

## CALCULATING FORMULAS

### 1. CALCULATION OF EMPIRICAL FORMULAS

#### a. INFORMATION REQUIRED

If the percent composition by elements is known for a compound, it is possible to calculate the empirical formula for a compound.

#### b. EXAMPLE

**Question:** Iron forms several different oxides, all of which are ionic compounds. One oxide of iron,  $\text{Fe}_x\text{O}_y$ , contains 69.940% Fe and 30.060% O. Calculate the empirical formula of this compound.

**Solution Process:** Assume that you have exactly 100 g of the compound so that the number of grams of each element is equal to its percent content in the compound. Calculate the number of moles of Fe and O in the sample, and then determine the simplest ratio of the number of moles.

$$69.940 \text{ g Fe} \times \frac{1.0000 \text{ mole Fe}}{55.847 \text{ g Fe}} = 1.2524 \text{ mole Fe}$$
$$30.060 \text{ g O} \times \frac{1.0000 \text{ mole O}}{15.999 \text{ g O}} = 1.8789 \text{ mole O}$$

Divide by the smallest number of moles, to obtain the mole ratio of the two elements. The O/Fe ratio is  $1.8789/1.2524 = 1.5003$ , which is essentially 1.5/1. Multiply by 2 to obtain the smallest whole number ratio of 3/2 for moles of O/Fe. When writing the chemical formula, the metal is written first.

**The empirical formula is  $\text{Fe}_2\text{O}_3$ .**

### 2. CALCULATION OF MOLECULAR FORMULAS

#### a. INFORMATION REQUIRED

If the molecular weight of a compound and its percent composition by elements are known, it is possible to calculate the molecular formula for a compound.

#### b. EXAMPLE

**Question:** A molecular covalent compound,  $\text{C}_x\text{H}_y$ , contains 85.636% C and 14.364% H and has a molecular weight of 140.268. Calculate the molecular formula of this compound.

**Solution Process:** Consider a one mole sample of the compound and use dimensional analysis to calculate the number of moles of each element in one mole of the compound. The answers will be very close to whole numbers; round these answers to the nearest whole number. The number of moles of each element in one mole of the compound is the same as the number of atoms of each element in one molecule.

If MW = 140.268 amu, the molar mass is 140.268 g/mole.

$$140.268 \text{ g C}_x\text{H}_y \times \frac{85.636 \text{ g C}}{100.00 \text{ g C}_x\text{H}_y} \times \frac{1.0000 \text{ mole C}}{12.011 \text{ g C}} = 10.001 \text{ mole C}$$

$$140.268 \text{ g C}_x\text{H}_y \times \frac{14.364 \text{ g H}}{100.00 \text{ g C}_x\text{H}_y} \times \frac{1.0000 \text{ mole H}}{1.0079 \text{ g H}} = 19.990 \text{ mole H}$$

**The molecular formula is  $\text{C}_{10}\text{H}_{20}$ .**