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In this chapter we consider *molecular structure* and the concepts of *electron bonding*. We will see how information about molecular structure and ideas about bonds can be used to interpret and predict physical properties and chemical reactivity. *Structural formulas* are a key tool for describing both structure and reactivity. At a minimum, they indicate *molecular connectivity* by specifying the *connectivity* among the atoms in the molecule. Structural formulas also give a rough indication of electron distribution by representing electron pairs in bonds by lines and unshared electrons as dots, although the latter are usually omitted in printed structures. The reader is undoubtedly familiar with structural formulas for molecules such as those shown in Scheme 1.1.

In quantitative terms, molecular structure specifies the relative position of all atoms in a molecule. These data provide the bond lengths and bond angles. There are a number of experimental means for precise determination of molecular structure, primarily based on spectroscopic and diffraction methods, and structural data are available for thousands of molecules. Structural information and interpretation is also provided by *computational chemistry*. In later sections of this chapter, we describe how molecular orbital theory and density functional theory can be applied to the calculation of molecular structure and properties.

The *distribution of electrons* is another element of molecular structure that is very important for understanding chemical reactivity. It is considerably more difficult to obtain experimental data on *electron density*, but fortunately, in recent years the rapid development of both structural theory and computational methods has allowed such calculations. We make use of computational electron density data in describing molecular structure, properties, and reactivity. In this chapter, we focus on the minimum energy structure of individual molecules. In Chapter 2, we consider other elements of molecular geometry, including dynamic processes involving *conformation*, that is, the variation of molecular shape as a result of bond rotation. In Chapter 3, we discuss