## Chapter 3

## Composition of Substances and Solutions



Figure 3.1 The water in a swimming pool is a complex mixture of substances whose relative amounts must be carefully maintained to ensure the health and comfort of people using the pool. (credit: modification of work by Vic Brincat)

## Chapter Outline

3.1 Formula Mass and the Mole Concept<br>3.2 Determining Empirical and Molecular Formulas<br>3.3 Molarity<br>3.4 Other Units for Solution Concentrations

## Introduction

Swimming pools have long been a popular means of recreation, exercise, and physical therapy. Since it is impractical to refill large pools with fresh water on a frequent basis, pool water is regularly treated with chemicals to prevent the growth of harmful bacteria and algae. Proper pool maintenance requires regular additions of various chemical compounds in carefully measured amounts. For example, the relative amount of calcium ion, $\mathrm{Ca}^{2+}$, in the water should be maintained within certain limits to prevent eye irritation and avoid damage to the pool bed and plumbing. To maintain proper calcium levels, calcium cations are added to the water in the form of an ionic compound that also contains anions; thus, it is necessary to know both the relative amount of $\mathrm{Ca}^{2+}$ in the compound and the volume of water in the pool in order to achieve the proper calcium level. Quantitative aspects of the composition of substances (such as the calcium-containing compound) and mixtures (such as the pool water) are the subject of this chapter.

### 3.1 Formula Mass and the Mole Concept

By the end of this section, you will be able to:

- Calculate formula masses for covalent and ionic compounds
- Define the amount unit mole and the related quantity Avogadro's number Explain the relation between mass, moles, and numbers of atoms or molecules, and perform calculations deriving these quantities from one another

We can argue that modern chemical science began when scientists started exploring the quantitative as well as the qualitative aspects of chemistry. For example, Dalton's atomic theory was an attempt to explain the results of measurements that allowed him to calculate the relative masses of elements combined in various compounds. Understanding the relationship between the masses of atoms and the chemical formulas of compounds allows us to quantitatively describe the composition of substances.

## Formula Mass

In an earlier chapter, we described the development of the atomic mass unit, the concept of average atomic masses, and the use of chemical formulas to represent the elemental makeup of substances. These ideas can be extended to calculate the formula mass of a substance by summing the average atomic masses of all the atoms represented in the substance's formula.

## Formula Mass for Covalent Substances

For covalent substances, the formula represents the numbers and types of atoms composing a single molecule of the substance; therefore, the formula mass may be correctly referred to as a molecular mass. Consider chloroform $\left(\mathrm{CHCl}_{3}\right)$, a covalent compound once used as a surgical anesthetic and now primarily used in the production of the "anti-stick" polymer, Teflon. The molecular formula of chloroform indicates that a single molecule contains one carbon atom, one hydrogen atom, and three chlorine atoms. The average molecular mass of a chloroform molecule is therefore equal to the sum of the average atomic masses of these atoms. Figure 3.2 outlines the calculations used to derive the molecular mass of chloroform, which is 119.37 amu .

| Element | Quantity |  | Average atomic <br> mass (amu) | Subtotal <br> (amu) |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| C | 1 | $\times$ | 12.01 | $=$ | 12.01 |
| H | 1 | $\times$ | 1.008 | $=$ | 1.008 |
| Cl | 3 | $\times$ | 35.45 | $=$ | 106.35 |
| Molecular mass |  |  |  |  | 119.37 |

Figure 3.2 The average mass of a chloroform molecule, $\mathrm{CHCl}_{3}$, is 119.37 amu , which is the sum of the average atomic masses of each of its constituent atoms. The model shows the molecular structure of chloroform.

Likewise, the molecular mass of an aspirin molecule, $\mathrm{C}_{9} \mathrm{H}_{8} \mathrm{O}_{4}$, is the sum of the atomic masses of nine carbon atoms, eight hydrogen atoms, and four oxygen atoms, which amounts to 180.15 amu (Figure 3.3).

| Element | Quantity | Average atomic <br> mass (amu) | Subtotal <br> $(\mathbf{a m u})$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| C | 9 | $\times$ | 12.01 | $=$ | 108.09 |
| H | 8 | $\times$ | 1.008 | $=$ | 8.064 |
| O | 4 | $\times$ | 16.00 | $=$ | 64.00 |
| Molecular mass |  |  |  |  | 180.15 |

Figure 3.3 The average mass of an aspirin molecule is 180.15 amu . The model shows the molecular structure of aspirin, $\mathrm{C}_{9} \mathrm{H}_{8} \mathrm{O}_{4}$.

## Example 3.1

## Computing Molecular Mass for a Covalent Compound

Ibuprofen, $\mathrm{C}_{13} \mathrm{H}_{18} \mathrm{O}_{2}$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Advil and Motrin. What is the molecular mass (amu) for this compound?

## Solution

Molecules of this compound are comprised of 13 carbon atoms, 18 hydrogen atoms, and 2 oxygen atoms. Following the approach described above, the average molecular mass for this compound is therefore:

| Element | Quantity | Average atomic <br> mass (amu) | Subtotal <br> $(\mathbf{a m u})$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| C | 13 | $\times$ | 12.01 | $=$ | 156.13 |
| H | 18 | $\times$ | 1.008 | $=$ | 18.114 |
| O | 2 | $\times$ | 16.00 | $=$ | 32.00 |
| Molecular mass |  |  |  |  | 206.27 |

## Check Your Learning

Acetaminophen, $\mathrm{C}_{8} \mathrm{H}_{9} \mathrm{NO}_{2}$, is a covalent compound and the active ingredient in several popular nonprescription pain medications, such as Tylenol. What is the molecular mass (amu) for this compound?

Answer: 151.16 amu

## Formula Mass for Ionic Compounds

Ionic compounds are composed of discrete cations and anions combined in ratios to yield electrically neutral bulk matter. The formula mass for an ionic compound is calculated in the same way as the formula mass for covalent compounds: by summing the average atomic masses of all the atoms in the compound's formula. Keep in mind, however, that the formula for an ionic compound does not represent the composition of a discrete molecule, so it may not correctly be referred to as the "molecular mass."

As an example, consider sodium chloride, NaCl , the chemical name for common table salt. Sodium chloride is an ionic compound composed of sodium cations, $\mathrm{Na}^{+}$, and chloride anions, $\mathrm{Cl}^{-}$, combined in a 1:1 ratio. The formula mass for this compound is computed as 58.44 amu (see Figure 3.4).

| Element | Quantity |  | Average atomic <br> mass (amu) | Subtotal |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Na | 1 | $\times$ | 22.99 | $=$ | 22.99 |
| Cl | 1 | $\times$ | 35.45 | $=$ | 35.45 |
|  |  |  |  |  |  |
| Formula mass |  |  |  |  | 58.44 |

Figure 3.4 Table salt, NaCl , contains an array of sodium and chloride ions combined in a 1:1 ratio. Its formula mass is 58.44 amu .

Note that the average masses of neutral sodium and chlorine atoms were used in this computation, rather than the masses for sodium cations and chlorine anions. This approach is perfectly acceptable when computing the formula mass of an ionic compound. Even though a sodium cation has a slightly smaller mass than a sodium atom (since it is missing an electron), this difference will be offset by the fact that a chloride anion is slightly more massive than a chloride atom (due to the extra electron). Moreover, the mass of an electron is negligibly small with respect to the mass of a typical atom. Even when calculating the mass of an isolated ion, the missing or additional electrons can generally be ignored, since their contribution to the overall mass is negligible, reflected only in the nonsignificant digits that will be lost when the computed mass is properly rounded. The few exceptions to this guideline are very light ions derived from elements with precisely known atomic masses.

## Example 3.2

## Computing Formula Mass for an Ionic Compound

Aluminum sulfate, $\mathrm{Al}_{2}\left(\mathrm{SO}_{4}\right)_{3}$, is an ionic compound that is used in the manufacture of paper and in various water purification processes. What is the formula mass (amu) of this compound?

## Solution

The formula for this compound indicates it contains $\mathrm{Al}^{3+}$ and $\mathrm{SO}_{4}{ }^{2-}$ ions combined in a $2: 3$ ratio. For purposes of computing a formula mass, it is helpful to rewrite the formula in the simpler format, $\mathrm{Al}_{2} \mathrm{~S}_{3} \mathrm{O}_{12}$. Following the approach outlined above, the formula mass for this compound is calculated as follows:

| Element | Quantity | Average atomic <br> mass (amu) | Subtotal <br> $(\mathbf{a m u})$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Al | 2 | $\times$ | 26.98 | $=$ | 53.96 |
| S | 3 | $\times$ | 32.06 | $=$ | 96.18 |
| O | 12 | $\times$ | 16.00 | 192.00 |  |
| Molecular mass |  |  |  |  | 342.14 |

## Check Your Learning

Calcium phosphate, $\mathrm{Ca} 3\left(\mathrm{PO}_{4}\right)_{2}$, is an ionic compound and a common anti-caking agent added to food products. What is the formula mass (amu) of calcium phosphate?

Answer: 310.18 amu

## The Mole

The identity of a substance is defined not only by the types of atoms or ions it contains, but by the quantity of each type of atom or ion. For example, water, $\mathrm{H}_{2} \mathrm{O}$, and hydrogen peroxide, $\mathrm{H}_{2} \mathrm{O}_{2}$, are alike in that their respective molecules are composed of hydrogen and oxygen atoms. However, because a hydrogen peroxide molecule contains two oxygen atoms, as opposed to the water molecule, which has only one, the two substances exhibit very different properties. Today, we possess sophisticated instruments that allow the direct measurement of these defining microscopic traits; however, the same traits were originally derived from the measurement of macroscopic properties (the masses and volumes of bulk quantities of matter) using relatively simple tools (balances and volumetric glassware). This experimental approach required the introduction of a new unit for amount of substances, the mole, which remains indispensable in modern chemical science.

The mole is an amount unit similar to familiar units like pair, dozen, gross, etc. It provides a specific measure of the number of atoms or molecules in a bulk sample of matter. A mole is defined as the amount of substance containing the same number of discrete entities (such as atoms, molecules, and ions) as the number of atoms in a sample of pure ${ }^{12} \mathrm{C}$ weighing exactly 12 g . One Latin connotation for the word "mole" is "large mass" or "bulk," which is consistent with its use as the name for this unit. The mole provides a link between an easily measured macroscopic property, bulk mass, and an extremely important fundamental property, number of atoms, molecules, and so forth.

The number of entities composing a mole has been experimentally determined to be $6.02214179 \times 10^{23}$, a fundamental constant named Avogadro's number ( $\mathbf{N}_{\mathbf{A}}$ ) or the Avogadro constant in honor of Italian scientist Amedeo Avogadro. This constant is properly reported with an explicit unit of "per mole," a conveniently rounded version being $6.022 \times 10^{23} / \mathrm{mol}$.

Consistent with its definition as an amount unit, 1 mole of any element contains the same number of atoms as 1 mole of any other element. The masses of 1 mole of different elements, however, are different, since the masses of the individual atoms are drastically different. The molar mass of an element (or compound) is the mass in grams of 1 mole of that substance, a property expressed in units of grams per mole (g/mol) (see Figure 3.5).


Figure 3.5 Each sample contains $6.022 \times 10^{23}$ atoms -1.00 mol of atoms. From left to right (top row): 65.4 g zinc, 12.0 g carbon, 24.3 g magnesium, and 63.5 g copper. From left to right (bottom row): 32.1 g sulfur, 28.1 g silicon, 207 g lead, and 118.7 g tin. (credit: modification of work by Mark Ott)

Because the definitions of both the mole and the atomic mass unit are based on the same reference substance, ${ }^{12} \mathrm{C}$, the molar mass of any substance is numerically equivalent to its atomic or formula weight in amu. Per the amu definition, a single ${ }^{12} \mathrm{C}$ atom weighs 12 amu (its atomic mass is 12 amu ). According to the definition of the mole, 12 g of ${ }^{12} \mathrm{C}$ contains 1 mole of ${ }^{12} \mathrm{C}$ atoms (its molar mass is $12 \mathrm{~g} / \mathrm{mol}$ ). This relationship holds for all elements, since their atomic masses are measured relative to that of the amu-reference substance, ${ }^{12}$. Extending this principle, the molar mass of a compound in grams is likewise numerically equivalent to its formula mass in amu (Figure 3.6).


Figure 3.6 Each sample contains $6.02 \times 10^{23}$ molecules or formula units-1.00 mol of the compound or element. Clock-wise from the upper left: 130.2 g of $\mathrm{C}_{8} \mathrm{H}_{17} \mathrm{OH}$ (1-octanol, formula mass 130.2 amu ), 454.9 g of Hgl2 (mercury(II) iodide, formula mass 459.9 amu ), 32.0 g of $\mathrm{CH}_{3} \mathrm{OH}$ (methanol, formula mass 32.0 amu ) and 256.5 g of S8 (sulfur, formula mass 256.6 amu ). (credit: Sahar Atwa)

| Element | Average Atomic Mass (amu) | Molar Mass (g/mol) | Atoms/Mole |
| :---: | :---: | :---: | :---: |
| C | 12.01 | 12.01 | $6.022 \times 10^{23}$ |
| H | 1.008 | 1.008 | $6.022 \times 10^{23}$ |
| O | 16.00 | 16.00 | $6.022 \times 10^{23}$ |
| Na | 22.99 | 22.99 | $6.022 \times 10^{23}$ |
| Cl | 33.45 | 33.45 | $6.022 \times 10^{23}$ |

While atomic mass and molar mass are numerically equivalent, keep in mind that they are vastly different in terms of scale, as represented by the vast difference in the magnitudes of their respective units (amu versus g). To appreciate the enormity of the mole, consider a small drop of water weighing about 0.03 g (see Figure 3.7). Although this represents just a tiny fraction of 1 mole of water ( $\sim 18 \mathrm{~g}$ ), it contains more water molecules than can be clearly imagined. If the molecules were distributed equally among the roughly seven billion people on earth, each person would receive more than 100 billion molecules.


Figure 3.7 The number of molecules in a single droplet of water is roughly 100 billion times greater than the number of people on earth. (credit: "tanakawho"/Wikimedia commons)

## Link to Learning



The mole is used in chemistry to represent $6.022 \times 10^{23}$ of something, but it can be difficult to conceptualize such a large number. Watch this video (http://openstaxcollege.org/I/16molevideo) and then complete the "Think" questions that follow. Explore more about the mole by reviewing the information under "Dig Deeper."

The relationships between formula mass, the mole, and Avogadro's number can be applied to compute various quantities that describe the composition of substances and compounds. For example, if we know the mass and chemical composition of a substance, we can determine the number of moles and calculate number of atoms or molecules in the sample. Likewise, if we know the number of moles of a substance, we can derive the number of atoms or molecules and calculate the substance's mass.

## Example 3.3

## Deriving Moles from Grams for an Element

According to nutritional guidelines from the US Department of Agriculture, the estimated average requirement for dietary potassium is 4.7 g . What is the estimated average requirement of potassium in moles?

## Solution

The mass of K is provided, and the corresponding amount of K in moles is requested. Referring to the periodic table, the atomic mass of K is 39.10 amu , and so its molar mass is $39.10 \mathrm{~g} / \mathrm{mol}$. The given mass of
$\mathrm{K}(4.7 \mathrm{~g})$ is a bit more than one-tenth the molar mass ( 39.10 g ), so a reasonable "ballpark" estimate of the number of moles would be slightly greater than 0.1 mol .

The molar amount of a substance may be calculated by dividing its mass (g) by its molar mass (g/mol):


The factor-label method supports this mathematical approach since the unit " g " cancels and the answer has units of "mol:"

$$
4.7 \frac{\mathrm{~g}}{\mathrm{~g}}\left(\frac{\mathrm{~mol} \mathrm{~K}}{39.10 \frac{\mathrm{~g}}{8}}\right)=0.12 \mathrm{~mol} \mathrm{~K}
$$

The calculated magnitude ( 0.12 mol K ) is consistent with our ballpark expectation, since it is a bit greater than 0.1 mol.

## Check Your Learning

Beryllium is a light metal used to fabricate transparent X-ray windows for medical imaging instruments. How many moles of Be are in a thin-foil window weighing 3.24 g ?

Answer: 0.360 mol

## Example 3.4

## Deriving Grams from Moles for an Element

A liter of air contains $9.2 \times 10^{-4} \mathrm{~mol}$ argon. What is the mass of Ar in a liter of air?

## Solution

The molar amount of Ar is provided and must be used to derive the corresponding mass in grams. Since the amount of Ar is less than 1 mole, the mass will be less than the mass of 1 mole of Ar , approximately 40 g . The molar amount in question is approximately one-one thousandth $\left(\sim 10^{-3}\right)$ of a mole, and so the corresponding mass should be roughly one-one thousandth of the molar mass ( $\sim 0.04 \mathrm{~g}$ ):


In this case, logic dictates (and the factor-label method supports) multiplying the provided amount (mol) by the molar mass ( $\mathrm{g} / \mathrm{mol}$ ):

$$
9.2 \times 10^{-4} \operatorname{Ar}\left(\frac{39.95 \mathrm{~g}}{\mathrm{mot} \mathrm{Ar}}\right)=0.037 \mathrm{~g} \mathrm{Ar}
$$

The result is in agreement with our expectations, around 0.04 g Ar .

## Check Your Learning

What is the mass of 2.561 mol of gold?
Answer: 504.4 g

## Example 3.5

## Deriving Number of Atoms from Mass for an Element

Copper is commonly used to fabricate electrical wire (Figure 3.8). How many copper atoms are in 5.00 g of copper wire?


Figure 3.8 Copper wire is composed of many, many atoms of Cu. (credit: Emilian Robert Vicol)

## Solution

The number of Cu atoms in the wire may be conveniently derived from its mass by a two-step computation: first calculating the molar amount of Cu , and then using Avogadro's number ( $N_{A}$ ) to convert this molar amount to number of Cu atoms:


Considering that the provided sample mass $(5.00 \mathrm{~g})$ is a little less than one-tenth the mass of 1 mole of Cu ( $\sim 64 \mathrm{~g}$ ), a reasonable estimate for the number of atoms in the sample would be on the order of one-tenth $N_{A}$, or approximately $10^{22} \mathrm{Cu}$ atoms. Carrying out the two-step computation yields:

$$
5.00 \frac{\mathrm{~g}}{8} \mathrm{Cu}\left(\frac{\operatorname{mot~Cu}}{63.55 \frac{9}{8}}\right)\left(\frac{6.022 \times 10^{23} \text { atoms }}{\text { mot }}\right)=4.74 \times 10^{22} \text { atoms of copper }
$$

The factor-label method yields the desired cancellation of units, and the computed result is on the order of $10^{22}$ as expected.

## Check Your Learning

A prospector panning for gold in a river collects 15.00 g of pure gold. How many Au atoms are in this quantity of gold?

Answer: $4.586 \times 10^{22} \mathrm{Au}$ atoms

## Example 3.6

## Deriving Moles from Grams for a Compound

Our bodies synthesize protein from amino acids. One of these amino acids is glycine, which has the molecular formula $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{O}_{2} \mathrm{~N}$. How many moles of glycine molecules are contained in 28.35 g of glycine?

## Solution

We can derive the number of moles of a compound from its mass following the same procedure we used for an element in Example 3.3:

| Mass of <br> $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{O}_{2} \mathrm{~N}(\mathrm{~g})$ | Divide by molar <br> mass (g/mol) |
| :--- | :--- | | Moles of |
| :--- |
| $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{O}_{2} \mathrm{~N}(\mathrm{~mol})$ |

The molar mass of glycine is required for this calculation, and it is computed in the same fashion as its molecular mass. One mole of glycine, $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{O}_{2} \mathrm{~N}$, contains 2 moles of carbon, 5 moles of hydrogen, 2 moles of oxygen, and 1 mole of nitrogen:

| Element | Quantity <br> (mol element/ <br> mol compound) | Molar mass <br> (g/mol element) | Subtotal <br> (g/mol compound) |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| C | 2 | $\times$ | 12.01 | $=$ | 24.02 |
| H | 5 | $\times$ | 1.008 | $=$ | 5.040 |
| O | 2 | $\times$ | 16.00 | $=$ | 32.00 |
| N | 1 | $\times$ | 14.007 | $=$ | 14.007 |
| Molecular mass (g/mol compound) |  |  |  |  | 75.07 |

The provided mass of glycine ( $\sim 28 \mathrm{~g}$ ) is a bit more than one-third the molar mass ( $\sim 75 \mathrm{~g} / \mathrm{mol}$ ), so we would expect the computed result to be a bit greater than one-third of a mole ( $\sim 0.33 \mathrm{~mol}$ ). Dividing the compound's mass by its molar mass yields:

$$
28.35 \frac{\mathrm{~g}}{8} \text { glycine }\left(\frac{\text { mol glycine }}{75.07 \frac{\mathrm{~g}}{8}}\right)=0.378 \mathrm{~mol} \text { glycine }
$$

This result is consistent with our rough estimate.

## Check Your Learning

How many moles of sucrose, $\mathrm{C}_{12} \mathrm{H}_{22} \mathrm{O}_{11}$, are in a 25 -g sample of sucrose?
Answer: 0.073 mol

## Example 3.7

## Deriving Grams from Moles for a Compound

Vitamin C is a covalent compound with the molecular formula $\mathrm{C}_{6} \mathrm{H}_{8} \mathrm{O}_{6}$. The recommended daily dietary allowance of vitamin $C$ for children aged 4-8 years is $1.42 \times 10^{-4} \mathrm{~mol}$. What is the mass of this allowance in grams?

## Solution

As for elements, the mass of a compound can be derived from its molar amount as shown:


The molar mass for this compound is computed to be $176.124 \mathrm{~g} / \mathrm{mol}$. The given number of moles is a very small fraction of a mole ( $\sim 10^{-4}$ or one-ten thousandth); therefore, we would expect the corresponding mass to be about one-ten thousandth of the molar mass $(\sim 0.02 \mathrm{~g})$. Performing the calculation, we get:

$$
1.42 \times 10^{-4} \text { vitamin } C\left(\frac{176.124 \mathrm{~g}}{\text { vitamin C }}\right)=0.0250 \mathrm{~g} \text { vitamin } \mathrm{C}
$$

This is consistent with the anticipated result.

## Check Your Learning

What is the mass of 0.443 mol of hydrazine, $\mathrm{N}_{2} \mathrm{H}_{4}$ ?
Answer: 14.2 g

## Example 3.8

## Deriving the Number of Atoms and Molecules from the Mass of a Compound

A packet of an artificial sweetener contains 40.0 mg of saccharin $\left(\mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S}\right)$, which has the structural formula:


Given that saccharin has a molar mass of $183.18 \mathrm{~g} / \mathrm{mol}$, how many saccharin molecules are in a $40.0-\mathrm{mg}$ ( $0.0400-\mathrm{g}$ ) sample of saccharin? How many carbon atoms are in the same sample?

## Solution

The number of molecules in a given mass of compound is computed by first deriving the number of moles, as demonstrated in Example 3.6, and then multiplying by Avogadro's number:


Using the provided mass and molar mass for saccharin yields:

$$
\begin{aligned}
& 0.0400 \text { \& } \mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S}\left(\frac{\mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S}}{\left.183.18 \frac{\mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S}}{}\right)\left(\frac{6.022 \times 10^{23} \mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S} \text { molecules }}{1 . \mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S}}\right)}\right. \\
& =1.31 \times 10^{20} \mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S} \text { molecules }
\end{aligned}
$$

The compound's formula shows that each molecule contains seven carbon atoms, and so the number of C atoms in the provided sample is:

$$
1.31 \times 10^{20} \mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S} \text { molecules }\left(\frac{7 \mathrm{C} \text { atoms }}{1 \mathrm{C}_{7} \mathrm{H}_{5} \mathrm{NO}_{3} \mathrm{~S} \text { molecule }}\right)=9.20 \times 10^{21} \mathrm{C} \text { atoms }
$$

## Check Your Learning

How many $\mathrm{C}_{4} \mathrm{H}_{10}$ molecules are contained in 9.213 g of this compound? How many hydrogen atoms?
Answer: $9.545 \times 10^{22}$ molecules $\mathrm{C}_{4} \mathrm{H}_{10} ; 9.545 \times 10^{23}$ atoms H

## How Sciences Interconnect

## Counting Neurotransmitter Molecules in the Brain

The brain is the control center of the central nervous system (Figure 3.9). It sends and receives signals to and from muscles and other internal organs to monitor and control their functions; it processes stimuli detected by sensory organs to guide interactions with the external world; and it houses the complex physiological processes that give rise to our intellect and emotions. The broad field of neuroscience spans all aspects of the structure and function of the central nervous system, including research on the anatomy and physiology of the brain. Great progress has been made in brain research over the past few decades, and the BRAIN Initiative, a federal initiative announced in 2013, aims to accelerate and capitalize on these advances through the concerted efforts of various industrial, academic, and government agencies (more details available at www.whitehouse.gov/share/brain-initiative).


Figure 3.9 (a) A typical human brain weighs about 1.5 kg and occupies a volume of roughly 1.1 L . (b) Information is transmitted in brain tissue and throughout the central nervous system by specialized cells called neurons (micrograph shows cells at 1600× magnification).

Specialized cells called neurons transmit information between different parts of the central nervous system by way of electrical and chemical signals. Chemical signaling occurs at the interface between different neurons when one of the cells releases molecules (called neurotransmitters) that diffuse across the small gap between the cells (called the synapse) and bind to the surface of the other cell. These neurotransmitter molecules are stored in small intracellular structures called vesicles that fuse to the cell wall and then break open to release their contents when the neuron is appropriately stimulated. This process is called exocytosis (see Figure 3.10).

One neurotransmitter that has been very extensively studied is dopamine, $\mathrm{C}_{8} \mathrm{H}_{11} \mathrm{NO}_{2}$. Dopamine is involved in various neurological processes that impact a wide variety of human behaviors. Dysfunctions in the dopamine systems of the brain underlie serious neurological diseases such as Parkinson's and schizophrenia.


Figure 3.10 (a) Chemical signals are transmitted from neurons to other cells by the release of neurotransmitter molecules into the small gaps (synapses) between the cells. (b) Dopamine, $\mathrm{C}_{8} \mathrm{H}_{11} \mathrm{NO}_{2}$, is a neurotransmitter involved in a number of neurological processes.

One important aspect of the complex processes related to dopamine signaling is the number of neurotransmitter molecules released during exocytosis. Since this number is a central factor in determining neurological response (and subsequent human thought and action), it is important to know how this number changes with certain controlled stimulations, such as the administration of drugs. It is also important to understand the mechanism responsible for any changes in the number of neurotransmitter molecules released-for example, some dysfunction in exocytosis, a change in the number of vesicles in the neuron, or a change in the number of neurotransmitter molecules in each vesicle.

Significant progress has been made recently in directly measuring the number of dopamine molecules stored in individual vesicles and the amount actually released when the vesicle undergoes exocytosis. Using miniaturized probes that can selectively detect dopamine molecules in very small amounts, scientists have determined that the vesicles of a certain type of mouse brain neuron contain an average of 30,000 dopamine molecules per vesicle (about $5 \times 10^{-20} \mathrm{~mol}$ or 50 zmol ). Analysis of these neurons from mice subjected to various drug therapies shows significant changes in the average number of dopamine molecules contained in individual vesicles, increasing or decreasing by up to three-fold, depending on the specific drug used. These studies also indicate that not all of the dopamine in a given vesicle is released during exocytosis, suggesting that it may be possible to regulate the fraction released using pharmaceutical therapies. ${ }^{[1]}$

1. Omiatek, Donna M., Amanda J. Bressler, Ann-Sofie Cans, Anne M. Andrews, Michael L. Heien, and Andrew G. Ewing. "The Real Catecholamine Content of Secretory Vesicles in the CNS Revealed by Electrochemical Cytometry." Scientific Report 3 (2013): 1447, accessed January 14, 2015, doi:10.1038/srep01447.

### 3.2 Determining Empirical and Molecular Formulas

By the end of this section, you will be able to:

- Compute the percent composition of a compound
- Determine the empirical formula of a compound
- Determine the molecular formula of a compound

In the previous section, we discussed the relationship between the bulk mass of a substance and the number of atoms or molecules it contains (moles). Given the chemical formula of the substance, we were able to determine the amount of the substance (moles) from its mass, and vice versa. But what if the chemical formula of a substance is unknown? In this section, we will explore how to apply these very same principles in order to derive the chemical formulas of unknown substances from experimental mass measurements.

## Percent Composition

The elemental makeup of a compound defines its chemical identity, and chemical formulas are the most succinct way of representing this elemental makeup. When a compound's formula is unknown, measuring the mass of each of its constituent elements is often the first step in the process of determining the formula experimentally. The results of these measurements permit the calculation of the compound's percent composition, defined as the percentage by mass of each element in the compound. For example, consider a gaseous compound composed solely of carbon and hydrogen. The percent composition of this compound could be represented as follows:

$$
\begin{aligned}
& \% \mathrm{H}=\frac{\text { mass } \mathrm{H}}{\text { mass compound }} \times 100 \% \\
& \% \mathrm{C}=\frac{\text { mass } \mathrm{C}}{\text { mass compound }} \times 100 \%
\end{aligned}
$$

If analysis of a $10.0-\mathrm{g}$ sample of this gas showed it to contain 2.5 g H and 7.5 g C , the percent composition would be calculated to be $25 \% \mathrm{H}$ and $75 \% \mathrm{C}$ :

$$
\begin{aligned}
& \% \mathrm{H}=\frac{2.5 \mathrm{~g} \mathrm{H}}{10.0 \mathrm{~g} \text { compound }} \times 100 \%=25 \% \\
& \% \mathrm{C}=\frac{7.5 \mathrm{~g} \mathrm{C}}{10.0 \mathrm{~g} \text { compound }} \times 100 \%=75 \%
\end{aligned}
$$

## Example 3.9

## Calculation of Percent Composition

Analysis of a $12.04-\mathrm{g}$ sample of a liquid compound composed of carbon, hydrogen, and nitrogen showed it to contain $7.34 \mathrm{~g} \mathrm{C}, 1.85 \mathrm{~g} \mathrm{H}$, and 2.85 g N . What is the percent composition of this compound?

## Solution

To calculate percent composition, we divide the experimentally derived mass of each element by the overall mass of the compound, and then convert to a percentage:

$$
\begin{aligned}
\% \mathrm{C} & =\frac{7.34 \mathrm{~g} \mathrm{C}}{12.04 \mathrm{~g} \text { compound }} \times 100 \%=61.0 \% \\
\% \mathrm{H} & =\frac{1.85 \mathrm{~g} \mathrm{H}}{12.04 \mathrm{~g} \text { compound }} \times 100 \%=15.4 \% \\
\% \mathrm{~N} & =\frac{2.85 \mathrm{~g} \mathrm{~N}}{12.04 \mathrm{~g} \text { compound }} \times 100 \%=23.7 \%
\end{aligned}
$$

The analysis results indicate that the compound is $61.0 \% \mathrm{C}, 15.4 \% \mathrm{H}$, and $23.7 \% \mathrm{~N}$ by mass.

## Check Your Learning

A 24.81-g sample of a gaseous compound containing only carbon, oxygen, and chlorine is determined to contain $3.01 \mathrm{~g} \mathrm{C}, 4.00 \mathrm{~g} \mathrm{O}$, and 17.81 g Cl . What is this compound's percent composition?

Answer: $12.1 \% \mathrm{C}, 16.1 \% \mathrm{O}, 71.8 \% \mathrm{Cl}$

## Determining Percent Composition from Formula Mass

Percent composition is also useful for evaluating the relative abundance of a given element in different compounds of known formulas. As one example, consider the common nitrogen-containing fertilizers ammonia ( $\mathrm{NH}_{3}$ ), ammonium nitrate $\left(\mathrm{NH}_{4} \mathrm{NO}_{3}\right)$, and urea $\left(\mathrm{CH}_{4} \mathrm{~N}_{2} \mathrm{O}\right)$. The element nitrogen is the active ingredient for agricultural purposes, so the mass percentage of nitrogen in the compound is a practical and economic concern for consumers choosing among these fertilizers. For these sorts of applications, the percent composition of a compound is easily derived from its formula mass and the atomic masses of its constituent elements. A molecule of $\mathrm{NH}_{3}$ contains one N atom weighing 14.01 amu and three H atoms weighing a total of $(3 \times 1.008 \mathrm{amu})=3.024 \mathrm{amu}$. The formula mass of ammonia is therefore $(14.01 \mathrm{amu}+3.024 \mathrm{amu})=17.03 \mathrm{amu}$, and its percent composition is:

$$
\begin{aligned}
& \% \mathrm{~N}=\frac{14.01 \mathrm{amu} \mathrm{~N}}{17.03 \mathrm{amu} \mathrm{NH}} 33 \\
& \% \mathrm{H}=\frac{3.024 \mathrm{amu} \mathrm{~N}}{17.03 \mathrm{amu} \mathrm{NH}_{3} \times 100 \%=82.27 \%}=17.76 \%
\end{aligned}
$$

This same approach may be taken considering a pair of molecules, a dozen molecules, or a mole of molecules, etc. The latter amount is most convenient and would simply involve the use of molar masses instead of atomic and formula masses, as demonstrated Example 3.10. As long as we know the chemical formula of the substance in question, we can easily derive percent composition from the formula mass or molar mass.

## Example 3.10

## Determining Percent Composition from a Molecular Formula

Aspirin is a compound with the molecular formula $\mathrm{C}_{9} \mathrm{H}_{8} \mathrm{O}_{4}$. What is its percent composition?

## Solution

To calculate the percent composition, we need to know the masses of $\mathrm{C}, \mathrm{H}$, and O in a known mass of $\mathrm{C}_{9} \mathrm{H}_{8} \mathrm{O}_{4}$. It is convenient to consider 1 mol of $\mathrm{C}_{9} \mathrm{H}_{8} \mathrm{O}_{4}$ and use its molar mass ( $180.159 \mathrm{~g} / \mathrm{mole}$, determined from the chemical formula) to calculate the percentages of each of its elements:

$$
\begin{aligned}
& \% \mathrm{C}=\frac{9 \text { mol C } \times \text { molar mass C }}{\text { molar mass C }{ }_{9} \mathrm{H}_{18} \mathrm{O}_{4}} \times 100=\frac{9 \times 12.01 \mathrm{~g} / \mathrm{mol}}{180.159 \mathrm{~g} / \mathrm{mol}} \times 100=\frac{108.09 \mathrm{~g} / \mathrm{mol}}{180.159 \mathrm{~g} / \mathrm{mol}} \times 100 \\
& \% \mathrm{C}=60.00 \% \mathrm{C} \\
& \% \mathrm{H}=\frac{8 \text { mol } \mathrm{C} \times \text { molar mass } \mathrm{H}}{\text { molar mass C }{ }_{9} \mathrm{H}_{18} \mathrm{O}_{4}} \times 100=\frac{8 \times 1.008 \mathrm{~g} / \mathrm{mol}}{180.159 \mathrm{~g} / \mathrm{mol}} \times 100=\frac{8.064 \mathrm{~g} / \mathrm{mol}}{180.159 \mathrm{~g} / \mathrm{mol}} \times 100 \\
& \% \mathrm{H}=4.476 \% \mathrm{H} \\
& \% \mathrm{O}=\frac{4 \text { mol O } \times \text { molar mass O}}{\text { molar mass C }{ }_{9} \mathrm{H}_{18} \mathrm{O}_{4}} \times 100=\frac{4 \times 16.00 \mathrm{~g} / \mathrm{mol}}{180.159 \mathrm{~g} / \mathrm{mol}} \times 100=\frac{64.00 \mathrm{~g} / \mathrm{mol}}{180.159 \mathrm{~g} / \mathrm{mol}} \times 100 \\
& \% \mathrm{O}=35.52 \%
\end{aligned}
$$

Note that these percentages sum to equal $100.00 \%$ when appropriately rounded.

## Check Your Learning

To three significant digits, what is the mass percentage of iron in the compound $\mathrm{Fe}_{2} \mathrm{O}_{3}$ ?
Answer: 69.9\% Fe

## Determination of Empirical Formulas

As previously mentioned, the most common approach to determining a compound’s chemical formula is to first measure the masses of its constituent elements. However, we must keep in mind that chemical formulas represent the relative numbers, not masses, of atoms in the substance. Therefore, any experimentally derived data involving mass must be used to derive the corresponding numbers of atoms in the compound. To accomplish this, we can use molar masses to convert the mass of each element to a number of moles. We then consider the moles of each element relative to each other, converting these numbers into a whole-number ratio that can be used to derive the empirical formula of the substance. Consider a sample of compound determined to contain 1.71 g C and 0.287 g H. The corresponding numbers of atoms (in moles) are:

$$
\begin{aligned}
& 1.17 \mathrm{~g} \mathrm{C} \times \frac{1 \mathrm{~mol} \mathrm{C}}{12.01 \mathrm{~g} \mathrm{C}}=0.142 \mathrm{~mol} \mathrm{C} \\
& 0.287 \mathrm{~g} \mathrm{H} \times \frac{1 \mathrm{~mol} \mathrm{H}}{1.008 \mathrm{~g} \mathrm{H}}=0.284 \mathrm{~mol} \mathrm{H}
\end{aligned}
$$

Thus, we can accurately represent this compound with the formula C 0.142 H 0.248 . Of course, per accepted convention, formulas contain whole-number subscripts, which can be achieved by dividing each subscript by the smaller subscript:

$$
\mathrm{C}_{\frac{0.142}{0.142}} \mathrm{H}_{\frac{0.248}{0.142}} \text { or } \mathrm{CH}_{2}
$$

(Recall that subscripts of " 1 " are not written but rather assumed if no other number is present.)
The empirical formula for this compound is thus $\mathrm{CH}_{2}$. This may or not be the compound's molecular formula as well; however, we would need additional information to make that determination (as discussed later in this section).

Consider as another example a sample of compound determined to contain 5.31 g Cl and 8.40 g O . Following the same approach yields a tentative empirical formula of:

$$
\mathrm{C}_{0.150} \mathrm{O}_{0.525}=\mathrm{Cl}_{\frac{0.150}{0.150}} \mathrm{O}_{\frac{0.525}{0.150}}=\mathrm{ClO}_{3.5}
$$

In this case, dividing by the smallest subscript still leaves us with a decimal subscript in the empirical formula. To convert this into a whole number, we must multiply each of the subscripts by two, retaining the same atom ratio and yielding $\mathrm{Cl}_{2} \mathrm{O}_{7}$ as the final empirical formula.

In summary, empirical formulas are derived from experimentally measured element masses by:

1. Deriving the number of moles of each element from its mass
2. Dividing each element's molar amount by the smallest molar amount to yield subscripts for a tentative empirical formula
3. Multiplying all coefficients by an integer, if necessary, to ensure that the smallest whole-number ratio of subscripts is obtained
Figure 3.11 outlines this procedure in flow chart fashion for a substance containing elements A and X .


Figure 3.11 The empirical formula of a compound can be derived from the masses of all elements in the sample.

## Example 3.11

## Determining a Compound's Empirical Formula from the Masses of Its Elements

A sample of the black mineral hematite (Figure 3.12), an oxide of iron found in many iron ores, contains 34.97 g of iron and 15.03 g of oxygen. What is the empirical formula of hematite?


Figure 3.12 Hematite is an iron oxide that is used in jewelry. (credit: Mauro Cateb)

## Solution

For this problem, we are given the mass in grams of each element. Begin by finding the moles of each:

$$
\begin{aligned}
& 34.97 \mathrm{~g} \mathrm{Fe}\left(\frac{\mathrm{~mol} \mathrm{Fe}}{55.85 \mathrm{~g}}\right)=0.6261 \mathrm{~mol} \mathrm{Fe} \\
& 15.03 \mathrm{~g} \mathrm{O}\left(\frac{\mathrm{~mol} \mathrm{O}}{16.00 \mathrm{~g}}\right)=0.9394 \mathrm{~mol} \mathrm{O}
\end{aligned}
$$

Next, derive the iron-to-oxygen molar ratio by dividing by the lesser number of moles:

$$
\begin{aligned}
& \frac{0.6261}{0.6261}=1.000 \mathrm{~mol} \mathrm{Fe} \\
& \frac{0.0394}{0.6261}=1.500 \mathrm{~mol} \mathrm{O}
\end{aligned}
$$

The ratio is 1.000 mol of iron to 1.500 mol of oxygen $\left(\mathrm{Fe}_{1} \mathrm{O}_{1.5}\right)$. Finally, multiply the ratio by two to get the smallest possible whole number subscripts while still maintaining the correct iron-to-oxygen ratio:

$$
2\left(\mathrm{Fe}_{1} \mathrm{O}_{1.5}\right)=\mathrm{Fe}_{2} \mathrm{O}_{3}
$$

The empirical formula is $\mathrm{Fe}_{2} \mathrm{O}_{3}$.

## Check Your Learning

What is the empirical formula of a compound if a sample contains 0.130 g of nitrogen and 0.370 g of oxygen?

Answer: $\mathrm{N}_{2} \mathrm{O}_{5}$

## Link to Learning



For additional worked examples illustrating the derivation of empirical formulas, watch the brief video (http://openstaxcollege.org/I/16empforms) clip.

## Deriving Empirical Formulas from Percent Composition

Finally, with regard to deriving empirical formulas, consider instances in which a compound's percent composition is available rather than the absolute masses of the compound's constituent elements. In such cases, the percent composition can be used to calculate the masses of elements present in any convenient mass of compound; these masses can then be used to derive the empirical formula in the usual fashion.

## Example 3.12

## Determining an Empirical Formula from Percent Composition

The bacterial fermentation of grain to produce ethanol forms a gas with a percent composition of 27.29\% C and 72.71\% O (Figure 3.13). What is the empirical formula for this gas?


Figure 3.13 An oxide of carbon is removed from these fermentation tanks through the large copper pipes at the top. (credit: "Dual Freq"/Wikimedia Commons)

## Solution

Since the scale for percentages is 100 , it is most convenient to calculate the mass of elements present in a sample weighing 100 g . The calculation is "most convenient" because, per the definition for percent composition, the mass of a given element in grams is numerically equivalent to the element's mass percentage. This numerical equivalence results from the definition of the "percentage" unit, whose name is derived from the Latin phrase per centum meaning "by the hundred." Considering this definition, the mass percentages provided may be more conveniently expressed as fractions:

$$
\begin{aligned}
27.29 \% \mathrm{C} & =\frac{27.29 \mathrm{~g} \mathrm{C}}{100 \mathrm{~g} \text { compound }} \\
72.71 \% \mathrm{O} & =\frac{72.71 \mathrm{~g} \mathrm{O}}{100 \mathrm{~g} \text { compound }}
\end{aligned}
$$

The molar amounts of carbon and hydrogen in a $100-\mathrm{g}$ sample are calculated by dividing each element's mass by its molar mass:

$$
\begin{aligned}
& 27.29 \mathrm{~g} \mathrm{C}\left(\frac{\mathrm{~mol} \mathrm{C}}{12.01 \mathrm{~g}}\right)=2.272 \mathrm{~mol} \mathrm{C} \\
& 72.71 \mathrm{~g} \mathrm{O}\left(\frac{\mathrm{~mol} \mathrm{O}}{16.00 \mathrm{~g}}\right)=4.544 \mathrm{~mol} \mathrm{O}
\end{aligned}
$$

Coefficients for the tentative empirical formula are derived by dividing each molar amount by the lesser of the two:

$$
\begin{aligned}
& \frac{2.272 \mathrm{~mol} \mathrm{C}}{2.272}=1 \\
& \frac{4.544 \mathrm{~mol} \mathrm{O}}{2.272}=2
\end{aligned}
$$

Since the resulting ratio is one carbon to two oxygen atoms, the empirical formula is $\mathrm{CO}_{2}$.

## Check Your Learning

What is the empirical formula of a compound containing $40.0 \% \mathrm{C}, 6.71 \% \mathrm{H}$, and $53.28 \% \mathrm{O}$ ?
Answer: $\mathrm{CH}_{2} \mathrm{O}$

## Derivation of Molecular Formulas

Recall that empirical formulas are symbols representing the relative numbers of a compound's elements. Determining the absolute numbers of atoms that compose a single molecule of a covalent compound requires knowledge of both its empirical formula and its molecular mass or molar mass. These quantities may be determined experimentally by various measurement techniques. Molecular mass, for example, is often derived from the mass spectrum of the compound (see discussion of this technique in the previous chapter on atoms and molecules). Molar mass can be measured by a number of experimental methods, many of which will be introduced in later chapters of this text.

Molecular formulas are derived by comparing the compound's molecular or molar mass to its empirical formula mass. As the name suggests, an empirical formula mass is the sum of the average atomic masses of all the atoms represented in an empirical formula. If we know the molecular (or molar) mass of the substance, we can divide this by the empirical formula mass in order to identify the number of empirical formula units per molecule, which we designate as $n$ :

$$
\frac{\text { molecular or molar mass }\left(\operatorname{amu} \text { or } \frac{\mathrm{g}}{\mathrm{~mol}}\right)}{\text { empirical formula mass }\left(\mathrm{amu} \text { or } \frac{\mathrm{g}}{\mathrm{~mol}}\right)}=n \text { formula units/molecule }
$$

The molecular formula is then obtained by multiplying each subscript in the empirical formula by $n$, as shown by the generic empirical formula $A_{x} B_{y}$ :

$$
\left(\mathrm{A}_{\mathrm{x}} \mathrm{~B}_{\mathrm{y}}\right)_{\mathrm{n}}=\mathrm{A}_{\mathrm{nx}} \mathrm{~B}_{\mathrm{nx}}
$$

For example, consider a covalent compound whose empirical formula is determined to be $\mathrm{CH}_{2} \mathrm{O}$. The empirical formula mass for this compound is approximately 30 amu (the sum of 12 amu for one C atom, 2 amu for two H atoms, and 16 amu for one O atom). If the compound's molecular mass is determined to be 180 amu , this indicates that molecules of this compound contain six times the number of atoms represented in the empirical formula:

$$
\frac{180 \mathrm{amu} / \text { molecule }}{30 \frac{\mathrm{amu}}{\text { formula unit }}}=6 \text { formula units } / \text { molecule }
$$

Molecules of this compound are then represented by molecular formulas whose subscripts are six times greater than those in the empirical formula:

$$
\left(\mathrm{CH}_{2} \mathrm{O}\right)_{6}=\mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}
$$

Note that this same approach may be used when the molar mass ( $\mathrm{g} / \mathrm{mol}$ ) instead of the molecular mass (amu) is used. In this case, we are merely considering one mole of empirical formula units and molecules, as opposed to single units and molecules.

## Example 3.13

## Determination of the Molecular Formula for Nicotine

Nicotine, an alkaloid in the nightshade family of plants that is mainly responsible for the addictive nature of cigarettes, contains $74.02 \% \mathrm{C}, 8.710 \% \mathrm{H}$, and $17.27 \% \mathrm{~N}$. If 40.57 g of nicotine contains 0.2500 mol nicotine, what is the molecular formula?

## Solution

Determining the molecular formula from the provided data will require comparison of the compound's empirical formula mass to its molar mass. As the first step, use the percent composition to derive the compound's empirical formula. Assuming a convenient, a $100-\mathrm{g}$ sample of nicotine yields the following molar amounts of its elements:

$$
\begin{aligned}
& (74.02 \mathrm{~g} \mathrm{C})\left(\frac{1 \mathrm{~mol} \mathrm{C}}{12.01 \mathrm{~g} \mathrm{C}}\right)=6.163 \mathrm{~mol} \mathrm{C} \\
& (8.710 \mathrm{~g} \mathrm{H})\left(\frac{1 \mathrm{~mol} \mathrm{H}}{1.01 \mathrm{~g} \mathrm{H}}\right)=8.624 \mathrm{~mol} \mathrm{H} \\
& (17.27 \mathrm{~g} \mathrm{~N})\left(\frac{1 \mathrm{~mol} \mathrm{~N}}{14.01 \mathrm{~g} \mathrm{~N}}\right)=1.233 \mathrm{~mol} \mathrm{~N}
\end{aligned}
$$

Next, we calculate the molar ratios of these elements.
The C-to- N and $\mathrm{H}-\mathrm{to}-\mathrm{N}$ molar ratios are adequately close to whole numbers, and so the empirical formula is $\mathrm{C}_{5} \mathrm{H}_{7} \mathrm{~N}$. The empirical formula mass for this compound is therefore $81.13 \mathrm{amu} /$ formula unit, or $81.13 \mathrm{~g} /$ mol formula unit.

We calculate the molar mass for nicotine from the given mass and molar amount of compound:

$$
\frac{40.57 \mathrm{~g} \text { nicotine }}{0.2500 \mathrm{~mol} \text { nicotine }}=\frac{162.3 \mathrm{~g}}{\mathrm{~mol}}
$$

Comparing the molar mass and empirical formula mass indicates that each nicotine molecule contains two formula units:

$$
\frac{162.3 \mathrm{~g} / \mathrm{mol}}{81.13 \frac{\mathrm{~g}}{\text { formula unit }}}=2 \text { formula units } / \text { molecule }
$$

Thus, we can derive the molecular formula for nicotine from the empirical formula by multiplying each subscript by two:

$$
\left(\mathrm{C}_{5} \mathrm{H}_{7} \mathrm{~N}\right)_{6}=\mathrm{C}_{10} \mathrm{H}_{14} \mathrm{~N}_{2}
$$

## Check Your Learning

What is the molecular formula of a compound with a percent composition of $49.47 \% \mathrm{C}, 5.201 \% \mathrm{H}, 28.84 \%$ N , and $16.48 \% \mathrm{O}$, and a molecular mass of 194.2 amu?

Answer: $\mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$

## Summary

### 3.1 Formula Mass and the Mole Concept

The formula mass of a substance is the sum of the average atomic masses of each atom represented in the chemical formula and is expressed in atomic mass units. The formula mass of a covalent compound is also called the molecular mass. A convenient amount unit for expressing very large numbers of atoms or molecules is the mole. Experimental measurements have determined the number of entities composing 1 mole of substance to be $6.022 \times 10^{23}$, a quantity called Avogadro's number. The mass in grams of 1 mole of substance is its molar mass. Due to the use of the same reference substance in defining the atomic mass unit and the mole, the formula mass (amu) and molar mass ( $\mathrm{g} / \mathrm{mol}$ ) for any substance are numerically equivalent (for example, one $\mathrm{H}_{2} \mathrm{O}$ molecule weighs approximately18 amu and 1 mole of $\mathrm{H}_{2} \mathrm{O}$ molecules weighs approximately 18 g ).

### 3.2 Determining Empirical and Molecular Formulas

The chemical identity of a substance is defined by the types and relative numbers of atoms composing its fundamental entities (molecules in the case of covalent compounds, ions in the case of ionic compounds). A compound's percent composition provides the mass percentage of each element in the compound, and it is often experimentally determined and used to derive the compound's empirical formula. The empirical formula mass of a covalent compound may be compared to the compound's molecular or molar mass to derive a molecular formula.

## Exercises

### 3.1 Formula Mass and the Mole Concept

1. What is the total mass (amu) of carbon in each of the following molecules?
(a) $\mathrm{CH}_{4}$
(b) $\mathrm{CHCl}_{3}$
(c) $\mathrm{C}_{12} \mathrm{H}_{10} \mathrm{O}_{6}$
(d) $\mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{CH}_{2} \mathrm{CH}_{2} \mathrm{CH}_{3}$
2. What is the total mass of hydrogen in each of the molecules?
(a) $\mathrm{CH}_{4}$
(b) $\mathrm{CHCl}_{3}$
(c) $\mathrm{C}_{12} \mathrm{H}_{10} \mathrm{O}_{6}$
(d) $\mathrm{CH}_{3} \mathrm{CH}_{2} \mathrm{CH}_{2} \mathrm{CH}_{2} \mathrm{CH}_{3}$
3. Calculate the molecular or formula mass of each of the following:
(a) $\mathrm{P}_{4}$
(b) $\mathrm{H}_{2} \mathrm{O}$
(c) $\mathrm{Ca}\left(\mathrm{NO}_{3}\right)_{2}$
(d) $\mathrm{CH}_{3} \mathrm{CO}_{2} \mathrm{H}$ (acetic acid)
(e) $\mathrm{C}_{12} \mathrm{H}_{22} \mathrm{O}_{11}$ (sucrose, cane sugar).
4. Determine the molecular mass of the following compounds:
(a)

(b)

$$
\mathrm{H}-\mathrm{C} \equiv \mathrm{C}-\mathrm{H}
$$

(c)

(d)

5. Determine the molecular mass of the following compounds:
(a)

(b)

(c)

(d)

6. Which molecule has a molecular mass of 28.05 amu ?
(a)

(b)

(c)

7. Write a sentence that describes how to determine the number of moles of a compound in a known mass of the compound if we know its molecular formula.
8. Compare 1 mole of $\mathrm{H}_{2}, 1$ mole of $\mathrm{O}_{2}$, and 1 mole of $\mathrm{F}_{2}$.
(a) Which has the largest number of molecules? Explain why.
(b) Which has the greatest mass? Explain why.
9. Which contains the greatest mass of oxygen: 0.75 mol of ethanol $\left(\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}\right), 0.60 \mathrm{~mol}$ of formic acid $\left(\mathrm{HCO}_{2} \mathrm{H}\right)$, or 1.0 mol of water $\left(\mathrm{H}_{2} \mathrm{O}\right)$ ? Explain why.
10. Which contains the greatest number of moles of oxygen atoms: 1 mol of ethanol $\left(\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{OH}\right), 1 \mathrm{~mol}$ of formic acid $\left(\mathrm{HCO}_{2} \mathrm{H}\right)$, or 1 mol of water $\left(\mathrm{H}_{2} \mathrm{O}\right)$ ? Explain why.
11. How are the molecular mass and the molar mass of a compound similar and how are they different?
12. Calculate the molar mass of each of the following compounds:
(a) hydrogen fluoride, HF
(b) ammonia, $\mathrm{NH}_{3}$
(c) nitric acid, $\mathrm{HNO}_{3}$
(d) silver sulfate, $\mathrm{Ag}_{2} \mathrm{SO}_{4}$
(e) boric acid, $\mathrm{B}(\mathrm{OH})_{3}$
13. Calculate the molar mass of each of the following:
(a) $\mathrm{S}_{8}$
(b) $\mathrm{C}_{5} \mathrm{H}_{12}$
(c) $\mathrm{Sc}_{2}\left(\mathrm{SO}_{4}\right)_{3}$
(d) $\mathrm{CH}_{3} \mathrm{COCH}_{3}$ (acetone)
(e) $\mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}$ (glucose)
14. Calculate the empirical or molecular formula mass and the molar mass of each of the following minerals:
(a) limestone, $\mathrm{CaCO}_{3}$
(b) halite, NaCl
(c) beryl, $\mathrm{Be}_{3} \mathrm{Al}_{2} \mathrm{Si}_{6} \mathrm{O}_{18}$
(d) malachite, $\mathrm{Cu}_{2}(\mathrm{OH})_{2} \mathrm{CO}_{3}$
(e) turquoise, $\mathrm{CuAl}_{6}\left(\mathrm{PO}_{4}\right)_{4}(\mathrm{OH})_{8}\left(\mathrm{H}_{2} \mathrm{O}\right)_{4}$
15. Calculate the molar mass of each of the following:
(a) the anesthetic halothane, $\mathrm{C}_{2} \mathrm{HBrClF}_{3}$
(b) the herbicide paraquat, $\mathrm{C}_{12} \mathrm{H}_{14} \mathrm{~N}_{2} \mathrm{Cl}_{2}$
(c) caffeine, $\mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$
(d) urea, $\mathrm{CO}\left(\mathrm{NH}_{2}\right)_{2}$
(e) a typical soap, $\mathrm{C}_{17} \mathrm{H}_{35} \mathrm{CO}_{2} \mathrm{Na}$
16. Determine the number of moles of compound and the number of moles of each type of atom in each of the following:
(a) 25.0 g of propylene, $\mathrm{C}_{3} \mathrm{H}_{6}$
(b) $3.06 \times 10^{-3} g$ of the amino acid glycine, $\mathrm{C}_{2} \mathrm{H}_{5} \mathrm{NO}_{2}$
(c) 25 lb of the herbicide Treflan, $\mathrm{C}_{13} \mathrm{H}_{16} \mathrm{~N}_{2} \mathrm{O}_{4} \mathrm{~F}(1 \mathrm{lb}=454 \mathrm{~g})$
(d) 0.125 kg of the insecticide Paris Green, $\mathrm{Cu}_{4}\left(\mathrm{AsO}_{3}\right)_{2}\left(\mathrm{CH}_{3} \mathrm{CO}_{2}\right)_{2}$
(e) 325 mg of aspirin, $\mathrm{C}_{6} \mathrm{H}_{4}\left(\mathrm{CO}_{2} \mathrm{H}\right)\left(\mathrm{CO}_{2} \mathrm{CH}_{3}\right)$
17. Determine the mass of each of the following:
(a) 0.0146 mol KOH
(b) 10.2 mol ethane, $\mathrm{C}_{2} \mathrm{H}_{6}$
(c) $1.6 \times 10^{-3} \mathrm{~mol} \mathrm{Na}_{2} \mathrm{SO}_{4}$
(d) $6.854 \times 10^{3}$ mol glucose, $\mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}$
(e) $2.86 \mathrm{~mol} \mathrm{Co}\left(\mathrm{NH}_{3}\right)_{6} \mathrm{Cl}_{3}$
18. Determine the number of moles of the compound and determine the number of moles of each type of atom in each of the following:
(a) 2.12 g of potassium bromide, KBr
(b) 0.1488 g of phosphoric acid, $\mathrm{H}_{3} \mathrm{PO}_{4}$
(c) 23 kg of calcium carbonate, $\mathrm{CaCO}_{3}$
(d) 78.452 g of aluminum sulfate, $\mathrm{Al}_{2}\left(\mathrm{SO}_{4}\right)_{3}$
(e) 0.1250 mg of caffeine, $\mathrm{C}_{8} \mathrm{H}_{10} \mathrm{~N}_{4} \mathrm{O}_{2}$
19. Determine the mass of each of the following:
(a) 2.345 mol LiCl
(b) 0.0872 mol acetylene, $\mathrm{C}_{2} \mathrm{H}_{2}$
(c) $3.3 \times 10^{-2} \mathrm{~mol} \mathrm{Na} 2 \mathrm{CO}_{3}$
(d) $1.23 \times 10^{3}$ mol fructose, $\mathrm{C}_{6} \mathrm{H}_{12} \mathrm{O}_{6}$
(e) $0.5758 \mathrm{~mol} \mathrm{FeSO}_{4}\left(\mathrm{H}_{2} \mathrm{O}\right)_{7}$
20. The approximate minimum daily dietary requirement of the amino acid leucine, $\mathrm{C}_{6} \mathrm{H}_{13} \mathrm{NO}_{2}$, is 1.1 g . What is this requirement in moles?
21. Determine the mass in grams of each of the following:
(a) 0.600 mol of oxygen atoms
(b) 0.600 mol of oxygen molecules, $\mathrm{O}_{2}$
(c) 0.600 mol of ozone molecules, $\mathrm{O}_{3}$
22. A $55-\mathrm{kg}$ woman has $7.5 \times 10^{-3} \mathrm{~mol}$ of hemoglobin (molar mass $=64,456 \mathrm{~g} / \mathrm{mol}$ ) in her blood. How many hemoglobin molecules is this? What is this quantity in grams?
23. Determine the number of atoms and the mass of zirconium, silicon, and oxygen found in 0.3384 mol of zircon, ZrSiO 4 , a semiprecious stone.
24. Determine which of the following contains the greatest mass of hydrogen: 1 mol of $\mathrm{CH}_{4}, 0.6 \mathrm{~mol}$ of $\mathrm{C}_{6} \mathrm{H}_{6}$, or 0.4 mol of $\mathrm{C}_{3} \mathrm{H}_{8}$.
25. Determine which of the following contains the greatest mass of aluminum: 122 g of $\mathrm{AlPO}_{4}, 266 \mathrm{~g}$ of $\mathrm{A}_{2} \mathrm{Cl}_{6}$, or 225 g of A 12 S 3 .
26. Diamond is one form of elemental carbon. An engagement ring contains a diamond weighing 1.25 carats ( 1 carat $=200 \mathrm{mg})$. How many atoms are present in the diamond?
27. The Cullinan diamond was the largest natural diamond ever found (January 25, 1905). It weighed 3104 carats ( 1 carat $=200 \mathrm{mg}$ ). How many carbon atoms were present in the stone?
28. One 55-gram serving of a particular cereal supplies 270 mg of sodium, $11 \%$ of the recommended daily allowance. How many moles and atoms of sodium are in the recommended daily allowance?
29. A certain nut crunch cereal contains 11.0 grams of sugar (sucrose, $\mathrm{C}_{12} \mathrm{H}_{22} \mathrm{O}_{11}$ ) per serving size of 60.0 grams. How many servings of this cereal must be eaten to consume 0.0278 moles of sugar?
30. A tube of toothpaste contains 0.76 g of sodium monofluorophosphate $\left(\mathrm{Na}_{2} \mathrm{PO}_{3} \mathrm{~F}\right)$ in 100 mL .
(a) What mass of fluorine atoms in mg was present?
(b) How many fluorine atoms were present?
31. Which of the following represents the least number of molecules?
(a) 20.0 g of $\mathrm{H}_{2} \mathrm{O}(18.02 \mathrm{~g} / \mathrm{mol})$
(b) 77.0 g of $\mathrm{CH}_{4}(16.06 \mathrm{~g} / \mathrm{mol})$
(c) 68.0 g of $\mathrm{CaH}_{2}(42.09 \mathrm{~g} / \mathrm{mol})$
(d) 100.0 g of $\mathrm{N}_{2} \mathrm{O}(44.02 \mathrm{~g} / \mathrm{mol})$
(e) 84.0 g of $\mathrm{HF}(20.01 \mathrm{~g} / \mathrm{mol})$

### 3.2 Determining Empirical and Molecular Formulas

32. What information do we need to determine the molecular formula of a compound from the empirical formula?
33. Calculate the following to four significant figures:
(a) the percent composition of ammonia, $\mathrm{NH}_{3}$
(b) the percent composition of photographic "hypo," $\mathrm{Na}_{2} \mathrm{~S}_{2} \mathrm{O}_{3}$
(c) the percent of calcium ion in $\mathrm{Ca3}\left(\mathrm{PO}_{4}\right) 2$
34. Determine the following to four significant figures:
(a) the percent composition of hydrazoic acid, $\mathrm{HN}_{3}$
(b) the percent composition of TNT, $\mathrm{C}_{6} \mathrm{H}_{2}\left(\mathrm{CH}_{3}\right)\left(\mathrm{NO}_{2}\right)_{3}$
(c) the percent of $\mathrm{SO}_{4}{ }^{2-}$ in $\mathrm{Al}_{2}\left(\mathrm{SO}_{4}\right)_{3}$
35. Determine the percent ammonia, $\mathrm{NH}_{3}$, in $\mathrm{Co}\left(\mathrm{NH}_{3}\right)_{6} \mathrm{Cl}_{3}$, to three significant figures.
36. Determine the percent water in $\mathrm{CuSO}_{4} \cdot 5 \mathrm{H}_{2} \mathrm{O}$ to three significant figures.
37. Determine the empirical formulas for compounds with the following percent compositions:
(a) $15.8 \%$ carbon and $84.2 \%$ sulfur
(b) $40.0 \%$ carbon, $6.7 \%$ hydrogen, and $53.3 \%$ oxygen
38. Determine the empirical formulas for compounds with the following percent compositions:
(a) $43.6 \%$ phosphorus and $56.4 \%$ oxygen
(b) $28.7 \% \mathrm{~K}, 1.5 \% \mathrm{H}, 22.8 \% \mathrm{P}$, and $47.0 \% \mathrm{O}$
39. A compound of carbon and hydrogen contains $92.3 \% \mathrm{C}$ and has a molar mass of $78.1 \mathrm{~g} / \mathrm{mol}$. What is its molecular formula?
40. Dichloroethane, a compound that is often used for dry cleaning, contains carbon, hydrogen, and chlorine. It has a molar mass of $99 \mathrm{~g} / \mathrm{mol}$. Analysis of a sample shows that it contains $24.3 \%$ carbon and $4.1 \%$ hydrogen. What is its molecular formula?
41. Determine the empirical and molecular formula for chrysotile asbestos. Chrysotile has the following percent composition: $28.03 \% \mathrm{Mg}, 21.60 \% \mathrm{Si}, 1.16 \% \mathrm{H}$, and $49.21 \% \mathrm{O}$. The molar mass for chrysotile is $520.8 \mathrm{~g} / \mathrm{mol}$.
42. Polymers are large molecules composed of simple units repeated many times. Thus, they often have relatively simple empirical formulas. Calculate the empirical formulas of the following polymers:
(a) Lucite (Plexiglas); 59.9\% C, $8.06 \% \mathrm{H}, 32.0 \% \mathrm{O}$
(b) Saran; $24.8 \% \mathrm{C}, 2.0 \% \mathrm{H}, 73.1 \% \mathrm{Cl}$
(c) polyethylene; $86 \% \mathrm{C}, 14 \% \mathrm{H}$
(d) polystyrene; $92.3 \% \mathrm{C}, 7.7 \% \mathrm{H}$
(e) Orlon; $67.9 \% \mathrm{C}, 5.70 \% \mathrm{H}, 26.4 \% \mathrm{~N}$
43. A major textile dye manufacturer developed a new yellow dye. The dye has a percent composition of $75.95 \%$ C, $17.72 \% \mathrm{~N}$, and $6.33 \% \mathrm{H}$ by mass with a molar mass of about $240 \mathrm{~g} / \mathrm{mol}$. Determine the molecular formula of the dye.
