Chapter Outline

A Look Ahead

- We begin by studying the mass of an atom, which is based on the carbon-12 isotope scale. An atom of the carbon-12 isotope is assigned a mass of exactly 12 atomic mass unit (amu). To work with the more convenient scale of grams, we use the molar mass. The molar mass of carbon-12 has a mass of exactly 12 grams and contains an Avogadro's number (6.022×10^{23}) of atoms. The molar masses of other elements are also expressed in grams and contain the same number of atoms. (3.1 and 3.2)
- Our discussion of atomic mass leads to molecular mass, which is the sum of the masses of the constituent atoms present. We learn that the most direct way to determine atomic and molecular mass is by the use of a mass spectrometer. (3.3 and 3.4)
- To continue our study of molecules and ionic compounds, we learn how to calculate the percent composition of these species from their chemical formulas. (3.5)
- We will see how the empirical and molecular formulas of a compound are determined by experiment. (3.6)
- Next, we learn how to write a chemical equation to describe the outcome of a chemical reaction. A chemical equation must be balanced so that we have the same number and type of atoms for the reactants, the starting materials, and the products, the substances formed at the end of the reaction. (3.7)
- Building on our knowledge of chemical equations, we then proceed to study the mass relationships of chemical reactions. A chemical equation enables us to use the mole method to predict the amount of product(s) formed, knowing how much the reactant(s) was used. We will see that a reaction's yield depends on the amount of limiting reagent (a reactant that is used up first) present. (3.8 and 3.9)
- We will learn that the actual yield of a reaction is almost always less than that predicted from the equation, called the theoretical yield, because of various complications. (3.10)

In this chapter we will consider the masses of atoms and molecules and what happens to them when chemical changes occur. Our guide for this discussion will be the law of conservation of mass.

3.1 Atomic Mass

In this chapter, we will use what we have learned about chemical structure and formulas in studying the mass relationships of atoms and molecules. These relationships in turn will help us to explain the composition of compounds and the ways in which composition changes.

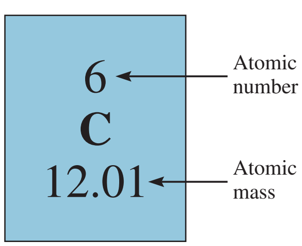
Section 3.4 describes a method for determining atomic mass.

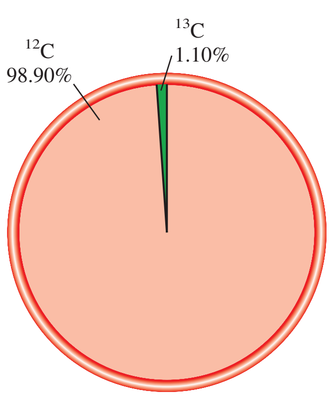
The mass of an atom depends on the number of electrons, protons, and neutrons it contains. Knowledge of an atom's mass is important in laboratory work. But atoms are extremely small particles—even the smallest speck of dust that our unaided eyes can detect contains as many as 1×10^{16} atoms! Clearly we cannot weigh a single atom, but it is possible to determine the mass of one atom *relative* to another experimentally. The first step is to assign a value to the mass of one atom of a given element so that it can be used as a standard.

One atomic mass unit is also called one dalton.

By international agreement, ***atomic mass*** (sometimes called *atomic weight*) is *the mass of the atom in atomic mass units (amu)*. One ***atomic mass unit*** is defined as *a mass exactly equal to one-twelfth the mass of one carbon-12 atom.* Carbon-12 is the carbon isotope that has six protons and six neutrons. Setting the atomic mass of carbon-12 at 12 amu provides the standard for measuring the atomic mass of the other elements. For example, experiments have shown that, on average, a hydrogen atom is only 8.400 percent as massive as the carbon-12 atom. Thus, if the mass of one carbon-12 atom is exactly 12 amu, the atomic mass of hydrogen must be 0.084×12.00 amu or 1.008 amu. Similar calculations show that the atomic mass of oxygen is 16.00 amu and that of iron is 55.85 amu. Thus, although we do not know just how much an average iron atom's mass is, we know that it is approximately 56 times as massive as a hydrogen atom.

Average Atomic Mass





Natural abundances of C-12 and C-13 isotopes.

When you look up the atomic mass of carbon in a table such as the one on the inside front cover of this book, you will find that its value is not 12.00 amu but 12.01 amu. The reason for the difference is that most naturally occurring elements (including carbon) have more than one isotope. This means that when we measure the atomic mass of an element, we must generally settle for the *average* mass of the naturally occurring mixture of isotopes. For example, the natural abundances of carbon-12 and carbon-13 are 98.90 percent and 1.10 percent, respectively. The atomic mass of carbon-13 has been determined to be 13.00335 amu. Thus, the average atomic mass of carbon can be calculated as follows:

$$\begin{aligned}\text{average atomic mass}\\ \text{of natural carbon} &= (0.9890)(12.00000 \text{ amu}) + (0.0110)(13.00335 \text{ amu})\\ &= 12.01 \text{ amu}\end{aligned}$$

Note that in calculations involving percentages, we need to convert percentages to fractions. For example, 98.90 percent becomes 98.90/100, or 0.9890. Because there are many more carbon-12 atoms than carbon-13 atoms in naturally occurring carbon, the average atomic mass is much closer to 12 amu than to 13 amu.

It is important to understand that when we say that the atomic mass of carbon is 12.01 amu, we are referring to the *average* value. If carbon atoms could be examined individually, we would find either an atom of atomic mass 12.00000 amu or one of 13.00335 amu, but never one of 12.01 amu. Example 3.1 shows how to calculate the average atomic mass of an element.


Copper.

EXAMPLE 3.1

Copper, a metal known since ancient times, is used in electrical cables and pennies, among other things. The atomic masses of its two stable isotopes, $^{63}_{29}Cu$ (69.09 percent) and $^{65}_{29}Cu$ (30.91 percent), are 62.93 amu and 64.9278 amu, respectively. Calculate the average atomic mass of copper. The relative abundances are given in parentheses.

Strategy Each isotope contributes to the average atomic mass based on its relative abundance. Multiplying the mass of an isotope by its fractional abundance (not percent) will give the contribution to the average atomic mass of that particular isotope.

Solution First the percents are converted to fractions: 69.09 percent to 69.09/100 or 0.6909 and 30.91 percent to 30.91/100 or 0.3091. We find the contribution to the average atomic mass for each isotope, then add the contributions together to obtain the average atomic mass.

$$(0.6909)(62.93 \text{ amu}) + (0.3091)(64.9278 \text{ amu}) = \boxed{63.55 \text{ amu}}$$

Check The average atomic mass should be between the two isotopic masses; therefore, the answer is reasonable. Note that because there are more $^{63}_{29}Cu$ than $^{65}_{29}Cu$ isotopes, the average atomic mass is closer to 62.93 amu than to 64.9278 amu.

Practice Exercise The atomic masses of the two stable isotopes of boron, $^{10}_{5}B$ (19.78 percent) and $^{11}_{5}B$ (80.22 percent), are 10.0129 amu and 11.0093 amu, respectively. Calculate the average atomic mass of boron.

The atomic masses of many elements have been accurately determined to five or six significant figures. However, for our purposes we will normally use atomic masses accurate only to four significant figures (see table of atomic masses inside the front cover). For simplicity, we will omit the word "average" when we discuss the atomic masses of the elements.

3.2 Avogadro's Number and the Molar Mass of an Element

Atomic mass units provide a relative scale for the masses of the elements. But because atoms have such small masses, no usable scale can be devised to weigh them in calibrated units of atomic mass units. In any real situation, we deal with macroscopic samples containing enormous numbers of atoms. Therefore, it is convenient to have a special unit to describe a very large number of atoms. The idea of a unit to denote a particular number of objects is not new. For example, the pair (2 items), the dozen (12 items), and the gross (144 items) are all familiar units. Chemists measure atoms and molecules in moles.

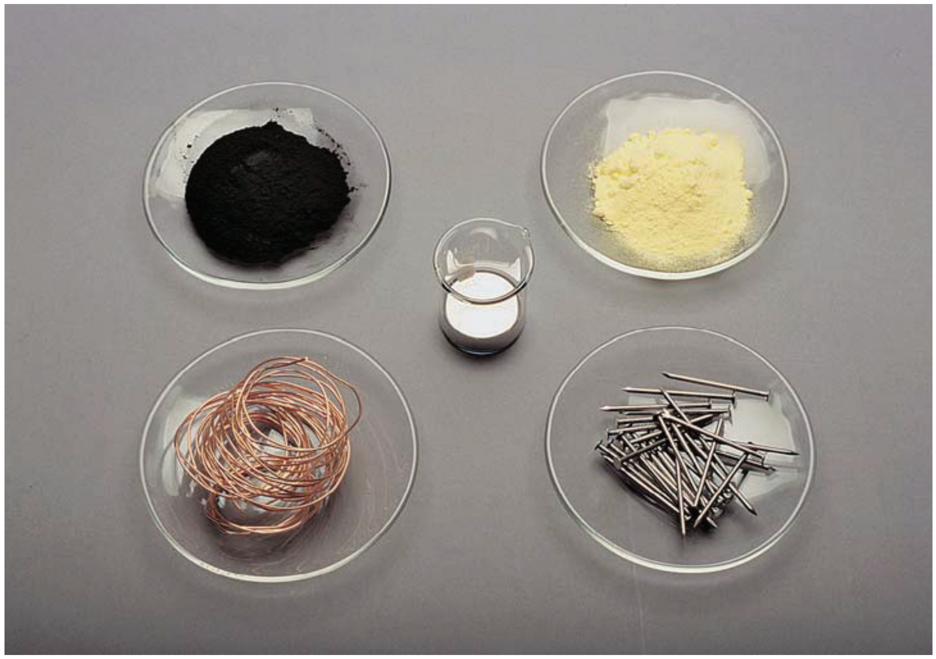


Figure 3.1 *One mole each of several common elements. Carbon (black charcoal powder), sulfur (yellow powder), iron (as nails), copper wires, and mercury (shiny liquid metal).*

This number is called ***Avogadro's number*** (N_A),[†] The currently accepted value of the number of particles in a mole is exactly

$$N_{\mathrm{A}} = 6.022140786 \times 10^{23}$$

Generally, we round Avogadro's number to 6.022×10^{23}. Thus, just as one dozen oranges contains 12 oranges, 1 mole of hydrogen atoms contains 6.022×10^{23} H atoms. Figure 3.1 shows samples containing 1 mole each of several common elements.

The enormity of Avogadro's number is difficult to imagine. For example, spreading 6.022×10^{23} oranges over the entire surface of Earth would produce a layer 9 mi into space! Because atoms (and molecules) are so tiny, we need a huge number to study them in manageable quantities.

In calculations, the units of molar mass are g/mol or kg/mol.

The molar masses of the elements are given on the inside front cover of the book.

[†]Lorenzo Romano Amedeo Carlo Avogadro di Quaregua e di Cerreto (1776–1856). Italian mathematical physicist. He practiced law for many years before he became interested in science. His most famous work, now known as Avogadro's law (see Chapter 5), was largely ignored during his lifetime, although it became the basis for determining atomic masses in the late nineteenth century.

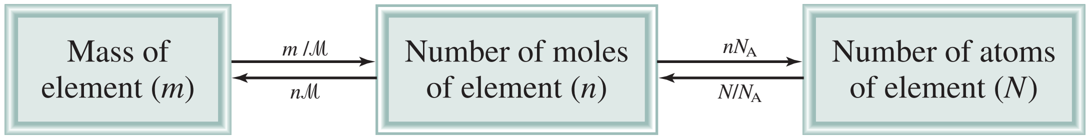


Figure 3.2 *The relationships between mass (m in grams) of an element and number of moles of an element (n) and between number of moles of an element and number of atoms (N) of an element. ℳ is the molar mass (g/mol) of the element and N_A is Avogadro's number.*

$$\frac{1 \text{ mol X}}{\text{molar mass of X}} \quad \text{and} \quad \frac{1 \text{ mol X}}{6.022 \times 10^{23} \text{ X atoms}}$$

After some practice, you can use the equations in Figure 3.2 in calculations: $n = m/\mathcal{M}$ and $N = nN_A$.

where X represents the symbol of an element. Using the proper conversion factors we can convert one quantity to another, as Examples 3.2–3.4 show.

EXAMPLE 3.2

Helium (He) is a valuable gas used in industry, low-temperature research, deep-sea diving tanks, and balloons. How many moles of He atoms are in 6.46 g of He?

Strategy We are given grams of helium and asked to solve for moles of helium. What conversion factor do we need to convert between grams and moles? Arrange the appropriate conversion factor so that grams cancel and the unit moles is obtained for your answer.

Solution The conversion factor needed to convert between grams and moles is the molar mass. In the periodic table (see inside front cover) we see that the molar mass of He is 4.003 g. This can be expressed as

$$1 \text{ mol He} = 4.003 \text{ g He}$$

From this equality, we can write two conversion factors

$$\frac{1 \text{ mol He}}{4.003 \text{ g He}} \quad \text{and} \quad \frac{4.003 \text{ g He}}{1 \text{ mol He}}$$

(Continued)

A scientific research helium balloon.

The conversion factor on the left is the correct one. Grams will cancel, leaving the unit mol for the answer, that is,

$$6.46\ \cancel{\text{g He}} \times \frac{1\ \text{mol He}}{4.003\ \cancel{\text{g He}}} = \boxed{1.61\ \text{mol He}}$$

Thus, there are 1.61 moles of He atoms in 6.46 g of He.

Check Because the given mass (6.46 g) is larger than the molar mass of He, we expect to have more than 1 mole of He.

Practice Exercise How many moles of magnesium (Mg) are there in 87.3 g of Mg?

Zinc.

EXAMPLE 3.3

Zinc (Zn) is a silvery metal that is used in making brass (with copper) and in plating iron to prevent corrosion. How many grams of Zn are in 0.356 mole of Zn?

Strategy We are trying to solve for grams of zinc. What conversion factor do we need to convert between moles and grams? Arrange the appropriate conversion factor so that moles cancel and the unit grams are obtained for your answer.

Solution The conversion factor needed to convert between moles and grams is the molar mass. In the periodic table (see inside front cover) we see the molar mass of Zn is 65.39 g. This can be expressed as

$$1\ \text{mol Zn} = 65.39\ \text{g Zn}$$

From this equality, we can write two conversion factors

$$\frac{1\ \text{mol Zn}}{65.39\ \text{g Zn}} \quad \text{and} \quad \frac{65.39\ \text{g Zn}}{1\ \text{mol Zn}}$$

The conversion factor on the right is the correct one. Moles will cancel, leaving unit of grams for the answer. The number of grams of Zn is

$$0.356\ \cancel{\text{mol Zn}} \times \frac{65.39\ \text{g Zn}}{1\ \cancel{\text{mol Zn}}} = \boxed{23.3\ \text{g Zn}}$$

Thus, there are 23.3 g of Zn in 0.356 mole of Zn.

Check Does a mass of 23.3 g for 0.356 mole of Zn seem reasonable? What is the mass of 1 mole of Zn?

Practice Exercise Calculate the number of grams of lead (Pb) in 12.4 moles of lead.

EXAMPLE 3.4

Sulfur (S) is a nonmetallic element that is present in coal. When coal is burned, sulfur is converted to sulfur dioxide and eventually to sulfuric acid that gives rise to the acid rain phenomenon. How many atoms are in 16.3 g of S?

Strategy The question asks for atoms of sulfur. We cannot convert directly from grams to atoms of sulfur. What unit do we need to convert grams of sulfur to in order to convert to atoms? What does Avogadro's number represent?

(Continued)

Solution We need two conversions: first from grams to moles and then from moles to number of particles (atoms). The first step is similar to Example 3.2. Because

$$1 \text{ mol S} = 32.07 \text{ g S}$$

the conversion factor is

$$\frac{1 \text{ mol S}}{32.07 \text{ g S}}$$

Avogadro's number is the key to the second step. We have

$$1 \text{ mol} = 6.022 \times 10^{23} \text{ particles (atoms)}$$

and the conversion factors are

$$\frac{6.022 \times 10^{23} \text{ S atoms}}{1 \text{ mol S}} \quad \text{and} \quad \frac{1 \text{ mol S}}{6.022 \times 10^{23} \text{ S atoms}}$$

The conversion factor on the left is the one we need because it has number of S atoms in the numerator. We can solve the problem by first calculating the number of moles contained in 16.3 g of S, and then calculating the number of S atoms from the number of moles of S:

$$\text{grams of S} \longrightarrow \text{moles of S} \longrightarrow \text{number of S atoms}$$

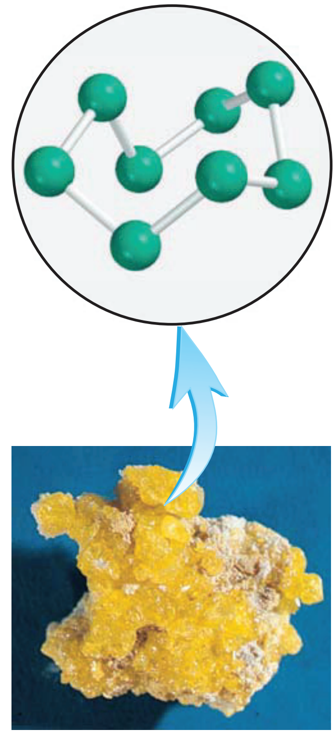
We can combine these conversions in one step as follows:

$$16.3 \cancel{\text{g S}} \times \frac{1 \cancel{\text{mol S}}}{32.07 \cancel{\text{g S}}} \times \frac{6.022 \times 10^{23} \text{ S atoms}}{1 \cancel{\text{mol S}}} = \boxed{3.06 \times 10^{23} \text{ S atoms}}$$

Thus, there are 3.06×10^{23} atoms of S in 16.3 g of S.

Check Should 16.3 g of S contain fewer than Avogadro's number of atoms? What mass of S would contain Avogadro's number of atoms?

Practice Exercise Calculate the number of atoms in 0.551 g of potassium (K).



Elemental sulfur (S_8) consists of eight S atoms joined in a ring.

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3.3 Molecular Mass

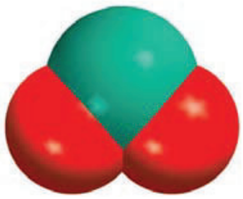
If we know the atomic masses of the component atoms, we can calculate the mass of a molecule. The ***molecular mass*** (sometimes called *molecular weight*) is *the sum of the atomic masses (in amu) in the molecule.* For example, the molecular mass of H_2O is

$$2(\text{atomic mass of H}) + \text{atomic mass of O}$$

or

$$2(1.008 \text{ amu}) + 16.00 \text{ amu} = 18.02 \text{ amu}$$

In general, we need to multiply the atomic mass of each element by the number of atoms of that element present in the molecule and sum over all the elements. Example 3.5 illustrates this approach.



SO_2

EXAMPLE 3.5

Calculate the molecular masses (in amu) of the following compounds: (a) sulfur dioxide (SO_2) and (b) caffeine ($C_8H_{10}N_4O_2$).

Strategy How do atomic masses of different elements combine to give the molecular mass of a compound?

Solution To calculate molecular mass, we need to sum all the atomic masses in the molecule. For each element, we multiply the atomic mass of the element by the number of atoms of that element in the molecule. We find atomic masses in the periodic table (inside front cover).

(a) There are two O atoms and one S atom in SO_2, so that

$$\begin{aligned}\text{molecular mass of } SO_2 &= 32.07 \text{ amu} + 2(16.00 \text{ amu})\\ &= 64.07 \text{ amu}\end{aligned}$$

(b) There are eight C atoms, ten H atoms, four N atoms, and two O atoms in caffeine, so the molecular mass of $C_8H_{10}N_4O_2$ is given by

$$8(12.01 \text{ amu}) + 10(1.008 \text{ amu}) + 4(14.01 \text{ amu}) + 2(16.00 \text{ amu}) = 194.20 \text{ amu}$$

Practice Exercise What is the molecular mass of methanol (CH_4O)?

From the molecular mass we can determine the molar mass of a molecule or compound. The molar mass of a compound (in grams) is numerically equal to its molecular mass (in amu). For example, the molecular mass of water is 18.02 amu, so its molar mass is 18.02 g. Note that 1 mole of water weighs 18.02 g and contains 6.022×10^{23} H_2O *molecules,* just as 1 mole of elemental carbon contains 6.022×10^{23} carbon *atoms.*

As Examples 3.6 and 3.7 show, a knowledge of the molar mass enables us to calculate the numbers of moles and individual atoms in a given quantity of a compound.

CH_4

Methane gas burning on a cooking range.

EXAMPLE 3.6

Methane (CH_4) is the principal component of natural gas. How many moles of CH_4 are present in 6.07 g of CH_4?

Strategy We are given grams of CH_4 and asked to solve for moles of CH_4. What conversion factor do we need to convert between grams and moles? Arrange the appropriate conversion factor so that grams cancel and the unit moles are obtained for your answer.

Solution The conversion factor needed to convert between grams and moles is the molar mass. First we need to calculate the molar mass of CH_4, following the procedure in Example 3.5:

$$\begin{aligned}\text{molar mass of } CH_4 &= 12.01 \text{ g} + 4(1.008 \text{ g})\\ &= 16.04 \text{ g}\end{aligned}$$

Because

$$1 \text{ mol } CH_4 = 16.04 \text{ g } CH_4$$

(Continued)

the conversion factor we need should have grams in the denominator so that the unit g will cancel, leaving the unit mol in the numerator:

$$\frac{1 \text{ mol } CH_4}{16.04 \text{ g } CH_4}$$

We now write

$$6.07 \cancel{\text{g } CH_4} \times \frac{1 \text{ mol } CH_4}{16.04 \cancel{\text{g } CH_4}} = \boxed{0.378 \text{ mol } CH_4}$$

Thus, there is 0.378 mole of CH_4 in 6.07 g of CH_4.

Check Should 6.07 g of CH_4 equal less than 1 mole of CH_4? What is the mass of 1 mole of CH_4?

Practice Exercise Calculate the number of moles of chloroform ($CHCl_3$) in 198 g of chloroform.

EXAMPLE 3.7

How many hydrogen atoms are present in 25.6 g of urea [$(NH_2)_2CO$], which is used as a fertilizer, in animal feed, and in the manufacture of polymers? The molar mass of urea is 60.06 g.

Strategy We are asked to solve for atoms of hydrogen in 25.6 g of urea. We cannot convert directly from grams of urea to atoms of hydrogen. How should molar mass and Avogadro's number be used in this calculation? How many moles of H are in 1 mole of urea?

Solution To calculate the number of H atoms, we first must convert grams of urea to moles of urea using the molar mass of urea. This part is similar to Example 3.2. The molecular formula of urea shows there are four moles of H atoms in one mole of urea molecule, so the mole ratio is 4:1. Finally, knowing the number of moles of H atoms, we can calculate the number of H atoms using Avogadro's number. We need two conversion factors: molar mass and Avogadro's number. We can combine these conversions

$$\text{grams of urea} \longrightarrow \text{moles of urea} \longrightarrow \text{moles of H} \longrightarrow \text{atoms of H}$$

into one step:

$$25.6 \cancel{\text{g } (NH_2)_2CO} \times \frac{1 \cancel{\text{mol } (NH_2)_2CO}}{60.06 \cancel{\text{g } (NH_2)_2CO}} \times \frac{4 \cancel{\text{mol H}}}{1 \cancel{\text{mol } (NH_2)_2CO}} \times \frac{6.022 \times 10^{23} \text{ H atoms}}{1 \cancel{\text{mol H}}}$$
$$= \boxed{1.03 \times 10^{24} \text{ H atoms}}$$

Check Does the answer look reasonable? How many atoms of H would 60.06 g of urea contain?

Practice Exercise How many H atoms are in 72.5 g of isopropanol (rubbing alcohol), C_3H_8O?

Urea.

Finally, note that for ionic compounds like NaCl and MgO that do not contain discrete molecular units, we use the term *formula mass* instead. The formula unit of NaCl consists of one Na^+ ion and one Cl^- ion. Thus, the formula mass of NaCl is the mass of one formula unit:

$$\begin{aligned}\text{formula mass of NaCl} &= 22.99 \text{ amu} + 35.45 \text{ amu} \\ &= 58.44 \text{ amu}\end{aligned}$$

Note that the combined mass of a Na^+ ion and a Cl^- ion is equal to the combined mass of a Na atom and a Cl atom.

and its molar mass is 58.44 g.

3.4 The Mass Spectrometer

The most direct and most accurate method for determining atomic and molecular masses is mass spectrometry, which is depicted in Figure 3.3. In one type of a *mass spectrometer,* a gaseous sample is bombarded by a stream of high-energy electrons. Collisions between the electrons and the gaseous atoms (or molecules) produce positive ions by dislodging an electron from each atom or molecule. These positive ions (of mass *m* and charge *e*) are accelerated by two oppositely charged plates as they pass through the plates. The emerging ions are deflected into a circular path by a magnet. The radius of the path depends on the charge-to-mass ratio (that is, *e/m*). Ions of smaller *e/m* ratio trace a wider curve than those having a larger *e/m* ratio, so that ions with equal charges but different masses are separated from one another. The mass of each ion (and hence its parent atom or molecule) is determined from the magnitude of its deflection. Eventually the ions arrive at the detector, which registers a current for each type of ion. The amount of current generated is directly proportional to the number of ions, so it enables us to determine the relative abundance of isotopes.

The first mass spectrometer, developed in the 1920s by the English physicist F. W. Aston,† was crude by today's standards. Nevertheless, it provided indisputable evidence of the existence of isotopes—neon-20 (atomic mass 19.9924 amu and natural abundance 90.92 percent) and neon-22 (atomic mass 21.9914 amu and natural abundance 8.82 percent). When more sophisticated and sensitive mass spectrometers became available, scientists were surprised to discover that neon has a third stable isotope with an atomic mass of 20.9940 amu and natural abundance 0.257 percent (Figure 3.4). This example illustrates how very important experimental accuracy is to a quantitative science like chemistry. Early experiments failed to detect neon-21 because its natural abundance is just 0.257 percent. In other words, only 26 in 10,000 Ne atoms are neon-21. The masses of molecules can be determined in a similar manner by the mass spectrometer.

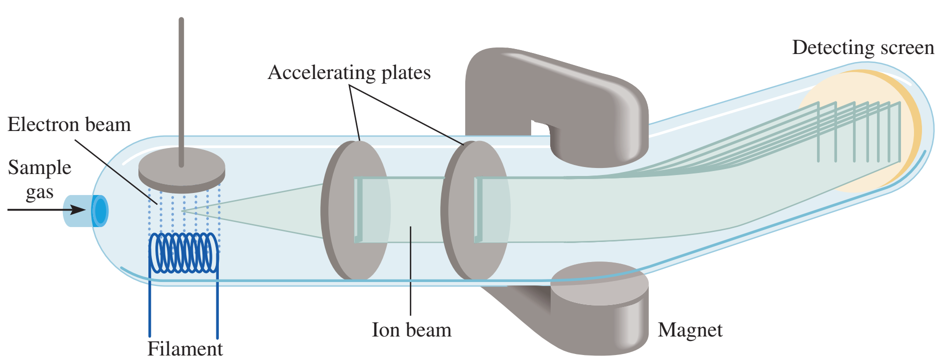
Note that it is possible to determine the molar mass of a compound without knowing its chemical formula.

3.5 Percent Composition of Compounds

As we have seen, the formula of a compound tells us the numbers of atoms of each element in a unit of the compound. However, suppose we needed to verify the purity of a compound for use in a laboratory experiment. From the formula we could calculate what percent of the total mass of the compound is contributed by each element. Then, by comparing the result to the percent composition obtained experimentally for our sample, we could determine the purity of the sample.

†Francis William Aston (1877–1945). English chemist and physicist. He was awarded the Nobel Prize in Chemistry in 1922 for developing the mass spectrometer.

Figure 3.3 *Schematic diagram of one type of mass spectrometer.*



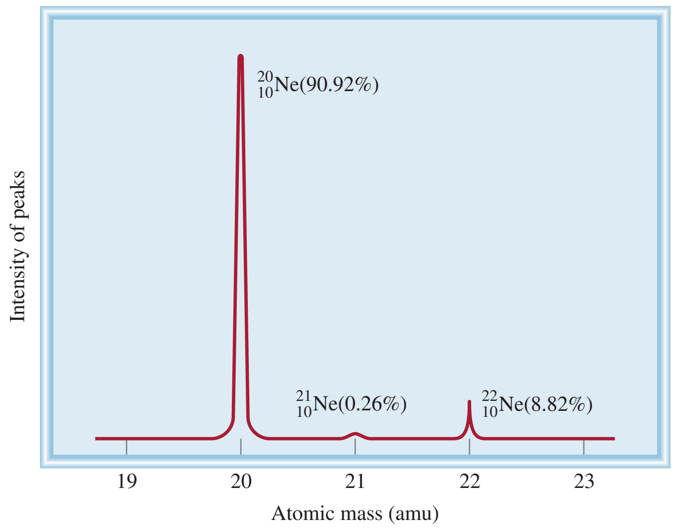
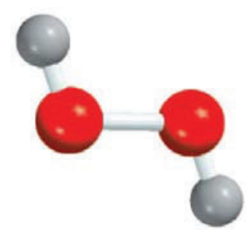


Figure 3.4 *The mass spectrum of the three isotopes of neon.*

The ***percent composition by mass*** is the *percent by mass of each element in a compound.* Percent composition is obtained by dividing the mass of each element in 1 mole of the compound by the molar mass of the compound and multiplying by 100 percent. Mathematically, the percent composition of an element in a compound is expressed as

$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\% \qquad (3.1)$$

where n is the number of moles of the element in 1 mole of the compound. For example, in 1 mole of hydrogen peroxide (H_2O_2) there are 2 moles of H atoms and 2 moles of O atoms. The molar masses of H_2O_2, H, and O are 34.02 g, 1.008 g, and 16.00 g, respectively. Therefore, the percent composition of H_2O_2 is calculated as follows:



H_2O_2

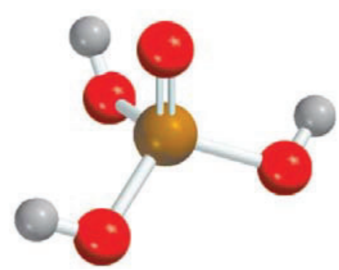
$$\%\text{H} = \frac{2 \times 1.008 \text{ g H}}{34.02 \text{ g } H_2O_2} \times 100\% = 5.926\%$$

$$\%\text{O} = \frac{2 \times 16.00 \text{ g O}}{34.02 \text{ g } H_2O_2} \times 100\% = 94.06\%$$

The sum of the percentages is 5.926% + 94.06% = 99.99%. The small discrepancy from 100 percent is due to the way we rounded off the molar masses of the elements. If we had used the empirical formula HO for the calculation, we would have obtained the same percentages. This is so because both the molecular formula and empirical formula tell us the percent composition by mass of the compound.

EXAMPLE 3.8

Phosphoric acid (H_3PO_4) is a colorless, syrupy liquid used in detergents, fertilizers, toothpastes, and in carbonated beverages for a "tangy" flavor. Calculate the percent composition by mass of H, P, and O in this compound.



H_3PO_4

Strategy Recall the procedure for calculating a percentage. Assume that we have 1 mole of H_3PO_4. The percent by mass of each element (H, P, and O) is given by the combined molar mass of the atoms of the element in 1 mole of H_3PO_4 divided by the molar mass of H_3PO_4, then multiplied by 100 percent.

(Continued)

Solution The molar mass of H_3PO_4 is 97.99 g. The percent by mass of each of the elements in H_3PO_4 is calculated as follows:

$$\%H = \frac{3(1.008 \text{ g) H}}{97.99 \text{ g } H_3PO_4} \times 100\% = \boxed{3.086\%}$$

$$\%P = \frac{30.97 \text{ g P}}{97.99 \text{ g } H_3PO_4} \times 100\% = \boxed{31.61\%}$$

$$\%O = \frac{4(16.00 \text{ g) O}}{97.99 \text{ g } H_3PO_4} \times 100\% = \boxed{65.31\%}$$

Check Do the percentages add to 100 percent? The sum of the percentages is (3.086% + 31.61% + 65.31%) = 100.01%. The small discrepancy from 100 percent is due to the way we rounded off.

Practice Exercise Calculate the percent composition by mass of each of the elements in sulfuric acid (H_2SO_4).

The procedure used in the example can be reversed if necessary. Given the percent composition by mass of a compound, we can determine the empirical formula of the compound (Figure 3.5). Because we are dealing with percentages and the sum of all the percentages is 100 percent, it is convenient to assume that we started with 100 g of a compound, as Example 3.9 shows.

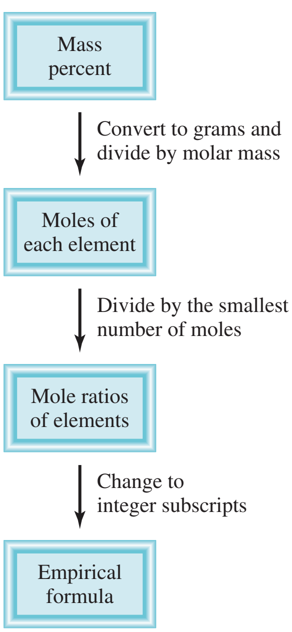


Figure 3.5 *Procedure for calculating the empirical formula of a compound from its percent compositions.*

EXAMPLE 3.9

Ascorbic acid (vitamin C) cures scurvy. It is composed of 40.92 percent carbon (C), 4.58 percent hydrogen (H), and 54.50 percent oxygen (O) by mass. Determine its empirical formula.

Strategy In a chemical formula, the subscripts represent the ratio of the number of moles of each element that combine to form one mole of the compound. How can we convert from mass percent to moles? If we assume an exactly 100-g sample of the compound, do we know the mass of each element in the compound? How do we then convert from grams to moles?

Solution If we have 100 g of ascorbic acid, then each percentage can be converted directly to grams. In this sample, there will be 40.92 g of C, 4.58 g of H, and 54.50 g of O. Because the subscripts in the formula represent a mole ratio, we need to convert the grams of each element to moles. The conversion factor needed is the molar mass of each element. Let n represent the number of moles of each element so that

$$n_C = 40.92 \cancel{\text{g C}} \times \frac{1 \text{ mol C}}{12.01 \cancel{\text{g C}}} = 3.407 \text{ mol C}$$

$$n_H = 4.58 \cancel{\text{g H}} \times \frac{1 \text{ mol H}}{1.008 \cancel{\text{g H}}} = 4.54 \text{ mol H}$$

$$n_O = 54.50 \cancel{\text{g O}} \times \frac{1 \text{ mol O}}{16.00 \cancel{\text{g O}}} = 3.406 \text{ mol O}$$

Thus, we arrive at the formula $C_{3.407}H_{4.54}O_{3.406}$, which gives the identity and the mole ratios of atoms present. However, chemical formulas are written with whole numbers.

(Continued)

Try to convert to whole numbers by dividing all the subscripts by the smallest subscript (3.406):

$$\text{C: } \frac{3.407}{3.406} \approx 1 \qquad \text{H: } \frac{4.54}{3.406} = 1.33 \qquad \text{O: } \frac{3.406}{3.406} = 1$$

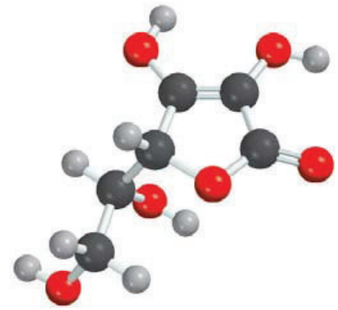
where the ≈ sign means "approximately equal to." This gives $CH_{1.33}O$ as the formula for ascorbic acid. Next, we need to convert 1.33, the subscript for H, into an integer. This can be done by a trial-and-error procedure:

$$1.33 \times 1 = 1.33$$
$$1.33 \times 2 = 2.66$$
$$1.33 \times 3 = 3.99 \approx 4$$

Because 1.33 × 3 gives us an integer (4), we multiply all the subscripts by 3 and obtain $\boxed{C_3H_4O_3}$ as the empirical formula for ascorbic acid.

Check Are the subscripts in $C_3H_4O_3$ reduced to the smallest whole numbers?

Practice Exercise Determine the empirical formula of a compound having the following percent composition by mass: K: 24.75 percent; Mn: 34.77 percent; O: 40.51 percent.



The molecular formula of ascorbic acid is $C_6H_8O_6$.

Similar problems: 3.49, 3.50.

Chemists often want to know the actual mass of an element in a certain mass of a compound. For example, in the mining industry, this information will tell the scientists about the quality of the ore. Because the percent composition by mass of the elements in the substance can be readily calculated, such a problem can be solved in a rather direct way.

EXAMPLE 3.10

Chalcopyrite ($CuFeS_2$) is a principal mineral of copper. Calculate the number of kilograms of Cu in 3.71×10^3 kg of chalcopyrite.

Strategy Chalcopyrite is composed of Cu, Fe, and S. The mass due to Cu is based on its percentage by mass in the compound. How do we calculate mass percent of an element?

Solution The molar masses of Cu and $CuFeS_2$ are 63.55 g and 183.5 g, respectively. The mass percent of Cu is therefore

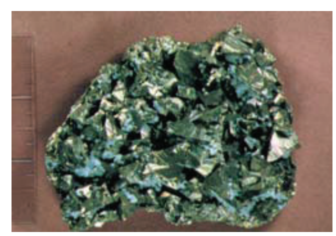
$$\begin{aligned}\%\text{Cu} &= \frac{\text{molar mass of Cu}}{\text{molar mass of CuFeS}_2} \times 100\% \\ &= \frac{63.55\text{ g}}{183.5\text{ g}} \times 100\% = 34.63\%\end{aligned}$$

To calculate the mass of Cu in a 3.71×10^3 kg sample of $CuFeS_2$, we need to convert the percentage to a fraction (that is, convert 34.63 percent to 34.63/100, or 0.3463) and write

$$\text{mass of Cu in CuFeS}_2 = 0.3463 \times (3.71 \times 10^3\text{ kg}) = \boxed{1.28 \times 10^3\text{ kg}}$$

Check As a ball-park estimate, note that the mass percent of Cu is roughly 33 percent, so that a third of the mass should be Cu; that is, $\frac{1}{3} \times 3.71 \times 10^3\text{ kg} \approx 1.24 \times 10^3\text{ kg}$. This quantity is quite close to the answer.

Practice Exercise Calculate the number of grams of Al in 371 g of Al_2O_3.



Chalcopyrite.

Similar problem: 3.45.

3.6 Experimental Determination of Empirical Formulas

The fact that we can determine the empirical formula of a compound if we know the percent composition enables us to identify compounds experimentally. The procedure is as follows. First, chemical analysis tells us the number of grams of each element present in a given amount of a compound. Then, we convert the quantities in grams to number of moles of each element. Finally, using the method given in Example 3.9, we find the empirical formula of the compound.

As a specific example, let us consider the compound ethanol. When ethanol is burned in an apparatus such as that shown in Figure 3.6, carbon dioxide (CO_2) and water (H_2O) are given off. Because neither carbon nor hydrogen was in the inlet gas, we can conclude that both carbon (C) and hydrogen (H) were present in ethanol and that oxygen (O) may also be present. (Molecular oxygen was added in the combustion process, but some of the oxygen may also have come from the original ethanol sample.)

The masses of CO_2 and of H_2O produced can be determined by measuring the increase in mass of the CO_2 and H_2O absorbers, respectively. Suppose that in one experiment the combustion of 11.5 g of ethanol produced 22.0 g of CO_2 and 13.5 g of H_2O. We can calculate the mass of carbon and hydrogen in the original 11.5-g sample of ethanol as follows:

$$\begin{aligned}
\text{mass of C} &= 22.0\ \cancel{\text{g CO}_2} \times \frac{1\ \cancel{\text{mol CO}_2}}{44.01\ \cancel{\text{g CO}_2}} \times \frac{1\ \cancel{\text{mol C}}}{1\ \cancel{\text{mol CO}_2}} \times \frac{12.01\ \text{g C}}{1\ \cancel{\text{mol C}}} \\
&= 6.00\ \text{g C} \\
\text{mass of H} &= 13.5\ \cancel{\text{g H}_2\text{O}} \times \frac{1\ \cancel{\text{mol H}_2\text{O}}}{18.02\ \cancel{\text{g H}_2\text{O}}} \times \frac{2\ \cancel{\text{mol H}}}{1\ \cancel{\text{mol H}_2\text{O}}} \times \frac{1.008\ \text{g H}}{1\ \cancel{\text{mol H}}} \\
&= 1.51\ \text{g H}
\end{aligned}$$

Thus, 11.5 g of ethanol contains 6.00 g of carbon and 1.51 g of hydrogen. The remainder must be oxygen, whose mass is

$$\begin{aligned}
\text{mass of O} &= \text{mass of sample} - (\text{mass of C} + \text{mass of H}) \\
&= 11.5\ \text{g} - (6.00\ \text{g} + 1.51\ \text{g}) \\
&= 4.0\ \text{g}
\end{aligned}$$

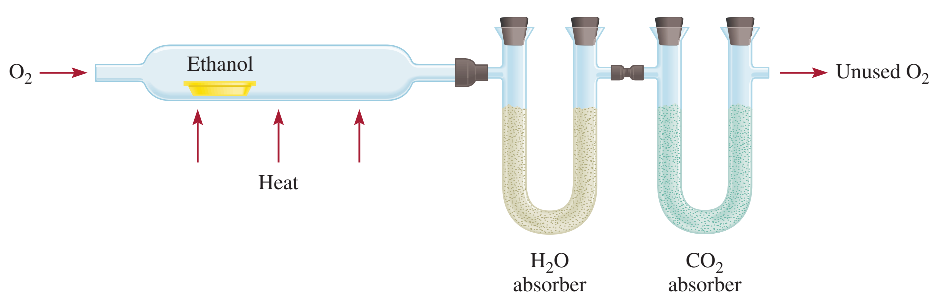


Figure 3.6 *Apparatus for determining the empirical formula of ethanol. The absorbers are substances that can retain water and carbon dioxide, respectively.*

The number of moles of each element present in 11.5 g of ethanol is

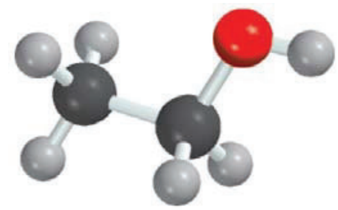
$$\text{moles of C} = 6.00\ \cancel{\text{g C}} \times \frac{1\ \text{mol C}}{12.01\ \cancel{\text{g C}}} = 0.500\ \text{mol C}$$

$$\text{moles of H} = 1.51\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.008\ \cancel{\text{g H}}} = 1.50\ \text{mol H}$$

$$\text{moles of O} = 4.0\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = 0.25\ \text{mol O}$$

The formula of ethanol is therefore $C_{0.50}H_{1.5}O_{0.25}$ (we round off the number of moles to two significant figures). Because the number of atoms must be an integer, we divide the subscripts by 0.25, the smallest subscript, and obtain for the empirical formula C_2H_6O.

Now we can better understand the word "empirical," which literally means "based only on observation and measurement." The empirical formula of ethanol is determined from analysis of the compound in terms of its component elements. No knowledge of how the atoms are linked together in the compound is required.


It happens that the molecular formula of ethanol is the same as its empirical formula.

Determination of Molecular Formulas

The formula calculated from percent composition by mass is always the empirical formula because the subscripts in the formula are always reduced to the smallest whole numbers. To calculate the actual, molecular formula we must know the *approximate* molar mass of the compound in addition to its empirical formula. Knowing that the molar mass of a compound must be an integral multiple of the molar mass of its empirical formula, we can use the molar mass to find the molecular formula, as Example 3.11 demonstrates.

EXAMPLE 3.11

A sample of a compound contains 1.52 g of nitrogen (N) and 3.47 g of oxygen (O). The molar mass of this compound is between 90 g and 95 g. Determine the molecular formula and the accurate molar mass of the compound.

Strategy To determine the molecular formula, we first need to determine the empirical formula. How do we convert between grams and moles? Comparing the empirical molar mass to the experimentally determined molar mass will reveal the relationship between the empirical formula and molecular formula.

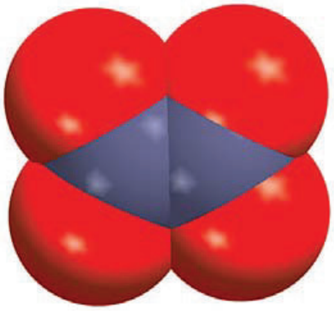
Solution We are given grams of N and O. Use molar mass as a conversion factor to convert grams to moles of each element. Let n represent the number of moles of each element. We write

$$n_N = 1.52\ \cancel{\text{g N}} \times \frac{1\ \text{mol N}}{14.01\ \cancel{\text{g N}}} = 0.108\ \text{mol N}$$

$$n_O = 3.47\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = 0.217\ \text{mol O}$$

Thus, we arrive at the formula $N_{0.108}O_{0.217}$, which gives the identity and the ratios of atoms present. However, chemical formulas are written with whole numbers. Try to convert to whole numbers by dividing the subscripts by the smaller subscript (0.108). After rounding off, we obtain NO_2 as the empirical formula.

(Continued)



N_2O_4

The molecular formula might be the same as the empirical formula or some integral multiple of it (for example, two, three, four, or more times the empirical formula). Comparing the ratio of the molar mass to the molar mass of the empirical formula will show the integral relationship between the empirical and molecular formulas. The molar mass of the empirical formula NO_2 is

$$\text{empirical molar mass} = 14.01 \text{ g} + 2(16.00 \text{ g}) = 46.01 \text{ g}$$

Next, we determine the ratio between the molar mass and the empirical molar mass

$$\frac{\text{molar mass}}{\text{empirical molar mass}} = \frac{90 \text{ g}}{46.01 \text{ g}} \approx 2$$

The molar mass is twice the empirical molar mass. This means that there are two NO_2 units in each molecule of the compound, and the molecular formula is $(NO_2)_2$ or N_2O_4.

The actual molar mass of the compound is two times the empirical molar mass, that is, 2(46.01 g) or 92.02 g, which is between 90 g and 95 g.

Check Note that in determining the molecular formula from the empirical formula, we need only know the *approximate* molar mass of the compound. The reason is that the true molar mass is an integral multiple (1×, 2×, 3×, . . .) of the empirical molar mass. Therefore, the ratio (molar mass/empirical molar mass) will always be close to an integer.

Practice Exercise A sample of a compound containing boron (B) and hydrogen (H) contains 6.444 g of B and 1.803 g of H. The molar mass of the compound is about 30 g. What is its molecular formula?

3.7 Chemical Reactions and Chemical Equations

Having discussed the masses of atoms and molecules, we turn next to what happens to atoms and molecules in a ***chemical reaction,*** *a process in which a substance (or substances) is changed into one or more new substances.* To communicate with one another about chemical reactions, chemists have devised a standard way to represent them using chemical equations. A ***chemical equation*** *uses chemical symbols to show what happens during a chemical reaction.* In this section we will learn how to write chemical equations and balance them.

Writing Chemical Equations

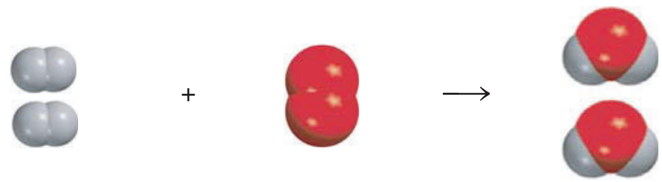
Consider what happens when hydrogen gas (H_2) burns in air (which contains oxygen, O_2) to form water (H_2O). This reaction can be represented by the chemical equation

$$H_2 + O_2 \longrightarrow H_2O \tag{3.2}$$

where the "plus" sign means "reacts with" and the arrow means "to yield." Thus, this symbolic expression can be read: "Molecular hydrogen reacts with molecular oxygen to yield water." The reaction is assumed to proceed from left to right as the arrow indicates.

We use the law of conservation of mass as our guide in balancing chemical equations.

Equation (3.2) is not complete, however, because there are twice as many oxygen atoms on the left side of the arrow (two) as on the right side (one). To conform with the law of conservation of mass, there must be the same number of each type of atom on both sides of the arrow; that is, we must have as many atoms after the reaction



Two hydrogen molecules + One oxygen molecule ⟶ Two water molecules

$$2H_2 + O_2 \longrightarrow 2H_2O$$

Figure 3.7 *Three ways of representing the combustion of hydrogen. In accordance with the law of conservation of mass, the number of each type of atom must be the same on both sides of the equation.*

ends as we did before it started. We can *balance* Equation (3.2) by placing the appropriate coefficient (2 in this case) in front of H_2 and H_2O:

$$2H_2 + O_2 \longrightarrow 2H_2O$$

When the coefficient is 1, as in the case of O_2, it is not shown.

This *balanced chemical equation* shows that "two hydrogen molecules can combine or react with one oxygen molecule to form two water molecules" (Figure 3.7). Because the ratio of the number of molecules is equal to the ratio of the number of moles, the equation can also be read as "2 moles of hydrogen molecules react with 1 mole of oxygen molecules to produce 2 moles of water molecules." We know the mass of a mole of each of these substances, so we can also interpret the equation as "4.04 g of H_2 react with 32.00 g of O_2 to give 36.04 g of H_2O." These three ways of reading the equation are summarized in Table 3.1.

We refer to H_2 and O_2 in Equation (3.2) as ***reactants,*** which are *the starting materials in a chemical reaction.* Water is the ***product,*** which is *the substance formed as a result of a chemical reaction.* A chemical equation, then, is just the chemist's shorthand description of a reaction. In a chemical equation, the reactants are conventionally written on the left and the products on the right of the arrow:

$$\text{reactants} \longrightarrow \text{products}$$

To provide additional information, chemists often indicate the physical states of the reactants and products by using the letters *g, l,* and *s* to denote gas, liquid, and solid, respectively. For example,

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$
$$2HgO(s) \longrightarrow 2Hg(l) + O_2(g)$$

The procedure for balancing chemical equations is shown on p. 96.

To represent what happens when sodium chloride (NaCl) is added to water, we write

$$NaCl(s) \xrightarrow{H_2O} NaCl(aq)$$

where *aq* denotes the aqueous (that is, water) environment. Writing H_2O above the arrow symbolizes the physical process of dissolving a substance in water, although it is sometimes left out for simplicity.

TABLE 3.1 Interpretation of a Chemical Equation

$2H_2$	$+ O_2$	$\longrightarrow$	$2H_2O$
Two molecules	+ one molecule	$\longrightarrow$	two molecules
2 moles	+ 1 mole	$\longrightarrow$	2 moles
$\underbrace{2(2.02\ g) = 4.04\ g + 32.00\ g}_{36.04\ g\ \text{reactants}}$		$\longrightarrow$	$\underbrace{2(18.02\ g) = 36.04\ g}_{36.04\ g\ \text{product}}$

Knowing the states of the reactants and products is especially useful in the laboratory. For example, when potassium bromide (KBr) and silver nitrate ($AgNO_3$) react in an aqueous environment, a solid, silver bromide (AgBr), is formed. This reaction can be represented by the equation:

$$KBr(aq) + AgNO_3(aq) \longrightarrow KNO_3(aq) + AgBr(s)$$

If the physical states of reactants and products are not given, an uninformed person might try to bring about the reaction by mixing solid KBr with solid $AgNO_3$. These solids would react very slowly or not at all. Imagining the process on the microscopic level, we can understand that for a product like silver bromide to form, the Ag^+ and Br^- ions would have to come in contact with each other. However, these ions are locked in place in their solid compounds and have little mobility. (Here is an example of how we explain a phenomenon by thinking about what happens at the molecular level, as discussed in Section 1.2.)

Balancing Chemical Equations

Suppose we want to write an equation to describe a chemical reaction that we have just carried out in the laboratory. How should we go about doing it? Because we know the identities of the reactants, we can write their chemical formulas. The identities of products are more difficult to establish. For simple reactions it is often possible to guess the product(s). For more complicated reactions involving three or more products, chemists may need to perform further tests to establish the presence of specific compounds.

Once we have identified all the reactants and products and have written the correct formulas for them, we assemble them in the conventional sequence—reactants on the left separated by an arrow from products on the right. The equation written at this point is likely to be *unbalanced;* that is, the number of each type of atom on one side of the arrow differs from the number on the other side. In general, we can balance a chemical equation by the following steps:

1. Identify all reactants and products and write their correct formulas on the left side and right side of the equation, respectively.
2. Begin balancing the equation by trying different coefficients to make the number of atoms of each element the same on both sides of the equation. We can change the coefficients (the numbers preceding the formulas) but not the subscripts (the numbers within formulas). Changing the subscripts would change the identity of the substance. For example, $2NO_2$ means "two molecules of nitrogen dioxide," but if we double the subscripts, we have N_2O_4, which is the formula of dinitrogen tetroxide, a completely different compound.
3. First, look for elements that appear only once on each side of the equation with the same number of atoms on each side: The formulas containing these elements must have the same coefficient. Therefore, there is no need to adjust the coefficients of these elements at this point. Next, look for elements that appear only once on each side of the equation but in unequal numbers of atoms. Balance these elements. Finally, balance elements that appear in two or more formulas on the same side of the equation.
4. Check your balanced equation to be sure that you have the same total number of each type of atoms on both sides of the equation arrow.


Heating potassium chlorate produces oxygen, which supports the combustion of wood splint.

Let's consider a specific example. In the laboratory, small amounts of oxygen gas can be prepared by heating potassium chlorate ($KClO_3$). The products are oxygen gas (O_2) and potassium chloride (KCl). From this information, we write

$$KClO_3 \longrightarrow KCl + O_2$$

(For simplicity, we omit the physical states of reactants and products.) All three elements (K, Cl, and O) appear only once on each side of the equation, but only for K and Cl do we have equal numbers of atoms on both sides. Thus, $KClO_3$ and KCl must have the same coefficient. The next step is to make the number of O atoms the same on both sides of the equation. Because there are three O atoms on the left and two O atoms on the right of the equation, we can balance the O atoms by placing a 2 in front of $KClO_3$ and a 3 in front of O_2.

$$2KClO_3 \longrightarrow KCl + 3O_2$$

Finally, we balance the K and Cl atoms by placing a 2 in front of KCl:

$$2KClO_3 \longrightarrow 2KCl + 3O_2 \tag{3.3}$$

As a final check, we can draw up a balance sheet for the reactants and products where the number in parentheses indicates the number of atoms of each element:

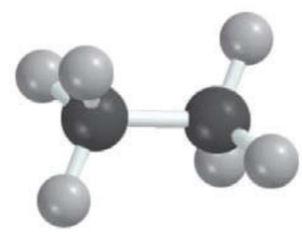
Reactants	Products
K (2)	K (2)
Cl (2)	Cl (2)
O (6)	O (6)

Note that this equation could also be balanced with coefficients that are multiples of 2 (for $KClO_3$), 2 (for KCl), and 3 (for O_2); for example,

$$4KClO_3 \longrightarrow 4KCl + 6O_2$$

However, it is common practice to use the *simplest* possible set of whole-number coefficients to balance the equation. Equation (3.3) conforms to this convention.

Now let us consider the combustion (that is, burning) of the natural gas component ethane (C_2H_6) in oxygen or air, which yields carbon dioxide (CO_2) and water. The unbalanced equation is


C_2H_6

$$C_2H_6 + O_2 \longrightarrow CO_2 + H_2O$$

We see that the number of atoms is not the same on both sides of the equation for any of the elements (C, H, and O). In addition, C and H appear only once on each side of the equation; O appears in two compounds on the right side (CO_2 and H_2O). To balance the C atoms, we place a 2 in front of CO_2:

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + H_2O$$

To balance the H atoms, we place a 3 in front of H_2O:

$$C_2H_6 + O_2 \longrightarrow 2CO_2 + 3H_2O$$

At this stage, the C and H atoms are balanced, but the O atoms are not because there are seven O atoms on the right-hand side and only two O atoms on the left-hand side of the equation. This inequality of O atoms can be eliminated by writing $\frac{7}{2}$ in front of the O_2 on the left-hand side:

$$C_2H_6 + \tfrac{7}{2}O_2 \longrightarrow 2CO_2 + 3H_2O$$

The "logic" for using $\frac{7}{2}$ as a coefficient is that there were seven oxygen atoms on the right-hand side of the equation, but only a pair of oxygen atoms (O_2) on the left. To balance them we ask how many *pairs* of oxygen atoms are needed to equal seven oxygen atoms. Just as 3.5 pairs of shoes equal seven shoes, $\frac{7}{2}O_2$ molecules equal seven O atoms. As the following tally shows, the equation is now balanced:

Reactants	Products
C (2)	C (2)
H (6)	H (6)
O (7)	O (7)

However, we normally prefer to express the coefficients as whole numbers rather than as fractions. Therefore, we multiply the entire equation by 2 to convert $\frac{7}{2}$ to 7:

$$2C_2H_6 + 7O_2 \longrightarrow 4CO_2 + 6H_2O$$

The final tally is

Reactants	Products
C (4)	C (4)
H (12)	H (12)
O (14)	O (14)

Note that the coefficients used in balancing the last equation are the smallest possible set of whole numbers.

In Example 3.12 we will continue to practice our equation-balancing skills.

EXAMPLE 3.12

When aluminum metal is exposed to air, a protective layer of aluminum oxide (Al_2O_3) forms on its surface. This layer prevents further reaction between aluminum and oxygen, and it is the reason that aluminum beverage cans do not corrode. [In the case of iron, the rust, or iron(III) oxide, that forms is too porous to protect the iron metal underneath, so rusting continues.] Write a balanced equation for the formation of Al_2O_3.

Strategy Remember that the formula of an element or compound cannot be changed when balancing a chemical equation. The equation is balanced by placing the appropriate coefficients in front of the formulas. Follow the procedure described on p. 96.

Solution The unbalanced equation is

$$Al + O_2 \longrightarrow Al_2O_3$$

In a balanced equation, the number and types of atoms on each side of the equation must be the same. We see that there is one Al atom on the reactants side and there are two Al atoms on the product side. We can balance the Al atoms by placing a coefficient of 2 in front of Al on the reactants side.

$$2Al + O_2 \longrightarrow Al_2O_3$$

There are two O atoms on the reactants side, and three O atoms on the product side of the equation. We can balance the O atoms by placing a coefficient of $\frac{3}{2}$ in front of O_2 on the reactants side.

$$2Al + \frac{3}{2}O_2 \longrightarrow Al_2O_3$$

This is a balanced equation. However, equations are normally balanced with the smallest set of *whole* number coefficients. Multiplying both sides of the equation by 2 gives whole number coefficients.

$$2(2Al + \frac{3}{2}O_2 \longrightarrow Al_2O_3)$$

or

$$\boxed{4Al + 3O_2 \longrightarrow 2Al_2O_3}$$

(Continued)

Check For an equation to be balanced, the number and types of atoms on each side of the equation must be the same. The final tally is

Reactants	Products
Al (4)	Al (4)
O (6)	O (6)

The equation is balanced. Also, the coefficients are reduced to the simplest set of whole numbers.

Practice Exercise Balance the equation representing the reaction between iron(III) oxide, Fe_2O_3, and carbon monoxide (CO) to yield iron (Fe) and carbon dioxide (CO_2).

3.8 Amounts of Reactants and Products

A basic question raised in the chemical laboratory is "How much product will be formed from specifi c amounts of starting materials (reactants)?" Or in some cases, we might ask the reverse question: "How much starting material must be used to obtain a specifi c amount of product?" To interpret a reaction quantitatively, we need to apply our knowledge of molar masses and the mole concept. ***Stoichiometry*** is *the quantitative study of reactants and products in a chemical reaction.*

Whether the units given for reactants (or products) are moles, grams, liters (for gases), or some other units, we use moles to calculate the amount of product formed in a reaction. This approach is called the ***mole method,*** which means simply that *the stoichiometric coeffi c ients in a chemical equation can be interpreted as the number of moles of each substance.* For example, industrially ammonia is synthesized from hydrogen and nitrogen as follows:

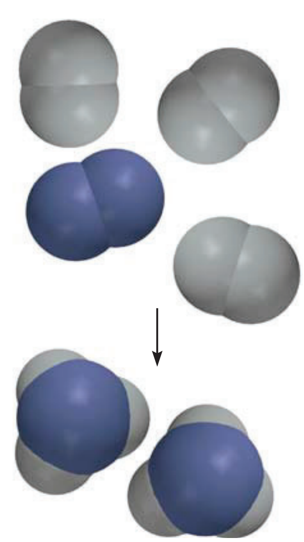
$$N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$$

The stoichiometric coeffi c ients show that one molecule of N_2 reacts with three molecules of H_2 to form two molecules of NH_3. It follows that the relative numbers of moles are the same as the relative number of molecules:

$N_2(g)$	+	$3H_2(g)$	$\longrightarrow$	$2NH_3(g)$
1 molecule		3 molecules		2 molecules
6.022×10^{23} molecules		$3(6.022 \times 10^{23}$ molecules)		$2(6.022 \times 10^{23}$ molecules)
1 mol		3 mol		2 mol

Thus, this equation can also be read as "1 mole of N_2 gas combines with 3 moles of H_2 gas to form 2 moles of NH_3 gas." In stoichiometric calculations, we say that three moles of H_2 are equivalent to two moles of NH_3, that is,

$$3 \text{ mol } H_2 \simeq 2 \text{ mol } NH_3$$



The synthesis of NH_3 from H_2 and N_2.

where the symbol $\simeq$ means "stoichiometrically equivalent to" or simply "equivalent to." This relationship enables us to write the conversion factors

$$\frac{3 \text{ mol } H_2}{2 \text{ mol } NH_3} \quad \text{and} \quad \frac{2 \text{ mol } NH_3}{3 \text{ mol } H_2}$$

Similarly, we have 1 mol $N_2 \simeq$ 2 mol NH_3 and 1 mol $N_2 \simeq$ 3 mol H_2.

Let's consider a simple example in which 6.0 moles of H_2 react completely with N_2 to form NH_3. To calculate the amount of NH_3 produced in moles, we use the conversion factor that has H_2 in the denominator and write

$$\begin{aligned} \text{moles of } NH_3 \text{ produced} &= 6.0 \cancel{\text{mol } H_2} \times \frac{2 \text{ mol } NH_3}{3 \cancel{\text{mol } H_2}} \\ &= 4.0 \text{ mol } NH_3 \end{aligned}$$

Now suppose 16.0 g of H_2 react completely with N_2 to form NH_3. How many grams of NH_3 will be formed? To do this calculation, we note that the link between H_2 and NH_3 is the mole ratio from the balanced equation. So we need to first convert grams of H_2 to moles of H_2, then to moles of NH_3, and finally to grams of NH_3. The conversion steps are

$$\text{grams of } H_2 \longrightarrow \text{moles of } H_2 \longrightarrow \text{moles of } NH_3 \longrightarrow \text{grams of } NH_3$$

First, we convert 16.0 g of H_2 to number of moles of H_2, using the molar mass of H_2 as the conversion factor:

$$\begin{aligned} \text{moles of } H_2 &= 16.0 \cancel{\text{g } H_2} \times \frac{1 \text{ mol } H_2}{2.016 \cancel{\text{g } H_2}} \\ &= 7.94 \text{ mol } H_2 \end{aligned}$$

Next, we calculate the number of moles of NH_3 produced.

$$\begin{aligned} \text{moles of } NH_3 &= 7.94 \cancel{\text{mol } H_2} \times \frac{2 \text{ mol } NH_3}{3 \cancel{\text{mol } H_2}} \\ &= 5.29 \text{ mol } NH_3 \end{aligned}$$

Finally, we calculate the mass of NH_3 produced in grams using the molar mass of NH_3 as the conversion factor

$$\begin{aligned} \text{grams of } NH_3 &= 5.29 \cancel{\text{mol } NH_3} \times \frac{17.03 \text{ g } NH_3}{1 \cancel{\text{mol } NH_3}} \\ &= 90.1 \text{ g } NH_3 \end{aligned}$$

These three separate calculations can be combined in a single step as follows:

$$\begin{aligned} \text{grams of } NH_3 &= 16.0 \cancel{\text{g } H_2} \times \frac{1 \cancel{\text{mol } H_2}}{2.016 \cancel{\text{g } H_2}} \times \frac{2 \cancel{\text{mol } NH_3}}{3 \cancel{\text{mol } H_2}} \times \frac{17.03 \text{ g } NH_3}{1 \cancel{\text{mol } NH_3}} \\ &= 90.1 \text{ g } NH_3 \end{aligned}$$

Similarly, we can calculate the mass in grams of N_2 consumed in this reaction. The conversion steps are

$$\text{grams of } H_2 \longrightarrow \text{moles of } H_2 \longrightarrow \text{moles of } N_2 \longrightarrow \text{grams of } N_2$$

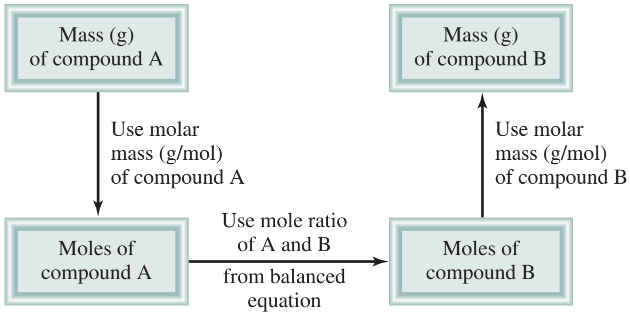


Figure 3.8 *The procedure for calculating the amounts of reactants or products in a reaction using the mole method.*

By using the relationship 1 mol N_2 $\simeq$ 3 mol H_2, we write

$$\begin{aligned}\text{grams of } N_2 &= 16.0\ \cancel{\text{g } H_2} \times \frac{1\ \cancel{\text{mol } H_2}}{2.016\ \cancel{\text{g } H_2}} \times \frac{1\ \cancel{\text{mol } N_2}}{3\ \cancel{\text{mol } H_2}} \times \frac{28.02\text{ g } N_2}{1\ \cancel{\text{mol } N_2}} \\ &= 74.1\text{ g } N_2\end{aligned}$$

The general approach for solving stoichiometry problems is summarized next.

1. Write a balanced equation for the reaction.
2. Convert the given amount of the reactant (in grams or other units) to number of moles.
3. Use the mole ratio from the balanced equation to calculate the number of moles of product formed.
4. Convert the moles of product to grams (or other units) of product.

Figure 3.8 shows these steps. Sometimes we may be asked to calculate the amount of a reactant needed to form a specific amount of product. In those cases, we can reverse the steps shown in Figure 3.8.

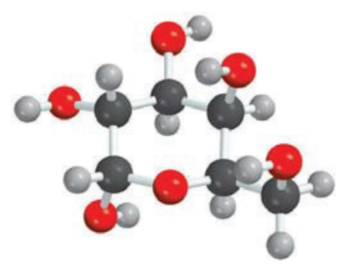
Examples 3.13 and 3.14 illustrate the application of this approach.

EXAMPLE 3.13

The food we eat is degraded, or broken down, in our bodies to provide energy for growth and function. A general overall equation for this very complex process represents the degradation of glucose ($C_6H_{12}O_6$) to carbon dioxide (CO_2) and water (H_2O):

$$C_6H_{12}O_6 + 6O_2 \longrightarrow 6CO_2 + 6H_2O$$

If 856 g of $C_6H_{12}O_6$ is consumed by a person over a certain period, what is the mass of CO_2 produced?



$C_6H_{12}O_6$

Strategy Looking at the balanced equation, how do we compare the amounts of $C_6H_{12}O_6$ and CO_2? We can compare them based on the *mole ratio* from the balanced equation. Starting with grams of $C_6H_{12}O_6$, how do we convert to moles of $C_6H_{12}O_6$? Once moles of CO_2 are determined using the mole ratio from the balanced equation, how do we convert to grams of CO_2?

Solution We follow the preceding steps and Figure 3.8.

(Continued)

Step 1: The balanced equation is given in the problem.

Step 2: To convert grams of $C_6H_{12}O_6$ to moles of $C_6H_{12}O_6$, we write

$$856 \cancel{\text{g } C_6H_{12}O_6} \times \frac{1 \text{ mol } C_6H_{12}O_6}{180.2 \cancel{\text{g } C_6H_{12}O_6}} = 4.750 \text{ mol } C_6H_{12}O_6$$

Step 3: From the mole ratio, we see that 1 mol $C_6H_{12}O_6 \simeq$ 6 mol CO_2. Therefore, the number of moles of CO_2 formed is

$$4.750 \cancel{\text{mol } C_6H_{12}O_6} \times \frac{6 \text{ mol } CO_2}{1 \cancel{\text{mol } C_6H_{12}O_6}} = 28.50 \text{ mol } CO_2$$

Step 4: Finally, the number of grams of CO_2 formed is given by

$$28.50 \cancel{\text{mol } CO_2} \times \frac{44.01 \text{ g } CO_2}{1 \cancel{\text{mol } CO_2}} = 1.25 \times 10^3 \text{ g } CO_2$$

After some practice, we can combine the conversion steps

$$\text{grams of } C_6H_{12}O_6 \longrightarrow \text{moles of } C_6H_{12}O_6 \longrightarrow \text{moles of } CO_2 \longrightarrow \text{grams of } CO_2$$

into one equation:

$$\begin{aligned}\text{mass of } CO_2 &= 856 \cancel{\text{g } C_6H_{12}O_6} \times \frac{1 \cancel{\text{mol } C_6H_{12}O_6}}{180.2 \cancel{\text{g } C_6H_{12}O_6}} \times \frac{6 \cancel{\text{mol } CO_2}}{1 \cancel{\text{mol } C_6H_{12}O_6}} \times \frac{44.01 \text{ g } CO_2}{1 \cancel{\text{mol } CO_2}} \\ &= 1.25 \times 10^3 \text{ g } CO_2\end{aligned}$$

Check Does the answer seem reasonable? Should the mass of CO_2 produced be larger than the mass of $C_6H_{12}O_6$ reacted, even though the molar mass of CO_2 is considerably less than the molar mass of $C_6H_{12}O_6$? What is the mole ratio between CO_2 and $C_6H_{12}O_6$?

Practice Exercise Methanol (CH_3OH) burns in air according to the equation

$$2CH_3OH + 3O_2 \longrightarrow 2CO_2 + 4H_2O$$

If 209 g of methanol are used up in a combustion process, what is the mass of H_2O produced?

Lithium reacting with water to produce hydrogen gas.

EXAMPLE 3.14

All alkali metals react with water to produce hydrogen gas and the corresponding alkali metal hydroxide. A typical reaction is that between lithium and water:

$$2Li(s) + 2H_2O(l) \longrightarrow 2LiOH(aq) + H_2(g)$$

How many grams of Li are needed to produce 9.89 g of H_2?

Strategy The question asks for number of grams of reactant (Li) to form a specific amount of product (H_2). Therefore, we need to reverse the steps shown in Figure 3.8. From the equation we see that 2 mol Li $\simeq$ 1 mol H_2.

Solution The conversion steps are

$$\text{grams of } H_2 \longrightarrow \text{moles of } H_2 \longrightarrow \text{moles of Li} \longrightarrow \text{grams of Li}$$

(Continued)

Combining these steps into one equation, we write

$$9.89\ \cancel{g\ H_2} \times \frac{1\ \cancel{mol\ H_2}}{2.016\ \cancel{g\ H_2}} \times \frac{2\ \cancel{mol\ Li}}{1\ \cancel{mol\ H_2}} \times \frac{6.941\ g\ Li}{1\ \cancel{mol\ Li}} = \boxed{68.1\ g\ Li}$$

Check There are roughly 5 moles of H_2 in 9.89 g H_2, so we need 10 moles of Li. From the approximate molar mass of Li (7 g), does the answer seem reasonable?

Practice Exercise The reaction between nitric oxide (NO) and oxygen to form nitrogen dioxide (NO_2) is a key step in photochemical smog formation:

$$2NO(g) + O_2(g) \longrightarrow 2NO_2(g)$$

How many grams of O_2 are needed to produce 2.21 g of NO_2?

3.9 Limiting Reagents

When a chemist carries out a reaction, the reactants are usually not present in exact ***stoichiometric amounts,*** that is, *in the proportions indicated by the balanced equation.* Because the goal of a reaction is to produce the maximum quantity of a useful compound from the starting materials, frequently a large excess of one reactant is supplied to ensure that the more expensive reactant is completely converted to the desired product. Consequently, some reactant will be left over at the end of the reaction. *The reactant used up first in a reaction* is called the ***limiting reagent,*** because the maximum amount of product formed depends on how much of this reactant was originally present. When this reactant is used up, no more product can be formed. ***Excess reagents*** are the *reactants present in quantities greater than necessary to react with the quantity of the limiting reagent.*

The concept of the limiting reagent is analogous to the relationship between men and women in a dance contest at a club. If there are 14 men and only 9 women, then only 9 female/male pairs can compete. Five men will be left without partners. The number of women thus *limits* the number of men that can dance in the contest, and there is an *excess* of men.

Consider the industrial synthesis of methanol (CH_3OH) from carbon monoxide and hydrogen at high temperatures:

$$CO(g) + 2H_2(g) \longrightarrow CH_3OH(g)$$

Suppose initially we have 4 moles of CO and 6 moles of H_2 (Figure 3.9). One way to determine which of two reactants is the limiting reagent is to calculate the number

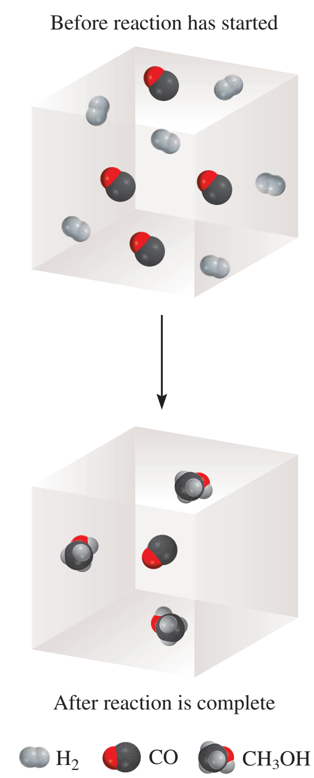


Figure 3.9 *At the start of the reaction, there were six H_2 molecules and four CO molecules. At the end, all the H_2 molecules are gone and only one CO molecule is left. Therefore, the H_2 molecule is the limiting reagent and CO is the excess reagent. Each molecule can also be treated as one mole of the substance in this reaction.*

of moles of CH_3OH obtained based on the initial quantities of CO and H_2. From the preceding definition, we see that only the limiting reagent will yield the *smaller* amount of the product. Starting with 4 moles of CO, we find the number of moles of CH_3OH produced is

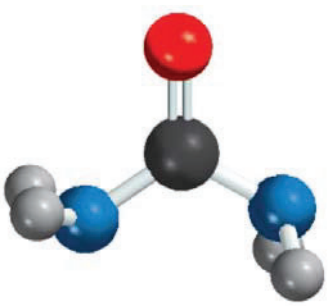
$$4\ \cancel{\text{mol CO}} \times \frac{1\ \text{mol CH}_3\text{OH}}{1\ \cancel{\text{mol CO}}} = 4\ \text{mol CH}_3\text{OH}$$

and starting with 6 moles of H_2, the number of moles of CH_3OH formed is

$$6\ \cancel{\text{mol H}_2} \times \frac{1\ \text{mol CH}_3\text{OH}}{2\ \cancel{\text{mol H}_2}} = 3\ \text{mol CH}_3\text{OH}$$

Because H_2 results in a smaller amount of CH_3OH, it must be the limiting reagent. Therefore, CO is the excess reagent.

In stoichiometric calculations involving limiting reagents, the first step is to decide which reactant is the limiting reagent. After the limiting reagent has been identified, the rest of the problem can be solved as outlined in Section 3.8. Example 3.15 illustrates this approach.



$(NH_2)_2CO$

EXAMPLE 3.15

Urea $[(NH_2)_2CO]$ is prepared by reacting ammonia with carbon dioxide:

$$2\text{NH}_3(g) + \text{CO}_2(g) \longrightarrow (\text{NH}_2)_2\text{CO}(aq) + \text{H}_2\text{O}(l)$$

In one process, 637.2 g of NH_3 are treated with 1142 g of CO_2. (a) Which of the two reactants is the limiting reagent? (b) Calculate the mass of $(NH_2)_2CO$ formed. (c) How much excess reagent (in grams) is left at the end of the reaction?

(a) Strategy The reactant that produces fewer moles of product is the limiting reagent because it limits the amount of product that can be formed. How do we convert from the amount of reactant to amount of product? Perform this calculation for each reactant, then compare the moles of product, $(NH_2)_2CO$, formed by the given amounts of NH_3 and CO_2 to determine which reactant is the limiting reagent.

Solution We carry out two separate calculations. First, starting with 637.2 g of NH_3, we calculate the number of moles of $(NH_2)_2CO$ that could be produced if all the NH_3 reacted according to the following conversions:

$$\text{grams of NH}_3 \longrightarrow \text{moles of NH}_3 \longrightarrow \text{moles of (NH}_2)_2\text{CO}$$

Combining these conversions in one step, we write

$$\begin{aligned}\text{moles of (NH}_2)_2\text{CO} &= 637.2\ \cancel{\text{g NH}_3} \times \frac{1\ \cancel{\text{mol NH}_3}}{17.03\ \cancel{\text{g NH}_3}} \times \frac{1\ \text{mol (NH}_2)_2\text{CO}}{2\ \cancel{\text{mol NH}_3}} \\ &= 18.71\ \text{mol (NH}_2)_2\text{CO}\end{aligned}$$

Second, for 1142 g of CO_2, the conversions are

$$\text{grams of CO}_2 \longrightarrow \text{moles of CO}_2 \longrightarrow \text{moles of (NH}_2)_2\text{CO}$$

(Continued)

The number of moles of $(NH_2)_2CO$ that could be produced if all the CO_2 reacted is

$$\text{moles of } (NH_2)_2CO = 1142 \cancel{\text{ g } CO_2} \times \frac{1 \cancel{\text{ mol } CO_2}}{44.01 \cancel{\text{ g } CO_2}} \times \frac{1 \text{ mol } (NH_2)_2CO}{1 \cancel{\text{ mol } CO_2}}$$
$$= 25.95 \text{ mol } (NH_2)_2CO$$

It follows, therefore, that NH_3 must be the limiting reagent because it produces a smaller amount of $(NH_2)_2CO$.

(b) Strategy We determined the moles of $(NH_2)_2CO$ produced in part (a), using NH_3 as the limiting reagent. How do we convert from moles to grams?

Solution The molar mass of $(NH_2)_2CO$ is 60.06 g. We use this as a conversion factor to convert from moles of $(NH_2)_2CO$ to grams of $(NH_2)_2CO$:

$$\text{mass of } (NH_2)_2CO = 18.71 \cancel{\text{ mol } (NH_2)_2CO} \times \frac{60.06 \text{ g } (NH_2)_2CO}{1 \cancel{\text{ mol } (NH_2)_2CO}}$$
$$= \boxed{1124 \text{ g } (NH_2)_2CO}$$

Check Does your answer seem reasonable? 18.71 moles of product are formed. What is the mass of 1 mole of $(NH_2)_2CO$?

(c) Strategy Working backward, we can determine the amount of CO_2 that reacted to produce 18.71 moles of $(NH_2)_2CO$. The amount of CO_2 left over is the difference between the initial amount and the amount reacted.

Solution Starting with 18.71 moles of $(NH_2)_2CO$, we can determine the mass of CO_2 that reacted using the mole ratio from the balanced equation and the molar mass of CO_2. The conversion steps are

$$\text{moles of } (NH_2)_2CO \longrightarrow \text{moles of } CO_2 \longrightarrow \text{grams of } CO_2$$

so that

$$\text{mass of } CO_2 \text{ reacted} = 18.71 \cancel{\text{ mol } (NH_2)_2CO} \times \frac{1 \cancel{\text{ mol } CO_2}}{1 \cancel{\text{ mol } (NH_2)_2CO}} \times \frac{44.01 \text{ g } CO_2}{1 \cancel{\text{ mol } CO_2}}$$
$$= 823.4 \text{ g } CO_2$$

The amount of CO_2 remaining (in excess) is the difference between the initial amount (1142 g) and the amount reacted (823.4 g):

$$\text{mass of } CO_2 \text{ remaining} = 1142 \text{ g} - 823.4 \text{ g} = \boxed{319 \text{ g}}$$

Practice Exercise The reaction between aluminum and iron(III) oxide can generate temperatures approaching 3000°C and is used in welding metals:

$$2Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2Fe$$

In one process, 124 g of Al are reacted with 601 g of Fe_2O_3. (a) Calculate the mass (in grams) of Al_2O_3 formed. (b) How much of the excess reagent is left at the end of the reaction?

Example 3.15 brings out an important point. In practice, chemists usually choose the more expensive chemical as the limiting reagent so that all or most of it will be consumed in the reaction. In the synthesis of urea, NH_3 is invariably the limiting reagent because it is much more expensive than CO_2.

3.10 Reaction Yield

Keep in mind that the theoretical yield is the yield that you calculate using the balanced equation. The actual yield is the yield obtained by carrying out the reaction.

The amount of limiting reagent present at the start of a reaction determines the ***theoretical yield*** of the reaction, that is, *the amount of product that would result if all the limiting reagent reacted.* The theoretical yield, then, is the *maximum* obtainable yield, predicted by the balanced equation. In practice, the ***actual yield,*** or *the amount of product actually obtained from a reaction,* is almost always less than the theoretical yield. There are many reasons for the difference between actual and theoretical yields. For instance, many reactions are reversible, and so they do not proceed 100 percent from left to right. Even when a reaction is 100 percent complete, it may be difficult to recover all of the product from the reaction medium (say, from an aqueous solution). Some reactions are complex in the sense that the products formed may react further among themselves or with the reactants to form still other products. These additional reactions will reduce the yield of the first reaction.

To determine how efficient a given reaction is, chemists often figure the ***percent yield,*** which describes *the proportion of the actual yield to the theoretical yield.* It is calculated as follows:

$$\%\text{yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% \tag{3.4}$$

Percent yields may range from a fraction of 1 percent to 100 percent. Chemists strive to maximize the percent yield in a reaction. Factors that can affect the percent yield include temperature and pressure. We will study these effects later.

In Example 3.16 we will calculate the yield of an industrial process.

The frame of this bicycle is made of titanium.

EXAMPLE 3.16

Titanium is a strong, lightweight, corrosion-resistant metal that is used in rockets, aircraft, jet engines, and bicycle frames. It is prepared by the reaction of titanium(IV) chloride with molten magnesium between 950°C and 1150°C:

$$TiCl_4(g) + 2Mg(l) \longrightarrow Ti(s) + 2MgCl_2(l)$$

In a certain industrial operation 3.54×10^7 g of $TiCl_4$ are reacted with 1.13×10^7 g of Mg. (a) Calculate the theoretical yield of Ti in grams. (b) Calculate the percent yield if 7.91×10^6 g of Ti are actually obtained.

(Continued)

(a) Strategy Because there are two reactants, this is likely to be a limiting reagent problem. The reactant that produces fewer moles of product is the limiting reagent. How do we convert from amount of reactant to amount of product? Perform this calculation for each reactant, then compare the moles of product, Ti, formed.

Solution Carry out two separate calculations to see which of the two reactants is the limiting reagent. First, starting with 3.54×10^7 g of $TiCl_4$, calculate the number of moles of Ti that could be produced if all the $TiCl_4$ reacted. The conversions are

$$\text{grams of TiCl}_4 \longrightarrow \text{moles of TiCl}_4 \longrightarrow \text{moles of Ti}$$

so that

$$\begin{aligned}\text{moles of Ti} &= 3.54 \times 10^7\ \cancel{\text{g TiCl}_4} \times \frac{1\ \cancel{\text{mol TiCl}_4}}{189.7\ \cancel{\text{g TiCl}_4}} \times \frac{1\ \text{mol Ti}}{1\ \cancel{\text{mol TiCl}_4}}\\ &= 1.87 \times 10^5\ \text{mol Ti}\end{aligned}$$

Next, we calculate the number of moles of Ti formed from 1.13×10^7 g of Mg. The conversion steps are

$$\text{grams of Mg} \longrightarrow \text{moles of Mg} \longrightarrow \text{moles of Ti}$$

and we write

$$\begin{aligned}\text{moles of Ti} &= 1.13 \times 10^7\ \cancel{\text{g Mg}} \times \frac{1\ \cancel{\text{mol Mg}}}{24.31\ \cancel{\text{g Mg}}} \times \frac{1\ \text{mol Ti}}{2\ \cancel{\text{mol Mg}}}\\ &= 2.32 \times 10^5\ \text{mol Ti}\end{aligned}$$

Therefore, $TiCl_4$ is the limiting reagent because it produces a smaller amount of Ti. The mass of Ti formed is

$$1.87 \times 10^5\ \cancel{\text{mol Ti}} \times \frac{47.88\ \text{g Ti}}{1\ \cancel{\text{mol Ti}}} = \boxed{8.95 \times 10^6\ \text{g Ti}}$$

(b) Strategy The mass of Ti determined in part (a) is the theoretical yield. The amount given in part (b) is the actual yield of the reaction.

Solution The percent yield is given by

$$\begin{aligned}\%\text{yield} &= \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\%\\ &= \frac{7.91 \times 10^6\ \text{g}}{8.95 \times 10^6\ \text{g}} \times 100\%\\ &= \boxed{88.4\%}\end{aligned}$$

Check Should the percent yield be less than 100 percent?

Practice Exercise Industrially, vanadium metal, which is used in steel alloys, can be obtained by reacting vanadium(V) oxide with calcium at high temperatures:

$$5\text{Ca} + \text{V}_2\text{O}_5 \longrightarrow 5\text{CaO} + 2\text{V}$$

In one process, 1.54×10^3 g of V_2O_5 react with 1.96×10^3 g of Ca. (a) Calculate the theoretical yield of V. (b) Calculate the percent yield if 803 g of V are obtained.

Industrial processes usually involve huge quantities (thousands to millions of tons) of products. Thus, even a slight improvement in the yield can significantly reduce the cost of production. A case in point is the manufacture of chemical fertilizers, discussed in the Chemistry in Action essay on p. 108.

KeyEquations

percent composition of an element in a compound =

$$\frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\% \quad (3.1)$$

$$\%\text{yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% \quad (3.4)$$

Summary of Facts and Concepts

1. Atomic masses are measured in atomic mass units (amu), a relative unit based on a value of exactly 12 for the C-12 isotope. The atomic mass given for the atoms of a particular element is the average of the naturally occurring isotope distribution of that element. The molecular mass of a molecule is the sum of the atomic masses of the atoms in the molecule. Both atomic mass and molecular mass can be accurately determined with a mass spectrometer.
2. A mole is Avogadro's number (6.022×10^{23}) of atoms, molecules, or other particles. The molar mass (in grams) of an element or a compound is numerically equal to its mass in atomic mass units (amu) and contains Avogadro's number of atoms (in the case of elements), molecules (in the case of molecular substances), or simplest formula units (in the case of ionic compounds).
3. The percent composition by mass of a compound is the percent by mass of each element present. If we know the percent composition by mass of a compound, we can deduce the empirical formula of the compound and also the molecular formula of the compound if the approximate molar mass is known.
4. Chemical changes, called chemical reactions, are represented by chemical equations. Substances that undergo change—the reactants—are written on the left and the substances formed—the products—appear to the right of the arrow. Chemical equations must be balanced, in accordance with the law of conservation of mass. The number of atoms of each element in the reactants must equal the number in the products.
5. Stoichiometry is the quantitative study of products and reactants in chemical reactions. Stoichiometric calculations are best done by expressing both the known and unknown quantities in terms of moles and then converting to other units if necessary. A limiting reagent is the reactant that is present in the smallest stoichiometric amount. It limits the amount of product that can be formed. The amount of product obtained in a reaction (the actual yield) may be less than the maximum possible amount (the theoretical yield). The ratio of the two multiplied by 100 percent is expressed as the percent yield.

KeyWords

Answers to Practice Exercises

3.1 10.81 amu. **3.2** 3.59 moles. **3.3** 2.57×10^3 g. **3.4** 8.49×10^{21} K atoms. **3.5** 32.04 amu. **3.6** 1.66 moles. **3.7** 5.81×10^{24} H atoms. **3.8** H: 2.055%; S: 32.69%; O: 65.25%. **3.9** $KMnO_4$ (potassium permanganate). **3.10** 196 g. **3.11** B_2H_6. **3.12** $Fe_2O_3 + 3CO \longrightarrow 2Fe + 3CO_2$. **3.13** 235 g. **3.14** 0.769 g. **3.15** (a) 234 g, (b) 234 g. **3.16** (a) 863 g, (b) 93.0%.