Determining Chemical Formulas

SECTION 4

OBJECTIVES

- Define *empirical formula,* and explain how the term applies to ionic and molecular compounds.
- Determine an empirical formula from either a percentage or a mass composition.
- Explain the relationship between the empirical formula and the molecular formula of a given compound.
- Determine a molecular formula from an empirical formula.

When a new substance is synthesized or is discovered, it is analyzed quantitatively to reveal its percentage composition. From these data, the empirical formula is then determined. *An* **empirical formula** *consists of the symbols for the elements combined in a compound, with subscripts showing the smallest whole-number mole ratio of the different atoms in the compound.* For an ionic compound, the formula unit is usually the compound's empirical formula. For a molecular compound, however, the empirical formula does not necessarily indicate the actual numbers of atoms present in each molecule. For example, the empirical formula of the gas diborane is BH_3, but the molecular formula is B_2H_6. In this case, the number of atoms given by the molecular formula corresponds to the empirical ratio multiplied by two.

Calculation of Empirical Formulas

To determine a compound's empirical formula from its percentage composition, begin by converting percentage composition to a mass composition. Assume that you have a 100.0 g sample of the compound. Then calculate the amount of each element in the sample. For example, the percentage composition of diborane is 78.1% B and 21.9% H. Therefore, 100.0 g of diborane contains 78.1 g of B and 21.9 g of H.

Next, the mass composition of each element is converted to a composition in moles by dividing by the appropriate molar mass.

$$78.1 \text{ g B} \times \frac{1 \text{ mol B}}{10.81 \text{ g B}} = 7.22 \text{ mol B}$$

$$21.9 \text{ g H} \times \frac{1 \text{ mol H}}{1.01 \text{ g H}} = 21.7 \text{ mol H}$$

These values give a mole ratio of 7.22 mol B to 21.7 mol H. However, this is not a ratio of smallest whole numbers. To find such a ratio, divide each number of moles by the smallest number in the existing ratio.

$$\frac{7.22 \text{ mol B}}{7.22} : \frac{21.7 \text{ mol H}}{7.22} = 1 \text{ mol B} : 3.01 \text{ mol H}$$