SECTION 6.2

Empirical and Molecular Formulas

Key Terms

molecular formula
empirical formula
ratio

molecular formula the formula for a compound that shows the number of atoms of each element that make up a molecule of that compound

empirical formula a formula that shows the smallest whole-number ratio of the elements in a compound

ratio relative amount; proportional relationship

In Section 6.1, you read that chemists can determine the percentage composition of a compound from mass data alone. However, the percentage composition only tells chemists which elements the compound contains and the relative masses of these elements. For more specific information about the composition of a compound, you need to know the relative number of atoms of each element.

Comparing Molecular and Empirical Formulas of Compounds

Chemical formulas communicate which elements are found in a compound, as well as their proportions. For example, the formula for hydrogen peroxide, H_2O_2, indicates that a molecule of hydrogen peroxide contains two atoms of hydrogen and two atoms of oxygen. Thus, this formula shows the actual number of atoms of each element in one molecule of the compound. Such a formula is known as the **molecular formula**. Molecular formulas can often be quite complex, as some molecules, such as glucose, $C_6H_{12}O_6$, contain many atoms.

A simpler method of writing a chemical formula involves showing only the proportional relationship or relative number of the atoms of each element in a compound. Such a formula, known as an **empirical formula**, shows the smallest whole-number **ratio**, or proportional relationship, of the elements in a compound. For instance, the molecular formula for hydrogen peroxide is H_2O_2, and the ratio of hydrogen to oxygen atoms is 2:2. The ratio 2:2 is not the smallest ratio because you can reduce it to 1:1. Thus, the empirical formula for this compound is HO,

Note that, for some compounds, the empirical formula may be the same as the molecular formula. For example, water has two hydrogen atoms and one oxygen atom, as shown in **Figure 6.6**. Thus, the molecular formula for water is H_2O. As this formula shows the smallest whole-number ratio of the elements in this molecule, it is also the molecule's empirical formula. Additionally, it is important to recognize, as you learned in Chapter 2, that ionic compounds only have one possible atomic configuration. As a result, they are always represented by empirical formulas. They never have a molecular formula. As the name indicates, molecular formulas apply only to molecules.

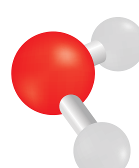


Figure 6.6 The empirical and molecular formulas for water are the same, as the molecular formula for water already shows the smallest whole-number molar ratio of the elements in this molecule.

Chemical Formulas and Specific Composition

The empirical formula for a compound gives a very basic glimpse into the composition of the compound. For this reason, the empirical formula is a very good start in an experimental analysis to determine the formula for a new or unknown compound. However, would determining the empirical formula for an unknown substance be enough to identify that substance? Because more than one compound can have the same empirical formula, it is often necessary to know the molecular formula in order to distinguish between compounds.

Applications of Empirical and Molecular Formulas

Suppose a thief has robbed a home but left behind some tracks on the floor. The residue is analyzed and found to contain an unknown compound. An initial analysis reveals that the compound contains carbon, hydrogen, and oxygen. Further analysis reveals that its empirical formula is CH_2O. Could the investigators conclude that the unknown substance is formaldehyde, which has the molecular formula $CH_2O(g)$, and that the thief is someone who comes in contact with formaldehyde? This would be a hasty decision. Formaldehyde is one of several compounds that have the same empirical formula, as shown in **Table 6.1**. These compounds have the same *relative* amount of each element. However, their molecular formulas differ, as the compounds are composed of different *actual* amounts of each element.

Suggested Investigation

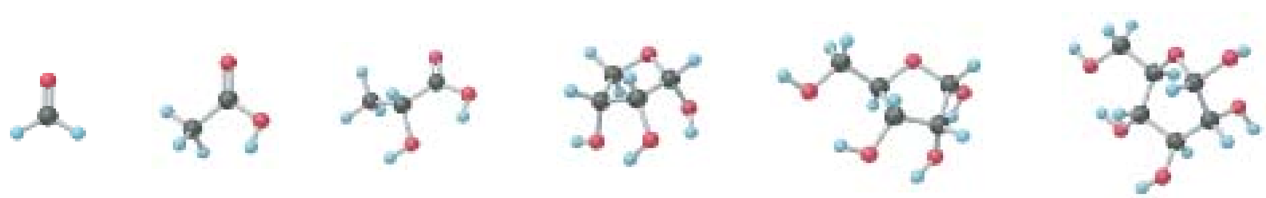
Inquiry Investigation 6-B, Chemical Analysis Simulation

Although the compounds in **Table 6.1** have the same proportions of the same elements, their chemical properties are quite different. For example, formaldehyde is toxic to humans whereas acetic acid is the main component in vinegar which we eat on salads and french fries. Ribose is an important biological compound that is found in Vitamin B. It is also a component the genetic material, DNA (*deoxyribo*nucleic acid). Erythrose is an intermediate in the conversion from glucose to ribose. Glucose is the main source of energy for most animals. During intense exercise, as shown in **Figure 6.7**, muscles breakdown glucose into lactic acid which causes sore muscles.

Figure 6.7 This runner's muscles are using glucose so rapidly that lactic acid builds up before it can be broken down into carbon dioxide and water.

Table 6.1 Six Compounds with the Empirical Formula CH_2O

Name	Empirical Formula	Molecular Formula	Whole-Number Multiple	*M* (g/mol)	Use or Function
Formaldehyde	CH_2O	CH_2O	1	30.03	Is used as a disinfectant and biological preservative
Acetic acid	CH_2O	$C_2H_4O_2$	2	60.06	Is used to produce acetate polymers; is a component of vinegar (5% solution)
Lactic acid	CH_2O	$C_3H_6O_3$	3	90.09	Causes milk to sour; forms in muscles during exercise
Erythrose	CH_2O	$C_4H_8O_4$	4	120.12	Forms during sugar metabolism
Ribose	CH_2O	$C_5H_{10}O_5$	5	150.15	Is a component of many nucleic acids and vitamin B_2
Glucose	CH_2O	$C_6H_{12}O_6$	6	180.18	Is a major nutrient for energy in cells



CH_2O $C_2H_4O_2$ $C_3H_6O_3$ $C_4H_8O_4$ $C_5H_{10}O_5$ $C_6H_{12}O_6$

Compounds with the Same Empirical Formula and Different Molecular Formulas

In the thief scenario, you compared compounds that have the same relative amount of each element, but different actual amounts of each element. Such compounds share the same empirical formula, but have different molecular formulas. As a result, they tend to have very different properties. Consider nitrogen dioxide, $NO_2(g)$, and dinitrogen tetroxide, $N_2O_4(g)$.

Nitrogen dioxide, is an orange-brown gas with a sharp, biting odour. In high concentrations, it is extremely toxic and corrosive. Recall that nitrogen dioxide is a common product in internal combustion engine exhaust, and it is released from power plants that burn fossil fuels to generate electrical power. Nitrogen dioxide is one of the main components of smog. It is the component that is responsible for making a visible smog haze above polluted urban centres, as shown in **Figure 6.8 (A)**.

Note that the ratio of nitrogen to oxygen in this gas is the simplest possible, so its empirical formula is also its molecular formula. That is, one molecule of this gas contains one nitrogen atom and two oxygen atoms.

Dinitrogen tetroxide has the same empirical formula as nitrogen dioxide, but a different molecular formula. As a result, its properties differ. For example, dinitrogen tetroxide in conjunction with hydrazine, H_2N_4([el]), make an important rocket propellant, as shown in **Figure 6.8 (B)**, because they burn on contact, without the need for a separate ignition source. Like nitrogen dioxide, it is very toxic and corrosive in high concentrations. The dinitrogen tetroxide molecule contains two nitrogen atoms and four oxygen atoms.

Figure 6.8 **(A)** Nitrogen dioxide is one of the main components of smog. **(B)** Dinitrogen tetroxide is used as a rocket propellant. The two compounds have the same empirical formulas but different molecular formulas, chemical properties, and applications.

Learning Check

7. State the ratio of carbon to hydrogen in one molecule of methane, $CH_4(g)$.

8. Both the percentage composition and the molecular formula for a compound provide information about the proportions of the elements in the compound. How are these proportions similar, and how are they different?

9. What information does a molecular formula tell you about a compound that an empirical formula does not?

10. When is the molecular formula for a compound the same as its empirical formula?

11. Why is it important to know the molecular formula for a compound? Use the chemicals in **Figure 6.8** as examples.

12. The following formulas contain only nitrogen and oxygen: NO, N_2O, NO_2, N_2O_4, and N_2O_5. Which formulas represent the empirical and molecular formulas for the same compound? Explain your answer.

Determining the Empirical Formula

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You can determine the empirical formula for a compound from the percentage composition. For example, assume that a compound is 50.91% zinc, 16.04% phosphorus, and 33.15% oxygen. Because only relative amounts of the elements are needed for an empirical formula, *any amount of the compound can be used*. Therefore, assume that you have a 100 g sample. Using the percentage composition, 100 g of the compound contains 50.91 g of zinc, 16.04 g of phosphorus, and 33.15 g of oxygen. Next, determine the amount in moles of each element. You can find the amount of an element by dividing the mass by the molar mass of the element, as shown below.

$$n_{\mathrm{Zn}} = \frac{50.81\ \cancel{\mathrm{g}}}{65.41\ \cancel{\mathrm{g}}/\mathrm{mol}} = 0.777\ \mathrm{mol\ (Zn)}$$

$$n_{\mathrm{P}} = \frac{16.04\ \cancel{\mathrm{g}}}{30.97\ \cancel{\mathrm{g}}/\mathrm{mol}} = 0.518\ \mathrm{mol\ (P)}$$

$$n_{\mathrm{O}} = \frac{33.15\ \cancel{\mathrm{g}}}{16.00\ \cancel{\mathrm{g}}/\mathrm{mol}} = 2.072\ \mathrm{mol\ (O)}$$

These values give you the ratio of the amounts of each element in the substance in moles, or 0.777 mol Zn : 0.518 mol P : 2.072 mol O. This ratio is the same as the subscripts in an empirical formula. Therefore, you could write the empirical formula as:

$$Zn_{0.777}P_{0.518}O_{2.072}$$

However, you cannot have fractions of an atom. You can obtain whole number subscripts in one or two more steps. First, divide each subscript by the smallest subscript, or 0.518.

$$Zn_{\frac{0.777}{0.518}}P_{\frac{0.518}{0.518}}O_{\frac{2.072}{0.518}}$$

$$Zn_{1.5}P_1O_4$$

In many calculations, the subscripts are all whole numbers at this step. However, the subscript for zinc is 1.5. In cases like this, you can multiply all subscripts by a whole number that will make the decimal subscript into a whole number. To complete this calculation, multiply all of the subscripts by 2. Your empirical formula becomes

$$Zn_{1.5\times 2}P_{1\times 2}O_{4\times 2}$$

$$Zn_3P_2O_8$$

Because this formula contains a metal, Zn, and two non-metals, P and O, the substance must be an ionic compound which has a polyatomic ion for the non-metal. Therefore, the empirical formula is the same as the formula for the compound. However, P_2O_8 is not a familiar polyatomic ion but it has the same ratio of elements as the phosphate ion. Therefore, your formula is $Zn_3(PO_4)_2$.

Rules for Determining Empirical Formulas

1. Convert percentage composition data into mass data by assuming that the total mass of the sample is 100 g.
2. Determine the number of moles of each element in the sample by dividing the mass by the molar mass of each element.
3. Convert the number of moles of each element into whole numbers that become subscripts in the empirical formula by dividing each amount in moles by the smallest amount.
4. If the subscripts are not yet whole numbers, determine the least common multiple that will make the decimal values into whole numbers. Multiply all subscripts by this least common multiple. Use these numbers as subscripts to complete the empirical formula.

Sample Problem

Determining the Empirical Formula for a Compound with More Than Two Elements from Percentage Composition

Problem

Determine the empirical formula for a compound that is found by analysis to contain 27.37% sodium, 1.200% hydrogen, 14.30% carbon, and 57.14% oxygen.

What Is Required?

You need to determine the empirical formula for the sample that contains sodium, hydrogen, carbon, and oxygen.

What Is Given?

You know the composition of the compound: 27.37% sodium, 1.200% hydrogen, 14.30% carbon, and 57.14% oxygen.

Plan Your Strategy	Act on Your Strategy
Assume that the mass of the sample is 100 g.	In a 100 g sample of the compound, there will be 27.37 g sodium, 1.200 g of hydrogen, 14.30 g carbon, and 57.14 g oxygen.
Determine the molar masses of sodium, hydrogen, carbon, and oxygen using the periodic table	The molar mass of sodium is 22.99 g/mol. The molar mass of hydrogen is 1.01 g/mol. The molar mass of carbon is 12.01 g/mol. The molar mass of oxygen is 16.00 g/mol.
Convert each mass to moles	$n_{Na} = \frac{27.37\ \cancel{g}}{22.99\ \cancel{g}/mol} = 1.190518\text{ mol}$ $n_{H} = \frac{1.200\ \cancel{g}}{1.01\ \cancel{g}/mol} = 1.188119\text{ mol}$ $n_{C} = \frac{14.30\ \cancel{g}}{12.01\ \cancel{g}/mol} = 1.190674\text{ mol}$ $n_{O} = \frac{57.14\ \cancel{g}}{16.00\ \cancel{g}/mol} = 3.57125\text{ mol}$
Divide all the mole amounts by the lowest mole amount.	$\frac{1.190518}{1.188119} : \frac{1.188119}{1.188119} : \frac{1.190674}{1.188119} : \frac{3.57125}{1.188119}$ ratios: 1:1:1:3 Therefore, the empirical formula is $Na_1H_1C_1O_3$ or $NaHCO_3$

Check Your Solution

Work backward. Calculate the percentage composition of $NaHCO_3$.

The molar mass of $NaHCO_3$ is:

$$\begin{aligned} M_{NaHCO_3} &= 1M_{Na} + 1M_{H} + 1M_{C} + 3M_{O} \\ &= 1(22.99\text{ g/mol}) + 1(1.01\text{ g/mol}) + 1(12.01\text{ g/mol}) + 3(16.00\text{ g/mol}) = 84.01\text{ g/mol} \end{aligned}$$

mass percent of Na: $\frac{22.99\ \cancel{g/mol}}{84.01\ \cancel{g/mol}} \times 100\% = 27.37\%$

mass percent of H: $\frac{1.01\ \cancel{g/mol}}{84.01\ \cancel{g/mol}} \times 100\% = 1.202\%$

mass percent of C: $\frac{12.01\ \cancel{g/mol}}{84.01\ \cancel{g/mol}} \times 100\% = 14.30\%$

mass percent of O: $\frac{3(16.00\ \cancel{g/mol})}{84.01\ \cancel{g/mol}} \times 100\% = 57.14\%$

The percentage composition calculated from the empirical formula closely matches the given data. Therefore, the empirical formula $NaHCO_3$ is reasonable. The percentages do not add to 100% due to rounding.

Sample Problem

Determining the Empirical Formula from Mass Data when a Ratio Term Is Not Close to a Whole Number

Problem

Determine the empirical formula for a compound that contains 69.88 g of iron and 30.12 g of oxygen.

What Is Required

You need to determine the empirical formula from mass data.

What Is Given?

You know the mass data of the compound: 69.88 g iron and 30.12 g oxygen

Plan Your Strategy	Act on Your Strategy
Convert each mass to moles using the molar mass.	$\frac{69.88\ \cancel{g}\ Fe}{55.85\ \cancel{g}/mol} = 1.2512\ mol\ Fe$ $\frac{30.12\ \cancel{g}\ O}{16.00\ \cancel{g}/mol} = 1.882\ mol\ O$
Divide all the mole amounts by the lowest mole amount.	$Fe:O = \frac{1.2512}{1.2512}:\frac{1.882}{1.2512} = 1:1.5$ The incomplete formula is $Fe_1O_{1.5}$.
Determine the least common multiple that will make all of the subscripts whole numbers. Multiply all the subscripts by this whole-number multiple to determine the empirical formula.	The smallest whole-number multiple that makes all the subscripts small whole numbers is 2. Therefore, the empirical formula is Fe_2O_3.

Check Your Solution

Work backward. Determine the percentage composition. Assume there is a 100 g sample and compare the number of grams of each substance.

$M_{Fe_2O_3} = 2M_{Fe} + 3M_O = 2(55.85\ g/mol) + 3(16.00\ g/mol) = 159.7\ g/mol$

Determine the percentage composition:

$$\text{mass percent of Fe} = \frac{111.70\ \cancel{g/mol}}{159.7\ \cancel{g/mol}} \times 100\% = 69.94\%$$

$$\text{mass percent of O} = \frac{48.00\ \cancel{g/mol}}{159.7\ \cancel{g/mol}} \times 100\% = 30.06\%$$

In a 100 g sample, there is 69.94 g of iron and 30.06 g of oxygen. This closely matches the given data. The empirical formula is reasonable.

Practice Problems

Determine the empirical formulas for the compounds with the following percentage compositions.

31. 80.04% carbon and 19.96% hydrogen

32. 58.2 g of magnesium and 41.8 g of chlorine

33. 40.0% copper, 20.0% sulfur, and 40.0% oxygen

34. 26.61% K, 35.38% Cr, and 38.01% O

35. 17.6 g of hydrogen and 82.4 g of nitrogen

36. 46.3 g of lithium and 53.7 g of oxygen

37. 15.9% boron, and the rest is fluorine

38. 60.11% sulfur, and the rest is chlorine

39. 11.33% carbon, 45.29% oxygen, and the rest is sodium

40. 56.36% oxygen, and the rest is phosphorus

Determining the Molecular Formula

Because the molecular formula is so closely related to the empirical formula, you can determine the molecular formula for a compound using the empirical formula and the molar mass of the compound, as shown in the Sample Problem below. Recall that the empirical formula is multiplied by a whole number to get the molecular formula. For example, the empirical formula for benzene, $C_6H_6(\ell)$, is CH, as shown in **Figure 6.9**. This empirical formula is multiplied by the whole number 6 to get the molecular formula.

To determine the molecular formula for a compound, use the method you learned in Chapter 5 to determine the molar mass of the empirical formula. The molar mass of the actual compound must be determined experimentally using a device such as a mass spectrometer. Because it must be determined experimentally, the molar mass of the actual compound is usually given in problems where you determine the molecular formula for a compound.

To determine the molecular formula from percentage composition data, you determine the empirical formula for the compound as you did in previous problems. Then you use the molar masses of the empirical formula and the molecular formula to find the whole-number multiple, x, which relates the empirical formula to the molecular formula. The Sample Problem on the following page demonstrates how to solve this type of problem.

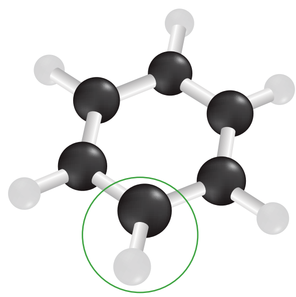


Figure 6.9 Benzene has six CH units joined together. The empirical formula for benzene is CH and the molecular formula is $C_6H_6(\ell)$.

Sample Problem

Molecular Formula from Empirical Formula and Molar Mass

Problem

A compound with the empirical formula CH was analyzed using a mass spectrometer. Its molar mass was found to be 78 g/mol. Determine the molecular formula.

What Is Required

You need to determine the the molecular formula.

What Is Given?

You know the empirical formula: CH

You know the molar mass of the actual compound: 78 g/mol

Plan Your Strategy	Act on Your Strategy
Determine the molar mass of CH.	$M_{CH} = M_C + M_H$ $= 12.01\text{ g/mol} + 1.01\text{ g/mol}$ $= 13.02\text{ g/mol}$
To find the whole-number multiple, x, divide the experimentally determined molar mass by the molar mass of the empirical formula. To determine the molecular formula, multiply each subscript of the empirical formula by the whole-number multiple.	$M_{\text{actual compound}} = x \times (M_{CH})$ $78\text{ g/mol} = x \times (13.02\text{ g/mol})$ $x = \frac{78\ \cancel{\text{g/mol}}}{13.02\ \cancel{\text{g/mol}}}$ $x = 6$ Therefore, the molecular formula is $C_6H_6(\ell)$.

Check Your Solution

Work backward by calculating the molar mass of $C_6H_6(\ell)$.

$(6 \times 12.01\text{ g/mol}) + (6 \times 1.01\text{ g/mol}) = 78.12\text{ g/mol}$

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

Sample Problem

Molecular Formula from Percentage Composition and Molar Mass

Problem

Chemical analysis indicates that a compound is 28.64% sulfur and 71.36% bromine. The molar mass of the compound is 223.94 g/mol. Determine the molecular formula.

What Is Required

You need to find the molecular formula for the compound composed of sulfur and bromine.

What Is Given?

You know the percentage composition: 28.64% sulfur and 71.36% bromine
You know the molar mass of the compound: 223.94 g/mol

Plan Your Strategy	Act on Your Strategy
Assume the mass of the sample is 100 g.	In 100 g of the compound, there will be 28.64 g of sulfur and 71.36 g of bromine.
Find the molar mass of sulfur. Find the molar mass of bromine.	The molar mass of sulfur is 32.07 g/mol. The molar mass of bromine is 79.90 g/mol.
Convert each mass to moles.	$\frac{28.64\ \cancel{g}\ S}{32.07\ \cancel{g}/mol} = 0.8930\ mol\ S$ $\frac{71.36\ \cancel{g}\ Br}{79.90\ \cancel{g}/mol} = 0.8931\ mol/Br$
Divide all the mole amounts by the lowest number of moles.	$S{:}Br = \frac{0.8930}{0.8930} : \frac{0.8931}{0.8930} = 1{:}1$
Determine the least common multiple that will make all of the subscripts whole numbers.	Because these subscripts are already whole numbers, you do not need to determine the least common multiple. The empirical formula is SBr.
Find the molar mass of the empirical formula.	$M_{SBr} = 1M_S + 1M_{Br}$ $= 1(32.07\ g/mol) + 1(79.90\ g/mol) = 111.97\ g/mol$
To find the whole-number multiple, *x*, divide the experimental molar mass by the molar mass of the empirical formula.	$x = \frac{\text{experimental molar mass}}{\text{empirical formula molar mass}} = \frac{223.94\ \cancel{g/mol}}{111.97\ \cancel{g/mol}} = 2$
To determine the molecular formula, multiply each subscript of the empirical formula by the whole-number multiple.	The molecular formula is S_2Br_2.

Practice Problems

41. The empirical formula for glucose is $CH_2O(s)$. The molar mass of glucose is 180.18 g/mol. Determine the molecular formula for glucose.

42. The empirical formula for xylene is $C_4H_5(\ell)$, and its molar mass is 106 g/mol. What is the molecular formula for xylene?

43. The empirical formula for 1,4-butanediol is $C_2OH_5(\ell)$. Its molar mass is 90.14 g/mol. What is its molecular formula?

44. The empirical formula for styrene is $CH(\ell)$, and its molar mass is 104 g/mol. What is its molecular formula?

45. Calomel is a compound that was once popular for treating syphilis. It contains 84.98% mercury and 15.02% chlorine. It has a molar mass of 472 g/mol. What is its empirical formula?

46. The molar mass of caffeine is 194 g/mol. Determine whether the molecular formula for caffeine is $C_4H_5N_2O(s)$ or $C_8H_{10}N_4O_2(s)$.

47. An unknown compound contains 42.6% oxygen, 32% carbon, 18.7% nitrogen, and the remainder hydrogen. Using mass spectrometry, its molar mass was determined to be 75.0 g/mol. What is the molecular formula for the compound?

Continued on next page

48. A compound that contains 6.44 g of boron and 1.80 g of hydrogen has a molar mass of approximately 28 g/mol. What is its molecular formula?

49. The molar mass of a compound is 148.20 g/mol. Its percentage composition is 48.63% carbon, 21.59% oxygen, 18.90% nitrogen, and the rest hydrogen.
 a. Find the empirical formula for the compound.
 b. Find its molecular formula.

50. Estradiol is the main estrogen compound that is found in humans. Its molar mass is 272.38 g/mol. The percentage composition of estradiol is 72.94% carbon, 10.80% oxygen, and 8.16% hydrogen. Determine whether its molecular formula is the same as its empirical formula. If not, what is each formula?

How to Determine Empirical and Molecular Formulas

The steps required to determine the empirical and molecular formulas for compounds are very similar. The flowchart in **Figure 6.10** illustrates these steps.

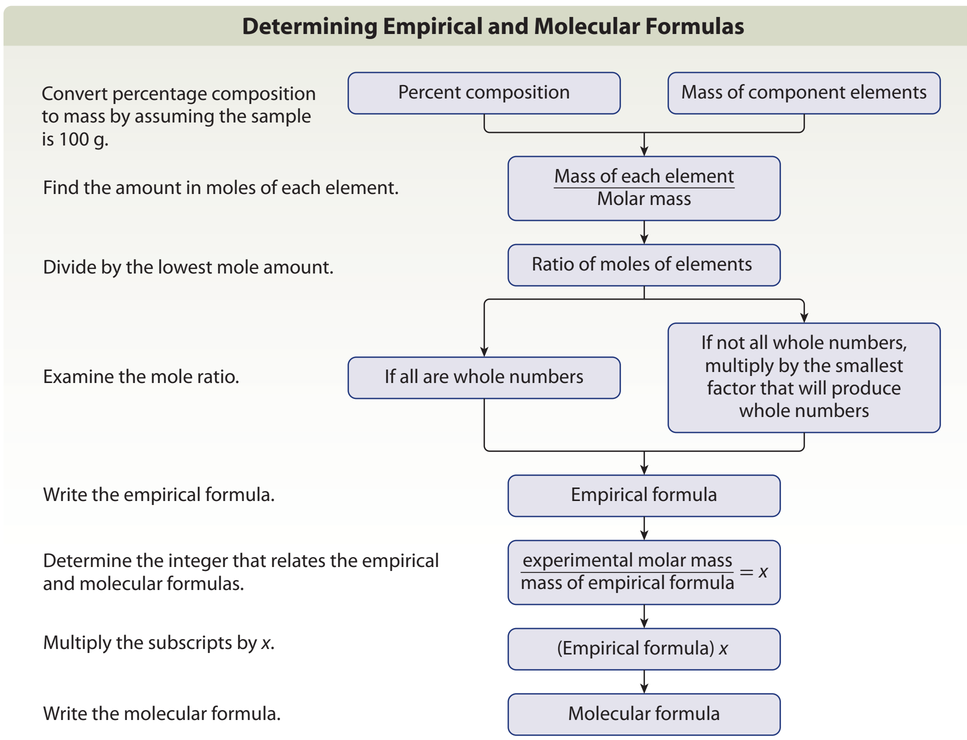


Figure 6.10 Use this flowchart as a guide to help you determine the empirical and molecular formulas for compounds.

Describe *How is the integer x related to the empirical and molecular formulas?*

Activity 6.2 Exploring Formulas Using Models

This activity will give you the opportunity to explore relationships between empirical and molecular formulas by building molecular models.

Materials

- molecular modelling kit
- reference sources

Procedure

1. Construct a table to record the names, molecular formulas, empirical formulas, and molar masses of ethylene, butane, and cyclohexane.
2. Research to find the molecular structure for ethylene, butane, and cyclohexane. Then build each molecule using the molecular modelling kit.
3. Examine each molecule you built. Record its molecular formula and empirical formula in your table.
4. Calculate and record the molar mass of each compound.

Questions

1. Compare and contrast the three molecules, based on their molecular and empirical formulas.
2. What is the relationship between the actual molar mass value of each molecule and the molar mass calculated for its empirical formula?

Hydrates and Their Chemical Formulas

A *hydrate* is a compound that has a specific number of water molecules bound to each formula unit. Often, when a crystal forms from a water solution, water molecules are trapped in the crystal in a specific arrangement. An example is the calcium sulfate, $CaSO_4(s)$, in gypsum, the white powder that is used to make drywall. When gypsum crystals form, as shown in **Figure 6.11**, each formula unit of calcium sulfate incorporates two water molecules into its structure. The chemical formula for gypsum is represented as $CaSO_4•2H_2O(s)$. This formula means that there are two water molecules for every formula unit of calcium sulfate.

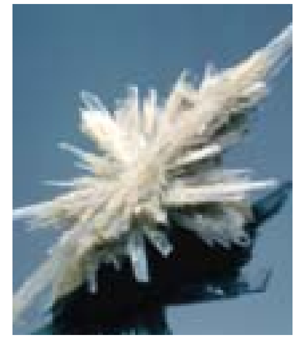


Figure 6.11 Gypsum crystals form when each formula unit of calcium sulfate incorporates two water molecules. Gypsum is a mineral that is used for making drywall and plaster of Paris.

Using Hydrates and Anhydrous Compounds

When chemists work with ionic compounds in the solid state, they need to know whether these compounds are hydrates or anhydrous compounds (without water molecules). The water molecules in the crystal structure of a hydrated ionic compound usually do not interfere with the chemical activity of the compound. However, the water molecules are part of the crystal structure and, therefore, add mass to the solid.

For example, consider a 1 g sample of magnesium sulfate heptahydrate, $MgSO_4•7H_2O(s)$, and a 1 g sample of anhydrous magnesium sulfate, $MgSO_4(s)$. Which sample do you think contains more magnesium atoms? If your answer is the anhydrous form, you are correct. The 1 g sample of the hydrate contains seven moles of water for every mole of magnesium sulfate. The anhydrous form, on the other hand, does not contain any water molecules, so there is more magnesium sulfate in the sample. As a result, there is more magnesium in the 1 g sample of the anhydrous form than in the 1 g sample of the hydrate.

Analyzing Hydrates

What analytical methods do chemists use to determine how many water molecules are attached to each formula unit in a hydrate? The simplest method is to convert the hydrated form of the compound to the anhydrous form by heating it and driving off the water molecules. The difference between the initial mass of the sample (the hydrate) and the final mass of the sample (the anhydrous form) is the mass of the water. As the Sample Problem on the following page shows, this is enough information for a chemist to determine both the percent by mass of water in a hydrate and the chemical formula for the hydrate.

Suggested Investigation

Inquiry Investigation 6-C, Determining the Chemical Formula for a Hydrate

Learning Check

13. Compare and contrast empirical and molecular formulas.

14. List the steps required to determine the empirical formula from mass data.

15. How is the molar mass usually determined for an unknown compound when you are trying to determine its empirical formula?

16. Explain the difference between a hydrate and the anhydrous form.

17. Why is it important for chemists to know if they are using a hydrate or the anhydrous form when they are performing investigations?

18. How can you determine the mass of water in a hydrate?

Sample Problem

Determining the Formula for a Hydrate

Problem

A 50.0 g sample of barium hydroxide, $Ba(OH)_2 \cdot xH_2O(s)$ contains 27.2 g of $Ba(OH)_2(s)$. Calculate the percent by mass of water in $Ba(OH)_2 \cdot xH_2O(s)$, and find the value of x.

What Is Required?

You need to calculate the percent by mass of water in the hydrate of barium hydroxide.
You need to determine how many water molecules are bonded to each formula unit of $Ba(OH)_2(s)$ to form the hydrate.

What Is Given?

You know the formula for the sample: $Ba(OH)_2 \cdot xH_2O(s)$.
You know the mass of the sample: 50.0 g
You know the mass of the $Ba(OH)_2(s)$ in the sample: 27.2 g

Plan Your Strategy	Act on Your Strategy
Find the mass of the water in the hydrate by finding the difference between the mass of the barium hydroxide and the total mass of the sample. Divide by the total mass of the sample, and multiply by 100%.	percent by mass of water in $Ba(OH)_2 \cdot xH_2O$ $= \frac{(\text{total mass of sample}) - (\text{mass of } Ba(OH)_2 \text{ in sample})}{\text{total mass of sample}} \times 100\%$ $= \frac{50.0\cancel{g} - 27.2\cancel{g}}{50.0\cancel{g}} \times 100\% = 45.6\%$
Find the amout in moles of barium hydroxide in the sample. Then find the amout in 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 amout in moles of barium hydroxide.	$n_{Ba(OH)_2} = \frac{m_{Ba(OH)_2}}{M_{Ba(OH)_2}} = \frac{27.2\cancel{g}}{171.35\cancel{g}} = 0.159 \text{ mol } Ba(OH)_2$ $n_{H_2O} = \frac{50.5\cancel{g} - 27.2\cancel{g}}{18.02\cancel{g}/\text{mol}} = 1.27 \text{ mol } H_2O$ $\frac{1.27 \text{ mol } H_2O}{0.129 \text{ mol } Ba(OH)_2} = \frac{8 \text{ mol } H_2O}{1 \text{ mol } Ba(OH)_2}$ Therefore, the formula for the hydrate is $Ba(OH)_2 \cdot 8H_2O(s)$.

Check Your Solution

The percent by mass of water in $Ba(OH)_2 \cdot 8H_2O(s)$ is $\frac{144.16 \cancel{\text{g/mol}}}{315.51 \cancel{\text{g/mol}}} \times 100\% = 45.691\%$

Using the given mass data, the percent by mass of water in the hydrate of $Ba(OH)_2(s)$ is

$$\frac{(50\cancel{g} - 27.2\cancel{g}/\text{mol})}{50.\cancel{0}\text{ g}} \times 100\% = 45.6\%.$$

The answer is reasonable.

Practice Problems

For the compounds in questions 61 to 64, calculate the percent by mass of water.

51. $MgSO_3 \cdot 6H_2O(s)$

52. $LiCl_2 \cdot 4H_2O(s)$

53. $Ca(SO_4)_2 \cdot 2H_2O(s)$

54. $Na_2CO_3 \cdot 10H_2O(s)$

55. List the following hydrates in order, from greatest to least percent by mass of water: $CaCl_2 \cdot 2H_2O(s)$, $MgSO_4 \cdot 7H_2O(s)$, $Ba(OH)_2 \cdot 8H_2O(s)$, $Mn(SO_4)_2 \cdot 2H_2O(s)$.

56. A 3.34 g sample of a hydrate, $SrS_2O_3 \cdot xH_2O(s)$, contains 2.30 g of $SrS_2O_3(s)$. Find the value of x.

57. A hydrate of zinc chlorate, $Zn(ClO_3)_2 \cdot xH_2O(s)$, contains 21.5% zinc by mass. Find the value of x.

58. Determine the formula for the hydrate of chromium(III) nitrate that is 40.50% water by mass.

59. The mass of a sample of a hydrate of magnesium iodide is 1.628 g. It is heated until it is anhydrous and its mass is 1.072 g. Determine the formula for the hydrate.

60. A chemist needs 1.28 g of sodium hypochlorite, $NaOCl(s)$, for an experiment, but she only has sodium hypochlorite pentahydrate, $NaOCl \cdot 5H_2O(s)$. How many grams of the hydrate should she use?

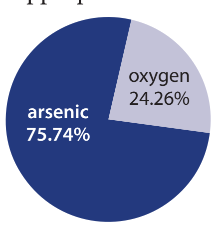
Section 6.2 REVIEW

Section Summary

- The empirical formula shows only the relative amounts of the elements, not the actual amounts.
- The molecular formula for a compound shows the actual number of each type of atom in the compound.
- The molecular formula is a whole-number multiple of the empirical formula. It can be determined from the empirical formula and molar mass of the compound or from the percentage composition and molar mass of the compound.
- The water content of a hydrate can be determined by measuring the mass of a sample before and after heating.
- Chemists need to know whether an ionic substance is a hydrate or in an anhydrous form in order to use the correct molecular formula in a calculation.

Review Questions

1. K/U Explain why you do not need to know the actual mass of a substance when you are determining the empirical formula for the substance from its percentage composition.
2. K/U Most analytical instruments require a very small sample of a substance—much smaller than 100 g—to determine the composition of the substance. Why is 100 g the most convenient mass to use when determining the empirical formula?
3. T/I Determine the empirical formula for a compound that contains 78.77% tin and 21.23% oxygen.
4. T/I Determine the empirical formula for a compound that contains 20.24% aluminum and 79.76% chlorine.
5. T/I Determine the empirical formula for a compound that is 24.74 % K, 34.76 % Mn, and the rest O.
6. T/I Determine the empirical formula for the compound that is represented by this pie graph, and give the graph an appropriate title.



7. T/I A compound that contains 22.35 g of lead and 7.65 g of chlorine has a molar mass of 278.11 g/mol. What is its empirical formula?
8. C Draw a Venn diagram to show the similarities and differences between the empirical formula and the molecular formula for a compound. Provide an example of a compound to show the differences.
9. T/I Turquoise, $CuAl_6(PO_4)_4(OH)_8{\cdot}5H_2O(s)$, is one of the most valuable non-transparent gemstones. It is made from a hydrate of copper aluminum phosphate. What percent by mass is the anhydrous form of the mineral?
10. T/I The formula for a hydrate of zinc sulfate is $ZnSO_4{\cdot}xH_2O(s)$. If 1 mol of anhydrous zinc sulfate is 56.14% of the mass of 1 mol of the hydrate, what is the value of x?
11. T/I Ikaite, $CaCO_3{\cdot}xH_2O(s)$, is a hydrate of a calcium carbonate that is found in stalagmites and stalactites, the limestone pillar formations that often form in underground caves. If 1 mol of anhydrous calcium carbonate is 48.08% of the mass of ikaite, what is the value of x?
12. A Imagine that you are a lawyer and you are representing an Olympic athlete who has been charged with taking anabolic steroids. The prosecutor presents, as forensic evidence, the empirical formula for the banned substance that was found in the athlete's urine sample. How might you deal with this evidence as the lawyer for the defence?
13. T/I Tetrafluoroethene, $C_2F_4(g)$, is the monomer found in the polymer polytetrafluorethene, more commonly known as Teflon™. Teflon™ is used as a coating on frying pans and other cookware.
    a. What is the empirical formula for Teflon™?
    b. How does the molar mass of Teflon™ compare with the molar mass of its empirical formula?
14. T/I EDTA, which is short for ethylenediaminetetraacetic acid, is a chemical used in the textile industry to prevent metal impurities from changing the colours of dyed products. The empirical formula for EDTA is $C_5H_8NO_4$. The molar mass of EDTA is 292.24 g/mol. What is its molecular formula?
15. T/I Acetone is an organic solvent that can mix with water and most organic solvents. Its empirical formula is C_3H_6O. Its molar mass is 58.08 g/mol. What is its molecular formula?
16. T/I An organic fuel has the empirical formula C_4H_4O. The molar mass of the fuel is 384.26 g/mol. What is the molecular formula for the fuel?