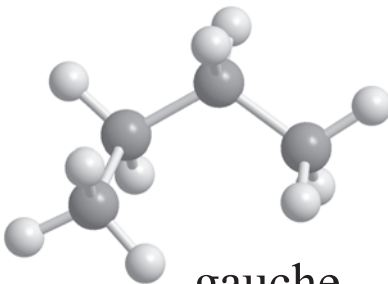
gauche

FIGURE 14.14. *Ethane, single bond, carbon tetrahedral bonds. Ethylene, double bond, carbon trigonal bonds. Acetylene, triple bond, carbon linear bonds.*

ethane

ethylene
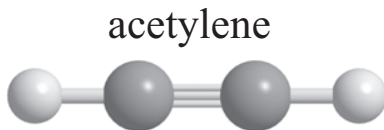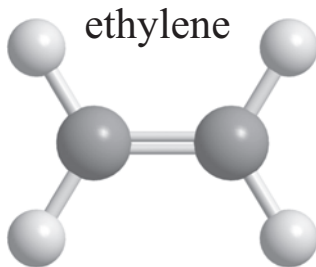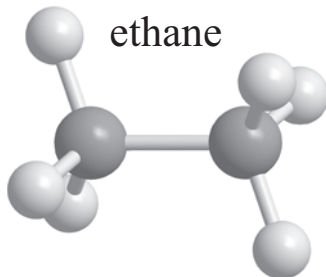
acetylene

TABLE 14.1. *Single, Double, and Triple C-C Bonds.*

	bond order	C-C bond length	C-C energy
ethane	single (1)	1.54 Å	5.8×10^{-19} J
ethylene	double (2)	1.35 Å	8.7×10^{-19} J
acetylene	triple (3)	1.21 Å	16×10^{-19} J

FIGURE 14.15. *Ethylene double bond orbitals. Top: Each carbon uses three sp² hybrids to make three σ bonds in a trigonal configuration. The page is the xy plane, with z out of the plane. Bottom: Each carbon has a 2pz orbital not used to form the sp² hybrids. The 2pz orbitals combine to make a π bonding molecular orbital to give a second bond between the carbons.*
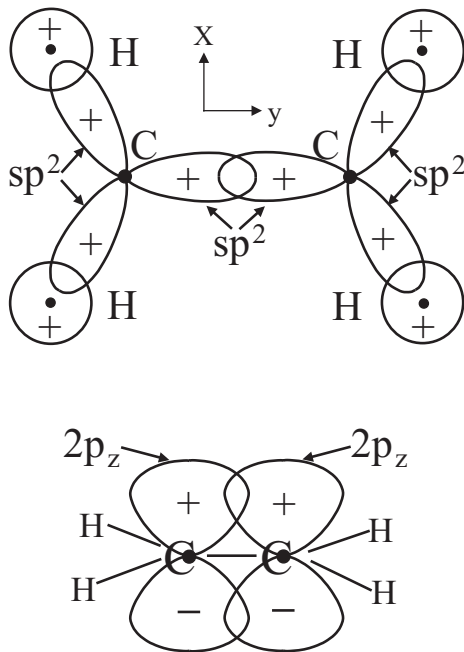
FIGURE 15.1. *Ethanol (ethyl alcohol) diagram showing atom connectivity (top), ball-and-stick model (bottom). The hydrogens are light gray, the carbons are dark gray, and the oxygen is black.*
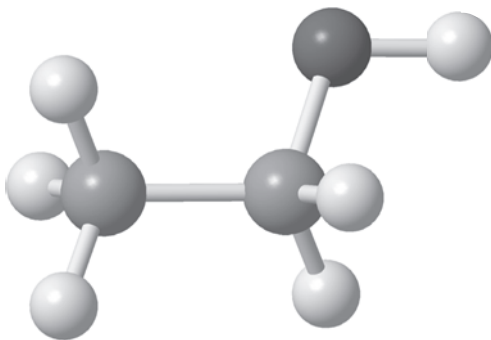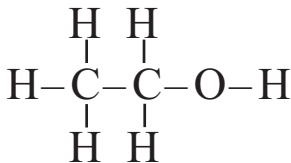
FIGURE 15.2. *Four ethanol molecules that form a chain. The oxygens are almost black in the figure. An oxygen has two lone pairs in addition to the hydrogen and carbon bonded to it. The dashed lines show hydrogen bonds that go from the hydroxyl's H on one ethanol to an oxygen lone pair on another ethanol.*
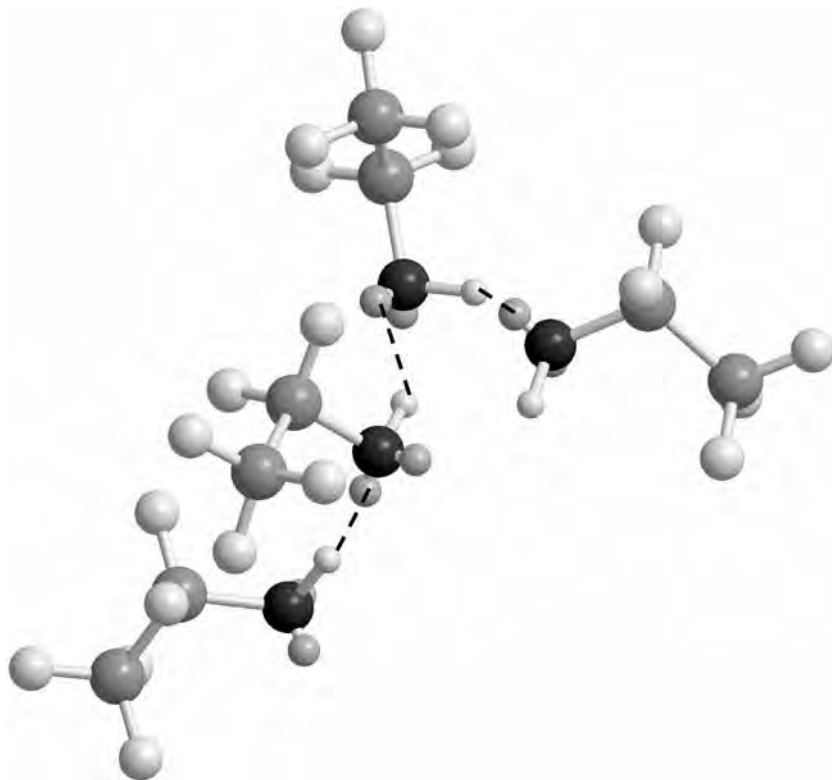
FIGURE 15.3. *A central water molecule hydrogen bonded to four surrounding water molecules. The central water's two hydroxyl hydrogens bond to two oxygens, and the central water's oxygen accepts two hydroxyl bonds from two other water molecules.*
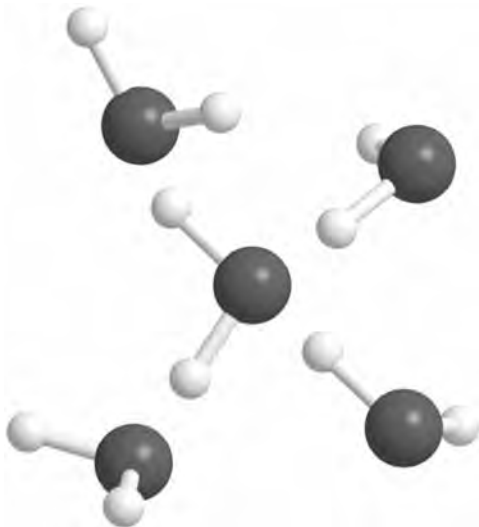
FIGURE 15.4. *Acetaldehyde (top) and acetic acid (bottom). Oxygens are the almost black spheres. Acetaldehyde C_2 carbon is bonded to C_1, a hydrogen, and double bonded to an oxygen. Acetic acid C_2 is bonded to C_1, double bonded to an oxygen and single bonded to another oxygen that is part of a hydroxyl group.*
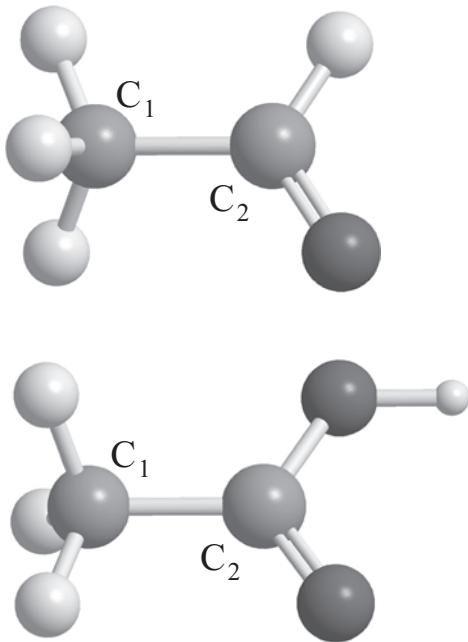
Figure 15.5. *n-tetradecane, $C_{14}H_{30}$, ball-and-stick model (top) and space-filling model (bottom). The molecule has 14 carbons connected one to the next without branching.*
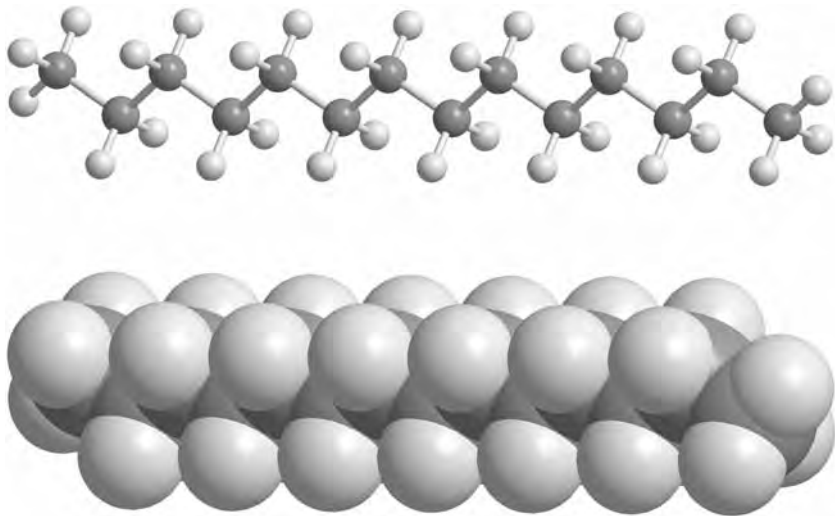
FIGURE 15.6. *2,8-dimethlydodecane, $C_{14}H_{30}$, ball-and-stick model (top) and space-filling model (bottom). The molecule has 14 carbons. There is a chain of 12 carbons, with two methyl groups branching off at the second and eighth carbons from the left.*
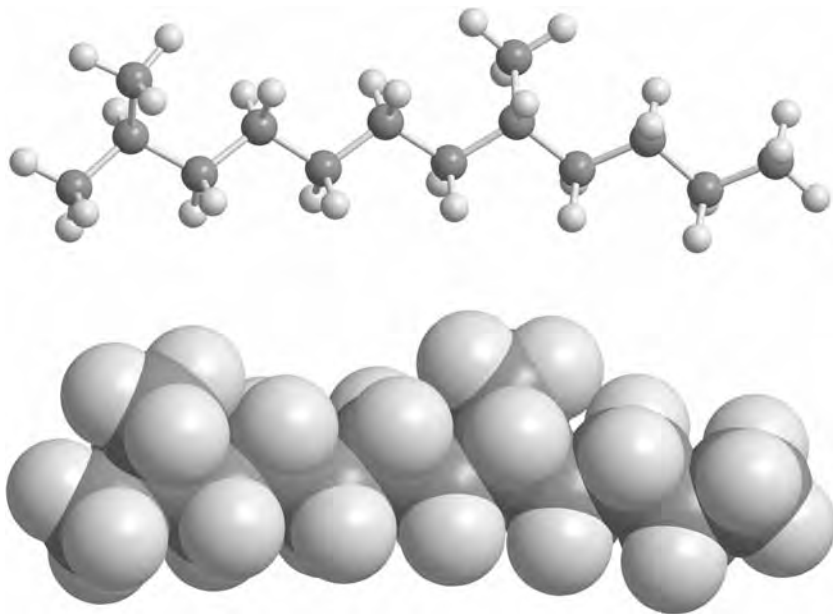
FIGURE 15.7. *Sodium heptadecaneacetate, $C_{18}H_{37}COO^- Na^+$, ball-and-stick model (top) and space-filling model (bottom). The dissociated sodium ion is not shown. The molecule has 19 carbons. There is a chain of 17 carbons and then an acetate group. The δ^- indicates that each oxygen (darkest spheres) carries an approximately negative one-half charge.*
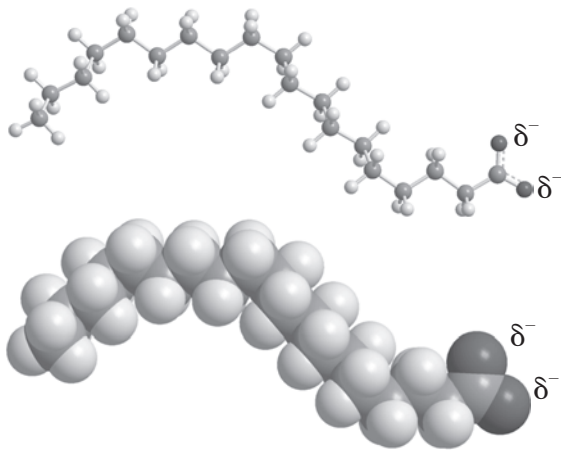
FIGURE 15.8. *A schematic of a spherical micelle. The balls represent the acetate anion head groups. Wiggly lines represent the hydrocarbon tails. The micelle is surrounded by water that hydrogen bonds to the head groups. The hydrocarbon chains clump together to form a nanodroplet of oil, which is protected from water by the head groups.*
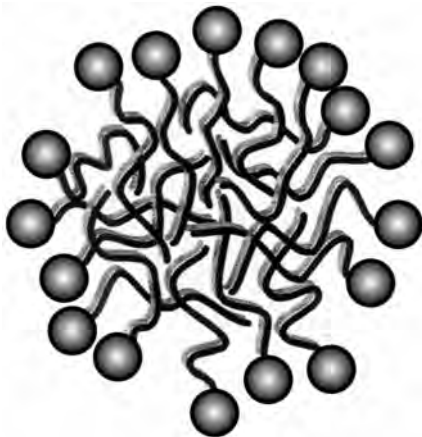
FIGURE 15.9. *A schematic of hydrocarbons from oil or grease (single spotted lines) contained in the interior of a soap micelle.*
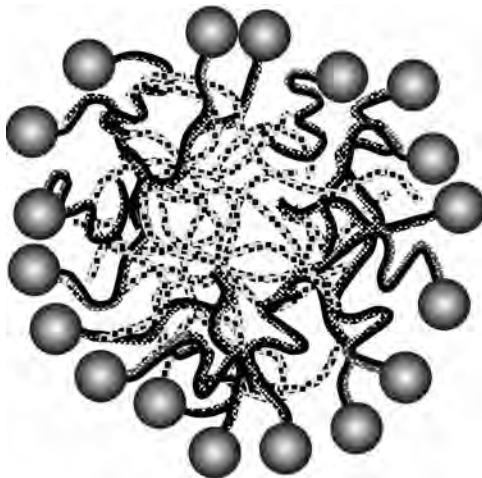
FIGURE 16.1. *Ball-and-stick (top) and space-filling models (bottom) of stearic acid. Stearic acid has 18 carbon atoms, 36 hydrogen atoms, and two oxygen atoms. It is a 17-carbon hydrocarbon with an acid group, −COOH, on the end (right side).*
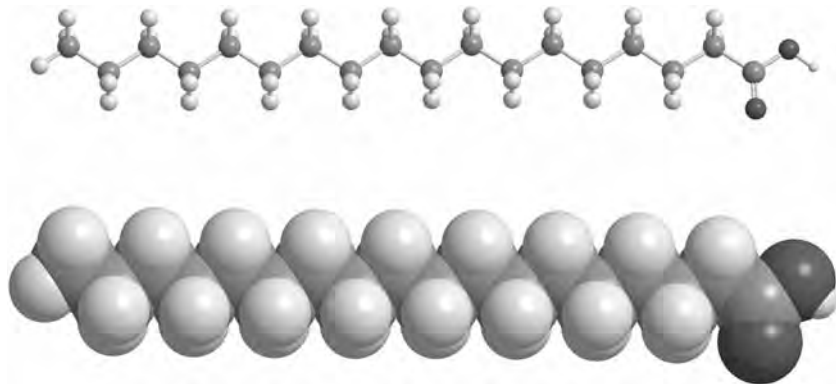
Figure 16.2. *Ball-and-stick model of oleic acid. Oleic acid has 18 carbon atoms like stearic acid in Figure 16.1, but it has one carbon-carbon double bond between carbons 9 and 10 counting from the acid group.*
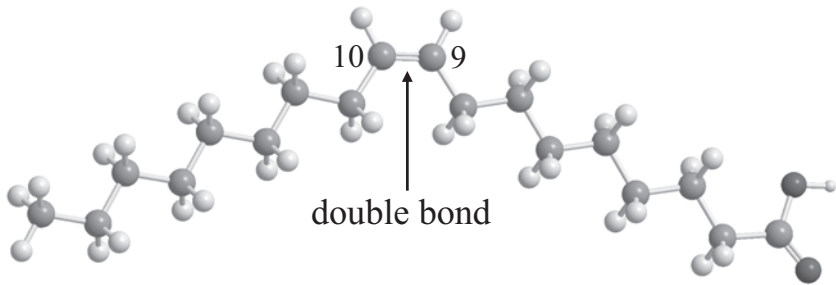
Figure 16.3. *Ball-and-stick model of α-linolenic acid, which has 18 carbon atoms and three carbon-carbon double bonds.*
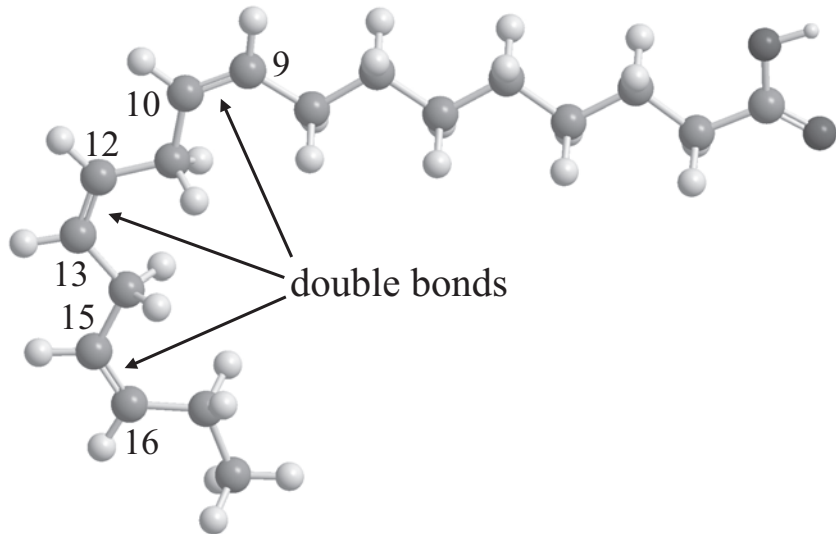
FIGURE 16.4. *Ball-and-stick models of cis-oleic acid and trans-oleic acid. Both have 18 carbons and one double bond. However, their geometries differ.*
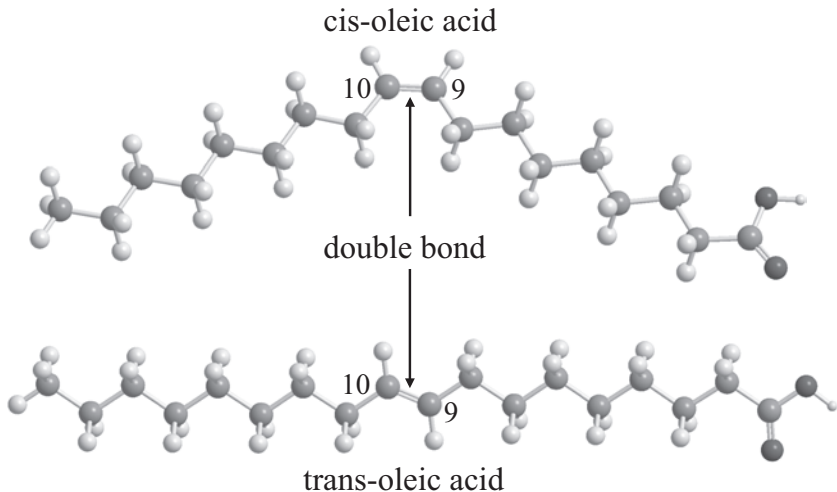
FIGURE 16.5. *Ball-and-stick model of docosahexaenoic acid (DHA). DHA is a polyunsaturated fat with 22 carbon atoms and six carbon-carbon double bonds all in the cis conformation.*
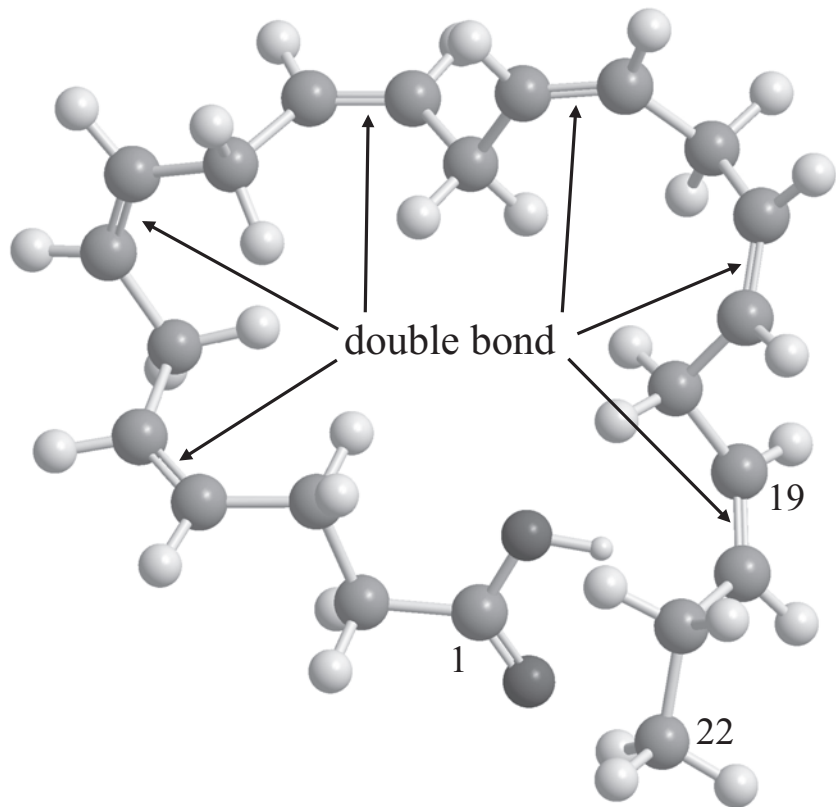
FIGURE 16.6. *Ball-and-stick model of capric acid triglyceride, which is composed of three capric acid chains. Each chain is a saturated fatty acid with 10 carbon atoms labeled 1 to 10. These are attached to three carbons labeled A, B, and C.*
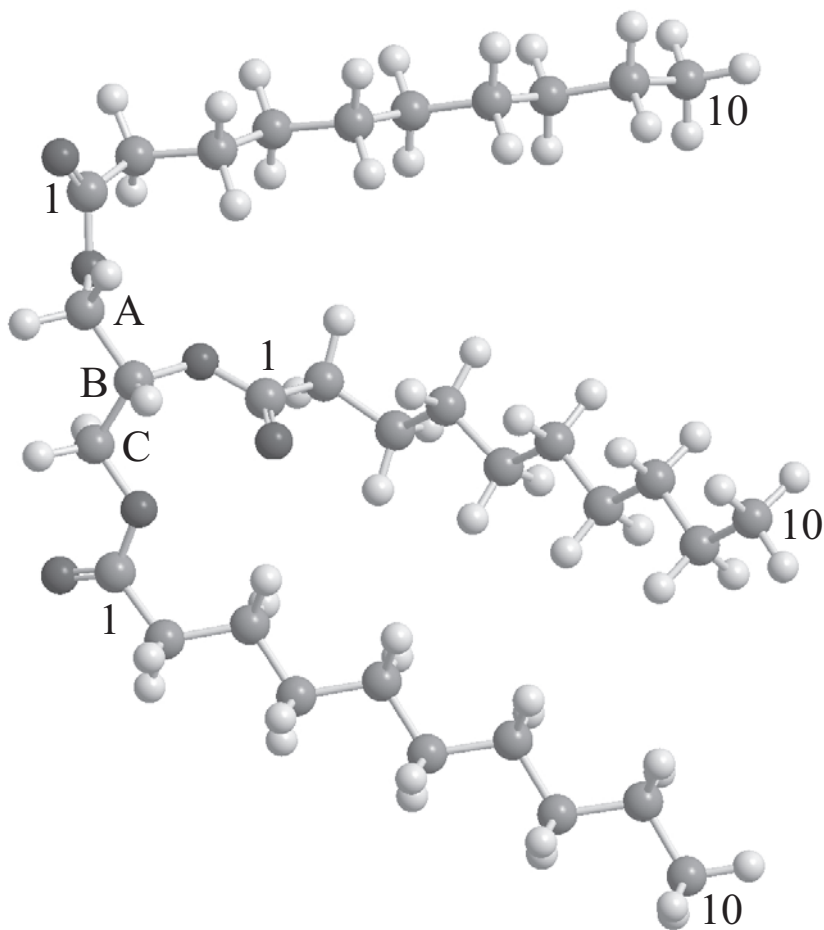
FIGURE 16.7. *Cholesterol. Top: Diagram of cholesterol. Middle: Ball-and-stick model. Bottom: Space-filling model. Cholesterol is an alcohol (−OH group) composed of four carbon rings, labeled 1 to 4, and a hydrocarbon chain.*
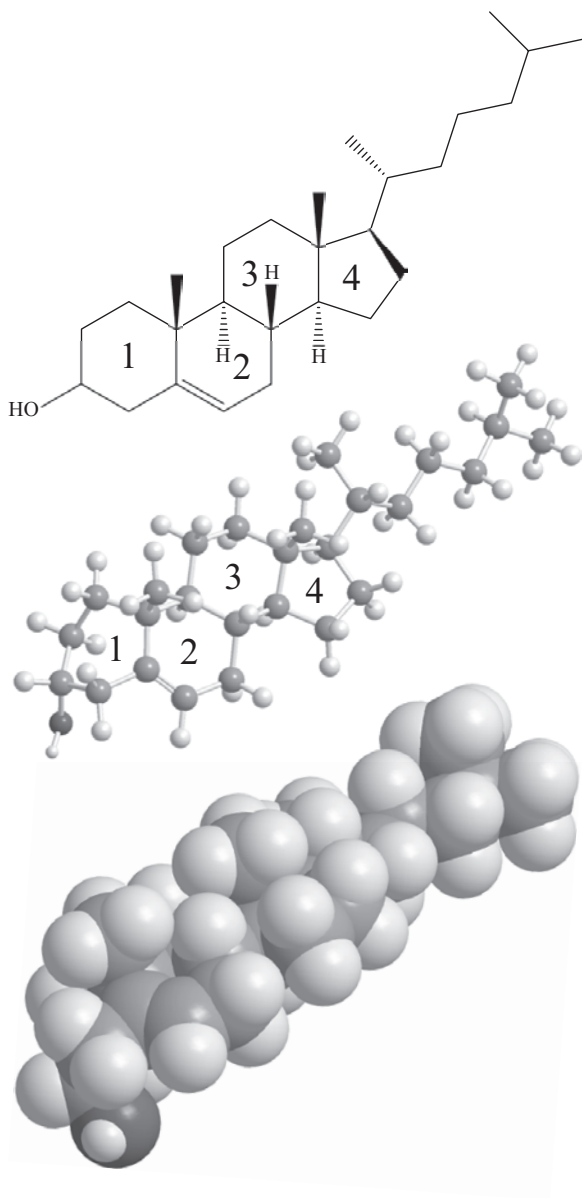
FIGURE 16.8. *Schematic of a portion of a phospholipid bilayer with two cholesterol molecules. The head groups (balls) are charged and want to be in water. The hydrocarbon tails avoid water by formation of the bilayer. The cholesterol hydroxyl is at the water interface.*

outside cell - water

inside cell - water
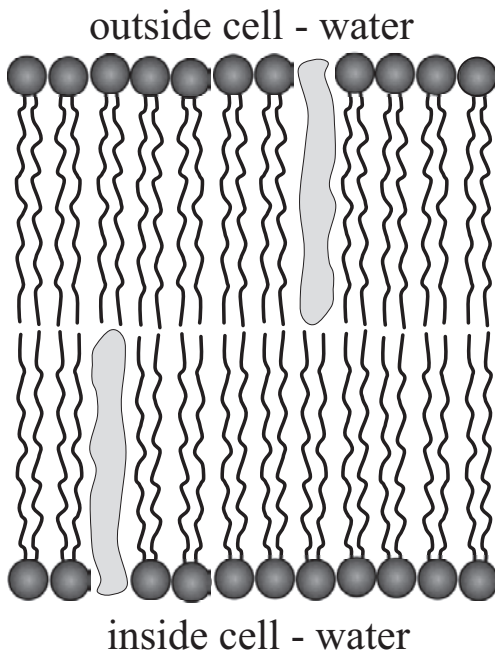
Figure 17.1. *Top: Calculated Earth black body spectra for three temperatures (solid curves). The shaded regions show the portions of the spectrum that are strongly absorbed by water and carbon dioxide in the atmosphere. Middle and bottom: spectra of the strong absorption by carbon dioxide and water in the range of 0 to 1000 cm^{-1}. Note the scale difference with the top part of the figure.*
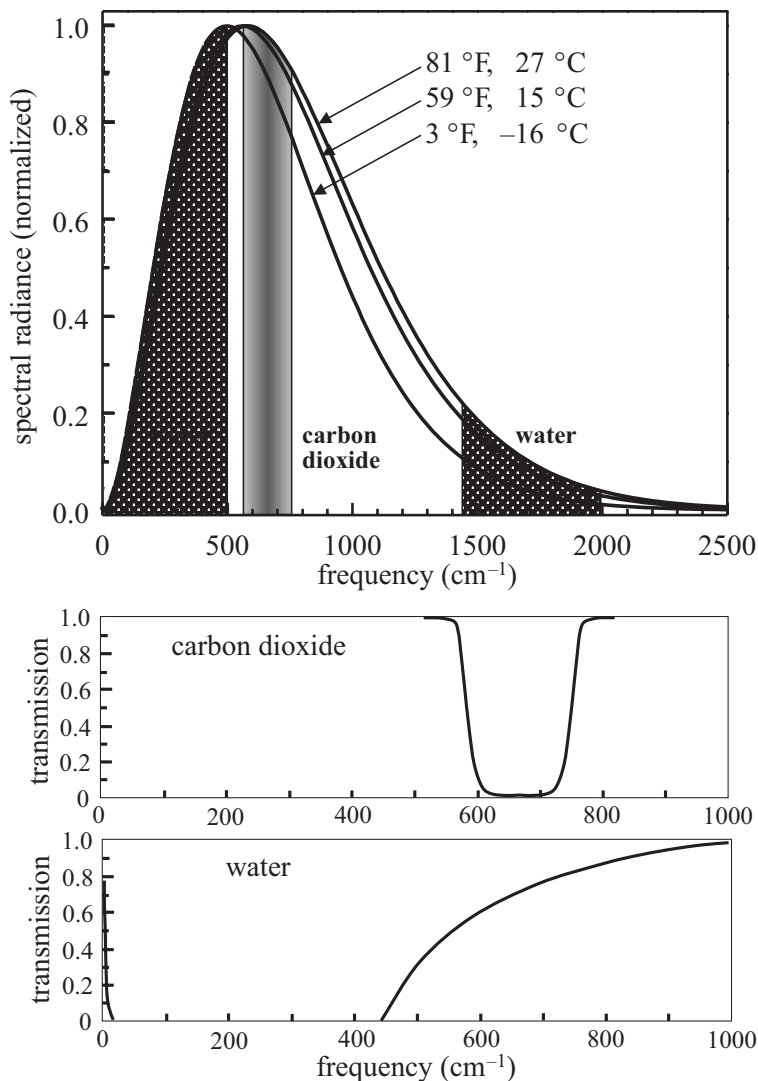
FIGURE 17.2. *Top: Ball-and-stick model of carbon dioxide (CO_2). Bottom: The three different vibration motions that the molecule can undergo. There are two bending modes: the one shown and the equivalent one with the atoms going in and out of the plane of the page.*

symmetric stretch

asymmetric stretch

bend (× 2)
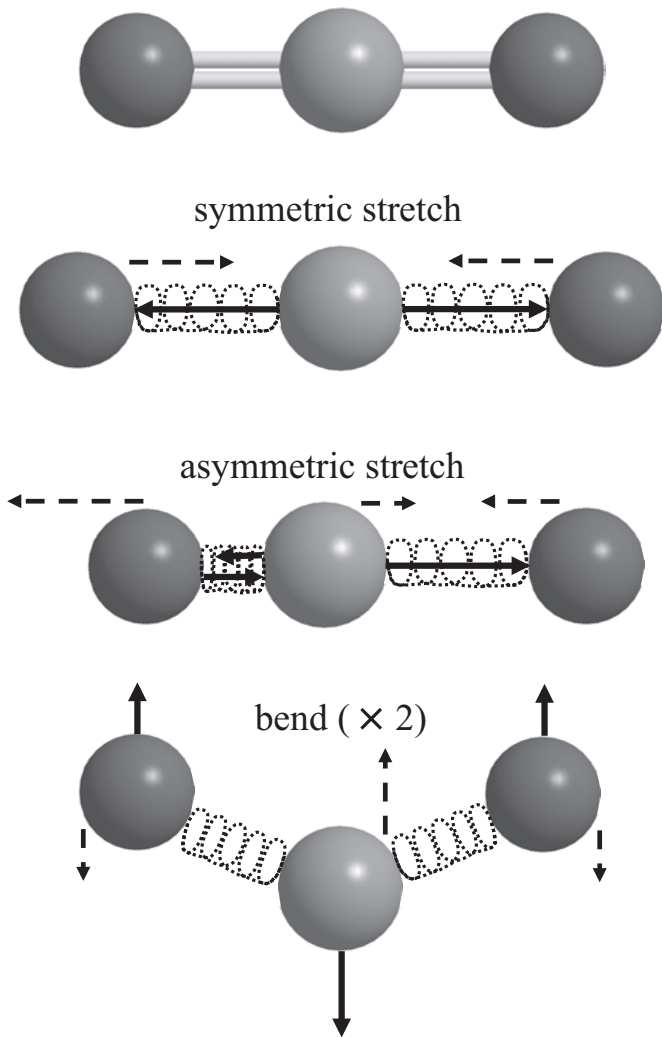
FIGURE 17.3. *Top: A potential energy curve showing the energy as a function of the bond lengths with the vibrational quantum levels. Only the first few energy levels are shown. Bottom: The lowest vibrational energy level ($n = 0$) and the first excited level ($n = 1$) for the CO_2 bending modes (Figure 17.2.). This transition (arrow) will absorb the Earth's black body radiation (see Figure 17.1).*
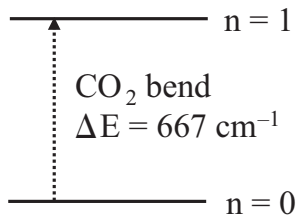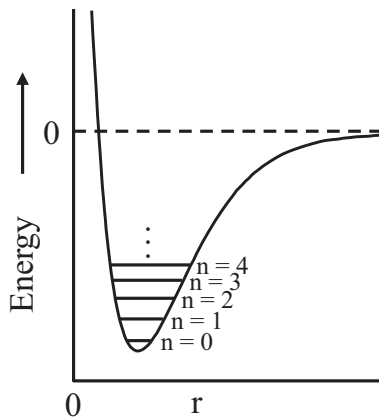
FIGURE 18.1. *The geometry of benzene, C_6H_6. Benzene is planar, and it is a perfect hexagon.*
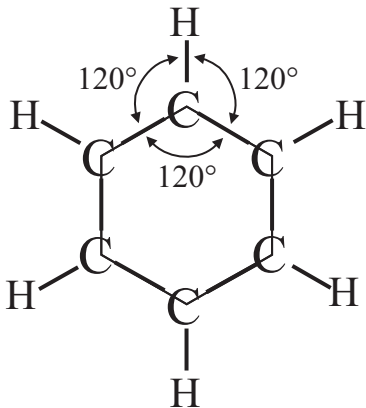
FIGURE 18.2. *Two possible configurations of double bonds in benzene. In both, each carbon makes four bonds.*
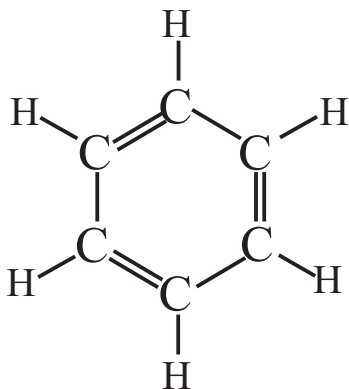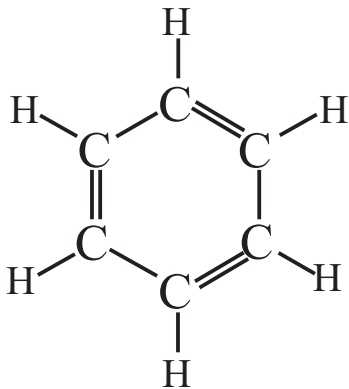
FIGURE 18.3. *Top: Benzene σ bonding. Each carbon makes three bonds using three sp² orbitals that lie in the xy plane. Each carbon has a p_z orbital perpendicular to the plane of the benzene ring. Bottom: The carbon p_z orbitals have positive and negative lobes that are above and below the plane of the ring. The bond lengths are exaggerated and the p_z lobes are made small for clarity of presentation. The lobes of adjacent p_z orbitals overlap.*
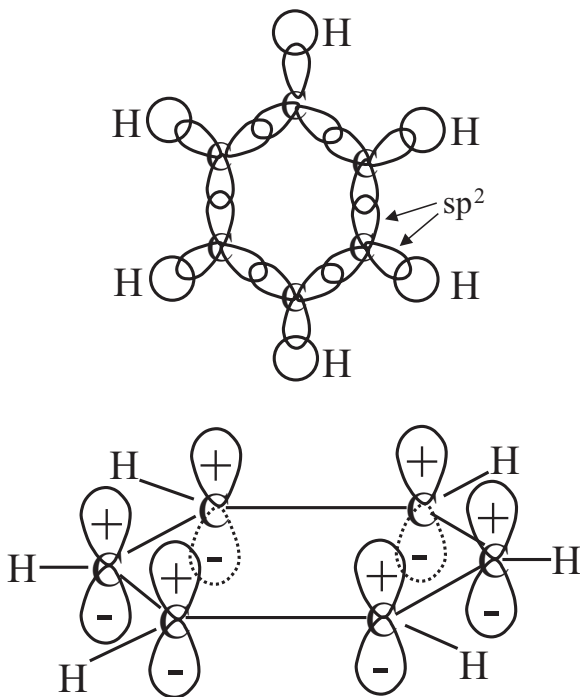
Figure 18.4. *Left: Benzene has six carbon atoms, each with a $2p_z$ orbital. These have identical energy, which is indicated by the six closely spaced lines. Right: The six p_z orbitals combine to form six π molecular orbitals, three bonding (b) and three antibonding (*) MOs.*

atomic orbitals   molecular orbitals

π_6^*

(6) $2p_z$ π_4^*, π_5^*

π_2^b, π_3^b

π_1^b
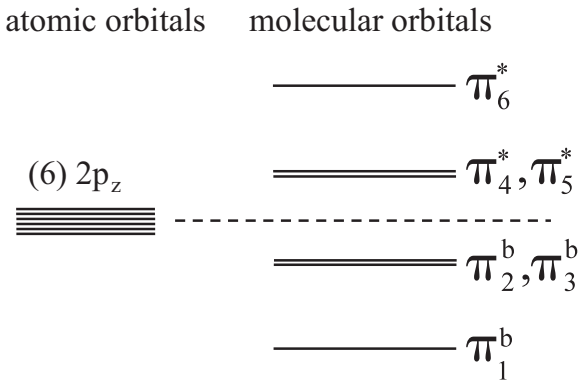
FIGURE 18.5. *Benzene π molecular orbital energy levels with the six electrons placed in the appropriate MOs in the lowest possible energy levels consistent with the Pauli Principle.*
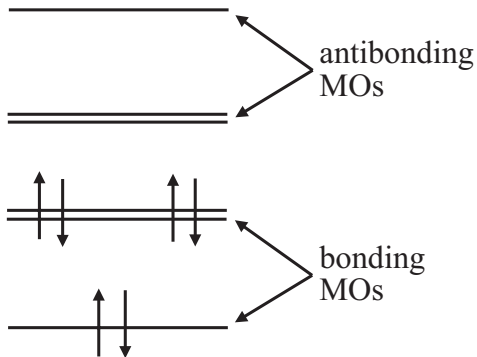
Figure 18.6. *Benzene chemical diagram. A carbon atom is at each vertex, and a hydrogen is at the end of each line from a carbon. The circle represents the delocalized π molecular orbitals.*
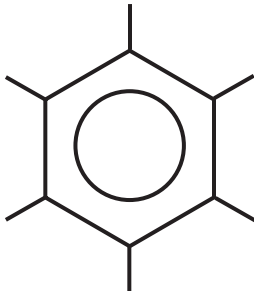
FIGURE 18.7. *Naphthalene chemical diagram. Naphthalene has 10 carbons and eight hydrogens. The circles represent the delocalized π molecular orbitals.*
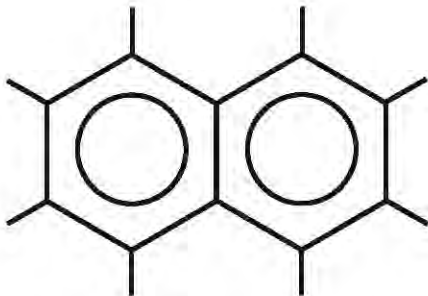
FIGURE 18.8. *Benzene* π *molecular orbital energy levels and schematics showing the shapes of the corresponding MOs. As the energy increases, the number of nodes increases. MOs with the same number of nodes have the same energy.*
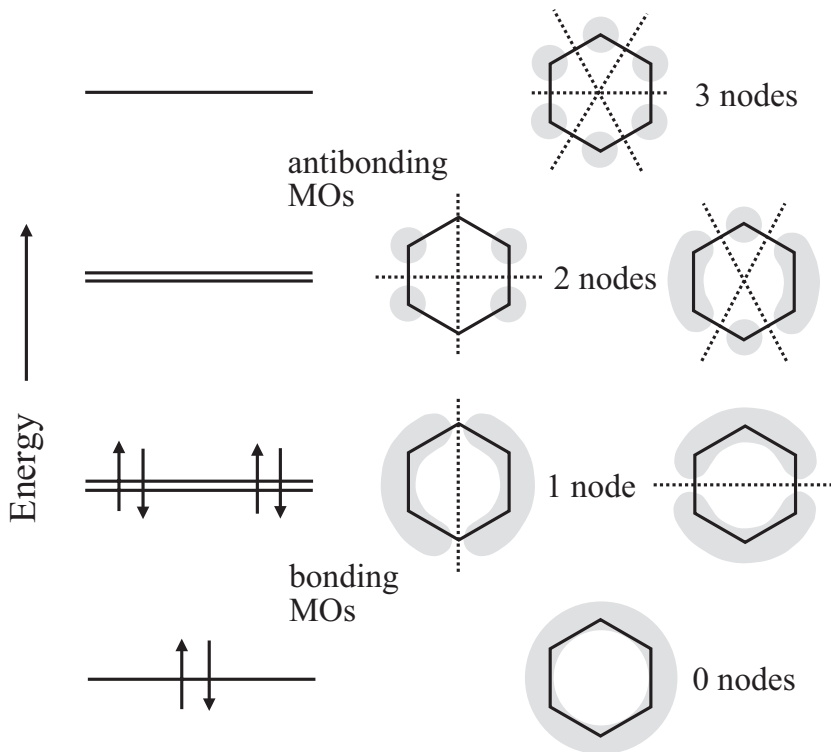
FIGURE 18.9. *A schematic of the naphthalene π molecular orbital energy levels. There are five bonding MOs and five antibonding MOs. The left side shows the 10 p electrons filling the five bonding MOs. The right side shows the result of absorption of light that raises the energy of a bonding electron into an antibonding MO.*
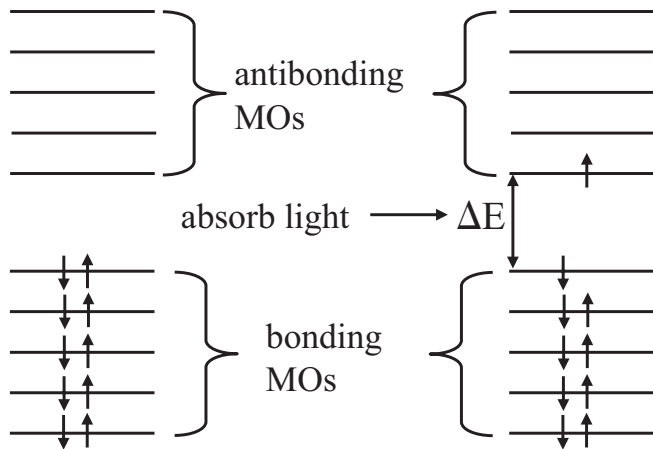
FIGURE 19.1. *A metal rod of sodium, for example, is connected by wires to a battery. Negatively charged electrons are pulled from the metal rod to the positive side of the battery. Electrons flow from the negative side of the battery back into the metal rod.*
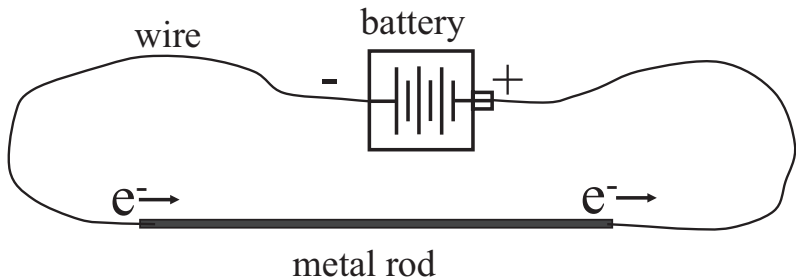
Figure 19.2. *Top: Two sodium 3s atomic orbitals interact to produce two molecular orbitals, one lower in energy (bonding) and one higher in energy (antibonding). Middle: Three 3s atomic orbitals interact to form three MOs. Bottom: Six 3s atomic orbitals interact to form six MOs.*
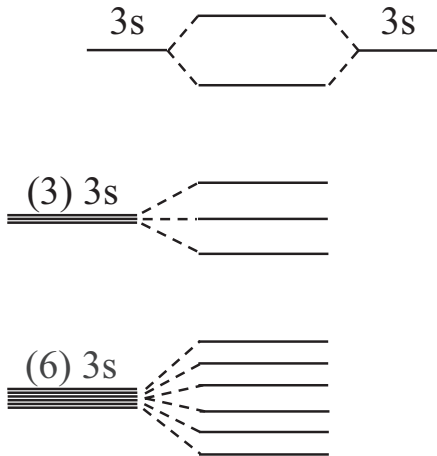
Figure 19.3. *In a piece of sodium metal, there are N atoms. Each has an electron in a 3s orbital, represented by the closely spaced lines on the left. These all have the same energy. The N 3s atomic orbitals interact to form N molecular orbitals with energy levels shown on the right. The MO energy levels are so close together that the energy is effectively a continuous band of states. The Fermi level marks the highest occupied molecular orbital.*
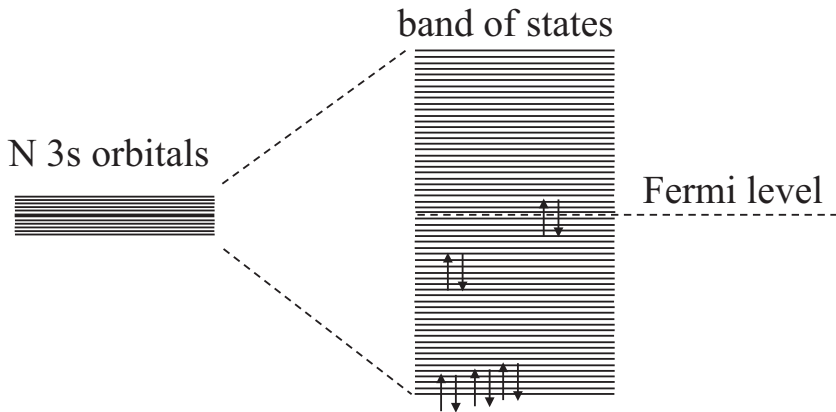
FIGURE 19.4. *Schematic of the sodium metal 3s band of levels as shown in Figure 19.3, but now with the influence of being connected to the battery. The effect is to put some electrons above the no battery Fermi level, taking them from filled MOs to empty MOs. These electrons are represented by the arrows above the Fermi level.*
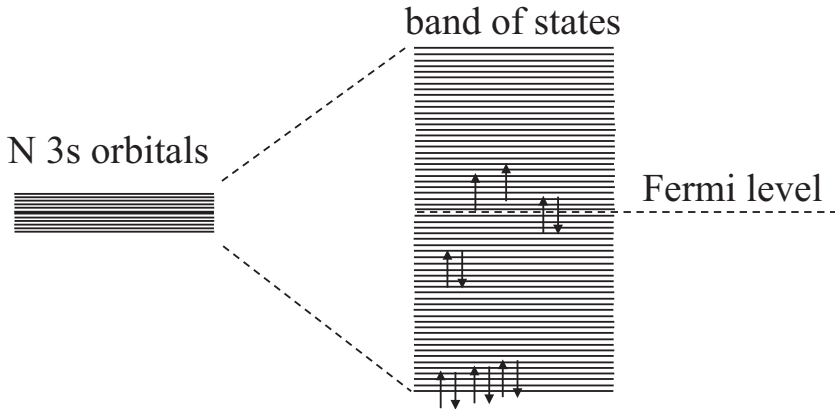
FIGURE 19.5. *Schematic of the band structure of an insulator. There is a filled band, with two electrons in each MO. At much higher energy, there is an empty band.*
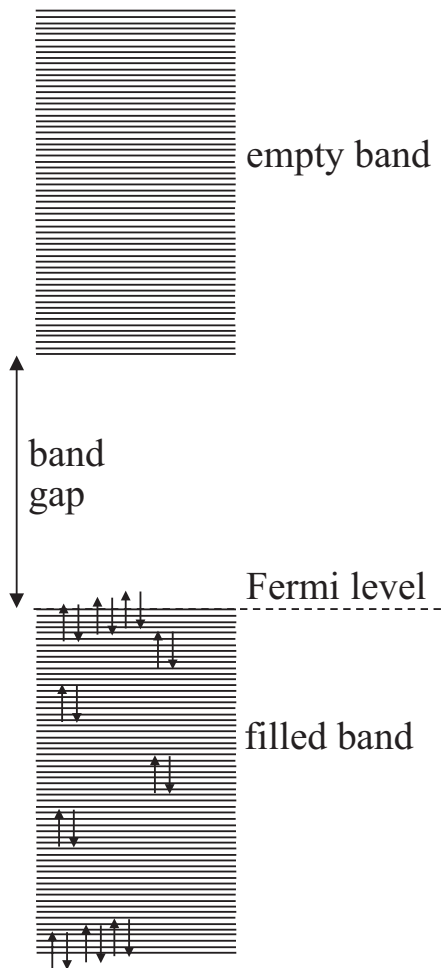
FIGURE 19.6. *Schematic of the band structure of a semiconductor. The valence band is essentially filled. The gap in energy to the next band is relatively small. Some electrons are thermally excited above the Fermi level into the conduction band.*
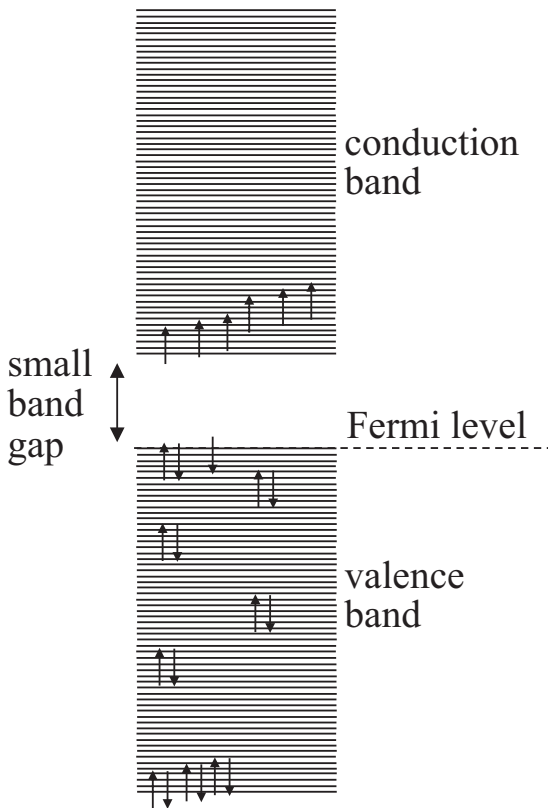
FIGURE 19.7. *Cartoon of an electron-phonon scattering event. The interaction of the electron and phonon causes the directions of the wave packet motions to change.*

phonon
wave packet

electron
wave packet

scattering
event
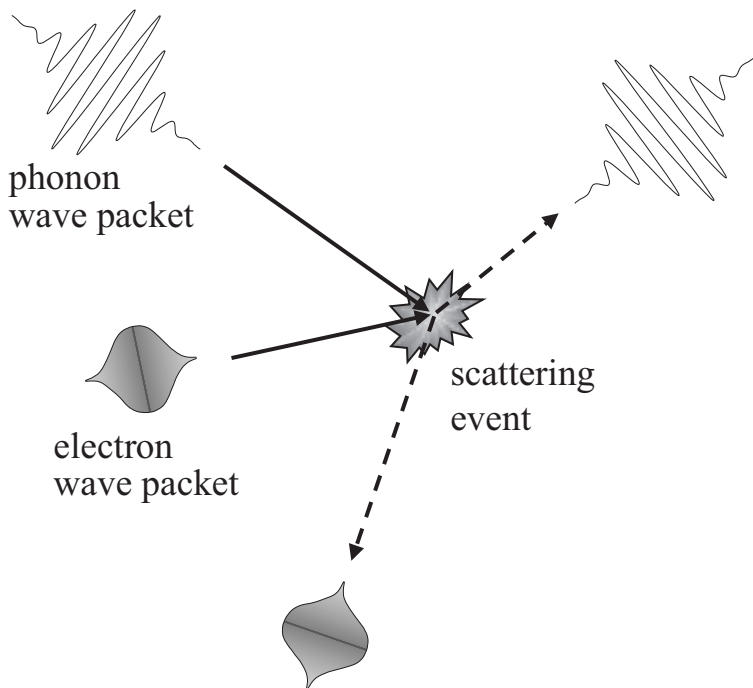
Glossary

absolute size—An object is large or small not by comparison to another object, but rather by comparison to the intrinsic minimum disturbance that accompanies a measurement. If the disturbance is negligible, the object is large in an absolute sense. If the intrinsic minimum disturbance is nonnegligible, the object is absolutely small.

absorption of light—The process by which the amount light is reduced, and the energy of an object is increased. Light (photons, particles of light) of the proper frequency (color) will cause the quantum state of an object to go to a higher energy state. The increase in energy of the object exactly matches the decrease in energy of the light. Absorption of light by objects is responsible for their color.

ångström—A unit of length that is 10^{-10} m (one ten billionth of a meter). The ångström unit has the symbol, Å.

anion—A negatively charged atom or molecule, such as Cl^-, the chloride anion. An anion is formed by adding one or more negatively charged electrons to a neutral atom or molecule.

atomic number—The number of protons (positively charged particles) in an atomic nucleus. A neutral atom (not an ion) has the same number of electrons (negatively charged particles) as protons.

atomic orbital—The name given a wavefunction (probability amplitude wave) that describes the probability distribution of an electron about an atomic nucleus.

black body radiation—The light given off by a hot object. The colors of the light depend on the temperature of the object. Black body radiation is the first physical phenomenon described with the ideas that became quantum mechanics by Max Planck in 1900.

Born interpretation—The description of quantum mechanical wavefunctions as probability amplitude waves. The Born interpretation, also referred to as the Copenhagen interpretation, states that the quantum mechanical wavefunctions obtained from solving the Schrödinger equation describe the probability of finding a particle in some region of space.

cation—a positively charged atom or molecule, such as Na^+, the sodium cation. A cation ion is formed by removing one or more negatively charged electrons from a neutral atom or molecule.

classical mechanics—The theory of matter and light that was developed before the advent of quantum mechanics. It treats size as relative and cannot describe absolutely small particles (electrons, photons, etc.). It is a powerful theory that works extremely well for the description of large objects such as airplanes, the trajectory of a rocket, or bridges.

classical waves—Waves, such as water waves and sound waves, that can be described with classical mechanics. Electromagnetic waves, which are classical mechanics' description of light, are also a type of classical wave. The classical description of light as waves works well for radio and other types of waves, but it cannot properly describe the particle nature of light (photons) responsible for such phenomena as the photoelectric effect.

closed shell configuration—An atom has the number of electrons associated with its nucleus that correspond to one of the noble gases, which comprise the right-hand column of the Periodic Table. A closed shell configuration is particularly stable. The noble gases, also called the inert gases, have the closed shell configuration, and are essentially chemically inert. An atom can obtain a closed shell configuration by gaining or losing electrons to become ions or by sharing electrons with another atom in a covalent bond.

constructive interference—Waves combine (add together) to make a new wave in a manner that increases the amplitude of the total

wave. For waves with different wavelengths, constructive interference will occur only in some regions of space. The wave can be large in some region because of constructive interference but small elsewhere.

Coulomb interaction—The interaction between electrically charged particles that gets smaller as the distance increases. The interaction decreases in proportion to the inverse of the distance. The Coulomb interaction causes particles with opposite charges (positive and negative) to attract each other (an electron and a proton), and like charges to repel (two electrons or two protons).

covalent bond—A chemical bond that holds atoms together because the atoms share electrons.

de Broglie wavelength—The wavelength associated with a particle that has mass. All particles have de Broglie wavelengths. For large particles like baseballs, the de Broglie wavelength is so small that it is negligible. So large particles do not act like waves. For small particles (electrons, etc.), the wavelength is comparable to the size of the particle. Therefore, small particles can exhibit properties that are wavelike.

destructive interference—Waves combine (add together) to make a new wave in a manner that decreases the amplitude of the total wave. For waves with different wavelengths, destructive interference will occur only in some regions of space. The wave can be large in some regions because of constructive interference but small elsewhere because of destructive interference.

Dirac's assumption—A minimum disturbance accompanies any measurement. This disturbance is not an artifact of the experimental method, but is intrinsic to nature. No improvement in technique can eliminate it. If the minimum disturbance is negligible, a particle is large in an absolute sense. If the disturbance is nonnegligible, the particle is absolutely small. Dirac's assumption has been demonstrated by many experiments to be true and is central to quantum theory.

double bond—A chemical bond in which two pairs of electrons are shared between two atoms. A double bond is stronger and shorter than a single bond.

eigenstate—A pure state of a system associated with a perfectly defined value of an observable called an eigenvalue. A system in an energy eigenstate, such as a hydrogen atom, has a perfectly defined energy. The hydrogen atom has many different energy eigenstates, which have different energies (energy eigenvalues). A system in a momentum eigenstate has a perfectly defined value of the momentum. Each eigenstate has a wavefunction associated with it. Eigenstates are the fundamental states of quantum theory.

electromagnetic wave—A wave composed of electric and magnetic fields that oscillate at the same frequency and propagate at the speed of light. Electromagnetic waves are the classical mechanics description of light. The classical theory of electromagnetic waves is useful in describing many aspects of light and radio waves, but it cannot describe many phenomena, such as the photoelectric effect.

electron—A subatomic particle that has a negative charge. It is one of the basic constituents of atoms and molecules. Its negative charge is the same size but opposite in sign from the positive charge of a proton. An atom has the same number of electrons and protons, so it has no overall charge. Adding an electron to an atom makes an anion with one unit of negative charge. Removing an electron from an atom makes a cation with one unit of positive charge.

energy levels—In atoms, molecules, and other quantum absolutely small systems, energy is not continuous. Energy changes can only occur in discreet steps. Each distinct discreet energy is an energy level.

excited state—The state of an atom or molecule that has a higher energy than the minimum. An excited state is created when an atom or molecule that starts in its lowest energy state absorbs a photon of the right frequency to place the system in an energy level above the lowest energy, which is referred to as the ground state. Excited states can also be generated by heat and other mechanisms to put energy into an atom or molecule.

free particle—A particle that has no forces acting on it. A moving free particle will go in a straight line because no forces, such as gravity or air resistance, affect its motion.

frequency—The number of repetitions of a recurring event per unit of

time. For a wave, the frequency is the number of wave peaks that pass by in a given time. For waves traveling at the same speed, a high frequency corresponds to a short wavelength and a low frequency corresponds to a long wavelength. The wavelength is the distance between peaks of a wave. For light waves, the frequency is the speed of light divided by the wavelength.

ground state—The lowest energy state of an atom or molecule. An excited state is created when an atom or molecule that starts in its lowest energy state absorbs a photon of the right frequency to place the system in an energy level above the lowest energy, the ground state. Excited states can also be generated by heat and other mechanisms to put energy into an atom or molecule.

Heisenberg Uncertainty Principle—The momentum and position of a particle cannot be known exactly simultaneously. If the momentum of a particle is known exactly, then the position is completely uncertain, that is, there can be no information on the position. If the position is known exactly, there can be no information on the magnitude of the momentum. In general, the principle states that the position and momentum can only be known within a certain degree of uncertainty. This is intrinsic to nature and not a consequence of experimental error.

hybrid atomic orbitals—Combinations (superpositions) of atomic orbitals that create new atomic orbitals with different shapes. Hybrid atomic orbitals are important in chemical bonding. Hybrid atomic orbitals will be formed to bond atoms together to produce a molecule with the lowest energy (most stable molecule). The shapes of the hybrid orbitals determine the shapes of molecules.

hydrocarbon—A molecule composed of only carbon and hydrogen, such as methane (natural gas) and oil.

inert gases (noble gases). Atoms such as helium, neon, argon, etc., that have closed electron shell configurations. They occupy the right-hand column of the Periodic Table of Elements. Because of closed shell configurations, they are essentially chemically inert. They do bond to other atoms to form molecules.

interference of waves—The combination of two or more waves to give a new wave. The waves can constructively interfere in some region

of space to give an increased amplitude (larger wave) and destructively interfere in other regions of space to produce decreased or zero amplitude.

Joule—A unit of energy. One Joule (J) is a meter times kilograms squared divided by seconds squared. $J = m\,kg^2/s^2$.

kinetic energy—The energy associated with motion. A moving particle has kinetic energy equal to one half times the mass times the velocity squared, as in $E_{ke} = 1/2mV^2$.

light quanta—A single particle of light. A phonon.

lone pair—A pair of electrons in a molecule that occupies an atomic orbital but does not participate in bonding. Lone pair electrons are not shared between atoms.

molecular orbital—A wavefunction for a molecule composed of a combination of atomic orbitals (atomic wavefunctions) that span the molecule. Molecular orbitals can be bonding (bonding MO). Electrons in bonding MOs make the energy of the molecule lower. Molecular orbitals can be antibonding (antibonding MO). Electrons in antibonding MOs increase the energy of a molecule. To have a stable molecule, there must be more electrons in bonding MOs than in antibonding MOs.

momentum eigenstate—The state of a particle with perfectly defined momentum. A momentum eigenstate of a free particle, like a photon or electron, has a wavefunction that is delocalized over all space. The momentum can be known exactly but the position is completely uncertain. Momentum eigenstates can be superimposed (added together) to make a wave packet that has a more or less well-defined position.

nanometer—A unit of length that is one billionth of a meter, 10^{-9} m.

node—For a one-dimensional wave, a point where the amplitude of the wave is zero. For a three-dimensional wave, a node is a plane or other shaped surface where the wave amplitude is zero. The sign of the wavefunction changes when a node is crossed. In quantum mechanics, a node in a wavefunction describing a particle, such as an electron, is a place where the probability of finding the particle is zero.

optical transition—The change in state from one energy level to an-

other in an atom or molecule caused by the absorption or emission of light.

orbital—Another name for the quantum mechanical wavefunction that describes an electron or pair of electrons in an atom or molecule. An atom has atomic orbitals, and a molecule has molecular orbitals.

particle in a box—A quantum mechanical problem in which a particle, such as an electron, is confined to a one-dimensional box with infinitely high and impenetrable walls. The energy levels of a particle in a box are quantized, that is, there are discreet energy levels. The particle in a box is the simplest quantum mechanical problem in which a particle is confined to a small region of space and has quantized energy levels.

Pauli Exclusion Principle—The principle that at most two electrons can be in an atomic or molecular orbital. If two electrons are in the same orbital, they must have opposite spins, that is, different electron quantum numbers s (one $+1/2$ and the other $-1/2$). The Pauli Exclusion Principle is important in determining the structure of the Periodic Table of Elements and the properties of atoms and molecules.

phase—The position along one cycle of a wave. The peak of the wave (point of maximum positive amplitude) is taken to have a phase of 0 degrees ($0°$), then the first node (point where the amplitude is zero) is $90°$. $90°$ is a quarter of a cycle of a wave. A phase of $180°$ is one half of a cycle. It is the point of maximum negative amplitude. Two waves of the same wavelength are said to be phase shifted if the peaks don't line up.

photoelectric effect—The effect explained by Einstein in which a single particle of light, a photon, can eject a single electron from a piece of metal. Einstein's explanation of the photoelectric effect showed that light is not a wave as described by classical electromagnetic theory.

photon—A particle of light.

Planck's constant—The fundamental constant of quantum theory. It is designated by the letter h. It appears in many of the mathematical equations found in quantum mechanics. For example, $E = h\nu$ says

that the energy is the frequency ν (Greek letter nu) multiplied by Planck's constant. Planck's constant has the value h $= 6.6 \times 10^{-34}$ J s (Joule times seconds). Planck introduced the constant in 1900 in his explanation of black body radiation.

potential energy well—A region in space where energy is lowered because of some type of attractive interaction. A hole in the ground is a gravitational potential energy well. A ball will fall to the bottom, lowering its gravitational energy. It will require energy to lift the ball out of the hole. Electrons are held in atoms by a Coulomb potential energy well, that is, by the electrical attraction of negatively charged electrons for the positively charged nucleus. It requires the addition of energy to remove an electron from an atom. Enough energy can raise the electron out of the Coulomb potential energy well created by the attraction to the positively charged nucleus.

probability amplitude wave—Quantum mechanical wave (wavefunction) that describes the probability of finding a particle in some region of space. A probability amplitude wave can go positive and negative. The probability of finding a particle in some region of space is related to the square (actually the absolute value squared) of the probability amplitude wave. The greater the probability in some region of space, the more likely the particle will be found there.

proton—A subatomic particle that has a positive charge. It is one of the basic constituents of atoms and molecules. Its positive charge is the same size but opposite in sign from the negative charge of an electron. An atom has the same number of electrons and protons, so it has no overall charge. The number of protons in an atomic nucleus, called the atomic number, determines the charge of the nucleus. Different atoms have different numbers of protons in their nuclei.

quantized energy levels—Energy levels that come in discreet steps. The energy is not continuous. Atoms and molecules have quantized energy levels.

quantum number—A number that defines the state of a quantum mechanical system. There can be more than one quantum number to

fully specify the state. In an atom, each electron has four quantum numbers, n, *l*, m, and s, which can only take on certain values. Quantum numbers arise from the mathematical description of quantum mechanical systems.

radial distribution function—The mathematical function that describes the probability of finding an electron a certain distance from the nucleus of an atom independent of the direction. It is obtained from the wavefunction for the electron in the atom.

Rydberg formula—The early empirical formula that gave the colors of light emitted or absorbed by hydrogen atoms.

Schrödinger Equation—A fundamental equation of quantum theory. Solution of the Schrödinger Equation for an atom or molecule gives the quantized energy levels and the wavefunctions that describe the probability amplitude of finding electrons in regions of space in an atom or molecule.

single bond—A chemical bond that holds two atoms together through the sharing of one pair of electrons.

size, absolute—An object is large or small depending on whether the intrinsic minimum disturbance that accompanies a measurement is negligible or nonnegligible. If the minimum disturbance is negligible, the object is large in an absolute sense. If it is nonnegligible, it is absolutely small. Absolutely small objects can be described by quantum mechanics, but not by classical mechanics.

size, relative—Size is determined by comparing one object to another. An object is big or small only in relation to another object. In classical mechanics it is assumed that size is relative. Classical mechanics cannot describe objects that are small in an absolute sense.

spatial probability distribution—The probability of finding a particle, such as an electron, in different regions of space. The spatial probability distribution can be calculated from the quantum mechanical wavefunction for a particle.

spectroscopy—The experimental measurement of the amount and colors of light that are absorbed or emitted by a system of atoms or molecules.

Superposition Principle—"Whenever a system is in one state, it can always be considered to be partly in each of two or more states."

This quantum mechanical principle says that a system in a particular quantum state can also be described by the superposition (addition) of two or more other states. In practice, this generally means that a particular wavefunction can be expressed as the sum of two or more other wavefunctions. For example, the wavefunctions for molecules can be formed by the superposition of atomic wavefunctions. A photon wave packet can be formed by the superposition of momentum eigenstates

triple bond—A chemical bond that holds two atoms together by sharing three pairs of electrons. A triple bond is shorter and stronger (harder to pull the atoms apart) than a double or a single bond.

Uncertainty Principle—The statement that the momentum and position of a particle cannot be known exactly simultaneously. If the momentum of a particle is known exactly, then the position is completely uncertain, that is, there can be no information on the position. If the position is known exactly, there can be no information on the magnitude of the momentum. In general, the principle states that the position and momentum can only be known within a certain degree of uncertainty. This is intrinsic to nature and not a consequence of experimental error.

vector—A directed line segment usually represented by an arrow. A vector is a quantity with both magnitude and direction. A car going 60 miles per hour has a speed, which is not a vector. A car going 60 miles per hour north has a velocity, which is a vector because it has a magnitude (60 miles per hour) and a direction (north).

velocity—A vector describing both the speed and the direction in which an object is moving.

wave packet—A superposition of waves that combine to make a particle more or less located in a region of space. The superposition of waves has regions of constructive and destructive interference. The probability of finding the particle is large where there is constructive interference. The superposition of waves more or less localizes a particle in some region of space. The location cannot be perfectly defined because of the Heisenberg Uncertainty Principle.

wavefunction—A solution to the Schrödinger Equation for a particular state of a system, such as an atom or molecule. A wavefunction is

a probability amplitude wave. It gives information on finding a particle in a particular region of space. For example, the wavefunctions for the hydrogen atom give the probabilities of finding the electron at different distances and directions from the nucleus.

wavefunction collapse—A state of a system is frequently a superposition of wavefunctions. Each wavefunction has associated with it a definite value of an observable, for example, the energy. Because a superposition is composed of many wavefunctions, it has associated with it many values of an observable. When a measurement is made, the system goes from being in a superposition of wavefunction to being in a single wavefunction with one value of the observable (e.g., the energy). It is said that the measurement causes the wavefunction to collapse from a superposition of states into a single state with one value of the observable. It is not possible to say beforehand which state the superposition will collapse into. Therefore, it is not possible to say ahead of time which value of the observable will be measured.

wavelength—The repeat distance in a wave, that is, the distance from one peak in the wave to another.