Practice! For more practice calculating percent composition, go to **Supplemental Practice Problems** in Appendix A.

Empirical Formula

Suppose that the identities of the elements in a sample of a new compound have been determined and the compound's percent composition is known. These data can be used to find the formula for the compound. First, you must determine the smallest whole number ratio of the moles of the elements in the compound. This ratio provides the subscripts in the empirical formula. The **empirical formula** for a compound is the formula with the smallest whole-number mole ratio of the elements. The empirical formula may or may not be the same as the actual molecular formula. If the two formulas are different, the molecular formula will always be a simple multiple of the empirical formula. The empirical formula for hydrogen peroxide is HO; the molecular formula is H_2O_2. In both formulas, the ratio of oxygen to hydrogen is 1:1.

The data used to determine the chemical formula for a compound may be in the form of percent composition or it may be the actual masses of the elements in a given mass of the compound. If percent composition is given, you can assume that the total mass of the compound is 100.00 g and that the percent by mass of each element is equal to the mass of that element in grams. For example, the percent composition of an oxide of sulfur is 40.05% S and 59.95% O. Thus, as you can see in **Figure 11-10**, 100.00 g of the oxide contains 40.05 g S and 59.95 g O. The mass of each element can be converted to a number of moles by multiplying by the inverse of the molar mass. Recall that the number of moles of S and O are calculated in this way.

$$40.05\ \cancel{g\ S} \times \frac{1\ \text{mol S}}{32.07\ \cancel{g\ S}} = 1.249\ \text{mol S}$$

$$59.95\ \cancel{g\ O} \times \frac{1\ \text{mol O}}{16.00\ \cancel{g\ O}} = 3.747\ \text{mol O}$$

The mole ratio of S atoms to O atoms in the oxide is 1.249 : 3.747. As you can see, these values are not whole numbers and cannot be used as subscripts in a chemical formula.

How, then, can the mole ratio be converted to whole numbers? As a starting point, recognize that the element with the smaller number of moles, in this case sulfur, might have the smallest subscript possible, 1. You can make the mole value of sulfur equal to 1 if you divide both mole values by the value of sulfur (1.249). In doing so, you do not change the ratio between the two elements because both are divided by the same number.

$$\frac{1.249\ \text{mol S}}{1.25} = 1\ \text{mol S}$$

$$\frac{3.747\ \text{mol O}}{1.25} = 3\ \text{mol O}$$

The simplest whole number mole ratio of S atoms to O atoms is 1:3. Thus, the empirical formula for the oxide of sulfur is SO_3.

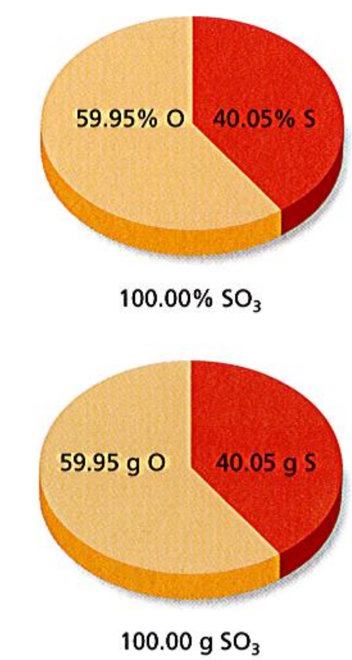

Figure 11-10

Keep this figure in mind when doing problems using percent composition. You can always assume that you have a 100-g sample of the compound and use the percents of the elements as masses of the elements.

Often in determining empirical formulas, the calculated mole values are still not whole numbers, as they are in the preceding example. In such cases, all the mole values must be multiplied by the smallest factor that will make them whole numbers. This is shown in Example Problem 11-11.

EXAMPLE PROBLEM 11-11

Calculating an Empirical Formula from Percent Composition

Methyl acetate is a solvent commonly used in some paints, inks, and adhesives. Determine the empirical formula for methyl acetate, which has the following chemical analysis: 48.64% carbon, 8.16% hydrogen, and 43.20% oxygen.

1. Analyze the Problem

You are given the percent composition of methyl acetate and must find the empirical formula. Because you can assume that each percent by mass represents the mass of the element in a 100.00-g sample, the percent sign can be replaced with the unit grams. Then, you can convert from grams to moles using the molar mass and find the smallest whole-number ratio of moles of the elements.

Known

percent by mass = 48.64% C

percent by mass = 8.16% H

percent by mass = 43.20% O

Unknown

empirical formula = ?

2. Solve for the Unknown

The mass of C is 48.64 g, the mass of H is 8.16 g, and the mass of O is 43.20 g. Multiply the mass of each element by the conversion factor that relates moles to grams based on molar mass.

$$48.64\ \cancel{g\ C} \times \frac{1\ mol\ C}{12.01\ \cancel{g\ C}} = 4.050\ mol\ C$$

$$8.16\ \cancel{g\ H} \times \frac{1\ mol\ H}{1.008\ \cancel{g\ H}} = 8.10\ mol\ H$$

$$43.20\ \cancel{g\ O} \times \frac{1\ mol\ O}{16.00\ \cancel{g\ O}} = 2.700\ mol\ O$$

Methyl acetate has a mole ratio of 4.050 mol C : 8.10 mol H : 2.700 mol O.

Calculate the simplest ratio of moles of the elements by dividing each number of moles by the smallest value in the mole ratio.

$$\frac{4.050\ mol\ C}{2.700} = 1.500\ mol\ C = 1.5\ mol\ C$$

$$\frac{8.10\ mol\ H}{2.700} = 3.00\ mol\ H = 3\ mol\ H$$

$$\frac{2.700\ mol\ O}{2.700} = 1.000\ mol\ O = 1\ mol\ O$$

3. Evaluate the Answer

The calculations are correct and significant figures have been observed. To check that the formula is correct, the percent composition represented by the formula can be calculated. The percent composition checks exactly with the data given in the problem.

PRACTICE PROBLEMS

46. A blue solid is found to contain 36.84% nitrogen and 63.16% oxygen. What is the empirical formula for this solid?

47. Determine the empirical formula for a compound that contains 35.98% aluminum and 64.02% sulfur.

48. Propane is a hydrocarbon, a compound composed only of carbon and hydrogen. It is 81.82% carbon and 18.18% hydrogen. What is the empirical formula?

49. The chemical analysis of aspirin indicates that the molecule is 60.00% carbon, 4.44% hydrogen, and 35.56% oxygen. Determine the empirical formula for aspirin.

50. What is the empirical formula for a compound that contains 10.89% magnesium, 31.77% chlorine, and 57.34% oxygen?

Practice!

For more practice calculating an empirical formula from percent composition, go to **Supplemental Practice Problems** in Appendix A.

Molecular Formula

Would it surprise you to learn that two or more substances with distinctly different properties can have the same percent composition and the same empirical formula? How is this possible? Remember that the subscripts in an empirical formula indicate the simplest whole-number ratio of moles of the elements in the compound. But the simplest ratio does not always indicate the actual number of moles in the compound. To identify a new compound, a chemist must go one step further and determine the **molecular formula**, which specifies the actual number of atoms of each element in one molecule or formula unit of the substance. **Figure 11-11** shows an important use of the gas, acetylene. It has the same percent composition and empirical formula, CH, as benzene which is a liquid. Yet chemically and structurally acetylene and benzene are very different.

To determine the molecular formula for a compound, the molar mass of the compound must be determined through experimentation and compared with the mass represented by the empirical formula. For example, the molar mass of acetylene is 26.04 g/mol and the mass of the empirical formula, CH, is13.02 g/mol. Dividing the actual molar mass by the mass of the empirical formula indicates that the molar mass of acetylene is two times the mass of the empirical formula.

Figure 11-11

Acetylene is a gas used for welding because of the high-temperature flame produced when it is burned with oxygen.

ChemistryOnline

Topic: Empirical Formulas
To learn more about empirical formulas, visit the Chemistry Web site at **chemistrymc.com**

Activity: Research how empirical formulas are used in mineral identification. Prepare a chart comparing the formulas of the minerals with their properties.

Similarly, when the experimentally determined molar mass of benzene, 78.12 g/mol, is compared with the mass of the empirical formula, the molar mass of benzene is found to be six times the mass of the empirical formula.

$$\frac{\text{experimentally determined molar mass of benzene}}{\text{mass of empirical formula CH}} =$$

$$\frac{78.12\ \cancel{\text{g/mol}}}{13.02\ \cancel{\text{g/mol}}} = 6.000$$

The molar mass of benzene is six times the mass represented by the empirical formula, so the molecular formula for benzene must represent six times the number of carbon and hydrogen atoms shown in the empirical formula. You can conclude that the molecular formula for acetylene is (CH)2 or C_2H_2 and the molecular formula for benezene is (CH)6 or C_6H_6.

A molecular formula can be represented as the empirical formula multiplied by an integer n.

$$\text{molecular formula} = (\text{empirical formula})n$$

The integer is the factor (6 in the example above) by which the subscripts in the empirical formula must be multiplied to obtain the molecular formula.

Succinic acid occurs naturally in fossils and fungi, and in lichens such as those shown. Succinic acid produced commercially is used to make compounds used in perfumes (esters) and in lacquers and dyes.

EXAMPLE PROBLEM 11-12

Determining a Molecular Formula

Succinic acid is a substance produced by lichens. Chemical analysis indicates it is composed of 40.68% carbon, 5.08% hydrogen, and 54.24% oxygen and has a molar mass of 118.1 g/mol. Determine the empirical and molecular formulas for succinic acid.

1. Analyze the Problem

You are given the percent composition that allows you to calculate the empirical formula. Assume that each percent by mass represents the mass of the element in a 100.00-g sample.You can compare the given molar mass with the mass represented by the empirical formula to find n.

Known	Unknown
percent by mass = 40.68% C	empirical formula = ?
percent by mass = 5.08% H	molecular formula = ?
percent by mass = 54.24 % O	
molar mass = 118.1 g/mol succinic acid	

2. Solve for the Unknown

Use the percents by mass as grams of elements and convert to the number of moles by multiplying by the conversion factor that relates moles to mass based on molar mass.

$$40.68\ \cancel{\text{g C}} \times \frac{1\text{ mol C}}{12.01\ \cancel{\text{g C}}} = 3.387\text{ mol C}$$

$$5.08\ \cancel{\text{g H}} \times \frac{1\text{ mol H}}{1.008\ \cancel{\text{g H}}} = 5.04\text{ mol H}$$

$$54.24\ \cancel{\text{g O}} \times \frac{1\text{ mol O}}{16.00\ \cancel{\text{g O}}} = 3.390\text{ mol O}$$

Succinic acid has a mole ratio of C : H : O of 3.387 : 5.04 : 3.390.

Calculate the simplest ratio among the elements by dividing each mole value by the smallest value in the mole ratio.

$$\frac{3.387\text{ mol C}}{3.387} = 1\text{ mol C}$$

$$\frac{5.040\text{ mol H}}{3.387} = 1.49\text{ mol H} = 1.5\text{ mol H}$$

$$\frac{3.390\text{ mol O}}{3.387} = 1.001\text{ mol O} = 1\text{ mol O}$$

The simplest ratio is 1 mol C : 1.5 mol H : 1 mol O.

The simplest mol ratio includes a fractional value that cannot be used as a subscript in a formula. Multiply all mole values by 2.

$2 \times 1\text{ mol C} = 2\text{ mol C}$

$2 \times 1.5\text{ mol H} = 3\text{ mol H}$

$2 \times 1\text{ mol O} = 2\text{ mol O}$

The simplest whole-number ratio of C atoms to H atoms to O atoms is 2 : 3 : 2. The empirical formula is $C_2H_3O_2$

Calculate the empirical formula mass using the molar mass of each element.

$$2\ \cancel{\text{mol C}} \times \frac{12.01\text{ g C}}{1\ \cancel{\text{mol C}}} = 24.02\text{ g C}$$

$$3\ \cancel{\text{mol H}} \times \frac{1.008\text{ g H}}{1\ \cancel{\text{mol H}}} = 3.024\text{ g H}$$

$$2\ \cancel{\text{mol O}} \times \frac{16.00\text{ g O}}{1\ \cancel{\text{mol O}}} = 32.00\text{ g O}$$

$$\text{molar mass } C_2H_3O_2 = 59.04\text{ g/mol } C_2H_3O_2$$

Divide the experimentally determined molar mass of succinic acid by the mass of the empirical formula to determine n.

$$n = \frac{\text{molar mass of succinic acid}}{\text{molar mass of } C_2H_3O_2}$$

$$n = \frac{118.1\ \cancel{\text{g/mol}}}{59.04\ \cancel{\text{g/mol}}} = 2.000$$

Multiply the subscripts in the empirical formula by 2 to determine the actual subscripts in the molecular formula.

$(C_2H_3O_2)(2) = C_4H_6O_4$

The molecular formula for succinic acid is $C_4H_6O_4$.

3. Evaluate the Answer

Calculation of the molar mass from the molecular formula gives the same result as the experimental molar mass.

Practice!

For more practice calculating a molecular formula from percent composition, go to **Supplemental Practice Problems** in Appendix A.