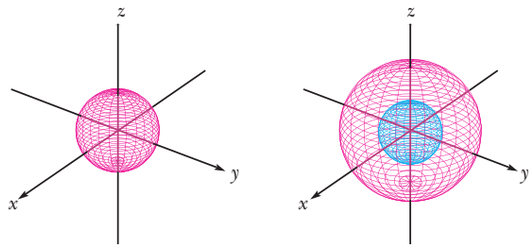
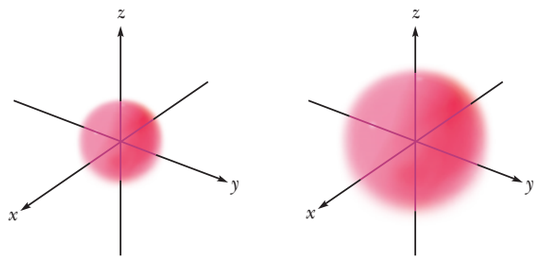
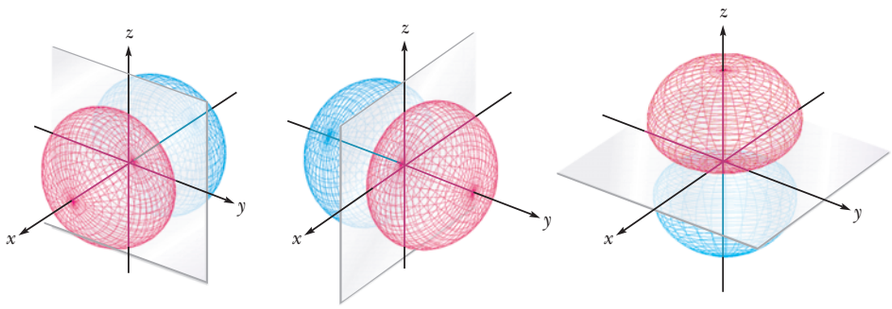


(a) 1*s* and 2*s* orbitals computed using the Schrödinger equation

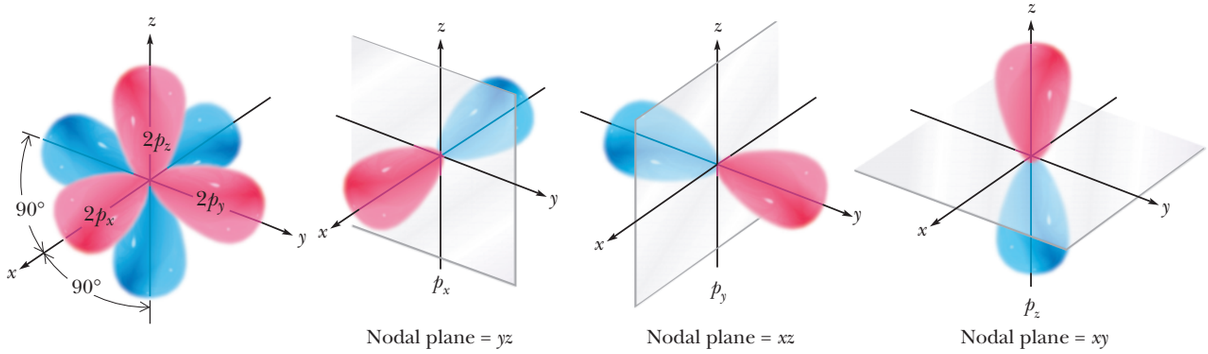


(b) Cartoon representations of 1*s* and 2*s* orbitals

Figure 1.8
(a) Calculated and (b) cartoon representations of the 1*s* and 2*s* atomic orbitals showing an arbitrary boundary containing about 95% of the electron density. Note that the 2*s* orbital has a phase change within the spherical electron density.



(a) 2*p* Orbitals computed using the Schrödinger equation



(b) Cartoon representations of 2*p* orbitals

Figure 1.9
Three-dimensional representations of the $2p_x$, $2p_y$, and $2p_z$ atomic orbitals and their orientation in space relative to one another. Nodal planes are shaded. Note that the lobes of the computed orbitals (a) are more spherical in appearance than the bowling-pin-like cartoon drawings (b) chemists routinely use to represent them.

Besides providing a way to determine the shapes of atomic orbitals, the Schrödinger equation also provides a way, at least approximately, to quantify the energetics of covalent bond formation. These approximations have taken two forms: (1) valence bond (VB) theory and (2) molecular orbital (MO) theory. Both theories of chemical bonding use the methods of quantum mechanics, but each