

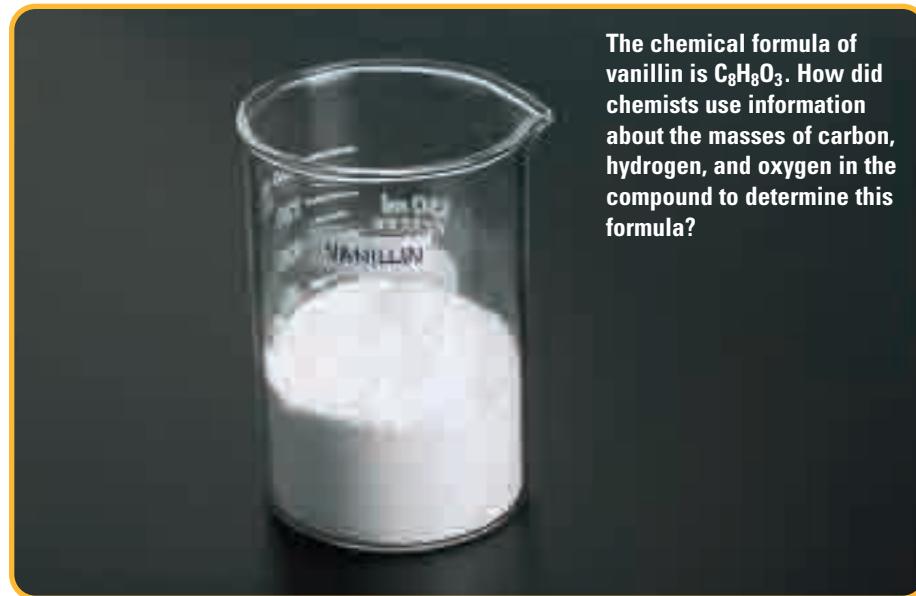
# Chemical Proportions in Compounds

**H**ow do chemists use what they know about molar masses? In Chapter 5, you learned how to use the periodic table and the mole to relate the mass of a compound to the number of particles in the compound. Chemists can use their understanding of molar mass to find out important information about compounds.

Sometimes chemists analyze a compound that is found in nature to learn how to produce it more cheaply in a laboratory. For example, consider the flavour used in vanilla ice cream, which may come from natural or artificial vanilla extract. Natural vanilla extract is made from vanilla seed pods, shown on the left. The seed pods must be harvested and processed before being sold as vanilla extract. The scent and flavour of synthetic vanilla come from a compound called vanillin, which can be produced chemically in bulk. Therefore its production is much cheaper. Similarly, many medicinal chemicals that are found in nature can be produced more cheaply and efficiently in a laboratory.

Suppose that you want to synthesize a compound such as vanillin in a laboratory. You must first determine the elements in the compound. Then you need to know the proportion of each element that is present. This information, along with your understanding of molar mass, will help you determine the chemical formula of the compound. Once you know the chemical formula, you are on your way to finding out how to produce the compound.

In this chapter, you will learn about the relationships between chemical formulas, molar masses, and the masses of elements in compounds.



The chemical formula of vanillin is  $C_8H_8O_3$ . How did chemists use information about the masses of carbon, hydrogen, and oxygen in the compound to determine this formula?

## Chapter Preview

- 6.1** Percentage Composition
- 6.2** The Empirical Formula of a Compound
- 6.3** The Molecular Formula of a Compound
- 6.4** Finding Empirical and Molecular Formulas by Experiment

## Concepts and Skills You Will Need

Before you begin this chapter, review the following concepts and skills:

- naming chemical compounds (Chapter 3, section 3.5)
- understanding the mole (Chapter 5, section 5.2)
- explaining the relationship between the mole and molar mass (Chapter 5, section 5.3)
- solving problems involving number of moles, number of particles, and mass (Chapter 5, section 5.3)

# 6.1

# Percentage Composition

## Section Preview/ Specific Expectations

In this section, you will

- **explain** the law of definite proportions
- **calculate** the percentage composition of a compound using the formula and the relative atomic masses of the elements
- **communicate** your understanding of the following terms: *law of definite proportions, mass percent, percentage composition*

## mind STRETCH

If a bicycle factory has 1000 wheels and 400 frames, how many bicycles can be made? How many wheels does each bicycle have? Is the number of wheels per bicycle affected by any extra wheels that the factory may have in stock? Relate these questions to the law of definite proportions.

When you calculate and use the molar mass of a compound, such as water, you are making an important assumption. You are assuming that every sample of water contains hydrogen and oxygen in the ratio of two hydrogen atoms to one oxygen atom. Thus you are also assuming that the masses of hydrogen and oxygen in pure water always exist in a ratio of 2 g:16 g. This may seem obvious to you, because you know that the molecular formula of water is always  $\text{H}_2\text{O}$ , regardless of whether it comes from any of the sources shown in Figure 6.1. When scientists first discovered that compounds contained elements in fixed mass proportions, they did not have the periodic table. In fact, the discovery of fixed mass proportions was an important step toward the development of atomic theory.

## The Law of Definite Proportions

In the late eighteenth century, Joseph Louis Proust, a French chemist, analyzed many samples of copper(II) carbonate,  $\text{CuCO}_3$ . He found that the samples contained the same proportion of copper, carbon, and oxygen, regardless of the source of the copper(II) carbonate. This discovery led Proust to propose the **law of definite proportions**: *the elements in a chemical compound are always present in the same proportions by mass*.



**Figure 6.1** Suppose that you distil pure water from each of these sources to purify it. Are the distilled water samples the same or different? What is the molar mass of the distilled water from each source?

Chemical formulas such as CO and CO<sub>2</sub> reflect an important law called the *law of multiple proportions*. This law applies when two elements (such as carbon and oxygen) combine to form two or more different compounds. In these cases, the masses of the element (such as O<sub>2</sub> in CO and CO<sub>2</sub>) that combine with a fixed amount of the second element are in ratios of small whole numbers. For example, two moles of carbon can combine with one mole of oxygen to form carbon monoxide, or with two moles of oxygen to form carbon dioxide. The ratio of the two different amounts of oxygen that combine with the fixed amount of carbon is 1:2.

The mass of an element in a compound, expressed as a percent of the total mass of the compound, is the element's **mass percent**. The mass percent of hydrogen in water from any of the sources shown in Figure 6.1 is 11.2%. Similarly, the mass percent of oxygen in water is always 88.8%. Whether the water sample is distilled from a lake, an ice floe, or a drinking fountain, the hydrogen and oxygen in pure water are always present in these proportions.

## Different Compounds from the Same Elements

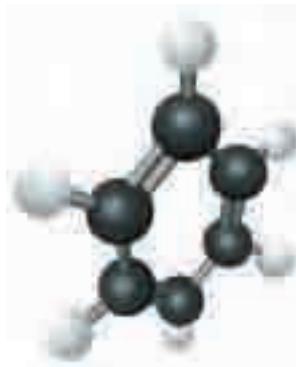
The law of definite proportions does not imply that elements in compounds are always present in the same relative amounts. It is possible to have different compounds made up of different amounts of the same elements. For example, water, H<sub>2</sub>O, and hydrogen peroxide, H<sub>2</sub>O<sub>2</sub>, are both made up of hydrogen and oxygen. Yet, as you can see in Figure 6.2, each compound has unique properties. Each compound has a different mass percent of oxygen and hydrogen. You may recognize hydrogen peroxide as a household chemical. It is an oxidizing agent that is used to bleach hair and treat minor cuts. It is also sold as an alternative to chlorine bleach.

Figure 6.3 shows a molecule of benzene, C<sub>6</sub>H<sub>6</sub>. Benzene contains 7.76% hydrogen and 92.2% carbon by mass. Octane, C<sub>8</sub>H<sub>18</sub>, is a major component of the fuel used for automobiles. It contains 84.1% carbon and 15.9% hydrogen.

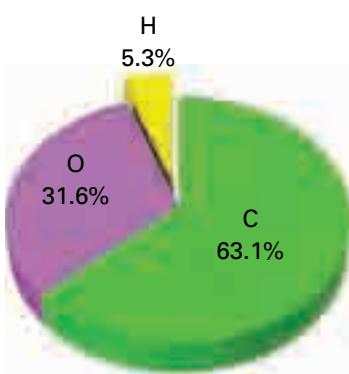


**Figure 6.2** Water contains hydrogen and oxygen, but it does not decompose in the presence of manganese dioxide. Hydrogen peroxide is also composed of hydrogen and oxygen. It is fairly unstable and decomposes vigorously in the presence of manganese(IV) oxide.

Similarly, carbon monoxide, CO, and carbon dioxide, CO<sub>2</sub>, are both made up of carbon and oxygen. Yet each compound is unique, with its own physical and chemical properties. Carbon dioxide is a product of cellular respiration and the complete combustion of fossil fuels. Carbon monoxide is a deadly gas formed when insufficient oxygen is present during the combustion of carbon-containing compounds. Carbon monoxide always contains 42.88% carbon by mass. Carbon dioxide always contains 27.29% carbon by mass.



**Figure 6.3** Benzene C<sub>6</sub>H<sub>6</sub>, is made up of six carbon atoms and six hydrogen atoms. Why does benzene not contain 50% of each element by mass?



**Figure 6.4** This pie graph shows the percentage composition of vanillin.

## Percentage Composition

Carbon dioxide and carbon monoxide contain the same elements but have different proportions of these elements. In other words, they are composed differently. Chemists express the composition of compounds in various ways. One way is to describe how many moles of each element make up a mole of a compound. For example, one mole of carbon dioxide contains one mole of carbon and two moles of oxygen. Another way is to describe the percent mass of each element in a compound.

The **percentage composition** of a compound refers to the relative mass of each element in the compound. In other words, percentage composition is a statement of the values for mass percent of every element in the compound. For example, the compound vanillin,  $C_8H_8O_3$ , has a percentage composition of 63.1% carbon, 5.3% hydrogen, and 31.6% oxygen, as shown in Figure 6.4.

A compound's percentage composition is an important piece of information. For example, percentage composition can be determined experimentally, and then used to help identify the compound.

Examine the following Sample Problem to learn how to calculate the percentage composition of a compound from the mass of the compound and the mass of the elements that make up the compound. Then do the Practice Problems to try expressing the composition of substances as mass percents.

### Sample Problem

#### Percentage Composition from Mass Data

##### Problem

A compound with a mass of 48.72 g is found to contain 32.69 g of zinc and 16.03 g of sulfur. What is the percentage composition of the compound?

##### What Is Required?

You need to find the mass percents of zinc and sulfur in the compound.

##### What Is Given?

You know the mass of the compound. You also know the mass of each element in the compound.

Mass of compound = 48.72 g

Mass of Zn = 32.69 g

Mass of S = 16.03 g

##### Plan Your Strategy

To find the percentage composition of the compound, find the mass percent of each element. To do this, divide the mass of each element by the mass of the compound and multiply by 100%.

### mind STRETCH

Does the unknown compound in the Sample Problem contain any elements other than zinc and sulfur? How do you know? Use the periodic table to predict the formula of the compound. Does the percentage composition support your prediction?

*Continued ...*

## mind STRETCH

Iron is commonly found as two oxides, with the general formula  $\text{Fe}_x\text{O}_y$ . One oxide is 77.7% iron. The other oxide is 69.9% iron. Use the periodic table to predict the formula of each oxide. Match the given values for the mass percent of iron to each compound. How can you use the molar mass of iron and the molar masses of the two iron oxides to check the given values for mass percent?

### Act on Your Strategy

$$\begin{aligned}\text{Mass percent of Zn} &= \frac{\text{Mass of Zn}}{\text{Mass of compound}} \times 100\% \\ &= \frac{32.69 \cancel{\text{g}}}{48.72 \cancel{\text{g}}} \times 100\% \\ &= 67.10\%\end{aligned}$$

$$\begin{aligned}\text{Mass percent of S} &= \frac{\text{Mass of S}}{\text{Mass of compound}} \times 100\% \\ &= \frac{16.03 \cancel{\text{g}}}{48.72 \cancel{\text{g}}} \times 100\% \\ &= 32.90\%\end{aligned}$$

The percentage composition of the compound is 67.10% zinc and 32.90% sulfur.

### Check Your Solution

The mass of zinc is about 32 g per 50 g of the compound. This is roughly 65%, which is close to the calculated value.

## Practice Problems

- A sample of a compound is analyzed and found to contain 0.90 g of calcium and 1.60 g of chlorine. The sample has a mass of 2.50 g. Find the percentage composition of the compound.
- Find the percentage composition of a pure substance that contains 7.22 g nickel, 2.53 g phosphorus, and 5.25 g oxygen only.
- A sample of a compound is analyzed and found to contain carbon, hydrogen, and oxygen. The mass of the sample is 650 mg, and the sample contains 257 mg of carbon and 50.4 mg of hydrogen. What is the percentage composition of the compound?
- A scientist analyzes a 50.0 g sample and finds that it contains 13.3 g of potassium, 17.7 g of chromium, and another element. Later the scientist learns that the sample is potassium dichromate,  $\text{K}_2\text{Cr}_2\text{O}_7$ . Potassium dichromate is a bright orange compound that is used in the production of safety matches. What is the percentage composition of potassium dichromate?

It is important to understand clearly the difference between percent by mass and percent by number. In the Thought Lab that follows, you will investigate the distinction between these two ways of describing composition.

### Web

### LINK

[www.school.mcgrawhill.ca/  
resources/](http://www.school.mcgrawhill.ca/resources/)

Vitamin C is the common name for ascorbic acid,  $\text{C}_6\text{H}_8\text{O}_6$ . To learn about this vitamin, go to the web site above. Go to **Science Resources**, then to **Chemistry 11** to find out where to go next. Do you think there is a difference between natural and synthetic vitamin C? Both are ascorbic acid.

Natural vitamin C comes from foods we eat, especially citrus fruits. Synthetic vitamin C is made in a laboratory. Why do the prices of natural and synthetic products often differ? Make a list to show the pros and cons of vitamins from natural and synthetic sources.



A company manufactures gift boxes that contain two pillows and one gold brick. The gold brick has a mass of 20 kg. Each pillow has a mass of 1.0 kg.

### Procedure

1. You are a quality control specialist at the gift box factory. You need to know the following information:
  - (a) What is the percent of pillows, in terms of the number of items, in the gift box?
  - (b) What is the percent of pillows, by mass, in the gift box?
  - (c) What is the percent of gold, by mass, in the gift box?
2. You have a truckload of gift boxes to inspect. You now need to know this information:
  - (a) What is the percent of pillows, in terms of the number of items, in the truckload of gift boxes?
  - (b) What is the percent of pillows, by mass, in the truckload of gift boxes?
  - (c) What is the percent of gold, by mass, in the truckload of gift boxes?

### Analysis

1. The truckload of gift boxes, each containing 2 light pillows and 1 heavy gold brick, can be used to represent a pure substance, water, containing 2 mol of a “light” element, such as hydrogen, and 1 mol of a “heavy” element, such as oxygen.
  - (a) What is the percent of hydrogen, in terms of the number of atoms, in 1 mol of water?
  - (b) What is the mass percent of hydrogen in 1 mol of water?
  - (c) What is the mass percent of oxygen in 1 mol of water?
2. Would the mass percent of hydrogen or oxygen in question 1 change if you had 25 mol of water? Explain.
3. Why do you think chemists use mass percent rather than percent by number of atoms?



## Calculating Percentage Composition from a Chemical Formula

In the previous Practice Problems, you used mass data to calculate percentage composition. This skill is useful for interpreting experimental data when the chemical formula is unknown. Often, however, the percentage composition is calculated from a known chemical formula. This is useful when you are interested in extracting a certain element from a compound. For example, many metals, such as iron and mercury, exist in mineral form. Mercury is most often found in nature as mercury(II) sulfide,  $\text{HgS}$ . Knowing the percentage composition of  $\text{HgS}$  helps a metallurgist predict the mass of mercury that can be extracted from a sample of  $\text{HgS}$ .

When determining the percentage composition by mass of a homogeneous sample, the size of the sample does not matter. According to the law of definite proportions, there is a fixed proportion of each element in the compound, no matter how much of the compound you have. This means that you can choose a convenient sample size when calculating percentage composition from a formula.

If you assume that you have one mole of a compound, you can use the molar mass of the compound, with its chemical formula, to calculate its percentage composition. For example, suppose that you want to find the

percentage composition of HgS. You can assume that you have one mole of HgS and find the mass percents of mercury and sulfur in one mole of the compound.

$$\begin{aligned}\text{Mass percent of Hg in HgS} &= \frac{\text{Mass of Hg in 1 mol of HgS}}{\text{Mass of 1 mol of HgS}} \times 100\% \\ &= \frac{200.6 \text{ g}}{228.68 \text{ g}} \times 100\% \\ &= 87.7\%\end{aligned}$$

Mercury(II) sulfide is 87.7% mercury by mass. Since there are only two elements in HgS, you can subtract the mass percent of mercury from 100 percent to find the mass percent of sulfur.

$$\text{Mass percent of S in HgS} = 100\% - 87.7\% = 12.3\%$$

Therefore, the percentage composition of mercury(II) sulfide is 87.7% mercury and 12.3% sulfur.

Sometimes there are more than two elements in a compound, or more than one atom of each element. This makes determining percentage composition more complex than in the example above. Work through the Sample Problem below to learn how to calculate the percentage composition of a compound from its molecular formula.

## Sample Problem

### Finding Percentage Composition from a Chemical Formula

#### Problem

Cinnamaldehyde, C<sub>9</sub>H<sub>8</sub>O, is responsible for the characteristic odour of cinnamon. Determine the percentage composition of cinnamaldehyde by calculating the mass percents of carbon, hydrogen, and oxygen.

#### What Is Required?

You need to find the mass percents of carbon, hydrogen, and oxygen in cinnamaldehyde.

#### What Is Given?

The molecular formula of cinnamaldehyde is C<sub>9</sub>H<sub>8</sub>O.

Molar mass of C = 12.01 g/mol

Molar mass of H = 1.01 g/mol

Molar mass of O = 16.00 g/mol

#### Plan Your Strategy

From the molar masses of carbon, hydrogen, and oxygen, calculate the molar mass of cinnamaldehyde.

Then find the mass percent of each element. To do this, divide the mass of each element in 1 mol of cinnamaldehyde by the molar mass of cinnamaldehyde, and multiply by 100%. Remember that

Before AD 1500, many alchemists thought that matter was composed of two “elements”: mercury and sulfur. To impress their patrons, they performed an experiment with mercury sulfide, also called cinnabar, HgS. They heated the red cinnabar, which drove off the sulfur and left the shiny liquid mercury. On further heating, the mercury reacted to form a red compound again. Alchemists wrongly thought that the mercury had been converted back to cinnabar. What Hg(II) compound do you think was really formed when the mercury was heated in the air? What is the mass percent of mercury in this new compound? What is the mass percent of mercury in cinnabar?

*Continued ...*

there are 9 mol carbon, 8 mol hydrogen, and 1 mol oxygen in each mole of cinnamaldehyde.

### Act on Your Strategy

$$\begin{aligned} M_{\text{C}_9\text{H}_8\text{O}} &= (9 \times M_{\text{C}}) + (8 \times M_{\text{H}}) + (M_{\text{O}}) \\ &= (9 \times 12.01 \text{ g}) + (8 \times 1.01 \text{ g}) + 16.00 \text{ g} \\ &= 132 \text{ g} \end{aligned}$$

$$\begin{aligned} \text{Mass percent of C} &= \frac{9 \times M_{\text{C}}}{M_{\text{C}_9\text{H}_8\text{O}}} \times 100\% \\ &= \frac{9 \times 12.01 \text{ g/mol}}{132 \text{ g/mol}} \times 100\% \\ &= 81.9\% \end{aligned}$$

$$\begin{aligned} \text{Mass percent of H} &= \frac{8 \times M_{\text{H}}}{M_{\text{C}_9\text{H}_8\text{O}}} \times 100\% \\ &= \frac{8 \times 1.01 \text{ g/mol}}{132 \text{ g/mol}} \times 100\% \\ &= 6.12\% \end{aligned}$$

$$\begin{aligned} \text{Mass percent of O} &= \frac{1 \times M_{\text{O}}}{M_{\text{C}_9\text{H}_8\text{O}}} \times 100\% \\ &= \frac{1 \times 16.00 \text{ g/mol}}{132 \text{ g/mol}} \times 100\% \\ &= 12.1\% \end{aligned}$$

The percentage composition of cinnamaldehyde is 81.9% carbon, 6.12% hydrogen, and 12.1% oxygen.

### Check Your Solution

The mass percents add up to 100%.

## Practice Problems

5. Calculate the mass percent of nitrogen in each compound.  
 (a) N<sub>2</sub>O      (c) NH<sub>4</sub>NO<sub>3</sub>  
 (b) Sr(NO<sub>3</sub>)<sub>2</sub>      (d) HNO<sub>3</sub>
6. Sulfuric acid, H<sub>2</sub>SO<sub>4</sub>, is an important acid in laboratories and industries. Determine the percentage composition of sulfuric acid.
7. Potassium nitrate, KNO<sub>3</sub>, is used to make fireworks. What is the mass percent of oxygen in potassium nitrate?
8. A mining company wishes to extract manganese metal from pyrolusite ore, MnO<sub>2</sub>.
  - (a) What is the percentage composition of pyrolusite ore?
  - (b) Use your answer from part (a) to calculate the mass of pure manganese that can be extracted from 250 kg of pyrolusite ore.

### CHECKPOINT

When it is heated, solid potassium nitrate reacts to form solid potassium oxide, gaseous nitrogen, and gaseous oxygen. Write a balanced chemical equation for this reaction. What type of reaction is it?

## Section Wrap-up

In this section, you learned that you can calculate percentage composition using a chemical formula. Often, however, chemists do not know the chemical formula of the compound they are analyzing, as in Figure 6.5. Through experiment, they can determine the masses of the elements that make up the compound. Then they can use the masses to calculate the percentage composition. (You will learn about one example of this kind of experimental technique in section 6.4.) From the percentage composition, chemists can work backward to determine the formula of the unknown compound. In section 6.2, you will learn about the first step in using the percentage composition of a compound to determine its chemical formula.

## mind STRETCH

You know that both elements and compounds are pure substances. Write a statement, using the term “percentage composition,” to distinguish between elements and compounds.



**Figure 6.5** One of these compounds is vanillin,  $C_8H_8O_3$ , and one is glucose,  $C_6H_{12}O_6$ . How could a chemist use percentage composition to find out which is which?

## Section Review

- 1 **C** Acetylene,  $C_2H_2$ , is the fuel in a welder’s torch. It contains an equal number of carbon and hydrogen atoms. Explain why acetylene is not 50% carbon by mass.
- 2 **K/U** When determining percentage composition, why is it acceptable to work with either molar quantities, expressed in grams, or average molecular (or atomic or formula unit) quantities, expressed in atomic mass units?
- 3 **I** Indigo,  $C_{16}H_{10}N_2O_2$ , is the common name of the dye that gives blue jeans their characteristic colour. Calculate the mass of oxygen in 25.0 g of indigo.

### Unit Investigation Prep

Before you design your experiment to find the composition of a mixture, think about using mass percents in analysis. If you wanted to determine the percent by mass of each component in a mixture, what would you need to do first? Compare this situation to finding percentage composition of a pure substance.



- 4 **I** Potassium perchlorate,  $\text{KClO}_4$ , is used extensively in explosives. Calculate the mass of oxygen in a 24.5 g sample of potassium perchlorate.
- 5 **I** 18.4 g of silver oxide,  $\text{Ag}_2\text{O}$ , is decomposed into silver and oxygen by heating. What mass of silver will be produced?
- 6 **MC** The label on a box of baking soda (sodium hydrogen carbonate,  $\text{NaHCO}_3$ ) claims that there are 137 mg of sodium per 0.500 g of baking soda. Comment on the validity of this claim.
- 7 **I** A typical soap molecule consists of a polyatomic anion associated with a cation. The polyatomic anion contains hydrogen, carbon, and oxygen. One particular soap molecule has 18 carbon atoms. It contains 70.5% carbon, 11.5% hydrogen, and 10.4% oxygen by mass. It also contains one alkali metal cation. Identify the cation.
- 8 **I** Examine the photographs below. When concentrated sulfuric acid is added to sucrose,  $\text{C}_{12}\text{H}_{22}\text{O}_{11}$ , a column of pure carbon is formed, as well as some water vapour and other gases. How would you find the mass percent of carbon in sucrose using this reaction? You may assume that all the carbon in the sucrose is converted to carbon. Design an experiment to determine the mass percent of carbon in sucrose, based on this reaction. Do not try to perform this experiment. What difficulties might you encounter?

**A****B****C**

# The Empirical Formula of a Compound

## 6.2

As part of his atomic theory, John Dalton stated that atoms combine with one another in simple whole number ratios to form compounds. For example, the molecular formula of benzene,  $C_6H_6$ , indicates that one molecule of benzene contains 6 carbon atoms and 6 hydrogen atoms. The **empirical formula** (also known as the simplest formula) of a compound shows the lowest whole number ratio of the elements in the compound. The **molecular formula** (also known as the actual formula) describes the number of atoms of each element that make up a molecule or formula unit. Benzene, with a molecular formula of  $C_6H_6$ , has an empirical formula of CH. Table 6.1 shows the molecular formulas of several compounds, along with their empirical formulas.

**Table 6.1** Comparing Molecular Formulas and Empirical Formulas

Name of compound	Molecular (actual) formula	Empirical (simplest) formula	Lowest ratio of elements
hydrogen peroxide	$H_2O_2$	HO	1:1
glucose	$C_6H_{12}O_6$	CH <sub>2</sub> O	1:2:1
benzene	$C_6H_6$	CH	1:1
acetylene (ethyne)	$C_2H_2$	CH	1:1
aniline	$C_6H_7N$	$C_6H_7N$	6:7:1
water	$H_2O$	$H_2O$	2:1

It is possible for different compounds to have the same empirical formula, as you can see in Figure 6.6. For example, benzene and acetylene both have the empirical formula CH. Each, however, is a unique compound. Benzene,  $C_6H_6$ , is a clear liquid with a molar mass of 78 g/mol and a boiling point of 80°C. Acetylene,  $C_2H_2$ , has a molar mass of 26 g/mol. It is a highly flammable gas, commonly used in a welder's torch. There is, in fact, no existing compound with the molecular formula CH. The empirical formula of a compound shows the lowest whole number ratio of the atoms in the compound. It does not express the composition of a molecule.

Many compounds have molecular formulas that are the same as their empirical formulas. One example is ammonia,  $NH_3$ . Try to think of three other examples.

### Section Preview/ Specific Expectations

In this section, you will

- **perform** an experiment to determine the percentage composition and the empirical formula of a compound
- **calculate** the empirical formula of a compound using percentage composition
- **communicate** your understanding of the following terms:  
*empirical formula, molecular formula*

### Language LINK

The word “empirical” comes from the Greek word *empeirikos*, meaning, roughly, “by experiment.” Why do you think the simplest formula of a compound is called its empirical formula?



**Figure 6.6** The same empirical formula can represent more than one compound. These two compounds are different—at room temperature, one is a gas and one is a liquid. Yet they have the same empirical formula.

In mathematics, you frequently need to reduce an expression to lowest terms. For example,  $\frac{4x^2}{x}$  is equivalent to  $4x$ . A ratio of 5:10 is equivalent to 1:2. In chemistry, however, the “lowest terms” version of a chemical formula is not equivalent to its “real” molecular formula. Why not?

## mind STRETCH

How do the molar masses of  $C_6H_6$  and  $C_2H_2$  compare with the molar mass of their empirical formula? How does the molar mass of water compare with the molar mass of its empirical formula? Describe the relationship between the molar mass of a compound and the molar mass of the empirical formula of the compound.

The relationship between the molecular formula of a compound and its empirical formula can be expressed as

Molecular formula subscripts =  $n \times$  Empirical formula subscripts, where  $n = 1, 2, 3\dots$

This relationship shows that the molecular formula of a compound is the same as its empirical formula when  $n = 1$ . What information do you need in order to determine whether the molecular formula of a compound is the same as its empirical formula?

### Determining a Compound’s Empirical Formula

In the previous section, you learned how to calculate the percentage composition of a compound from its chemical formula. Now you will do the reverse. You will use the percentage composition of a compound, along with the concept of the mole, to calculate the empirical formula of the compound. Since the percentage composition can often be determined by experiment, chemists use this calculation when they want to identify a compound.

The following Sample Problem illustrates how to use percentage composition to obtain the empirical formula of a compound.

### Sample Problem

#### Finding a Compound’s Empirical Formula from Percentage Composition: Part A

##### Problem

Calculate the empirical formula of a compound that is 85.6% carbon and 14.4% hydrogen.

##### What Is Required?

You need to find the empirical formula of the compound.

##### What Is Given?

You know the percentage composition of the compound. You have access to a periodic table.

##### Plan Your Strategy

Since you know the percentage composition, it is convenient to assume that you have 100 g of the compound. This means that you have 85.6 g of carbon and 14.4 g of hydrogen. Convert each mass to moles. The number of moles can then be converted into a lowest terms ratio of the elements to get the empirical formula.

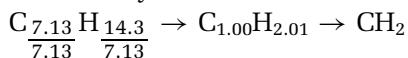
##### Act on Your Strategy

$$\text{Number of moles of C in 100 g sample} = \frac{85.6 \text{ g}}{12.01 \text{ g/mol}} = 7.13 \text{ mol}$$

$$\text{Number of moles of H in 100 g sample} = \frac{14.4 \text{ g}}{1.01 \text{ g/mol}} = 14.3 \text{ mol}$$

*Continued ...*

Now determine the lowest whole number ratio. Divide both molar amounts by the lowest molar amount.



Alternatively, you can set up your solution as a table.

Element	Mass percent (%)	Grams per 100 g sample (g)	Molar mass (g/mol)	Number of moles (mol)	Molar amount + lowest molar amount
C	85.6	85.6	12.01	7.13	$\frac{7.13}{7.13} = 1$
H	14.4	14.4	1.01	14.3	$\frac{14.3}{7.13} = 2.01$

The empirical formula of the compound is CH<sub>2</sub>.

### PROBLEM TIP

The fact that 2.01 was rounded to 2 in CH<sub>2</sub> is fine. The percentage composition is often determined by experiment, so it is unlikely to be exact.

### Check Your Solution

Work backward. Calculate the percentage composition of CH<sub>2</sub>.

$$\text{Mass percent of C} = \frac{12.01 \text{ g/mol}}{14.03 \text{ g/mol}} \times 100\% \\ = 85.6\%$$

$$\text{Mass percent of H} = \frac{2 \times 1.01 \text{ g/mol}}{14.03 \text{ g/mol}} \times 100\% \\ = 14.0\%$$

The percentage composition calculated from the empirical formula closely matches the given data. The formula is reasonable.

### Practice Problems

9. A compound consists of 17.6% hydrogen and 82.4% nitrogen. Determine the empirical formula of the compound.
10. Find the empirical formula of a compound that is 46.3% lithium and 53.7% oxygen.
11. What is the empirical formula of a compound that is 15.9% boron and 84.1% fluorine?
12. Determine the empirical formula of a compound made up of 52.51% chlorine and 47.48% sulfur.

### Tips for Solving Empirical Formula Problems

In the Sample Problem above, the numbers were rounded at each step to simplify the calculation. To calculate an empirical formula successfully, however, you should not round the numbers until you have completed the calculation. Use the maximum number of significant digits that your calculator will allow, throughout the calculation. Rounding too soon when calculating an empirical formula may result in getting the wrong answer.

**Table 6.2** Converting Subscripts in Empirical Formulas

When you see this decimal...	Try multiplying all subscripts by...
x.80 ( $\frac{4}{5}$ )	5
x.75 ( $\frac{3}{4}$ )	4
x.67 ( $\frac{2}{3}$ )	3
x.60 ( $\frac{3}{5}$ )	5
x.40 ( $\frac{2}{5}$ )	5
x.50 ( $\frac{1}{2}$ )	2
x.33 ( $\frac{1}{3}$ )	3
x.25 ( $\frac{1}{4}$ )	4
x.20 ( $\frac{1}{5}$ )	5
x.17 ( $\frac{1}{6}$ )	6

Often only one step is needed to determine the number of moles in an empirical formula. This is not always the case, however. Since you must divide by the lowest number of moles, initially one of your ratio terms will always be 1. If your other terms are quite close to whole numbers, as in the last Sample Problem, you can round them to the closest whole numbers. If your other terms are not close to whole numbers, you will need to do some additional steps. This is because empirical formulas do not always contain the subscript 1. For example,  $\text{Fe}_2\text{O}_3$  contains the subscripts 2 and 3.

Decimals such as 0.95 to 0.99 can be rounded up to the nearest whole number. Decimals such as 0.01 to 0.05 can be rounded down to the nearest whole number. Other decimals require additional manipulation. What if you have the empirical formula  $\text{C}_{1.5}\text{H}_3\text{O}_1$ ? To convert all subscripts to whole numbers, multiply each subscript by 2. This gives you the empirical formula  $\text{C}_3\text{H}_6\text{O}_2$ . Thus, a ratio that involves a decimal ending in 0.5 must be doubled. What if a decimal ends in 0.45 to 0.55? Round the decimal so that it ends in .5, and then double the ratio.

Table 6.2 gives you some strategies for converting subscripts to whole numbers. The variable x stands for any whole number. Examine the following Sample Problem to learn how to convert the empirical formula subscripts to the lowest possible whole numbers.

## Sample Problem

### Finding a Compound's Empirical Formula from Percentage Composition: Part B

#### Problem

The percentage composition of a fuel is 81.7% carbon and 18.3% hydrogen. Find the empirical formula of the fuel.

#### What Is Required?

You need to determine the empirical formula of the fuel.

#### What Is Given?

You know the percentage composition of the fuel. You have access to a periodic table.

#### Plan Your Strategy

Convert mass percent to mass, then to number of moles. Then find the lowest whole number ratio.

#### Act on Your Strategy

Element	Mass percent (%)	Grams per 100 g sample (g)	Molar mass (g/mol)	Number of moles (mol)	Molar amount ÷ lowest molar amount
C	81.7	81.7	12.0	6.81	$\frac{6.81}{6.81} = 1$
H	18.3	18.3	1.01	18.1	$\frac{18.1}{6.81} = 2.66$

*Continued ...*

You now have the empirical formula  $C_1H_{2.66}$ . Convert the subscript 2.66 ( $\frac{8}{3}$ ) to a whole number.  $C_{1 \times 3}H_{2.66 \times 3} = C_3H_8$ .

### Check Your Solution

Work backward. Calculate the percentage composition of  $C_3H_8$ .

$$\text{Mass percent of C} = \frac{3 \times 12.01 \text{ g/mol}}{44.09 \text{ g/mol}} \times 100\% \\ = 81.7\%$$

$$\text{Mass percent of H} = \frac{8 \times 1.008 \text{ g/mol}}{44.09 \text{ g/mol}} \times 100\% \\ = 18.3\%$$

The percentage composition calculated from the empirical formula matches the percentage composition given in the problem.

### PROBLEM TIP

Notice that Table 6.2 suggests multiplying by 3 when you obtain a subscript ending in .67, which is very close to .66.

## Practice Problems

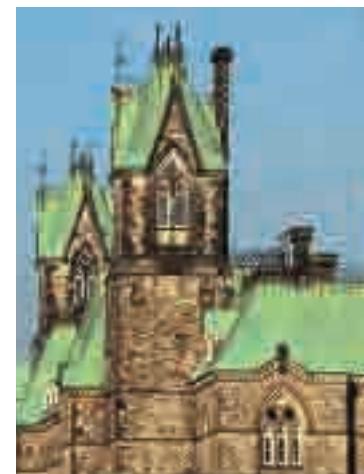
13. An oxide of chromium is made up of 68.4% chromium and 31.6% oxygen. What is the empirical formula of this oxide?
14. Phosphorus reacts with oxygen to give a compound that is 43.7% phosphorus and 56.4% oxygen. What is the empirical formula of the compound?
15. An inorganic salt is composed of 17.6% sodium, 39.7% chromium, and 42.8% oxygen. What is the empirical formula of this salt?
16. Compound X contains 69.9% carbon, 6.86% hydrogen, and 23.3% oxygen. Determine the empirical formula of compound X.

### Determining the Empirical Formula by Experiment

In practice, you can determine a compound's empirical formula by analyzing its percentage composition. There are several different ways to do this. One way is to use a synthesis reaction in which a sample of an element with a known mass reacts with another element to form a compound. Since you know the mass of one of the elements and you can measure the mass of the compound produced, you can calculate the percentage composition.

For example, copper reacts with the oxygen in air to form the green compound copper oxide. Many buildings in Canada, such as the Parliament buildings in Ottawa, have green roofs that contain some copper(II) oxide. (See Figure 6.7.) Imagine you have a 5.0 g sample of copper shavings. You allow the copper shavings to react completely with oxygen. If the resulting compound has a mass of 6.3 g, you know that the compound contains 5.0 g copper and 1.3 g oxygen. Although you can use the periodic table to predict that the formula for copper(II) oxide is  $CuO$ , the masses help you confirm your prediction. Try converting the masses given above into an empirical formula.

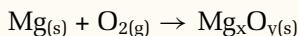
In Investigation 6-A, you will use a synthesis reaction to determine the empirical formula of magnesium oxide by experiment.



**Figure 6.7** Although this green roof may contain some copper(II) oxide, it is mostly composed of basic copper sulfates and carbonates that form when the copper reacts with acid precipitation.

# Determining the Empirical Formula of Magnesium Oxide

When magnesium metal is heated over a flame, it reacts with oxygen in the air to form magnesium oxide,  $Mg_xO_y$ :



In this investigation, you will react a strip of pure magnesium metal with oxygen,  $O_2$ , in the air to form magnesium oxide. Then you will measure the mass of the magnesium oxide produced to determine the percentage composition of magnesium oxide. You will use this percentage composition to calculate the empirical formula of magnesium oxide. **CAUTION** Do not perform this investigation unless welder's goggles are available.

## Question

What is the percentage composition and empirical formula of magnesium oxide?

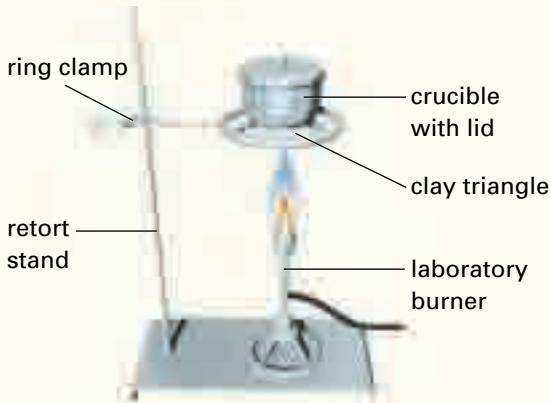
## Predictions

Using what you have learned about writing formulas, predict the molecular formula and percentage composition of magnesium oxide.

## Materials

electronic balance  
small square of sandpaper or emery paper  
8 cm strip of magnesium ribbon  
laboratory burner  
sparkler  
retort stand  
ring clamp  
clay triangle  
clean crucible with lid  
crucible tongs  
ceramic pad  
distilled water  
wash bottle  
disposal beaker  
welder's goggles

**Note:** Make sure that the mass of the magnesium ribbon is at least 0.10 g.



## Safety Precautions



- Do not look directly at the burning magnesium.
- Do not put a hot crucible on the bench or the balance.

## Procedure

1. Make a table like the one below.

## Observations

Mass of clean, empty crucible and lid	
Mass of crucible, lid, and magnesium	
Mass of crucible and magnesium oxide	

2. Assemble the apparatus as shown in the diagram.
3. Obtain a strip of magnesium, about 8 cm long, from your teacher. Clean the magnesium strip with sandpaper or emery paper to remove any oxide coating.
4. Measure and record the mass of the empty crucible and lid. Add the strip of cleaned magnesium to the crucible. Record the mass of the crucible, lid, and magnesium.

5. With the lid off, place the crucible containing the magnesium on the clay triangle. Heat the crucible with a strong flame. Using the crucible tongs, hold the lid of the crucible nearby.  
**CAUTION** When the magnesium ignites, quickly cover the crucible with the lid. Continue heating for about 1 min.
6. Carefully remove the lid. **CAUTION** Heat the crucible until the magnesium ignites once more. Again, quickly cover the crucible. Repeat this heating and covering of the crucible until the magnesium no longer ignites. Heat for a further 4 to 5 min with the lid off.
7. Using the crucible tongs, put the crucible on the ceramic pad to cool.
8. When the crucible is cool enough to touch, put it on the bench. Carefully grind the product into small particles using the glass rod. Rinse any particles on the glass rod into the crucible with distilled water from the wash bottle.
9. Add enough distilled water to the crucible to thoroughly wet the contents. The white product is magnesium oxide. The yellowish-orange product is magnesium nitride.
10. Return the crucible to the clay triangle. Place the lid slightly ajar. Heat the crucible gently until the water begins to boil. Continue heating until all the water has evaporated, and the product is completely dry. Allow the crucible to cool on the ceramic pad.
11. Using the crucible tongs, carry the crucible and lid to the balance. Measure and record the mass of the crucible and lid.
12. Do not put the magnesium oxide in the garbage or in the sink. Put it in the disposal beaker designated by your teacher.

## Analysis

1. (a) What mass of magnesium did you use in the reaction?  
(b) What mass of magnesium oxide was produced?  
(c) Calculate the mass of oxygen that reacted with the magnesium.

- (d) Use your data to calculate the percentage composition of magnesium oxide.
  - (e) Determine the empirical formula of magnesium oxide. Remember to round your empirical formula to the nearest whole number ratio, such as 1:1, 1:2, 2:1, or 3:3.
2. (a) Verify your empirical formula with your teacher. Use the empirical formula of magnesium oxide to determine the mass percent of magnesium in magnesium oxide.
  - (b) Calculate your percent error (PE) by finding the difference between the experimental mass percent (EP) of magnesium and the actual mass percent (AP) of magnesium. Then you divide the difference by the actual mass percent of magnesium and multiply by 100%.
- $$PE = \frac{EP - AP}{AP} \times 100\%$$
3. Why did you need to round the empirical formula you obtained to a whole number ratio?

## Conclusion

4. Compare the empirical formula you obtained with the empirical formula you predicted.

## Applications

5. Write a balanced chemical equation for the reaction of magnesium with oxygen gas, O<sub>2</sub>.
6. (a) Suppose that you had allowed some magnesium oxide smoke to escape during the investigation. How would the Mg:O ratio have been affected? Would the ratio have increased, decreased, or remained unchanged? Explain using sample calculations.  
(b) How would your calculated value for the empirical formula of magnesium oxide have been affected if all the magnesium in the crucible had not burned? Support your answer with sample calculations.  
(c) Could either of the situations mentioned in parts (a) and (b) have affected your results? Explain.

## Section Wrap-up

In section 6.2, you learned how to calculate the empirical formula of a compound based on percentage composition data obtained by experiment. In section 6.3, you will learn how chemists use the empirical formula of a compound and its molar mass to determine the molecular formula of a compound.

## Section Review

- 1 (a) K/U** Why is the empirical formula of a compound also referred to as its simplest formula?
- (b) K/U** Explain how the empirical formula of a compound is related to its molecular formula.
- 2 I** Methyl salicylate, or oil of wintergreen, is produced by the wintergreen plant. It can also be prepared easily in a laboratory. Methyl salicylate is 63.1% carbon, 5.31% hydrogen, and 31.6% oxygen. Calculate the empirical formula of methyl salicylate.
- 3 I** Determine the empirical formula of the compound that is formed by each of the following reactions.
  - (a)** 0.315 mol chlorine atoms react completely with 1.1 mol oxygen atoms
  - (b)** 4.90 g silicon react completely with 24.8 g chlorine
- 4 I** Muscle soreness from physical activity is caused by a buildup of lactic acid in muscle tissue. Analysis of lactic acid reveals it to be 40.0% carbon, 6.71% hydrogen, and 53.3% oxygen by mass. Calculate the empirical formula of lactic acid.
- 5 MC** Imagine that you are a lawyer. You are representing a client charged with possession of a controlled substance. The prosecutor introduces, as forensic evidence, the empirical formula of the substance that was found in your client's possession. How would you deal with this evidence as a lawyer for the defence?
- 6 I** Olive oil is used widely in cooking. Oleic acid, a component of olive oil, contains 76.54% carbon, 12.13% hydrogen and 11.33% oxygen by mass. What is the empirical formula of oleic acid?
- 7 I** Phenyl valerate is a colourless liquid that is used as a flavour and odorant. It contains 74.13% carbon, 7.92% hydrogen and 17.95% oxygen by mass. Determine the empirical formula of phenyl valerate.
- 8 I** Ferrocene is the common name given to a unique compound that consists of one iron atom sandwiched between two rings containing hydrogen and carbon. This orange, crystalline solid is added to fuel oil to improve combustion efficiency and eliminate smoke. As well, it is used as an industrial catalyst and a high-temperature lubricant.
  - (a)** Elemental analysis reveals ferrocene to be 64.56% carbon, 5.42% hydrogen and 30.02% iron by mass. Determine the empirical formula of ferrocene.
  - (b)** Read the description of ferrocene carefully. Does this description provide enough information for you to determine the molecular formula of ferrocene? Explain your answer.

# The Molecular Formula of a Compound

## 6.3

Determining the identity of an unknown compound is important in all kinds of research. It can even be used to solve crimes. **Forensic scientists** specialize in analyzing evidence for criminal and legal cases. To understand why forensic scientists might need to find out the molecular formula of a compound, consider the following example.

Suppose that a suspect in a theft investigation is a researcher in a biology laboratory. The suspect frequently works with formaldehyde,  $\text{CH}_2\text{O}$ . Police officers find traces of a substance at the crime scene, and send samples to the Centre for Forensic Science. The forensic analysts find that the substance contains a compound that has an empirical formula of  $\text{CH}_2\text{O}$ . Will this evidence help to convict the suspect? Not necessarily.

As you can see from Table 6.3, there are many compounds that have the empirical formula  $\text{CH}_2\text{O}$ . The substance might be formaldehyde, but it could also be lactic acid (found in milk) or acetic acid (found in vinegar). Neither lactic acid nor acetic acid connect the theft to the suspect. Further information is required to prove that the substance is formaldehyde. Analyzing the physical properties of the substance would help to discover whether it is formaldehyde. Another important piece of information is the molar mass of the substance. Continue reading to find out why.

**Table 6.3** Six Compounds with the Empirical Formula  $\text{CH}_2\text{O}$

Name	Molecular formula	Whole-number multiple	$M$ (g/mol)	Use or function
formaldehyde	$\text{CH}_2\text{O}$	1	30.03	disinfectant; biological preservative
acetic acid	$\text{C}_2\text{H}_4\text{O}_2$	2	60.05	acetate polymers; vinegar (5% solution)
lactic acid	$\text{C}_3\text{H}_6\text{O}_3$	3	90.08	causes milk to sour; forms in muscles during exercise
erythrose	$\text{C}_4\text{H}_8\text{O}_4$	4	120.10	forms during sugar metabolism
ribose	$\text{C}_5\text{H}_{10}\text{O}_5$	5	150.13	component of many nucleic acids and vitamin B <sub>2</sub>
glucose	$\text{C}_6\text{H}_{12}\text{O}_6$	6	180.16	major nutrient for energy in cells



CH<sub>2</sub>O      C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>      C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>      C<sub>4</sub>H<sub>8</sub>O<sub>4</sub>      C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>      C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>

## Determining a Molecular Formula

Recall the equation

Molecular formula subscripts =  $n \times$  Empirical formula subscripts,  
where  $n = 1, 2, 3\dots$

Additional information is required to obtain the molecular formula of a compound, given its empirical formula. We can use the molar mass and build on the above equation, as follows:

Molar mass of compound =  $n \times$  Molar mass of empirical formula,  
where  $n = 1, 2, 3\dots$

### Section Preview/ Specific Expectations

In this section, you will

- determine the molecular formula of a compound, given the empirical formula of the compound and some additional information
- identify real-life situations in which the analysis of unknown substances is important
- communicate your understanding of the following terms: *forensic scientists*



## Analytical Chemistry



Ben Johnson, Steve Vezina, Eric Lamaze—all of these athletes tested positive for performance-enhancing substances that are banned by the International Olympic Committee (IOC). Who conducts the tests for these substances? Meet Dr. Christiane Ayotte, head of Canada's Doping Control Laboratory since 1991.

### The Doping Control Lab

What happens to a urine sample after it arrives at the doping control lab? Technicians and scientists must be careful to ensure careful handling of the sample. Portions of the sample are taken for six different analytical procedures. More than 150 substances are banned by the IOC. These substances are grouped according to their physical and chemical properties. There are two main steps for analyzing a sample:

1. purification, which involves steps such as filtration and extraction using solvents, and
2. analysis by either gas chromatography, mass spectrometry, or high-performance liquid chromatography. Chromatography refers to certain methods by which chemists separate mixtures into pure substances.

For most substances, just their presence in a urine sample means a positive result. Other substances must be present in an amount higher than a certain threshold. According to Dr. Ayotte, a male athlete would have to consume “10 very strong French coffees within 15 min” to go over the 12 mg/L limit for caffeine. Ephedrines and pseudoephedrines, two decongestants that are found in cough remedies and that act as stimulants, have a cut-off level. This allows athletes to take them up to one or two days before a competition.

### Challenges

Dr. Ayotte and her team face many challenges. They look for reliable tests for natural substances, develop new analytical techniques, and determine the normal levels of banned substances for male and female athletes. Dr. Ayotte must defend her tests in hearings and with the press, especially when high-profile athletes get positive results. Her dreams include an independent international doping control agency and better drug-risk education for athletes.

For Dr. Ayotte, integrity and a logical mind are essential aspects of being a good scientist.

### Make Career Connections

1. For information about careers in analytical chemistry, contact university and college chemistry departments.
2. For information about doping control and the movement for drug-free sport, contact the Canadian Centre for Ethics in Sport (CCES), the World Anti-Doping Agency (WADA), and the Centre for Sport and Law.

Thus, the molar mass of a compound is a whole number multiple of the “molar mass” of the empirical formula.

Chemists can use a mass spectrometer to determine the molar mass of a compound. They can use the molar mass, along with the “molar mass” of a known empirical formula, to determine the compound’s molecular formula. For example, the empirical formula CH has a “molar mass” of 13 g/mol. We know, however, that acetylene,  $C_2H_2$ , and benzene,  $C_6H_6$ , both have the empirical formula CH. Suppose it is determined, through mass spectrometry,

that a sample has a molar mass of 78 g/mol. We know that the compound is C<sub>6</sub>H<sub>6</sub>, since  $6 \times 13\text{ g} = 78\text{ g}$ , as shown in Table 6.4.

Examine the Sample Problem and Practice Problems that follow to learn how to find the molecular formula of a compound using the empirical formula and the molar mass of the compound.

## Sample Problem

### Determining a Molecular Formula

#### Problem

The empirical formula of ribose (a sugar) is CH<sub>2</sub>O. In a separate experiment, using a mass spectrometer, the molar mass of ribose was determined to be 150 g/mol. What is the molecular formula of ribose?

#### What Is Required?

You need to find the molecular formula of ribose.

#### What Is Given?

You know the empirical formula and the molar mass of ribose.

#### Plan Your Strategy

Divide the molar mass of ribose by the “molar mass” of the empirical formula. The answer you get is the factor by which you multiply the empirical formula.

#### Act on Your Strategy

The “molar mass” of the empirical formula CH<sub>2</sub>O, determined using the periodic table, is

$$12\text{ g/mol} + 2(1)\text{ g/mol} + 16\text{ g/mol} = 30\text{ g/mol}$$

The molar mass of ribose is 150 g/mol.

$$\frac{150\text{ g/mol}}{30\text{ g/mol}} = 5$$

Molecular formula subscripts =  $5 \times$  Empirical formula subscripts  
= C<sub>1×5</sub>H<sub>2×5</sub>O<sub>1×5</sub>  
= C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>

Therefore, the molecular formula of ribose is C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>.

#### Check Your Solution

Work backward by calculating the molar mass of C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>.

$$(5 \times 12.01\text{ g/mol}) + (10 \times 1.01\text{ g/mol}) + (5 \times 16.00\text{ g/mol}) = 150\text{ g/mol}$$

The calculated molar mass matches the molar mass that is given in the problem. The answer is reasonable.

**Table 6.4** Relating Molecular and Empirical Formulas

Formula	Molar Mass (g)	Ratio
C <sub>6</sub> H <sub>6</sub> molecular	78	$\frac{78}{13} = 6$
CH empirical	13	



**CHEM**

**FACT**

Three classifications of food are proteins, fats, and carbohydrates. Many carbohydrates have the empirical formula CH<sub>2</sub>O. This empirical formula looks like a hydrate of carbon, hence the name “carbohydrate.” Glucose, fructose, galactose, mannose, and sorbose all have the empirical formula CH<sub>2</sub>O since they all have the same molecular formula, C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>. What makes these sugars different is the way in which their atoms are bonded to one another. In Chapter 13, you will learn more about different compounds with the same formulas.

*Continued ...*

## Practice Problems


**CHEM**
**FACT**

Codeine is a potent pain reliever. It acts on the pain centre in the brain, rather than interrupting pain messages from, for example, a headache or a sore arm. It is potentially habit-forming and classified as a narcotic.

17. The empirical formula of butane, the fuel used in disposable lighters, is  $C_2H_5$ . In an experiment, the molar mass of butane was determined to be 58 g/mol. What is the molecular formula of butane?
18. Oxalic acid has the empirical formula  $CHO_2$ . Its molar mass is 90 g/mol. What is the molecular formula of oxalic acid?
19. The empirical formula of codeine is  $C_{18}H_{21}NO_3$ . If the molar mass of codeine is 299 g/mol, what is its molecular formula?
20. A compound's molar mass is 240.28 g/mol. Its percentage composition is 75.0% carbon, 5.05% hydrogen, and 20.0% oxygen. What is the compound's molecular formula?

### Section Wrap-up

How do chemists obtain the data they use to identify compounds? In Investigation 6-A, you explored one technique for finding the percentage composition, and hence the empirical formula, of a compound containing magnesium and oxygen. In section 6.4, you will learn about another technique that chemists use to determine the empirical formula of compounds containing carbon and hydrogen. You will learn how chemists combine this technique with mass spectrometry to determine the compound's molecular formula. You will also learn about a new type of compound and perform an experiment to determine the molecular formula of one of these compounds.

### Section Review

#### Unit Investigation Prep

Before you design your experiment to find the composition of a mixture, think about the relationships between different compounds. Suppose you have 5.0 g of copper. This copper reacts to form copper(II) chloride, also containing 5.0 g of copper. How can you determine the mass of copper(II) chloride formed?

- 1 **K/U** Explain the role that a mass spectrometer plays in determining the molecular formula of an unknown compound.
- 2 **I** Tartaric acid, also known as cream of tartar, is used in baking. Its empirical formula is  $C_2H_3O_3$ . If 1.00 mol of tartaric acid contains  $3.61 \times 10^{24}$  oxygen atoms, what is the molecular formula of tartaric acid?
- 3 **MC** Why is the molecular formula of a compound much more useful to a forensic scientist than the empirical formula of the compound?
- 4 **K/U** Vinyl acetate,  $C_4H_6O_2$ , is an important industrial chemical. It is used to make some of the polymers in products such as adhesives, paints, computer discs, and plastic films.
  - (a) What is the empirical formula of vinyl acetate?
  - (b) How does the molar mass of vinyl acetate compare with the molar mass of its empirical formula?
- 5 **I** A compound has the formula  $C_{6x}H_{5x}O_x$ , where  $x$  is a whole number. Its molar mass is 186 g/mol; what is its molecular formula?

# Finding Empirical and Molecular Formulas by Experiment

## 6.4

You have learned how to calculate the percentage composition of a compound using its formula. Often, however, the formula of a compound is not known. Chemists must determine the percentage composition and molar mass of an unknown compound through experimentation. Then they use this information to determine the molecular formula of the compound. Determining the molecular formula is an important step in understanding the properties of the compound and developing a way to synthesize it in a laboratory.

In Investigation 6-A, you reacted a known mass of magnesium with oxygen and found the mass of the product. Then you determined the percentage composition and empirical formula of magnesium oxide. This is just one method for determining percentage composition. It is suitable for analyzing simple compounds that react in predictable ways. Chemists have developed other methods for analyzing different types of compounds, as you will learn in this section.

### The Carbon-Hydrogen Combustion Analyzer

A large number of important chemicals are composed of hydrogen, carbon, and oxygen. The **carbon-hydrogen combustion analyzer** is a useful instrument for analyzing these chemicals. It allows chemists to determine the percentage composition of compounds that are made up of carbon, hydrogen, and oxygen. The applications of this instrument include forensic science, food chemistry, pharmaceuticals and academic research—anywhere that an unknown compound needs to be analyzed.

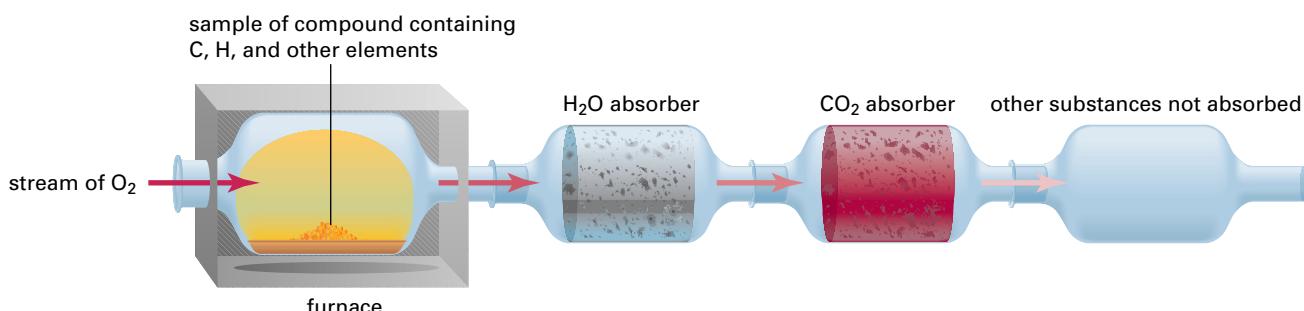
The carbon-hydrogen combustion analyzer works because we know that compounds containing carbon and hydrogen will burn in a stream of pure oxygen, O<sub>2</sub>, to yield only carbon dioxide and water. If we can find the mass of the carbon dioxide and water separately, we can determine the mass percent of carbon and hydrogen in the compound.

Examine Figure 6.8 to see how a carbon-hydrogen combustion analyzer works. A sample, made up of only carbon and hydrogen, is placed in a furnace. The sample is heated and simultaneously reacted with a stream

#### Section Preview/ Specific Expectations

In this section, you will

- **identify** real-life situations in which the analysis of unknown substances is important
- **determine** the empirical formula of a hydrate through experimentation
- **explain** how a carbon-hydrogen analyzer can be used to determine the empirical formula of a compound
- **communicate** your understanding of the following terms: *carbon-hydrogen combustion analyzer, hydrate, anhydrous*



**Figure 6.8** A schematic diagram of a carbon-hydrogen combustion analyzer. After the combustion, all the carbon in the sample is contained in the carbon dioxide. All the hydrogen in the sample is contained in the water.

## CHECKPOINT

Carbon dioxide reacts with sodium hydroxide to form sodium carbonate and water. Write a balanced chemical equation for this reaction.



### PROBEWARE

If you have access to probeware, do the Chemistry 11 lab, Determining Molecular Mass, or a similar lab available from a probeware company.

## CHECKPOINT

If you have a compound containing carbon, hydrogen, and oxygen, what two instruments would you need to determine its molecular formula?

of oxygen. Eventually the sample is completely combusted to yield only water vapour and carbon dioxide.

The water vapour is collected by passing it through a tube that contains magnesium perchlorate,  $Mg(ClO_4)_2$ . The magnesium perchlorate absorbs all of the water. The mass of the tube is determined before and after the reaction. The difference is the mass of the water that is produced in the reaction. We know that all the hydrogen in the sample is converted to water. Therefore, we can use the percentage composition of hydrogen in water to determine the mass of the hydrogen in the sample.

The carbon dioxide is captured in a second tube, which contains sodium hydroxide,  $NaOH$ . The mass of this tube is also measured before and after the reaction. The increase in the mass of the tube corresponds to the mass of the carbon dioxide that is produced. We know that all the carbon in the sample reacts to form carbon dioxide. Therefore, we can use the percentage composition of carbon in carbon dioxide to determine the mass of the carbon in the sample.

The carbon-hydrogen combustion analyzer can also be used to find the empirical formula of a compound that contains carbon, hydrogen, and one other element, such as oxygen. The difference between the mass of the sample and the mass of the hydrogen and carbon produced is the mass of the third element.

Examine the following Sample Problem to learn how to determine the empirical formula of a compound based on carbon-hydrogen combustion data.

### Sample Problem

#### Carbon-Hydrogen Combustion Analyzer Calculations

##### Problem

A 1.000 g sample of a pure compound, containing only carbon and hydrogen, was combusted in a carbon-hydrogen combustion analyzer. The combustion produced 0.6919 g of water and 3.338 g of carbon dioxide.

- Calculate the masses of the carbon and the hydrogen in the sample.
- Find the empirical formula of the compound.

##### What Is Required?

You need to find

- the mass of the carbon and the hydrogen in the sample
- the empirical formula of the compound

##### What Is Given?

You know the mass of the sample. You also know the masses of the water and the carbon dioxide produced in the combustion of the sample.

*Continued ...*

## Plan Your Strategy

All the hydrogen in the sample was converted to water. Multiply the mass percent (as a decimal) of hydrogen in water by the mass of the water to get the mass of the hydrogen in the sample.

Similarly, all the carbon in the sample has been incorporated into the carbon dioxide. Multiply the mass percent (as a decimal) of carbon in carbon dioxide by the mass of the carbon dioxide to get the mass of carbon in the sample. Convert to moles and determine the empirical formula.

## Act on Your Strategy

(a) Mass of H in sample

$$= \frac{2.02 \text{ g H}_2}{18.02 \text{ g H}_2\text{O}} \times 0.6919 \text{ g H}_2\text{O} = 0.07756 \text{ g H}_2$$

$$\text{Mass of C in sample} = \frac{12.01 \text{ g C}}{44.01 \text{ g CO}_2} \times 3.338 \text{ g CO}_2 = 0.9109 \text{ g C}$$

The sample contained 0.07756 g of hydrogen and 0.9109 g of carbon.

$$(b) \text{ Moles of H in sample} = \frac{0.07756 \text{ g}}{1.008 \text{ g/mol}} = 0.07694 \text{ mol}$$

$$\text{Moles of C in sample} = \frac{0.9109 \text{ g}}{12.01 \text{ g/mol}} = 0.07584 \text{ mol}$$

$$\begin{aligned} \text{Empirical formula} &= \text{C}_{\frac{0.07584}{0.07584}} \text{H}_{\frac{0.07584}{0.07694}} \\ &= \text{C}_{1.0} \text{H}_{1.0} \\ &= \text{CH} \end{aligned}$$

## Check Your Solution

The sum of the masses of carbon and hydrogen is 0.07756 g + 0.9109 g = 0.98846 g. This is close to the mass of the sample. Therefore your answers are reasonable.

## Practice Problems

21. A 0.539 g sample of a compound that contained only carbon and hydrogen was subjected to combustion analysis. The combustion produced 1.64 g of carbon dioxide and 0.807 g of water. Calculate the percentage composition and the empirical formula of the sample.
22. An 874 mg sample of cortisol was subjected to carbon-hydrogen combustion analysis. 2.23 g of carbon dioxide and 0.652 g of water were produced. The molar mass of cortisol was found to be 362 g/mol using a mass spectrometer. If cortisol contains carbon, hydrogen, and oxygen, determine its molecular formula.



### CHEM

### FACT

Cortisol is an important steroid hormone. It helps your body synthesize protein. Cortisol can also reduce inflammation, and is used to treat allergies and rheumatoid arthritis.

# Chemistry Bulletin

Science

Technology

Society

Environment

## Accident or Arson?

All chemists who try to identify unknown compounds are like detectives. Forensic chemists, however, actually work with investigators. They use their chemical knowledge to help explain evidence. Forensic chemists are especially helpful in an arson investigation.



## Investigating Arson

One of the main jobs of the investigator in a possible arson case is to locate and sample residual traces of accelerants. Accelerants are flammable substances that are used to quickly ignite and spread a fire. They include compounds called hydrocarbons, which contain hydrogen and carbon. Examples of hydrocarbons include petrol, kerosene and diesel.

Portable instruments called *sniffers* can be used to determine the best places to collect samples. These sniffers, however, are not able to determine the type of hydrocarbon present. As well, they can be set off by vapours from burnt plastics. Deciding whether or not a substance is an accelerant is best done by a chemist in a laboratory, using a technique called gas chromatography (GC).

## In the Forensic Laboratory

In the laboratory, the sample residue must be concentrated on charcoal or another material. Then the sample is ready for GC analysis. GC is used to separate and detect trace amounts of volatile hydrocarbons and separate them from a mixture. Most accelerants are complex mixtures. They have many components, in different but specific ratios.

GC involves taking the concentrated residue and passing it through a gas column. As the sample residue moves through the column, the different components separate based on their boiling points. The compound with the lowest boiling point emerges from the column and onto a detector first. The other components follow as they reach their boiling points. It is possible to identify each component of a mixture based on the time that it emerges from the column. A detector records this information on a chromatogram. Each component is represented by a peak on a graph. The overall pattern of peaks is always the same for a specific type of accelerant. Therefore, accelerants are identified by their components and the relative proportions of their components.

Only trace amounts of an accelerant need to be collected because current analytical tools are extremely sensitive. If an accelerant is used to start a fire, it is highly likely that there will be trace amounts left over after the fire. The presence of an accelerant at a fire scene strongly suggests that the fire was started intentionally.

## Making Connections

1. What other types of crime could be solved by a forensic chemist? Brainstorm a list.
2. What other instruments might a forensic chemist use to identify compounds? Using the Internet or reference books, do some research to find out.

## Hydrated Ionic Compounds

You have learned how to find the molecular formula of a compound that contains only hydrogen, carbon, and oxygen. When chemists use this method, they usually have no mass percent data for the compound when they begin. In some cases, however, chemists know most of the molecular formula of a compound, but one significant piece of information is missing.

For example, many ionic compounds crystallize from a water solution with water molecules incorporated into their crystal structure, forming a **hydrate**. Hydrates have a specific number of water molecules chemically bonded to each formula unit. A chemist may know the formula of the ionic part of the hydrate but not how many water molecules are present for each formula unit.

Epsom salts, for example, consist of crystals of magnesium sulfate heptahydrate,  $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ . Every formula unit of magnesium sulfate has seven molecules of water weakly bonded to it. A raised dot in a chemical formula, in front of one or more water molecules, denotes a hydrated compound. Note that the dot does not include multiplication, but rather a weak bond between an ionic compound and one or more water molecules. Some other examples of hydrates are shown in Table 6.4.

Compounds that have no water molecules incorporated into them are called **anhydrous** to distinguish them from their hydrated forms. For example, a chemist might refer to  $\text{CaSO}_4$  as anhydrous calcium sulfate. This is because it is often found in hydrated form as calcium sulfate dihydrate, shown in Figure 6.9.

**Table 6.4** Selected Hydrates

Formula	Chemical name
$\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$	calcium sulfate dihydrate (gypsum)
$\text{CaCl}_2 \cdot 2\text{H}_2\text{O}$	calcium chloride dihydrate
$\text{LiCl}_2 \cdot 4\text{H}_2\text{O}$	lithium chloride tetrahydrate
$\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$	magnesium sulfate heptahydrate (Epsom salts)
$\text{Ba}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$	barium hydroxide octahydrate
$\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O}$	sodium carbonate decahydrate
$\text{KAl}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	potassium aluminum sulfate dodecahydrate (alum)

The molar mass of a hydrated compound must include the mass of any water molecules that are in the compound. For example, the molar mass of magnesium sulfate heptahydrate includes the mass of 7 mol of water. It is very important to know whether a compound exists as a hydrate. For example, if a chemical reaction calls for 0.25 mol of copper(II) chloride, you need to know whether you are dealing with anhydrous copper(II) chloride or with copper(II) chloride dihydrate, shown in Figure 6.10. The mass of 0.25 mol of  $\text{CuCl}_2$  is 33.61 g. The mass of 0.25 mol of  $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$  is 38.11 g.

Calculations involving hydrates involve using the same techniques you have already practised for determining percent by mass, empirical formulas, and molecular formulas.

The following Sample Problem shows how to find the percent by mass of water in a hydrate. It also shows how to determine the formula of a hydrate based on an incomplete chemical formula.

### mind STRETCH

Suppose there is  $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$  in the chemistry prep room. The experiment you want to do, however, calls for  $\text{MgSO}_4$ . How do you think you might remove the water from  $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ ?



**Figure 6.9** Alabaster is a compact form of gypsum often used in sculpture. Gypsum is the common name for calcium sulfate dihydrate,  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ .



**Figure 6.10** If you need 5 mol of  $\text{CuCl}_2$ , how much of the compound above would you use?

## Sample Problem

### Determining the Formula of a Hydrate

#### Problem

A hydrate of barium hydroxide,  $\text{Ba}(\text{OH})_2 \cdot x\text{H}_2\text{O}$ , is used to make barium salts and to prepare certain organic compounds. Since it reacts with  $\text{CO}_2$  from the air to yield barium carbonate,  $\text{BaCO}_3$ , it must be stored in tightly stoppered bottles.

- (a) A 50.0 g sample of the hydrate contains 27.2 g of  $\text{Ba}(\text{OH})_2$ . Calculate the percent, by mass, of water in  $\text{Ba}(\text{OH})_2 \cdot x\text{H}_2\text{O}$ .
- (b) Find the value of  $x$  in  $\text{Ba}(\text{OH})_2 \cdot x\text{H}_2\text{O}$ .

#### What Is Required?

- (a) You need to calculate the percent, by mass, of water in the hydrate of barium hydroxide.
- (b) You need to find how many water molecules are bonded to each formula unit of  $\text{Ba}(\text{OH})_2$ .

#### What Is Given?

The formula of the sample is  $\text{Ba}(\text{OH})_2 \cdot x\text{H}_2\text{O}$ .  
The mass of the sample is 50.0 g.  
The sample contains 27.2 g of  $\text{Ba}(\text{OH})_2$ .

#### Plan Your Strategy

- (a) To find the mass of water in the hydrate, find the difference between the mass of barium hydroxide and the total mass of the sample. Divide by the total mass of the sample and multiply by 100%.
- (b) Find the number of moles of barium hydroxide in the sample. Then find the number of moles of water in the sample. To find out how many water molecules bond to each formula unit of barium hydroxide, divide each answer by the number of moles of barium hydroxide.

#### Act on Your Strategy

- (a) Mass percent of water in  $\text{Ba}(\text{OH})_2 \cdot x\text{H}_2\text{O}$
- $$= \frac{(\text{Total mass of sample}) - (\text{Mass of } \text{Ba}(\text{OH})_2 \text{ in sample})}{(\text{Total mass of sample})} \times 100\%$$
- $$= \frac{50.0 \cancel{\text{g}} - 27.2 \cancel{\text{g}}}{50.0 \cancel{\text{g}}} \times 100\%$$
- $$= 45.6\%$$
- (b) Moles of  $\text{Ba}(\text{OH})_2 = \frac{\text{Mass of } \text{Ba}(\text{OH})_2}{\text{Molar mass of } \text{Ba}(\text{OH})_2}$
- $$= \frac{27.2 \cancel{\text{g}}}{171.3 \cancel{\text{g/mol}}}$$
- $$= 0.159 \text{ mol } \text{Ba}(\text{OH})_2$$

*Continued ...*

$$\begin{aligned}\text{Moles of H}_2\text{O} &= \frac{\text{Mass of H}_2\text{O}}{\text{Molar mass of H}_2\text{O}} \\ &= \frac{50.0 \cancel{\text{g}} - 27.2 \cancel{\text{g}}}{18.02 \cancel{\text{g/mol}}} \\ &= 1.27 \text{ mol H}_2\text{O}\end{aligned}$$

$$\frac{0.159}{0.159} \text{ mol Ba(OH)}_2 : \frac{1.27}{0.159} \text{ mol H}_2\text{O} = 1.0 \text{ mol Ba(OH)}_2 : 8.0 \text{ mol H}_2\text{O}$$

The value of  $x$  in  $\text{Ba(OH)}_2 \cdot x\text{H}_2\text{O}$  is 8.

Therefore, the molecular formula of the hydrate is  $\text{Ba(OH)}_2 \cdot 8\text{H}_2\text{O}$ .

### PROBLEM TIP

This step is similar to finding an empirical formula based on percentage composition.

### Check Your Solution

Work backward.

According to the formula, the percent by mass of water in  $\text{Ba(OH)}_2 \cdot 8\text{H}_2\text{O}$  is:

$$\frac{144.16 \cancel{\text{g/mol}}}{315.51 \cancel{\text{g/mol}}} \times 100\% = 45.7\%$$

According to the question, the percent by mass of water in the hydrate of  $\text{Ba(OH)}_2$  is:

$$\frac{(50.0 \cancel{\text{g}} - 27.2 \cancel{\text{g}})}{50.0 \cancel{\text{g}}} \times 100\% = 45.6\%$$

Therefore, your answer is reasonable.

### Practice Problems

23. What is the percent by mass of water in magnesium sulfite hexahydrate,  $\text{MgSO}_3 \cdot 6\text{H}_2\text{O}$ ?
24. A 3.34 g sample of a hydrate has the formula  $\text{SrS}_2\text{O}_3 \cdot x\text{H}_2\text{O}$ , and contains 2.30 g of  $\text{SrS}_2\text{O}_3$ . Find the value of  $x$ .
25. A hydrate of zinc chlorate,  $\text{Zn}(\text{ClO}_3)_2 \cdot x\text{H}_2\text{O}$ , contains 21.5% zinc by mass. Find the value of  $x$ .

### CHECKPOINT

Write an equation that shows what happens when you heat magnesium sulfate hexahydrate enough to convert it to its anhydrous form.

### Determining the Molecular Formula of a Hydrate

As you have just discovered, calculations involving hydrates usually involve comparing the anhydrous form of the ionic compound to the hydrated form. Many chemicals are available in hydrated form. Usually chemists are only interested in how much of the ionic part of the hydrate they are working with. This is because, in most reactions involving hydrates, the water portion of the compound does not take part in the reaction. Only the ionic portion does.

How do chemists determine how many water molecules are bonded to each ionic formula unit in a hydrate? One method is to heat the compound in order to convert it to its anhydrous form. The bonds that join the water molecules to the ionic compound are very weak compared with the strong ionic bonds within the ionic compound. Heating a hydrate usually removes the water molecules, leaving the anhydrous compound behind. In Investigation 6-B, you will heat a hydrate to determine its formula.



#### Electronic Learning Partner

A video clip describing hydrated ionic compounds can be found on the Chemistry 11 Electronic Learning Partner.

# Determining the Chemical Formula of a Hydrate

Many ionic compounds exist as hydrates. Often you can convert hydrates to anhydrous ionic compounds by heating them. Thus, hydrates are well suited to determining percentage composition experimentally.

In this investigation, you will find the mass percent of water in a hydrate of copper(II) sulfate hydrate,  $\text{CuSO}_4 \cdot x\text{H}_2\text{O}$ . You will use copper(II) sulfate hydrate for an important reason: The crystals of the hydrate are blue, while anhydrous copper(II) sulfate is white.

## Question

What is the molecular formula of the hydrate of copper(II) sulfate,  $\text{CuSO}_4 \cdot x\text{H}_2\text{O}$ ?

## Prediction

Predict what reaction will occur when you heat the hydrate of copper(II) sulfate.

## Materials

400 mL beaker (if hot plate is used)  
tongs  
scoopula

electronic balance  
glass rod  
hot pad  
3 g to 5 g hydrated copper(II) sulfate

## Safety Precautions



Heat the hydrate at a low to medium temperature only.

## Procedure

**Note:** If you are using a hot plate as your heat source, use the 400 mL beaker. If you are using a laboratory burner, use the porcelain evaporating dish.

1. Make a table like the one below, for recording your observations.

## Observations

Mass of empty beaker or evaporating dish	
Mass of beaker or evaporating dish + hydrated copper(II) sulfate	
Mass of beaker or evaporating dish + anhydrous copper(II) sulfate	



A hydrate of copper(II) sulfate (far left) is light blue. It loses its colour on heating.

- Measure the mass of the beaker and stirring rod. Record the mass in your table.
- Add 3 g to 5 g hydrated copper(II) sulfate to the beaker.
- Measure the mass of the beaker with the hydrated copper(II) sulfate. Record the mass in your table.
- If you are using a hot plate, heat the beaker with the hydrated copper(II) sulfate until the crystals lose their blue colour. You may need to stir occasionally with the glass rod. Be sure to keep the heat at a medium setting. Otherwise, the beaker may break.
- When you see the colour change, stop heating the beaker. Turn off or unplug the hot plate. Remove the beaker with the beaker tongs. Allow the beaker and crystals to cool on a hot pad.
- Find the mass of the beaker with the white crystals. Record the mass in your table.
- Return the anhydrous copper(II) sulfate to your teacher when you are finished. Do not put it in the sink or in the garbage.

### Analysis

- (a) Determine the percent by mass of water in your sample of hydrated copper(II) sulfate. Show your calculations clearly.  
(b) Do you expect the mass percent of water that you determined to be similar to the mass percents that other groups determined? Explain.
- (a) On the chalkboard, write the mass of your sample of hydrated copper(II) sulfate, the mass of the anhydrous copper(II) sulfate, and the mass percent of water that you calculated.  
(b) How do your results compare with other groups' results?

### Conclusion

- Based on your observations, determine the molecular formula of  $\text{CuSO}_4 \cdot x\text{H}_2\text{O}$ .

### Applications

- Suppose that you heated a sample of a hydrated ionic compound in a test tube. What might you expect to see inside the test tube, near the mouth of the test tube? Explain.
- You obtained the mass percent of water in the copper sulfate hydrate.
  - Using your observations, calculate the percentage composition of the copper sulfate hydrate.
  - In the case of a hydrate, and assuming you know the formula of the associated anhydrous ionic compound, do you think it is more useful to have the mass percent of water in the hydrate or the percentage composition? Explain your answer.
- Compare the formula that you obtained for the copper sulfate hydrate with the formulas that other groups obtained. Are there any differences? How might these differences have occurred?
- Suppose that you did not completely convert the hydrate to the anhydrous compound. Explain how this would affect
  - the calculated percent by mass of water in the compound
  - the molecular formula you determined
- Suppose the hydrate was heated too quickly and some of it was lost as it spattered out of the container. Explain how this would affect
  - the calculated percent by mass of water in the compound
  - the molecular formula you determined
- Suggest a source of error (not already mentioned) that would result in a value of  $x$  that is
  - higher than the actual value
  - lower than the actual value

## Section Wrap-up

In section 6.4, you learned several practical methods for determining empirical and molecular formulas of compounds. You may have noticed that these methods work because compounds react in predictable ways. For example, you learned that a compound containing carbon and hydrogen reacts with oxygen to produce water and carbon dioxide. From the mass of the products, you can determine the amount of carbon and hydrogen in the reactant. You also learned that a hydrate decomposes when it is heated to form water and an anhydrous compound. Again, the mass of one of the products of this reaction helps you identify the reactant. In Chapter 7, you will learn more about how to use the information from chemical reactions in order to do quantitative calculations.

## Section Review



- 1 K/U** Many compounds that contain carbon and hydrogen also contain nitrogen. Can you find the nitrogen content by carbon-hydrogen analysis, if the nitrogen does not interfere with the combustion reaction? If so, explain how. If not, explain why not.
- 2 I** What would be the mass of a bag of anhydrous magnesium sulfate,  $\text{MgSO}_4$ , if it contained the same amount of magnesium as a 1.00 kg bag of Epsom salts,  $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$ ? Give your answer in grams.
- 3 K/U** A compound that contains carbon, hydrogen, chlorine, and oxygen is subjected to carbon-hydrogen analysis. Can the mass percent of oxygen in the compound be determined using this method? Explain your answer.
- 4 C** Imagine that you are an analytical chemist. You are presented with an unknown compound, in the form of a white powder, for analysis. Your job is to determine the molecular formula of the compound. Create a flow chart that outlines the questions that you would ask and the analyses you would carry out. Briefly explain why each question or analysis is needed.
- 5 MC** A carbon-hydrogen analyzer uses a water absorber (which contains magnesium perchlorate,  $\text{Mg}(\text{ClO}_4)_2$ ) and a carbon dioxide absorber (which contains sodium hydroxide,  $\text{NaOH}$ ). The water absorber is always located in front of the carbon dioxide absorber. What does this suggest about the sodium hydroxide that is contained in the  $\text{CO}_2$  absorber?
- 6 I** A hydrate of zinc nitrate has the formula  $\text{Zn}(\text{NO}_3)_2 \cdot x\text{H}_2\text{O}$ . If the mass of 1 mol of anhydrous zinc nitrate is 63.67% of the mass of 1 mol of the hydrate, what is the value of  $x$ ?
- 7 K/U** A 2.524 g sample of a compound contains carbon, hydrogen, and oxygen. The sample is subjected to carbon-hydrogen analysis. 3.703 g of carbon dioxide and 1.514 g of water are collected.
  - (a) Determine the empirical formula of the compound.
  - (b) If one molecule of the compound contains 12 atoms of hydrogen, what is the molecular formula of the compound?

## Reflecting on Chapter 6

Summarize this chapter in the format of your choice. Here are a few ideas to use as guidelines:

- Determine the mass percent of each element in a compound.
- Predict the empirical formula of a compound using the periodic table, and test your prediction through experimentation.
- Use experimental data to determine the empirical (simplest) formula of a compound.
- Use the molar mass and empirical formula of a compound to determine the molecular (actual) formula of the compound.
- Determine experimentally the percent by mass of water in a hydrate. Use this information to determine its molecular formula.
- Explain how a carbon-hydrogen combustion analyzer can be used to determine the mass percent of carbon, hydrogen, and oxygen in a compound.

## Reviewing Key Terms

For each of the following terms, write a sentence that shows your understanding of its meaning.

anhydrous

carbon-hydrogen combustion analyzer

empirical formula

forensic scientists

hydrate

law of definite proportions

mass percent

molecular formula

percentage composition

## Knowledge/Understanding

1. When determining the percentage composition of a compound from its formula, why do you base your calculations on a one mole sample?
2. The main engines of the space shuttle burn hydrogen and oxygen, with water as the product. Is this synthetic (human-made) water the same as water found in nature? Explain.
3. (a) What measurements need to be taken during a carbon-hydrogen combustion analysis?

(b) Acetylene,  $C_2H_2$ , and benzene,  $C_6H_6$ , both have the same empirical formula. How would their results compare in a carbon-hydrogen combustion analysis? Explain your answer.

4. If you know the molar mass of a substance, and the elements that make up the substance, can you determine its molecular formula? Explain your answer.

## Inquiry

5. A 5.00 g sample of borax (sodium tetraborate decahydrate,  $Na_2B_4O_7 \cdot 10H_2O$ ) was thoroughly heated to remove all the water of hydration. What mass of anhydrous sodium tetraborate remained?
6. Determine the percentage composition of each compound.
  - (a) freon-12,  $CCl_2F_2$
  - (b) white lead,  $Pb_3(OH)_2(CO_3)_2$
7. (a) What mass of water is present in 25.0 g of  $MgCl_2 \cdot 2H_2O$ ?  
(b) What mass of manganese is present in 5.00 g of potassium permanganate,  $KMnO_4$ ?
8. Silver nitrate,  $AgNO_3$ , can be used to test for the presence of halide ions in solution. It combines with the halide ions to form a silver halide precipitate. In medicine, it is used as an antiseptic and an antibacterial agent. Silver nitrate drops are placed in the eyes of newborn babies to protect them against an eye disease.
  - (a) Calculate the mass percent of silver in silver nitrate.
  - (b) What mass of pure silver is contained in  $2.00 \times 10^2$  kg of silver nitrate?
9. Barium sulfate,  $BaSO_4$ , is opaque to X-rays. For this reason, it is sometimes given to patients before X-rays of their intestines are taken. What mass of barium is contained in 45.8 g of barium sulfate?
10. Bismuth nitrate,  $Bi(NO_3)_2$ , is used in the production of some luminous paints. How many grams of pure bismuth are in a 268 g sample of bismuth nitrate?
11. The molar mass of a compound is approximately 121 g. The empirical formula of the

- compound is  $\text{CH}_2\text{O}$ . What is the molecular formula of the compound?
12. A complex organic compound, with the name 2,3,7,8-tetrachlorodibenz-p-*dioxin*, belongs to a family of toxic compounds called *dioxins*. The empirical formula of a certain dioxin is  $\text{C}_6\text{H}_2\text{OCl}_2$ . If the molar mass of this dioxin is 322 g/mol, what is its molecular formula?
13. A student obtains an empirical formula of  $\text{C}_1\text{H}_{2.67}$  for a gaseous compound.
- (a) Why is this not a valid empirical formula?
- (b) Use the student's empirical formula to determine the correct empirical formula.
14. Progesterone, a hormone, is made up of 80.2% carbon, 10.18% oxygen, and 9.62% hydrogen. Determine the empirical formula of progesterone.
15. An inorganic salt is composed of 17.6% sodium, 39.7% chromium, and 42.8% oxygen. What is the empirical formula of this salt?
16. What is the empirical formula of a compound that contains 67.6% mercury, 10.8% sulfur, and 21.6% oxygen?
17. (a) An inorganic salt is made up of 38.8% calcium, 20.0% phosphorus, and 41.2% oxygen. What is the empirical formula of this salt?
- (b) On further analysis, each formula unit of this salt is found to contain two phosphate ions. Predict the molecular formula of this salt.
18. Capsaicin is the compound that is responsible for the "hotness" of chili peppers. Chemical analysis reveals capsaicin to contain 71.0% carbon, 8.60% hydrogen, 15.8% oxygen, and 4.60% nitrogen.
- (a) Determine the empirical formula of capsaicin.
- (b) Each molecule of capsaicin contains one atom of nitrogen. What is the molecular formula of capsaicin?
19. A compound has the formula  $\text{X}_2\text{O}_5$ , where X is an unknown element. The compound is 44.0% oxygen by mass. What is the identity of element X?
20. A 1.254 g sample of an organic compound that contains only carbon, hydrogen, and oxygen reacts with a stream of chlorine gas,  $\text{Cl}_{2(g)}$ . After the reaction, 4.730 g of HCl and 9.977 g of  $\text{CCl}_4$  are obtained. Determine the empirical formula of the organic compound.
21. A 2.78 g sample of hydrated iron(II) sulfate,  $\text{FeSO}_4 \cdot x\text{H}_2\text{O}$ , was heated to remove all the water of hydration. The mass of the anhydrous iron(II) sulfate was 1.52 g. Calculate the number of water molecules associated with each formula unit of  $\text{FeSO}_4$ .
22. Citric acid is present in citrus fruits. It is composed of carbon, hydrogen, and oxygen. When a 0.5000 g sample of citric acid was subjected to carbon-hydrogen combustion analysis, 0.6871 g of carbon dioxide and 0.1874 g of water were produced. Using a mass spectrometer, the molar mass of citric acid was determined to be 192 g/mol.
- (a) What are the percentages of carbon, hydrogen, and oxygen in citric acid?
- (b) What is the empirical formula of citric acid?
- (c) What is the molecular formula of citric acid?
23. Methanol,  $\text{CH}_3\text{OH}$  (also known as methyl alcohol), is a common laboratory reagent. It can be purchased at a hardware store under the name "methyl hydrate" or "wood alcohol." If 1.00 g of methanol is subjected to carbon-hydrogen combustion analysis, what masses of carbon dioxide and water are produced?
24. Copper can form two different oxides: copper(II) oxide,  $\text{CuO}$ , and copper(I) oxide,  $\text{Cu}_2\text{O}$ . Suppose that you find a bottle labelled "copper oxide" in the chemistry prep room. You call this mystery oxide  $\text{Cu}_x\text{O}$ . Design an experiment to determine the empirical formula of  $\text{Cu}_x\text{O}$ . Assume that you have a fully equipped chemistry lab at your disposal. Keep in mind the following information:
- Both  $\text{CuO}$  and  $\text{Cu}_2\text{O}$  react with carbon to produce solid copper and carbon dioxide gas:  
$$\text{Cu}_x\text{O}_{(s)} + \text{C}_{(s)} \rightarrow \text{Cu}_{(s)} + \text{CO}_{2(g)}$$
This reaction proceeds with strong heating.
  - Carbon reacts with oxygen to produce carbon dioxide gas:  
$$\text{C}_{(s)} + \text{O}_{2(g)} \rightarrow \text{CO}_{2(g)}$$
This reaction also proceeds with strong heating.
  - Carbon is available in the form of activated charcoal.

- (a) State at least one safety precaution that you would take.

(b) State the materials required, and sketch your apparatus.

(c) Outline your procedure.

(d) What data do you need to collect?

(e) State any assumptions that you would make.

25. Magnesium sulfate,  $\text{MgSO}_4$ , is available as anhydrous crystals or as a heptahydrate. Assume that you are given a bottle of  $\text{MgSO}_4$ , but you are not sure whether or not it is the hydrate.

(a) What method could you use, in a laboratory, to determine whether this is the hydrate?

(b) If it is the hydrate, what results would you expect to see?

(c) If it is the anhydrous crystals, what results would you expect to see?

## Communication

- 26.** Draw a concept map to relate the following terms: molar mass of an element, molar mass of a compound, percentage composition, empirical formula, and molecular formula. Use an example for each term.

**27.** Draw a schematic diagram of a carbon-hydrogen combustion analyzer. Write a few sentences to describe each stage of the analysis as dimethyl ether,  $\text{C}_2\text{H}_6\text{O}$ , passes through the apparatus.

## Making Connections

- 28.** For many years, tetraethyl lead,  $\text{Pb}(\text{C}_2\text{H}_5)_4$ , a colourless liquid, was added to gasoline to improve engine performance. Over the last 20 years it has been replaced with non-lead-containing additives due to health risks associated with exposure to lead. Tetraethyl lead was added to gasoline up to 2.0 mL per 3.8 L (1.0 US gallon) of gasoline.

(a) Calculate the mass of tetraethyl lead in 1.0 L of gasoline. The density of  $\text{Pb}(\text{C}_2\text{H}_5)_4$  is 1.653 g/mL.

(b) Calculate the mass of elemental lead in 1.0 L of gasoline.

**29.** Natron is the name of the mixture of salts that was used by the ancient Egyptians to dehydrate corpses before mummification. Natron is com-

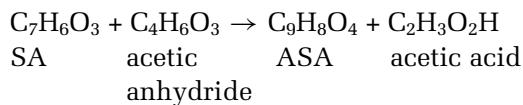
posed of  $\text{Na}_2\text{CO}_3$ ,  $\text{NaHCO}_3$ ,  $\text{NaCl}$ , and  $\text{CaCl}_2$ . The  $\text{Na}_2\text{CO}_3$  absorbs water from tissues to form  $\text{Na}_2\text{CO}_3 \cdot 7\text{H}_2\text{O}$ .

- (a) Name the compound  $\text{Na}_2\text{CO}_3 \cdot 7\text{H}_2\text{O}$ .

(b) Calculate the mass percent of water in  $\text{Na}_2\text{CO}_3 \cdot 7\text{H}_2\text{O}$ .

(c) What mass of anhydrous  $\text{Na}_2\text{CO}_3$  is required to dessicate (remove all the water) from an 80 kg body that is 78% water by mass?

9. Imagine that you are an analytical chemist at a pharmaceutical company. One of your jobs is to determine the purity of the acetylsalicylic acid (ASA),  $\text{C}_9\text{H}_8\text{O}_4$ . ASA is prepared by reacting salicylic acid (SA),  $\text{C}_7\text{H}_6\text{O}_3$ , with acetic anhydride,  $\text{C}_4\text{H}_6\text{O}_3$ . Acetic acid,  $\text{C}_2\text{H}_3\text{O}_2\text{H}$ , is also produced



ASA often contains unreacted SA. Since it is not acceptable to sell ASA contaminated with SA, one of your jobs is to analyze the ASA to check purity. Both ASA and SA are white powders.

- (a)** You analyze a sample that you believe to be pure ASA, but which is actually contaminated with some SA. How will this affect the empirical formula that you determine for the sample?

**(b)** Another sample contains ASA contaminated with 0.35 g SA. The mass of the sample is 5.73 g. What empirical formula will you obtain?

## **Answers to Practice Problems and**

## **Short Answers to Section Review Questions:**

**Practice Problems:** 1. 36% Ca; 64% Cl 2. 48.1% Ni; 16.9%

P; 35.0% O 3. 39.5% C; 7.8% H; 52.7% O

4. 26.6% K; 35.4% Cr; 38.0% O 5.(a) 63.6

**(b)** 13.24% N **(c)** 35.00% N **(d)** 22.23% N

6. 2.06% H; 32.69% S; 62.25% O 7. 47.47% O

**8.(a)** 63.19% Mn; 36.81% O **(b)** 158 g **9.** NH<sub>3</sub>

**10.** Li<sub>2</sub>O   **11.** BF<sub>3</sub>   **12.** SCl   **13.** Cr<sub>2</sub>O<sub>3</sub>   **14.** P<sub>2</sub>O<sub>5</sub>   **15.**

**16.** C<sub>12</sub>H<sub>14</sub>O<sub>3</sub>   **17.** C<sub>4</sub>H<sub>10</sub>   **18.** C<sub>2</sub>H<sub>2</sub>O<sub>4</sub>   **19.** C<sub>18</sub>H<sub>21</sub>NO

**20.** C<sub>15</sub>H<sub>12</sub>O<sub>3</sub>   **21.** C<sub>5</sub>H<sub>12</sub>; 83.3% C; 16.7% H.   **22.** C<sub>21</sub>

**23.** 50.9% **24.** 5 **25.** 4

**Section Review: 6.1:** 3. 3.05 g 4. 11.3 g 5. 17.1 g. 7.

6.2: 2. C<sub>8</sub>H<sub>8</sub>O<sub>3</sub> 3.(a) C

7.  $\text{C}_{11}\text{H}_{14}\text{O}_2$  8.(a)  $\text{FeC}_{10}\text{H}_{10}$  (b) Yes. 6.3: 2.  $\text{C}_4\text{H}_6\text{O}_6$

**4.(a)** C<sub>2</sub>H<sub>3</sub>O   **(b)** Double   **5.** C<sub>12</sub>H<sub>10</sub>O<sub>2</sub>   **6.4:** **1.** Yes   **2.** 488 g

**4.** No **6.** 6 **7.(a)**  $\text{CH}_2\text{O}$  **(b)**  $\text{C}_6\text{H}_{12}\text{O}_6$  **8.(a)**  $\text{CH}_2$  **(b)**  $\text{CH}_{12}$

