Chapter 3

Stoichiometry

3.1 Counting by Weighing
3.2 Atomic Masses
3.3 The Mole
3.4 Molar Mass
3.5 Learning to Solve Problems

3.6 Percent Composition of Compounds
3.7 Determining the Formula of a Compound
3.8 Chemical Equations
   Chemical Reactions
   The Meaning of a Chemical Equation

3.9 Balancing Chemical Equations
3.10 Stoichiometric Calculations:
    Amounts of Reactants and Products
3.11 The Concept of Limiting Reactant

*Fireworks provide a spectacular example of chemical reactions.* (DaffyDreamstime.com)
Chemical reactions have a profound effect on our lives. There are many examples: Food is converted to energy in the human body; nitrogen and hydrogen are combined to form ammonia, which is used as a fertilizier; fuels and plastics are produced from petroleum; the starch in plants is synthesized from carbon dioxide and water using energy from sunlight; human insulin is produced in laboratories by bacteria; cancer is induced in humans by substances from our environment; and so on, in a seemingly endless list. The central activity of chemistry is to understand chemical changes such as these, and the study of reactions occupies a central place in this book. We will examine why reactions occur, how fast they occur, and the specific pathways they follow.

In this chapter we will consider the quantities of materials consumed and produced in chemical reactions. This area of study is called chemical stoichiometry (pronounced stoy-kē-om'-uh-trē). To understand chemical stoichiometry, you must first understand the concept of relative atomic masses.

3.1 Counting by Weighing

Suppose you work in a candy store that sells gourmet jelly beans by the bean. People come in and ask for 50 beans, 100 beans, 1000 beans, and so on, and you have to count them out—a tedious process at best. As a good problem solver, you try to come up with a better system. It occurs to you that it might be far more efficient to buy a scale and count the jelly beans by weighing them. How can you count jelly beans by weighing them? What information about the individual beans do you need to know?

Assume that all of the jelly beans are identical and that each has a mass of 5 g. If a customer asks for 1000 jelly beans, what mass of jelly beans would be required? Each bean has a mass of 5 g, so you would need 1000 beans \( \times 5 \text{ g/bean} \), or 5000 g (5 kg). It takes just a few seconds to weigh out 5 kg of jelly beans. It would take much longer to count out 1000 of them.

In reality, jelly beans are not identical. For example, let's assume that you weigh 10 beans individually and get the following results:

<table>
<thead>
<tr>
<th>Bean</th>
<th>Mass (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.1</td>
</tr>
<tr>
<td>2</td>
<td>5.2</td>
</tr>
<tr>
<td>3</td>
<td>5.0</td>
</tr>
<tr>
<td>4</td>
<td>4.8</td>
</tr>
<tr>
<td>5</td>
<td>4.9</td>
</tr>
<tr>
<td>6</td>
<td>5.0</td>
</tr>
<tr>
<td>7</td>
<td>5.0</td>
</tr>
<tr>
<td>8</td>
<td>5.1</td>
</tr>
<tr>
<td>9</td>
<td>4.9</td>
</tr>
<tr>
<td>10</td>
<td>5.0</td>
</tr>
</tbody>
</table>

Can we count these nonidentical beans by weighing? Yes. The key piece of information we need is the average mass of the jelly beans. Let's compute the average mass for our 10-bean sample.

\[
\text{Average mass} = \frac{\text{total mass of beans}}{\text{number of beans}}
\]

\[
= \frac{5.1 \text{ g} + 5.2 \text{ g} + 5.0 \text{ g} + 4.8 \text{ g} + 4.9 \text{ g} + 5.0 \text{ g} + 5.1 \text{ g} + 4.9 \text{ g} + 5.0 \text{ g}}{10}
\]

\[
= \frac{50.0}{10} = 5.0 \text{ g}
\]
The average mass of a jelly bean is 5.0 g. Thus, to count out 1000 beans, we need to weigh out 5000 g of beans. This sample of beans, in which the beans have an average mass of 5.0 g, can be treated exactly like a sample where all of the beans are identical. Objects do not need to have identical masses to be counted by weighing. We simply need to know the average mass of the objects. For purposes of counting, the objects behave as though they were all identical, as though they each actually had the average mass.

We count atoms in exactly the same way. Because atoms are so small, we deal with samples of matter that contain huge numbers of atoms. Even if we could see the atoms, it would not be possible to count them directly. Thus we determine the number of atoms in a given sample by finding its mass. However, just as with jelly beans, to relate the mass to a number of atoms, we must know the average mass of the atoms.

3.2 Atomic Masses

As we saw in Chapter 2, the first quantitative information about atomic masses came from the work of Dalton, Gay-Lussac, Lavoisier, Avogadro, and Berzelius. By observing the proportions in which elements combine to form various compounds, nineteenth-century chemists calculated relative atomic masses. The modern system of atomic masses, instituted in 1961, is based on $^{12}$C ("carbon twelve") as the standard. In this system, $^{12}$C is assigned a mass of exactly 12 atomic mass units (u), and the masses of all other atoms are given relative to this standard.

The most accurate method currently available for comparing the masses of atoms involves the use of the mass spectrometer. In this instrument, diagramed in Fig. 3.1, atoms or molecules are passed into a beam of high-speed electrons, which knock electrons off the atoms or molecules being analyzed and change them into positive ions. An applied electric field then accelerates these ions into a magnetic field. Because an accelerating ion produces its own magnetic field, an interaction with the applied magnetic field occurs, which tends to change the path of the ion. The amount of path deflection for each ion depends on its mass—the most massive ions are deflected the smallest amount—which causes the ions to separate, as shown in Fig. 3.1. A comparison of the positions where the ions hit the detector plate gives very accurate values of their relative masses. For example, when $^{12}$C and $^{13}$C are analyzed in a mass spectrometer, the ratio of their masses is found to be

$$\frac{\text{Mass } ^{13}\text{C}}{\text{Mass } ^{12}\text{C}} = 1.0836129$$

Figure 3.1 (left) A scientist injecting a sample into a mass spectrometer. (right) Schematic diagram of a mass spectrometer.

Unless otherwise noted, all art on this page is © Cengage Learning 2014.
Since the atomic mass unit is defined such that the mass of $^{12}\text{C}$ is exactly 12 atomic mass units, then on this same scale,

$$\text{Mass of } ^{12}\text{C} = (1.0036129)(12 \text{ u}) = 13.003355 \text{ u}$$

This value, even though it is actually a mass, is sometimes called the atomic weight for each element.

The masses of other atoms can be determined in a similar fashion.

The mass for each element is given in the table inside the front cover of this text. This value, even though it is actually a mass, is sometimes called the atomic weight for each element.

The masses of other atoms can be determined in a similar fashion.

The mass for each element is given in the table inside the front cover of this text. This value, even though it is actually a mass, is sometimes called the atomic weight for each element.

Look at the value of the atomic mass of carbon given in this table. You might expect to see 12, since we said the system of atomic masses is based on $^{12}\text{C}$. However, the number given for carbon is not 12 but 12.01. Why? The reason for this apparent discrepancy is that the carbon found on earth (natural carbon) is a mixture of the isotopes $^{12}\text{C}$, $^{13}\text{C}$, and $^{14}\text{C}$. All three isotopes have six protons, but they have six, seven, and eight neutrons, respectively. Because natural carbon is a mixture of isotopes, the atomic mass we use for carbon is an average value reflecting the average of the isotopes composing it.

The average atomic mass for carbon is computed as follows: It is known that natural carbon is composed of 98.89% $^{12}\text{C}$ atoms and 1.11% $^{13}\text{C}$ atoms. The amount of $^{14}\text{C}$ is negligibly small at this level of precision. Using the masses of $^{12}\text{C}$ (exactly 12 u) and $^{13}\text{C}$ (13.003355 u), we can calculate the average atomic mass for natural carbon as follows:

$$98.89\% \text{ of } 12 \text{ u} + 1.11\% \text{ of } 13.0034 \text{ u} = (0.9889)(12 \text{ u}) + (0.0111)(13.0034 \text{ u}) = 12.01 \text{ u}$$

In this text we will call the average mass for an element the average atomic mass or, simply, the atomic mass for that element.

Even though natural carbon does not contain a single atom with mass 12.01, for stoichiometric purposes, we can consider carbon to be composed of only one type of atom with a mass of 12.01. This enables us to count atoms of natural carbon by weighing a sample of carbon.

Recall from Section 3.1 that counting by weighing works if you know the average mass of the units being counted. Counting by weighing works just the same for atoms as for jelly beans. For natural carbon with an average mass of 12.01 atomic mass units, to obtain 1000 atoms would require weighing out 12,010 atomic mass units of natural carbon (a mixture of $^{12}\text{C}$ and $^{13}\text{C}$).

**Figure 3.2** (a) Neon gas glowing in a discharge tube. The relative intensities of the signals recorded when natural neon is injected into a mass spectrometer, represented in terms of (b) "peaks" and (c) a bar graph. The relative areas of the peaks are 0.0902 $^{20}\text{Ne}$, 0.00257 $^{21}\text{Ne}$, and 0.0882 $^{22}\text{Ne}$; natural neon is therefore 90.92% $^{20}\text{Ne}$, 0.257% $^{21}\text{Ne}$, and 8.82% $^{22}\text{Ne}$.
As in the case of carbon, the mass for each element listed in the table inside the front cover of the text is an average value based on the isotopic composition of the naturally occurring element. For instance, the mass listed for hydrogen (1.008) is the average mass for natural hydrogen, which is a mixture of \( ^1\text{H} \) and \( ^2\text{H} \) (deuterium). No atom of hydrogen actually has the mass 1.008.

In addition to being useful for determining accurate mass values for individual atoms, the mass spectrometer is used to determine the isotopic composition of a natural element. For example, when a sample of natural neon is injected into a mass spectrometer, the mass spectrum shown in Fig. 3.2 is obtained. The areas of the “peaks” or the heights of the bars indicate the relative abundances of \( ^{20}\text{Ne}, ^{21}\text{Ne}, \) and \( ^{22}\text{Ne} \) atoms.

### Example 3.1

**The Average Mass of an Element**

When a sample of natural copper is vaporized and injected into a mass spectrometer, the results shown in Fig. 3.3 are obtained. Use these data to compute the average mass of natural copper. (The mass values for \( ^{63}\text{Cu} \) and \( ^{65}\text{Cu} \) are 62.93 u and 64.93 u, respectively.)

**Solution**

**Where are we going?**

To calculate the average mass of natural copper.

**What do we know?**

\[
\begin{align*}
\text{\( ^{63}\text{Cu} \) mass} &= 62.93 \text{ u} \\
\text{\( ^{65}\text{Cu} \) mass} &= 64.93 \text{ u}
\end{align*}
\]

**How do we get there?**

As shown by the graph, of every 100 atoms of natural copper, 69.09 are \( ^{63}\text{Cu} \) and 30.91 are \( ^{65}\text{Cu} \). Thus the mass of 100 atoms of natural copper is

\[
(69.09 \text{ atoms}) \left( 62.93 \frac{\text{u}}{\text{atom}} \right) + (30.91 \text{ atoms}) \left( 64.93 \frac{\text{u}}{\text{atom}} \right) = 6355 \text{ u}
\]

The average mass of a copper atom is

\[
\frac{6355 \text{ u}}{100 \text{ atoms}} = 63.55 \text{ u/atom}
\]

This mass value is used in doing calculations involving the reactions of copper and is the value given in the table inside the front cover of this book.

**Reality Check** | When you finish a calculation, you should always check whether your answer makes sense. In this case our answer of 63.55 u is between the masses of the atoms that make up natural copper. This makes sense. The answer could not be smaller than 62.93 u or larger than 64.93 u.

### 3.3 The Mole

Because samples of matter typically contain so many atoms, a unit of measure called the **mole** has been established for use in counting atoms. For our purposes, it is most convenient to define the mole (abbreviated mol) as the number equal to the number of carbon atoms in exactly 12 g of pure \( ^{12}\text{C} \). Techniques such as mass spectrometry, which count atoms very precisely, have been used to determine this number as \( 6.02214 \times 10^{23} \)

\[
N_A = \frac{6.02214 \times 10^{23}}{12 \text{ u}} = 5.00 \times 10^{23} \text{ atoms/mol}
\]

This number defines the **Avogadro constant** (\( N_A \)).

Using the Avogadro constant, we can easily calculate the mole with a simple ratio:

\[
\text{Number of atoms} = \frac{\text{mass in u}}{\text{atomic mass in u/atom}}
\]

If the mass is given in atomic mass units (u), the result is a number of atoms.

Using the atomic masses, we can calculate the number of atoms in a given mass of copper:

\[
\frac{62.93 \text{ g}}{\text{Cu}} \times \frac{\text{u}}{\text{Cu}} \times \frac{1 \text{ mol}}{N_A} = \frac{62.93 \text{ u}}{6.02214 \times 10^{23} \text{ atoms/mol}} = \frac{62.93 \text{ atoms}}{10^{23}}
\]

Thus the number of copper atoms in 62.93 g of copper is 6.293 \( \times 10^{23} \) atoms.

**Exercise:** Calculate the number of atoms in 100 g of copper.

**Answer:** 1.00 \( \times 10^{24} \) atoms.
The SI definition of the mole is the amount of a substance that contains as many entities as there are in exactly 12 g of carbon-12.

Avogadro’s number is $6.022 \times 10^{23}$. One mole of anything is $6.022 \times 10^{23}$ units of that substance.

(6.022 $\times 10^{23}$ will be sufficient for our purposes). This number is called Avogadro’s number to honor his contributions to chemistry. One mole of something consists of $6.022 \times 10^{23}$ units of that substance. Just as a dozen eggs is 12 eggs, a mole of eggs is $6.022 \times 10^{23}$ eggs.

The magnitude of the number $6.022 \times 10^{23}$ is very difficult to imagine. To give you some idea, 1 mole of seconds represents a span of time 4 million times as long as the earth has already existed, and 1 mole of marbles is enough to cover the entire earth to a depth of 50 miles! However, since atoms are so tiny, a mole of atoms or molecules is a perfectly manageable quantity to use in a reaction (Fig. 3.4).

**Critical Thinking**

What if you were offered $1 million to count from 1 to $6 \times 10^{23}$ at a rate of one number each second?

Determine your hourly wage. Would you do it? Could you do it?

How do we use the mole in chemical calculations? Recall that Avogadro’s number is defined as the number of atoms in exactly 12 g of $^{12}$C. This means that 12 g of $^{12}$C contains $6.022 \times 10^{23}$ atoms. It also means that a 12.01-g sample of natural carbon contains $6.022 \times 10^{23}$ atoms (a mixture of $^{12}$C, $^{13}$C, and $^{14}$C atoms, with an average atomic mass of 12.01). Since the ratio of the masses of the samples (12 g/12.01 g) is the same as the ratio of the masses of the individual components (12 u/12.01 u), the two samples contain the same number of atoms ($6.022 \times 10^{23}$).

To be sure this point is clear, think of oranges with an average mass of 0.5 lb each and grapefruit with an average mass of 1.0 lb each. Any two sacks for which the sack of grapefruit weighs twice as much as the sack of oranges will contain the same number of pieces of fruit. The same idea extends to atoms. Compare natural carbon (average mass of 12.01) and natural helium (average mass of 4.003). A sample of 12.01 g of natural carbon contains the same number of atoms as 4.003 g of natural helium. Both samples contain 1 mole of atoms ($6.022 \times 10^{23}$). Table 3.1 gives more examples that illustrate this basic idea.
Table 3.1 | Comparison of 1-Mole Samples of Various Elements

<table>
<thead>
<tr>
<th>Element</th>
<th>Number of Atoms Present</th>
<th>Mass of Sample (g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>$6.022 \times 10^{23}$</td>
<td>26.98</td>
</tr>
<tr>
<td>Copper</td>
<td>$6.022 \times 10^{23}$</td>
<td>63.55</td>
</tr>
<tr>
<td>Iron</td>
<td>$6.022 \times 10^{23}$</td>
<td>55.85</td>
</tr>
<tr>
<td>Sulfur</td>
<td>$6.022 \times 10^{23}$</td>
<td>32.07</td>
</tr>
<tr>
<td>Iodine</td>
<td>$6.022 \times 10^{23}$</td>
<td>126.9</td>
</tr>
<tr>
<td>Mercury</td>
<td>$6.022 \times 10^{23}$</td>
<td>200.6</td>
</tr>
</tbody>
</table>

The mass of 1 mole of an element is equal to its atomic mass in grams.

Thus the mole is defined such that a sample of a natural element with a mass equal to the element's atomic mass expressed in grams contains 1 mole of atoms. This definition also fixes the relationship between the atomic mass unit and the gram. Since $6.022 \times 10^{23}$ atoms of carbon (each with a mass of 12 u) have a mass of 12 g, then

$$\left(6.022 \times 10^{23} \text{ atoms} \right) \left(\frac{12 \text{ u}}{\text{atom}}\right) = 12 \text{ g}$$

and

$$6.022 \times 10^{23} \text{ u} = 1 \text{ g}$$

This relationship can be used to derive the unit factor needed to convert between atomic mass units and grams.

Critical Thinking

What if you discovered Avogadro's number was not $6.02 \times 10^{23}$ but $3.01 \times 10^{23}$? Would this affect the relative masses given on the periodic table? If so, how? If not, why not?

Interactive Example 3.2

Sign in at http://login.cengagebrain.com to try this Interactive Example in OWL.

Determining the Mass of a Sample of Atoms

Americium is an element that does not occur naturally. It can be made in very small amounts in a device known as a particle accelerator. Compute the mass in grams of a sample of americium containing six atoms.

Solution

Where are we going?

To calculate the mass of six americium atoms

What do we know?

> Mass of 1 atom of Am = 243 u (from the periodic table inside the front cover)

How do we get there?

The mass of six atoms is

$$6 \text{ atoms} \times \frac{243 \text{ u}}{\text{atom}} = 1.46 \times 10^3 \text{ u}$$

Using the relationship

$$6.022 \times 10^{23} \text{ u} = 1 \text{ g}$$
we write the conversion factor for converting atomic mass units to grams:

\[
\frac{1 \text{ g}}{6.022 \times 10^{23} \text{ u}}
\]

The mass of six americium atoms in grams is

\[
1.46 \times 10^3 \text{ u} \times \frac{1 \text{ g}}{6.022 \times 10^{23} \text{ u}} = 2.42 \times 10^{-21} \text{ g}
\]

Reality Check | Since this sample contains only six atoms, the mass should be very small as the amount \(2.42 \times 10^{-21} \text{ g}\) indicates.

To do chemical calculations, you must understand what the mole means and how to determine the number of moles in a given mass of a substance. These procedures are illustrated in Examples 3.3 and 3.4.

### Interactive Example 3.3

Sign in at http://login.cengagebrain .com to try this Interactive Example in OWL.

(Left) Pure aluminum. (Right) Aluminum alloys are used for many products used in our kitchens.

### Determining Moles of Atoms

Aluminum (Al) is a metal with a high strength-to-mass ratio and a high resistance to corrosion; thus it is often used for structural purposes. Compute both the number of moles of atoms and the number of atoms in a 10.0-g sample of aluminum.

#### Solution

**Where are we going?**

To calculate the moles and number of atoms in a sample of Al

**What do we know?**

\(\rightarrow\) Sample contains 10.0 g of Al

\(\rightarrow\) Mass of 1 mole \((6.022 \times 10^{23} \text{ atoms})\) of Al = 26.93 g

**How do we get there?**

We can calculate the number of moles of Al in a 10.0-g sample as follows:

\[
\frac{10.0 \text{ g-Al}}{26.98 \text{ g-Al}} \times 1 \text{ mol-Al} = 0.371 \text{ mol-Al atoms}
\]

The number of atoms in 10.0 g \((0.371 \text{ mole})\) of aluminum is

\[
0.371 \text{ mol-Al} \times \frac{6.022 \times 10^{23} \text{ atoms}}{1 \text{ mol-Al}} = 2.23 \times 10^{23} \text{ atoms}
\]
Reality Check | One mole of Al has a mass of 26.98 g and contains $6.022 \times 10^{23}$ atoms. Our sample is 10.0 g, which is roughly 1/3 of 26.98. Thus the calculated amount should be on the order of 1/3 of $6 \times 10^{20}$, which it is.

See Exercise 3.46

Calculating Numbers of Atoms

A silicon chip used in an integrated circuit of a microcomputer has a mass of 5.68 mg. How many silicon (Si) atoms are present in the chip?

Solution

Where are we going?

To calculate the atoms of Si in the chip

What do we know?

- The chip has 5.68 mg of Si
- Mass of 1 mole ($6.022 \times 10^{23}$ atoms) of Si = 28.09 g

How do we get there?

The strategy for doing this problem is to convert from milligrams of silicon to grams of silicon, then to moles of silicon, and finally to atoms of silicon:

\[
5.68 \text{ mg Si} \times \frac{1 \text{ g Si}}{1000 \text{ mg Si}} = 5.68 \times 10^{-3} \text{ g Si}
\]

\[
5.68 \times 10^{-3} \text{ g Si} \times \frac{1 \text{ mol Si}}{28.09 \text{ g Si}} = 2.02 \times 10^{-4} \text{ mol Si}
\]

\[
2.02 \times 10^{-4} \text{ mol Si} \times \frac{6.022 \times 10^{23} \text{ atoms}}{1 \text{ mol Si}} = 1.22 \times 10^{20} \text{ atoms}
\]

Reality Check | Note that 5.68 mg of silicon is clearly much less than 1 mole of silicon (which has a mass of 28.09 g), so the final answer of $1.22 \times 10^{20}$ atoms (compared with $6.022 \times 10^{23}$ atoms) is in the right direction.

See Exercise 3.47

Calculating the Number of Moles and Mass

Cobalt (Co) is a metal that is added to steel to improve its resistance to corrosion. Calculate both the number of moles in a sample of cobalt containing $5.00 \times 10^{20}$ atoms and the mass of the sample.

Solution

Where are we going?

To calculate the number of moles and the mass of a sample of Co

What do we know?

- Sample contains $5.00 \times 10^{20}$ atoms of Co

Fragments of cobalt metal.

Unless otherwise noted, all art on this page is © Cengage Learning 2016.
How do we get there?

Note that the sample of \(5.00 \times 10^{20}\) atoms of cobalt is less than 1 mole (6.022 \(\times\) 10\(^{23}\) atoms) of cobalt. What fraction of a mole it represents can be determined as follows:

\[
5.00 \times 10^{20} \text{ atoms Co} \times \frac{1 \text{ mol Co}}{6.022 \times 10^{23} \text{ atoms Co}} = 8.30 \times 10^{-4} \text{ mol Co}
\]

Since the mass of 1 mole of cobalt atoms is 58.93 g, the mass of \(5.00 \times 10^{20}\) atoms can be determined as follows:

\[
8.30 \times 10^{-4} \text{ mol Co} \times \frac{58.93 \text{ g Co}}{1 \text{ mol Co}} = 4.89 \times 10^{-2} \text{ g Co}
\]

Reality Check: In this case the sample contains \(5 \times 10^{20}\) atoms, which is approximately \(1/1000\) of a mole. Thus the sample should have a mass of about \((1/1000)(58.93) \approx 0.06\). Our answer of \(-0.05\) makes sense.

3.4 | Molar Mass

A chemical compound is, ultimately, a collection of atoms. For example, methane (the major component of natural gas) consists of molecules that each contain one carbon and four hydrogen atoms \((\text{CH}_4)\). How can we calculate the mass of 1 mole of methane; that is, what is the mass of \(6.022 \times 10^{23}\) \(\text{CH}_4\) molecules? Since each \(\text{CH}_4\) molecule contains one carbon atom and four hydrogen atoms, 1 mole of \(\text{CH}_4\) molecules contains 1 mole of carbon atoms and 4 moles of hydrogen atoms. The mass of 1 mole of methane can be found by summing the masses of carbon and hydrogen present:

- Mass of 1 mol C = 12.01 g
- Mass of 4 mol H = 4 \(\times\) 1.008 g
- Mass of 1 mol \(\text{CH}_4\) = 16.04 g

Because 16.04 g represents the mass of 1 mole of methane molecules, it makes sense to call it the molar mass for methane. Thus the molar mass of a substance is the mass in grams of 1 mole of the compound. Traditionally, the term molecular weight has been used for this quantity. However, we will use molar mass exclusively in this text. The molar mass of a known substance is obtained by summing the masses of the component atoms as we did for methane.

Methane is a molecular compound—its components are molecules. Many substances are ionic—they contain simple ions or polyatomic ions. Examples are \(\text{NaCl}\) (contains \(\text{Na}^+\) and \(\text{Cl}^-\)) and \(\text{CaCO}_3\) (contains \(\text{Ca}^{2+}\) and \(\text{CO}_3^{2-}\)). Because ionic compounds do not contain molecules, we need a special name for the fundamental unit of these materials. Instead of molecule, we use the term formula unit. Thus \(\text{CaCO}_3\) is the formula unit for calcium carbonate, and \(\text{NaCl}\) is the formula unit for sodium chloride.

Interactive Example 3.6

Sign in at http://login.cengagebrain.com to try this Interactive Example in OWL.

Calculating Molar Mass I

Juglone, a dye known for centuries, is produced from the husks of black walnuts. It is also a natural herbicide (weed killer) that kills off competitive plants around the black walnut tree but does not affect grass and other noncompetitive plants. The formula for juglone is \(\text{C}_{20}\text{H}_{30}\text{O}_3\).

a. Calculate the molar mass of juglone.

b. A sample of \(1.56 \times 10^{-2}\) g of pure juglone was extracted from black walnut husks. How many moles of juglone does this sample represent?
Solution

a. The molar mass is obtained by summing the masses of the component atoms. In 1 mole of juglone, there are 10 moles of carbon atoms, 6 moles of hydrogen atoms, and 3 moles of oxygen atoms:

- $10\text{ C: } 10 \times 12.01\text{ g} = 120.1\text{ g}$
- $6\text{ H: } 6 \times 1.008\text{ g} = 6.048\text{ g}$
- $3\text{ O: } 3 \times 16.00\text{ g} = 48.00\text{ g}$

Mass of 1 mol C$_{14}$H$_{16}$O$_{3}$ = 174.1 g

The mass of 1 mole of juglone is 174.1 g, which is the molar mass.

b. The mass of 1 mole of this compound is 174.1 g; thus $1.56 \times 10^{-2}\text{ g}$ is much less than a mole. The exact fraction of a mole can be determined as follows:

$$1.56 \times 10^{-2}\text{ g juglone} \times \frac{1\text{ mol juglone}}{174.1\text{ g juglone}} = 8.96 \times 10^{-3}\text{ mol juglone}$$

See Exercises 3.51 through 3.54.

---

**Interactive Example 3.7**

Sign in at http://login.cengagebrain.com to try this Interactive Example in OWL.

A calcite (CaCO$_3$) crystal.

---

**Calculating Molar Mass II**

Calcium carbonate (CaCO$_3$), also called calcite, is the principal mineral found in limestone, marble, chalk, pearls, and the shells of marine animals such as clams.

**a.** Calculate the molar mass of calcium carbonate.

**b.** A certain sample of calcium carbonate contains 4.86 moles. What is the mass in grams of this sample? What is the mass of the CO$_3^{2-}$ ions present?

**Solution**

**a.** Calcium carbonate is an ionic compound composed of Ca$^{2+}$ and CO$_3^{2-}$ ions. In 1 mole of calcium carbonate, there are 1 mole of Ca$^{2+}$ ions and 1 mole of CO$_3^{2-}$ ions. The molar mass is calculated by summing the masses of the components;

- $1\text{ Ca}^{2+}: 1 \times 40.08\text{ g} = 40.08\text{ g}$
- $1\text{ CO}_3^{2-}: 1 \times 12.01\text{ g} = 12.01\text{ g}$
- $3\text{ O: } 3 \times 16.00\text{ g} = 48.00\text{ g}$

Mass of 1 mol CaCO$_3$ = 100.09 g

Thus the mass of 1 mole of CaCO$_3$ (1 mole of Ca$^{2+}$ plus 1 mole of CO$_3^{2-}$) is 100.09 g. This is the molar mass.

**b.** The mass of 1 mole of CaCO$_3$ is 100.09 g. The sample contains nearly 5 moles, or close to 500 g. The exact amount is determined as follows:

$$4.86\text{ mol CaCO}_3 \times \frac{100.09\text{ g CaCO}_3}{1\text{ mol CaCO}_3} = 486\text{ g CaCO}_3$$

To find the mass of carbonate ions (CO$_3^{2-}$) present in this sample, we must realize that 4.86 moles of CaCO$_3$ contains 4.86 moles of Ca$^{2+}$ ions and 4.86 moles of CO$_3^{2-}$ ions. The mass of 1 mole of CO$_3^{2-}$ ions is

- $1\text{ C: } 1 \times 12.01\text{ g} = 12.01\text{ g}$
- $3\text{ O: } 3 \times 16.00\text{ g} = 48.00\text{ g}$

Mass of 1 mol CO$_3^{2-}$ = 60.01 g
Thus the mass of 4.86 moles of $\text{CO}_3^{2-}$ ions is
\[
4.86 \text{ mol} \cdot \text{CO}_3^{2-} \times \frac{60.01 \text{ g} \cdot \text{CO}_3^{2-}}{1 \text{ mol} \cdot \text{CO}_3^{2-}} = 292 \text{ g} \cdot \text{CO}_3^{2-}
\]

See Exercises 3.55 through 3.58.

### Interactive Example 3.8

Sign in at http://login.cengagebrain.com to try this Interactive Example in OWL.

Isopentyl acetate is released when a bee stings.

![Isopentyl acetate molecule](image)

**Isopentyl acetate**

- **Carbon**
- **Oxygen**
- **Hydrogen**

To show the correct number of significant figures in each calculation, we round after each step. In your calculations, always carry extra significant figures through to the end, then round.

#### Molar Mass and Numbers of Molecules

Isopentyl acetate ($\text{C}_7\text{H}_{14}\text{O}_2$) is the compound responsible for the scent of bananas. A molecular model of isopentyl acetate is shown in the margin below. Interestingly, bees release about 1 $\mu$g ($1 \times 10^{-6} \text{ g}$) of this compound when they sting. The resulting scent attracts other bees to join the attack. How many molecules of isopentyl acetate are released in a typical bee sting? How many atoms of carbon are present?

#### Solution

**Where are we going?**

To calculate the number of molecules of isopentyl acetate and the number of carbon atoms in a bee sting.

**What do we know?**

- Mass of isopentyl acetate in a typical bee sting is 1 microgram = $1 \times 10^{-6} \text{ g}$

**How do we get there?**

Since we are given a mass of isopentyl acetate and want to find the number of molecules, we must first compute the molar mass of $\text{C}_7\text{H}_{14}\text{O}_2$:

\[
7 \text{ mol} \cdot \text{C} \times 12.01 \frac{\text{g}}{\text{mol}} = 84.07 \text{ g} \cdot \text{C}
\]

\[
14 \text{ mol} \cdot \text{H} \times 1.008 \frac{\text{g}}{\text{mol}} = 14.11 \text{ g} \cdot \text{H}
\]

\[
2 \text{ mol} \cdot \text{O} \times 16.00 \frac{\text{g}}{\text{mol}} = 32.00 \frac{\text{g}}{\text{O}}
\]

This means that 1 mole of isopentyl acetate ($6.022 \times 10^{23}$ molecules) has a mass of 130.18 g.

To find the number of molecules released in a sting, we must first determine the number of moles of isopentyl acetate in $1 \times 10^{-6} \text{ g}$:

\[
1 \times 10^{-6} \text{ g} \cdot \text{C}_7\text{H}_{14}\text{O}_2 \times \frac{1 \text{ mol} \cdot \text{C}_7\text{H}_{14}\text{O}_2}{130.18 \text{ g} \cdot \text{C}_7\text{H}_{14}\text{O}_2} = 8 \times 10^{-9} \text{ mol} \cdot \text{C}_7\text{H}_{14}\text{O}_2
\]

Since 1 mole is $6.022 \times 10^{23}$ units, we can determine the number of molecules:

\[
8 \times 10^{-9} \text{ mol} \cdot \text{C}_7\text{H}_{14}\text{O}_2 \times \frac{6.022 \times 10^{23} \text{ molecules}}{1 \text{ mol} \cdot \text{C}_7\text{H}_{14}\text{O}_2} = 5 \times 10^{15} \text{ molecules}
\]

To determine the number of carbon atoms present, we must multiply the number of molecules by 7, since each molecule of isopentyl acetate contains seven carbon atoms:

\[
5 \times 10^{15} \text{ molecules} \times \frac{7 \text{ carbon atoms}}{\text{molecule}} = 4 \times 10^{16} \text{ carbon atoms}
\]

**Note:** In keeping with our practice of always showing the correct number of significant figures, we have rounded after each step. However, extra digits are carried throughout this problem, the final answer rounds to $3 \times 10^{16}$.

See Exercises 3.59 through 3.64.
3.5 Learning to Solve Problems

One of the great rewards of studying chemistry is to become a good problem solver. Being able to solve complex problems is a talent that will serve you well in all walks of life. It is our purpose in this text to help you learn to solve problems in a flexible, creative way based on understanding the fundamental ideas of chemistry. We call this approach conceptual problem solving.

The ultimate goal is to be able to solve new problems (that is, problems you have not seen before) on your own. In this text we will provide problems and offer solutions by explaining how to think about the problems. While the answers to these problems are important, it is perhaps even more important to understand the process—the thinking necessary to get the answer. Although at first we will be solving the problem for you, do not take a passive role. While studying the solution, it is crucial that you interactively think through the problem with us. Do not skip the discussion and jump to the answer. Usually, the solution will involve asking a series of questions. Make sure that you understand each step in the process. This active approach should apply to problems outside of chemistry as well. For example, imagine riding with someone in a car to an unfamiliar destination. If your goal is simply to have the other person get you to that destination, you probably will not pay much attention to how to get there (passive), and if you have to find this same place in the future on your own, you probably will not be able to do it. If, however, your goal is to learn how to get there, you would pay attention to distances, signs, and turns (active). This is how you should read the solutions in the text (and the text in general).

While actively studying our solutions to problems is helpful, at some point you will need to know how to think through these problems on your own. If we help you too much as you solve a problem, you won't really learn effectively. If we always "drive," you won't interact as meaningfully with the material. Eventually you need to learn to drive yourself. We will provide more help at the beginning of the text and less as we proceed to later chapters.

There are two fundamentally different ways you might use to approach a problem. One way emphasizes memorization. We might call this the "pigeonholing method." In this approach, the first step is to label the problem—to decide in which pigeonhole it fits. The pigeonholing method requires that you provide you with a set of steps that you memorize and store in the appropriate slot for each different problem you encounter. The difficulty with this method is that it requires a new pigeonhole each time a problem is changed by even a small amount.

Consider the driving analogy again. Suppose you have memorized how to drive from your house to the grocery store. Do you know how to drive back from the grocery store to your house? Not necessarily. If you have only memorized the directions and do not understand fundamental principles such as "I traveled north to get to the store, so my house is south of the store," you may find yourself stranded. In a more complicated example, suppose you know how to get from your house to the store (and back) and from your house to the library (and back). Can you get from the library to the store without having to go back home? Probably not if you have only memorized directions and you do not have a "big picture" of where your house, the store, and the library are relative to one another.

The second approach is conceptual problem solving, in which we help you get the "big picture"—a real understanding of the situation. This approach to problem solving looks within the problem for a solution. In this method we assume that the problem is a new one, and we let the problem guide us as we solve it. In this approach we ask a series of questions as we proceed and use our knowledge of fundamental principles to answer these questions. Learning this approach requires some patience, but the reward for learning to solve problems this way is that we become an effective solver of any new problem that confronts us in daily life or in our work in any field. In summary, instead of looking outside the problem for a memorized solution, we will look inside the problem and let the problem help us as we proceed to a solution.
As we have seen in problems we have already considered, there are several organizing principles to help you become a creative problem solver. Although we have been using these ideas in earlier problems, let’s review and expand on them. Because as we progress in our study of chemistry the problems become more complicated, we will need to rely on this approach even more.

1. We need to read the problem and decide on the final goal. Then we sort through the facts given, focusing on the key words and often drawing a diagram of the problem. In this part of the analysis we need to state the problem as simply and as visually as possible. We could summarize this entire process as “Where are we going?”

2. In order to reach our final goal, we need to decide where to start. For example, in a stoichiometry problem we always start with the chemical reaction. Then we ask a series of questions as we proceed, such as, “What are the reactants and products?” “What is the balanced equation?” “What are the amounts of the reactants?” and so on. Our understanding of the fundamental principles of chemistry will enable us to answer each of these simple questions and eventually will lead us to the final solution. We might summarize this process as “How do we get there?”

3. Once we get the solution of the problem, then we ask ourselves, “Does it make sense?” That is, does our answer seem reasonable? We call this the Reality Check. It always pays to check your answer.

Using a conceptual approach to problem solving will enable you to develop real confidence as a problem solver. You will no longer panic when you see a problem that is different in some ways from those you have solved in the past. Although you might be frustrated at times as you learn this method, we guarantee that it will pay dividends later and should make your experience with chemistry a positive one that will prepare you for any career you choose.

To summarize, one of our major goals in this text is to help you become a creative problem solver. We will do this by, at first, giving you lots of guidance in how to solve problems. We will “drive,” but we hope you will be paying attention instead of just “riding along.” As we move forward, we will gradually shift more of the responsibility to you. As you gain confidence in letting the problem guide you, you will be amazed at how effective you can be at solving some really complex problems—just like the ones you will confront in “real life.”

### 3.6 Percent Composition of Compounds

There are two common ways of describing the composition of a compound: in terms of the numbers of its constituent atoms and in terms of the percentages (by mass) of its elements. We can obtain the mass percents of the elements from the formula of the compound by comparing the mass of each element present in 1 mole of the compound to the total mass of 1 mole of the compound.

For example, for ethanol, which has the formula C₂H₅OH, the mass of each element present and the molar mass are obtained as follows:

\[
\text{Mass of C} = 2 \text{ mol} \times 12.01 \frac{g}{\text{mol}} = 24.02 \text{ g}
\]

\[
\text{Mass of H} = 6 \text{ mol} \times 1.008 \frac{g}{\text{mol}} = 6.048 \text{ g}
\]

\[
\text{Mass of O} = 1 \text{ mol} \times 16.00 \frac{g}{\text{mol}} = 16.00 \text{ g}
\]

Mass of 1 mol C₂H₅OH = 46.07 g
The mass percent (often called the weight percent) of carbon in ethanol can be computed by comparing the mass of carbon in 1 mole of ethanol to the total mass of 1 mole of ethanol and multiplying the result by 100:

\[
\text{Mass percent of C} = \frac{\text{mass of C in 1 mol \( \text{C}_2\text{H}_5\text{OH} \)}}{\text{mass of 1 mol \( \text{C}_2\text{H}_5\text{OH} \)}} \times 100\%
\]

\[
= \frac{24.02 \text{ g}}{46.07 \text{ g}} \times 100\% = 52.14\%
\]

The mass percents of hydrogen and oxygen in ethanol are obtained in a similar manner:

\[
\text{Mass percent of H} = \frac{\text{mass of H in 1 mol \( \text{C}_2\text{H}_5\text{OH} \)}}{\text{mass of 1 mol \( \text{C}_2\text{H}_5\text{OH} \)}} \times 100\%
\]

\[
= \frac{6.048 \text{ g}}{46.07 \text{ g}} \times 100\% = 13.13\%
\]

\[
\text{Mass percent of O} = \frac{\text{mass of O in 1 mol \( \text{C}_2\text{H}_5\text{OH} \)}}{\text{mass of 1 mol \( \text{C}_2\text{H}_5\text{OH} \)}} \times 100\%
\]

\[
= \frac{16.00 \text{ g}}{46.07 \text{ g}} \times 100\% = 34.73\%
\]

Reality Check | Notice that the percentages add up to 100.00%; this provides a check that the calculations are correct.

---

**Interactive Example 3.9**

Sign in at http://login.cengagebrain.com to try this Interactive Example in OWL.

---

**Calculating Mass Percent**

Carvone is a substance that occurs in two forms having different arrangements of the atoms but the same molecular formula \( \text{C}_{10}\text{H}_{14}\text{O} \) and mass. One type of carvone gives caraway seeds their characteristic smell, and the other type is responsible for the smell of spearmint oil. Compute the mass percent of each element in carvone.

**Solution**

*Where are we going?*

To find the mass percent of each element in carvone

*What do we know?*

\( \text{Molecular formula is \( \text{C}_{10}\text{H}_{14}\text{O} \)} \)

*What information do we need to find the mass percent?*

\( \text{Mass of each element (we'll use 1 mole of carvone)} \)

\( \text{Molar mass of carvone} \)

*How do we get there?*

*What is the mass of each element in 1 mole of \( \text{C}_{10}\text{H}_{14}\text{O} \)?*

\[
\text{Mass of C in 1 mol} = 10 \text{ mol} \times \frac{12.01 \text{ g}}{\text{mol}} = 120.1 \text{ g}
\]

\[
\text{Mass of H in 1 mol} = 14 \text{ mol} \times \frac{1.008 \text{ g}}{\text{mol}} = 14.11 \text{ g}
\]

\[
\text{Mass of O in 1 mol} = 1 \text{ mol} \times \frac{16.00 \text{ g}}{\text{mol}} = 16.00 \text{ g}
\]

*What is the molar mass of \( \text{C}_{10}\text{H}_{14}\text{O} \)?*

\[
120.1 \text{ g} + 14.11 \text{ g} + 16.00 \text{ g} = 150.2 \text{ g}
\]

\[
\text{C}_{10} + \text{H}_{14} + \text{O} = \text{C}_{10}\text{H}_{14}\text{O}
\]
3.7 Determining the Formula of a Compound

When a new compound is prepared, one of the first items of interest is the formula of the compound. This is most often determined by taking a weighed sample of the compound and either decomposing it into its component elements or reacting it with oxygen to produce substances such as CO₂, H₂O, and N₂, which are then collected and weighed. A device for doing this type of analysis is shown in Fig. 3.5. The results of such analyses provide the mass of each type of element in the compound, which can be used to determine the mass percent of each element.

We will see how information of this type can be used to compute the formula of a compound. Suppose a substance has been prepared that is composed of carbon, hydrogen, and nitrogen. When 0.1156 g of this compound is reacted with oxygen, 0.1638 g of carbon dioxide (CO₂) and 0.1676 g of water (H₂O) are collected. Assuming that all the carbon in the compound is converted to CO₂, we can determine the mass of carbon originally present in the 0.1156-g sample. To do this, we must use the fraction (by mass) of carbon in CO₂. The molar mass of CO₂ is

\[ C: \quad 1 \text{ mol} \times \frac{12.01 \text{ g}}{\text{mol}} = 12.01 \text{ g} \]

\[ O: \quad 2 \text{ mol} \times \frac{16.00 \text{ g}}{\text{mol}} = 32.00 \text{ g} \]

Molar mass of CO₂ = 44.01 g/mol

Figure 3.5 | A schematic diagram of the combustion device used to analyze substances for carbon and hydrogen. The sample is burned in the presence of excess oxygen, which converts all its carbon to carbon dioxide and all its hydrogen to water. These products are collected by absorption using appropriate materials, and their amounts are determined by measuring the increase in masses of the absorbents.
The fraction of carbon present by mass is

\[
\frac{\text{Mass of } C}{\text{Total mass of } \text{CO}_2} = \frac{12.01 \text{ g C}}{44.01 \text{ g } \text{CO}_2}
\]

This factor can now be used to determine the mass of carbon in 0.1638 g of \( \text{CO}_2 \):

\[
0.1638 \text{ g } \text{CO}_2 \times \frac{12.01 \text{ g C}}{44.01 \text{ g } \text{CO}_2} = 0.04470 \text{ g C}
\]

Remember that this carbon originally came from the 0.1156 g sample of unknown compound. Thus the mass percent of carbon in this compound is

\[
\frac{0.04470 \text{ g C}}{0.1156 \text{ g compound}} \times 100\% = 38.67\% \text{ C}
\]

The same procedure can be used to find the mass percent of hydrogen in the unknown compound. We assume that all the hydrogen present in the original 0.1156 g of compound was converted to \( \text{H}_2\text{O} \). The molar mass of \( \text{H}_2\text{O} \) is 18.02 g, and the fraction of hydrogen by mass in \( \text{H}_2\text{O} \) is

\[
\frac{\text{Mass of } H}{\text{Mass of } \text{H}_2\text{O}} = \frac{2.016 \text{ g } H}{18.02 \text{ g } \text{H}_2\text{O}}
\]

Therefore, the mass of hydrogen in 0.1676 g of \( \text{H}_2\text{O} \) is

\[
0.1676 \text{ g } \text{H}_2\text{O} \times \frac{2.016 \text{ g } H}{18.02 \text{ g } \text{H}_2\text{O}} = 0.01875 \text{ g H}
\]

The mass percent of hydrogen in the compound is

\[
\frac{0.01875 \text{ g H}}{0.1156 \text{ g compound}} \times 100\% = 16.22\% \text{ H}
\]

The unknown compound contains only carbon, hydrogen, and nitrogen. So far we have determined that it is 38.67% carbon and 16.22% hydrogen. The remainder must be nitrogen:

\[
100.00\% - (38.67\% + 16.22\%) = 45.11\% \text{ N}
\]

We have determined that the compound contains 38.67% carbon, 16.22% hydrogen, and 45.11% nitrogen. Next we use these data to obtain the formula.

Since the formula of a compound indicates the \textit{numbers} of atoms in the compound, we must convert the masses of the elements to numbers of atoms. The easiest way to do this is to work with 100.00 g of the compound. In the present case, 38.67% carbon by mass means 38.67 g of carbon per 100.00 g of compound; 16.22% hydrogen means 16.22 g of hydrogen per 100.00 g of compound; and so on. To determine the formula, we must calculate the number of carbon atoms in 38.67 g of carbon, the number of hydrogen atoms in 16.22 g of hydrogen, and the number of nitrogen atoms in 45.11 g of nitrogen. We can do this as follows:

\[
38.67 \text{ g C} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = 3.220 \text{ mol C}
\]

\[
16.22 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 16.09 \text{ mol H}
\]

\[
45.11 \text{ g N} \times \frac{1 \text{ mol N}}{14.01 \text{ g N}} = 3.220 \text{ mol N}
\]

Thus 100.00 g of this compound contains 3.220 moles of carbon atoms, 16.09 moles of hydrogen atoms, and 3.220 moles of nitrogen atoms.
We can find the smallest whole-number ratio of atoms in this compound by dividing each of the mole values above by the smallest of the three:

\[
\begin{align*}
C: & \quad \frac{3.220}{3.220} = 1.000 = 1 \\
H: & \quad \frac{16.09}{3.220} = 4.997 = 5 \\
N: & \quad \frac{3.220}{3.220} = 1.000 = 1
\end{align*}
\]

Thus the formula might well be \( \text{CH}_3\text{N} \). However, it also could be \( \text{C}_2\text{H}_6\text{N}_2 \) or \( \text{C}_2\text{H}_6\text{N}_3 \), and so on—that is, some multiple of the smallest whole-number ratio. Each of these alternatives also has the correct relative numbers of atoms. That is, any molecule that can be represented as \((\text{CH}_2\text{N})_n\), where \( n \) is an integer, has the empirical formula \( \text{CH}_3\text{N} \). To be able to specify the exact formula of the molecule involved, the molecular formula, we must know the molar mass.

Suppose we know that this compound with empirical formula \( \text{CH}_3\text{N} \) has a molar mass of 31.06 g/mol. How do we determine which of the possible choices represents the molecular formula? Since the molecular formula is always a whole-number multiple of the empirical formula, we must first find the empirical formula mass for \( \text{CH}_3\text{N} \):

\[
\begin{align*}
1 \text{ C}: & \quad 1 \times 12.01 \text{ g} = 12.01 \text{ g} \\
5 \text{ H}: & \quad 5 \times 1.008 \text{ g} = 5.040 \text{ g} \\
1 \text{ N}: & \quad 1 \times 14.01 \text{ g} = 14.01 \text{ g}
\end{align*}
\]

Formula mass of \( \text{CH}_3\text{N} \) = 31.06 g/mol

This is the same as the known molar mass of the compound. Thus in this case the empirical formula and the molecular formula are the same; this substance consists of molecules with the formula \( \text{CH}_3\text{N} \). It is quite common for the empirical and molecular formulas to be different; some examples where this is the case are shown in Fig. 3.6.

**Problem-Solving Strategy**

**Empirical Formula Determination**

> Since mass percentage gives the number of grams of a particular element per 100 g of compound, base the calculation on 100 g of compound. Each percent will then represent the mass in grams of that element.

> Determine the number of moles of each element present in 100 g of compound using the atomic masses of the elements present.

> Divide each value of the number of moles by the smallest of the values. If each resulting number is a whole number (after appropriate rounding), these numbers represent the subscripts of the elements in the empirical formula.

> If the numbers obtained in the previous step are not whole numbers; multiply each number by an integer so that the results are all whole numbers.

**Critical Thinking**

One part of the problem-solving strategy for empirical formula determination is to base the calculation on 100 g of compound. What if you chose a mass other than 100 g? Would this work? What if you chose to base the calculation on 100 moles of compound? Would this work?
Figure 3.6 | Examples of substances whose empirical and molecular formulas differ. Notice that molecular formula = (empirical formula)$^n$, where $n$ is an integer.

$C_4H_6 = (CH)^6$

$S_8 = (S)_8$

$C_6H_{12}O_6 = (CH_2O)^6$

Problem-Solving Strategy

**Determining Molecular Formula from Empirical Formula**

› Obtain the empirical formula.

› Compute the mass corresponding to the empirical formula.

› Calculate the ratio:

\[
\text{Molar mass} \quad \frac{\text{Empirical formula mass}}{\text{Molar mass}}
\]

› The integer from the previous step represents the number of empirical formula units in one molecule. When the empirical formula subscripts are multiplied by this integer, the molecular formula results. This procedure is summarized by the equation:

\[
\text{Molecular formula} = \text{empirical formula} \times \frac{\text{molar mass}}{\text{empirical formula mass}}
\]

Interactive Example 3.10

Sign in at [http://login.cengagebrain.com](http://login.cengagebrain.com) to try this Interactive Example in OWL.

Determining Empirical and Molecular Formulas I

Determine the empirical and molecular formulas for a compound that gives the following percentages on analysis (in mass percents):

71.65% Cl  24.27% C  4.07% H

The molar mass is known to be 98.96 g/mol.

Solution

Where are we going?

To find the empirical and molecular formulas for the given compound

What do we know?

› Percent of each element

› Molar mass of the compound is 98.96 g/mol

What information do we need to find the empirical formula?

› Mass of each element in 100.00 g of compound

› Moles of each element
How do we get there?

What is the mass of each element in 100.00 g of compound?

- Cl: 71.65 g
- C: 24.27 g
- H: 4.07 g

What are the moles of each element in 100.00 g of compound?

- Cl: \( \frac{71.65 \text{ g Cl}}{35.45 \text{ g Cl}} \times \frac{1 \text{ mol Cl}}{1} = 2.021 \text{ mol Cl} \)
- C: \( \frac{24.27 \text{ g C}}{12.01 \text{ g C}} \times \frac{1 \text{ mol C}}{1} = 2.021 \text{ mol C} \)
- H: \( \frac{4.07 \text{ g H}}{1.008 \text{ g H}} \times \frac{1 \text{ mol H}}{1} = 4.04 \text{ mol H} \)

What is the empirical formula for the compound?

Dividing each mole value by 2.021 (the smallest number of moles present), we find the empirical formula ClCH₂.

What is the molecular formula for the compound?

Compare the empirical formula mass to the molar mass.

Empirical formula mass = 49.48 g/mol (Confirm this!

Molar mass is given = 98.96 g/mol

\[
\frac{\text{Molar mass}}{\text{Empirical formula mass}} = \frac{98.96 \text{ g/mol}}{49.48 \text{ g/mol}} = 2
\]

Molecular formula = (ClCH₂)₂ = Cl₂C₂H₄

> This substance is composed of molecules with the formula Cl₂C₂H₄.

Note: The method we use here allows us to determine the molecular formula of a compound but not its structural formula. The compound Cl₂C₂H₄ is called dichloroethane. There are two forms of this compound, shown in Fig. 3.7. The form at the bottom was formerly used as an additive in leaded gasoline.

See Exercises 3.87 and 3.88.

---

**Interactive Example 3.11**

Sign in at [http://login.cengagebrain.com](http://login.cengagebrain.com) to try this Interactive Example in OWL.

---

**Determining Empirical and Molecular Formulas II**

A white powder is analyzed and found to contain 43.64% phosphorus and 56.36% oxygen by mass. The compound has a molar mass of 283.88 g/mol. What are the compound’s empirical and molecular formulas?

**Solution**

**Where are we going?**

To find the empirical and molecular formulas for the given compound.

**What do we know?**

- Percent of each element
- Molar mass of the compound is 283.88 g/mol

**What information do we need to find the empirical formula?**

- Mass of each element in 100.00 g of compound
- Moles of each element
How do we get there?

What is the mass of each element in 100.00 g of compound?

\[
P \quad 43.64 \text{ g} \\
O \quad 56.36 \text{ g}
\]

What are the moles of each element in 100.00 g of compound?

\[
\begin{align*}
43.64 \text{ g P} & \times \frac{1 \text{ mol P}}{30.97 \text{ g P}} = 1.409 \text{ mol P} \\
56.36 \text{ g O} & \times \frac{1 \text{ mol O}}{16.00 \text{ g O}} = 3.523 \text{ mol O}
\end{align*}
\]

What is the empirical formula for the compound?

Dividing each mole value by the smaller one gives

\[
\frac{1.409}{1.409} = 1 \text{ P} \quad \text{and} \quad \frac{3.523}{1.409} = 2.5 \text{ O}
\]

This yields the formula \( \text{P}_2\text{O}_{5.5} \). Since compounds must contain whole numbers of atoms, the empirical formula should contain only whole numbers. To obtain the simplest set of whole numbers, we multiply both numbers by 2 to give the empirical formula \( \text{P}_3\text{O}_6 \).

What is the molecular formula for the compound?

Compare the empirical formula mass to the molar mass.

Empirical formula mass = 141.94 g/mol (Confirm this!)

Molar mass is given = 283.88 g/mol

\[
\frac{\text{Molar mass}}{\text{Empirical formula mass}} = \frac{283.88}{141.94} = 2
\]

\( \triangleright \) The molecular formula is \( \text{P}_2\text{O}_5 \), or \( \text{P}_3\text{O}_{10} \).

Note: The structural formula for this interesting compound is given in Fig. 3.8.

See Exercise 3.89

In Examples 3.10 and 3.11 we found the molecular formula by comparing the empirical formula mass with the molar mass. There is an alternate way to obtain the molecular formula. For example, in Example 3.10 we know the molar mass of the compound is 98.96 g/mol. This means that 1 mole of the compound weighs 98.96 g. Since we also know the mass percentages of each element, we can compute the mass of each element present in 1 mole of compound:

- **Chlorine:**
  \[
  \frac{71.65 \text{ g Cl}}{100.0 \text{ g compound}} \times \frac{98.96 \text{ g}}{\text{mol}} = \frac{70.90 \text{ g Cl}}{\text{mol compound}}
  \]

- **Carbon:**
  \[
  \frac{24.27 \text{ g C}}{100.0 \text{ g compound}} \times \frac{98.96 \text{ g}}{\text{mol}} = \frac{24.02 \text{ g C}}{\text{mol compound}}
  \]

- **Hydrogen:**
  \[
  \frac{4.07 \text{ g H}}{100.0 \text{ g compound}} \times \frac{98.96 \text{ g}}{\text{mol}} = \frac{4.03 \text{ g H}}{\text{mol compound}}
  \]

Now we can compute moles of atoms present per mole of compound:

- **Chlorine:**
  \[
  \frac{70.90 \text{ g Cl}}{\text{mol compound}} \times \frac{1 \text{ mol Cl}}{35.45 \text{ g Cl}} = \frac{2.000 \text{ mol Cl}}{\text{mol compound}}
  \]

- **Carbon:**
  \[
  \frac{24.02 \text{ g C}}{\text{mol compound}} \times \frac{1 \text{ mol C}}{12.01 \text{ g C}} = \frac{2.000 \text{ mol C}}{\text{mol compound}}
  \]

- **Hydrogen:**
  \[
  \frac{4.03 \text{ g H}}{\text{mol compound}} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = \frac{4.00 \text{ mol H}}{\text{mol compound}}
  \]
Thus 1 mole of the compound contains 2 moles of Cl atoms, 2 moles of C atoms, and 4 moles of H atoms, and the molecular formula is $\text{Cl}_2\text{C}_2\text{H}_4$, as obtained in Example 3.10.

**Problem-Solving Strategy**

**Determining Molecular Formula from Mass Percent and Molar Mass**

- Using the mass percentages and the molar mass, determine the mass of each element present in 1 mole of compound.
- Determine the number of moles of each element present in 1 mole of compound.
- The integers from the previous step represent the subscripts in the molecular formula.

**Interactive Example 3.12**

Sign in at http://login.cengagebrain.com to try this Interactive Example in OWL.

**Determining a Molecular Formula**

Caffeine, a stimulant found in coffee, tea, and chocolate, contains 49.48% carbon, 5.15% hydrogen, 28.87% nitrogen, and 16.49% oxygen by mass and has a molar mass of 194.2 g/mol. Determine the molecular formula of caffeine.

**Solution**

**Where are we going?**

To find the molecular formula for caffeine

**What do we know?**

- Percent of each element
  - 49.48% C
  - 28.87% N
  - 5.15% H
  - 16.49% O
- Molar mass of caffeine is 194.2 g/mol

**What information do we need to find the molecular formula?**

- Mass of each element (in 1 mole of caffeine)
- Mole of each element (in 1 mole of caffeine)

**How do we get there?**

**What is the mass of each element in 1 mole (194.2 g) of caffeine?**

\[
\begin{align*}
\frac{49.48 \text{ g C}}{100.0 \text{ g caffeine}} & \times \frac{194.2 \text{ g}}{\text{mol}} = \frac{96.09 \text{ g C}}{\text{mol caffeine}} \\
\frac{5.15 \text{ g H}}{100.0 \text{ g caffeine}} & \times \frac{194.2 \text{ g}}{\text{mol}} = \frac{10.0 \text{ g H}}{\text{mol caffeine}} \\
\frac{28.87 \text{ g N}}{100.0 \text{ g caffeine}} & \times \frac{194.2 \text{ g}}{\text{mol}} = \frac{56.07 \text{ g N}}{\text{mol caffeine}} \\
\frac{16.49 \text{ g O}}{100.0 \text{ g caffeine}} & \times \frac{194.2 \text{ g}}{\text{mol}} = \frac{32.02 \text{ g O}}{\text{mol caffeine}}
\end{align*}
\]
3.8 Chemical Equations

Chemical Reactions

A chemical change involves a reorganization of the atoms in one or more substances. For example, when the methane (CH₄) in natural gas combines with oxygen (O₂) in the air and burns, carbon dioxide (CO₂) and water (H₂O) are formed. This process is represented by a chemical equation with the reactants (here methane and oxygen) on the left side of an arrow and the products (carbon dioxide and water) on the right side:

\[
\text{CH}_4 + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O}
\]

Notice that the atoms have been reorganized. Bonds have been broken, and new ones have been formed. It is important to recognize that in a chemical reaction, atoms are neither created nor destroyed. All atoms present in the reactants must be accounted for among the products. In other words, there must be the same number of each type of atom on the products side and on the reactants side of the arrow. Making sure that this rule is obeyed is called balancing a chemical equation for a reaction.

The equation (shown above) for the reaction between CH₄ and O₂ is not balanced. We can see this from the following representation of the reaction:

\[
\begin{align*}
\text{CH}_4 & \quad \rightarrow \quad \text{CO}_2 & \quad + & \quad \text{H}_2\text{O} \\
\text{Reactants} & & & \text{Products}
\end{align*}
\]

Notice that the number of oxygen atoms (in O₂) on the left of the arrow is two, while on the right there are three O atoms (in CO₂ and H₂O). Also, there are four hydrogen atoms (in CH₄) on the left and only two (in H₂O) on the right. Remember that a chemical reaction is simply a rearrangement of the atoms (a change in the way they are organized). Atoms are neither created nor destroyed in a chemical reaction. Thus the reactants and products must occur in numbers that give the same number of each type of atom among both the reactants and products. Simple trial and error will allow us to figure this out for the reaction of methane with oxygen. The needed numbers of molecules are

\[
\begin{align*}
\text{CH}_4 & \quad + \quad \text{O}_2 \rightarrow \quad 2\text{CO}_2 & \quad + & \quad 2\text{H}_2\text{O} \\
\text{Reactants} & & & \text{Products}
\end{align*}
\]
Notice that now we have the same number of each type of atom represented among the reactants and the products.

We can represent the preceding situation in a shorthand manner by the following chemical equation:

$$\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$$

We can check that the equation is balanced by comparing the number of each type of atom on both sides:

$$\begin{array}{ccc}
\text{CH}_4 & + & 2\text{O}_2 \\
\uparrow & & \uparrow \\
1 \text{C} & + & 4 \text{H} \\
\downarrow & & \downarrow \\
1 \text{C} & + & 4 \text{H} \\
\uparrow & & \uparrow \\
\text{CO}_2 & + & 2\text{H}_2\text{O} \\
\end{array}$$

To summarize, we have

<table>
<thead>
<tr>
<th>Reactants</th>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 C</td>
<td>1 C</td>
</tr>
<tr>
<td>4 H</td>
<td>4 H</td>
</tr>
<tr>
<td>4 O</td>
<td>4 O</td>
</tr>
</tbody>
</table>

### The Meaning of a Chemical Equation

The chemical equation for a reaction gives two important types of information: the nature of the reactants and products and the relative numbers of each.

The reactants and products in a specific reaction must be identified by experiment. Besides specifying the compounds involved in the reaction, the equation often gives the physical states of the reactants and products:

<table>
<thead>
<tr>
<th>State</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid</td>
<td>(s)</td>
</tr>
<tr>
<td>Liquid</td>
<td>(l)</td>
</tr>
<tr>
<td>Gas</td>
<td>(g)</td>
</tr>
<tr>
<td>Dissolved in water (in aqueous solution)</td>
<td>(aq)</td>
</tr>
</tbody>
</table>

For example, when hydrochloric acid in aqueous solution is added to solid sodium hydrogen carbonate, the products carbon dioxide gas, liquid water, and sodium chloride (which dissolves in the water) are formed:

$$\text{HCl(aq)} + \text{NaHCO}_3(s) \rightarrow \text{CO}_2(g) + \text{H}_2\text{O(l)} + \text{NaCl(aq)}$$

The relative numbers of reactants and products in a reaction are indicated by the coefficients in the balanced equation. (The coefficients can be determined because we know that the same number of each type of atom must occur on both sides of the equation.) For example, the balanced equation

$$\text{CH}_4(g) + 2\text{O}_2(g) \rightarrow \text{CO}_2(g) + 2\text{H}_2\text{O(g)}$$

can be interpreted in several equivalent ways, as shown in Table 3.2. Note that the total mass is 80 g for both reactants and products. We expect the mass to remain constant, since chemical reactions involve only a rearrangement of atoms. Atoms, and therefore mass, are conserved in a chemical reaction.

From this discussion you can see that a balanced chemical equation gives you a great deal of information.
3.9 | Balancing Chemical Equations

An unbalanced chemical equation is of limited use. Whenever you see an equation, you should ask yourself whether it is balanced. The principle that lies at the heart of the balancing process is that atoms are conserved in a chemical reaction. The same number of each type of atom must be found among the reactants and products. It is also important to recognize that the identities of the reactants and products of a reaction are determined by experimental observation. For example, when liquid ethanol is burned in the presence of sufficient oxygen gas, the products are always carbon dioxide and water. When the equation for this reaction is balanced, the identities of the reactants and products must not be changed. The formulas of the compounds must never be changed in balancing a chemical equation. That is, the subscripts in a formula cannot be changed, nor can atoms be added or subtracted from a formula.

Critical Thinking

What if a friend was balancing chemical equations by changing the values of the subscripts instead of using the coefficients? How would you explain to your friend that this was the wrong thing to do?

Most chemical equations can be balanced by inspection, that is, by trial and error. It is always best to start with the most complicated molecule (those containing the greatest number of atoms). For example, consider the reaction of ethanol with oxygen, given by the unbalanced equation

\[ \text{C}_2\text{H}_5\text{OH}(l) + \text{O}_2(g) \rightarrow \text{CO}_2(g) + \text{H}_2\text{O}(g) \]

which can be represented by the following molecular models:

\[ \text{C}_2\text{H}_5\text{OH} + \text{O}_2 \rightarrow \text{CO}_2 + \text{H}_2\text{O} \]

Notice that the carbon and hydrogen atoms are not balanced. There are two carbon atoms on the left and one on the right, and there are six hydrogens on the left and two on the right. We need to find the correct numbers of reactants and products so that we have the same number of all types of atoms among the reactants and products. We will balance the equation "by inspection" (a systematic trial-and-error procedure).

The most complicated molecule here is \( \text{C}_2\text{H}_5\text{OH} \). We will begin by balancing the products that contain the atoms in \( \text{C}_2\text{H}_5\text{OH} \). Since \( \text{C}_2\text{H}_5\text{OH} \) contains two carbon atoms, we place the coefficient 2 before the \( \text{CO}_2 \) to balance the carbon atoms:

\[ \text{C}_2\text{H}_5\text{OH}(l) + \text{O}_2(g) \rightarrow 2\text{CO}_2(g) + \text{H}_2\text{O}(g) \]

Unless otherwise noted, all art on this page is © Cengage Learning 2014.
Since \( C_2H_5OH \) contains six hydrogen atoms, the hydrogen atoms can be balanced by placing a 3 before the \( H_2O \):

\[
C_2H_5OH(l) + O_2(g) \rightarrow 2CO_2(g) + 3H_2O(g)
\]

\((5 + 1)H \quad (3 \times 2)H\)

Last, we balance the oxygen atoms. Note that the right side of the preceding equation contains seven oxygen atoms, whereas the left side has only three. We can correct this by putting a 3 before the \( O_2 \) to produce the balanced equation:

\[
C_2H_5OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(g)
\]

\( \frac{1O}{7O} \quad \frac{6O}{7O} \quad \frac{2O}{6O} \quad \frac{3O}{7O} \)

Now we check:

\[
C_2H_5OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(g)
\]

2 C atoms 6 H atoms 7 O atoms
2 C atoms 6 H atoms 7 O atoms

The equation is balanced.

The balanced equation can be represented as follows:

You can see that all the elements balance.

**Problem-Solving Strategy**

**Writing and Balancing the Equation for a Chemical Reaction**

1. Determine what reaction is occurring. What are the reactants, the products, and the physical states involved?

2. Write the *unbalanced* equation that summarizes the reaction described in Step 1.

3. Balance the equation by inspection, starting with the most complicated molecule(s). Determine what coefficients are necessary so that the same number of each type of atom appears on both reactant and product sides. Do not change the identities (formulas) of any of the reactants or products.

**Critical Thinking**

One part of the problem-solving strategy for balancing chemical equations is "starting with the most complicated molecule." What if you started with a different molecule? Could you still eventually balance the chemical equation? How would this approach be different from the suggested technique?
Balancing a Chemical Equation

Chromium compounds exhibit a variety of bright colors. When solid ammonium dichromate, \((\text{NH}_4)_2\text{Cr}_2\text{O}_7\), a vivid orange compound, is ignited, a spectacular reaction occurs, as shown in the two photographs. Although the reaction is actually somewhat more complex, let’s assume here that the products are solid chromium(III) oxide, nitrogen gas (consisting of \(N_2\) molecules), and water vapor. Balance the equation for this reaction.

**Solution**

1. From the description given, the reactant is solid ammonium dichromate, \((\text{NH}_4)_2\text{Cr}_2\text{O}_7(s)\), and the products are nitrogen gas, \(N_2(g)\), water vapor, \(H_2O(g)\), and solid chromium(III) oxide, \(\text{Cr}_2\text{O}_3(s)\). The formula for chromium(III) oxide can be determined by recognizing that the Roman numeral III means that \(\text{Cr}^{3+}\) ions are present. For a neutral compound, the formula must then be \(\text{Cr}_2\text{O}_3\), since each oxide ion is \(O^{2-}\).

2. The unbalanced equation is

\[
(\text{NH}_4)_2\text{Cr}_2\text{O}_7(s) \rightarrow \text{Cr}_2\text{O}_3(s) + N_2(g) + H_2O(g)
\]

3. Note that nitrogen and chromium are balanced (two nitrogen atoms and two chromium atoms on each side), but hydrogen and oxygen are not. A coefficient of 4 for \(H_2O\) balances the hydrogen atoms:

\[
(\text{NH}_4)_2\text{Cr}_2\text{O}_7(s) \rightarrow \text{Cr}_2\text{O}_3(s) + N_2(g) + 4H_2O(g)
\]

\[
(4 \times 2) \text{ H}
\]

Note that in balancing the hydrogen we also have balanced the oxygen, since there are seven oxygen atoms in the reactants and in the products.

**Reality Check**

\[
\begin{align*}
2 \text{ N, 8 H, 2 Cr, 7 O} & \rightarrow 2 \text{ N, 8 H, 2 Cr, 7 O} \\
\text{Reactant atoms} & \text{Product atoms}
\end{align*}
\]

The equation is balanced.

*Decomposition of ammonium dichromate.*
Balancing a Chemical Equation II

At 1000°C, ammonia gas, \( \text{NH}_3(g) \), reacts with oxygen gas to form gaseous nitric oxide, \( \text{NO}(g) \), and water vapor. This reaction is the first step in the commercial production of nitric acid by the Ostwald process. Balance the equation for this reaction.

Solution

1. The unbalanced equation for the reaction is

\[
\text{NH}_3(g) + \text{O}_2(g) \rightarrow \text{NO}(g) + \text{H}_2\text{O}(g)
\]

2. Because all the molecules in this equation are of about equal complexity, where we start in balancing it is rather arbitrary. Let's begin by balancing the hydrogen. A coefficient of 2 for \( \text{NH}_3 \) and a coefficient of 3 for \( \text{H}_2\text{O} \) give six atoms of hydrogen on both sides:

\[
2\text{NH}_3(g) + \text{O}_2(g) \rightarrow \text{NO}(g) + 3\text{H}_2\text{O}(g)
\]

The nitrogen can be balanced with a coefficient of 2 for \( \text{NO} \):

\[
2\text{NH}_3(g) + \text{O}_2(g) \rightarrow 2\text{NO}(g) + 3\text{H}_2\text{O}(g)
\]

Finally, note that there are two atoms of oxygen on the left and five on the right. The oxygen can be balanced with a coefficient of \( \frac{5}{2} \) for \( \text{O}_2 \):

\[
2\text{NH}_3(g) + \frac{5}{2}\text{O}_2(g) \rightarrow 2\text{NO}(g) + 3\text{H}_2\text{O}(g)
\]

However, the usual custom is to have whole-number coefficients. We simply multiply the entire equation by 2.

\[
4\text{NH}_3(g) + 5\text{O}_2(g) \rightarrow 4\text{NO}(g) + 6\text{H}_2\text{O}(g)
\]

Reality Check | There are 4 N, 12 H, and 10 O on both sides, so the equation is balanced.

We can represent this balanced equation visually as

![Balanced chemical equation diagram]

3.10 Stoichiometric Calculations: Amounts of Reactants and Products

As we have seen in previous sections of this chapter, the coefficients in chemical equations represent numbers of molecules, not masses of molecules. However, when a reaction is to be run in a laboratory or chemical plant, the amounts of substances needed...
The next time you visit a gas station, take a moment to note the octane rating that accompanies the grade of gasoline that you are purchasing. The gasoline is priced according to its octane rating—a measure of the fuel's antiknock properties. In a conventional internal combustion engine, gasoline vapors and air are drawn into the combustion cylinder on the downward stroke of the piston. This air–fuel mixture is compressed on the upward piston stroke (compression stroke), and a spark from the sparkplug ignites the mix. The rhythmic combustion of the air–fuel mix occurring sequentially in several cylinders furnishes the power to propel the vehicle down the road. Excessive heat and pressure (or poor-quality fuel) within the cylinder may cause the premature combustion of the mixture—commonly known as engine "knock" or "ping." Over time, this engine knock can damage the engine, resulting in inefficient performance and costly repairs.

A consumer typically is faced with three choices of gasoline, with octane ratings of 87 (regular), 89 (midgrade), and 93 (premium). But if you happen to travel or live in the higher elevations of the Rocky Mountain states, you might be surprised to find different octane ratings at the gasoline pumps. The reason for this provides a lesson in stoichiometry. At higher elevations the air is less dense—the volume of oxygen per unit volume of air is smaller. Most engines are designed to achieve a 14:1 oxygen-to-fuel ratio in the cylinder prior to combustion. If less oxygen is available, then less fuel is required to achieve this optimal ratio. In turn, the lower volumes of oxygen and fuel result in a lower pressure in the cylinder. Because high pressure tends to promote knocking, the lower pressure within engine cylinders at higher elevations promotes a more controlled combustion of the air–fuel mixture, and therefore octane requirements are lower. While consumers in the Rocky Mountain states can purchase three grades of gasoline, the octane ratings of these fuel blends are different from those in the rest of the United States. In Denver, Colorado, regular gasoline is 85 octane, midgrade is 87 octane, and premium is 91 octane—2 points lower than gasoline sold in most of the rest of the country.

Before doing any calculations involving a chemical reaction, be sure the equation for the reaction is balanced.

**Chemical connections**

**High Mountains—Low Octane**

Cannot be determined by counting molecules directly. Counting is always done by weighing. In this section we will see how chemical equations can be used to determine the masses of reacting chemicals.

To develop the principles for dealing with the stoichiometry of reactions, we will consider the reaction of propane with oxygen to produce carbon dioxide and water. We will consider the question: "What mass of oxygen will react with 96.1 g of propane?"

In doing stoichiometry, the first thing we must do is write the balanced chemical equation for the reaction. In this case the balanced equation is

\[
C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)
\]

which can be visualized as
This equation means that 1 mole of C₃H₈ reacts with 5 moles of O₂ to produce 3 moles of CO₂ and 4 moles of H₂O. To use this equation to find the masses of reactants and products, we must be able to convert between masses and moles of substances. Thus we must first ask: "How many moles of propane are present in 96.1 g of propane?" The molar mass of propane to three significant figures is 44.1 (that is, 3 × 12.01 + 8 × 1.008). The moles of propane can be calculated as follows:

\[
96.1 \text{ g C}_3\text{H}_8 \times \frac{1 \text{ mol C}_3\text{H}_8}{44.1 \text{ g C}_3\text{H}_8} = 2.18 \text{ mol C}_3\text{H}_8
\]

Next we must take into account the fact that each mole of propane reacts with 5 moles of oxygen. The best way to do this is to use the balanced equation to construct a mole ratio. In this case we want to convert from moles of propane to moles of oxygen. From the balanced equation, we see that 5 moles of O₂ are required for each mole of C₃H₈, so the appropriate ratio is

\[
\frac{5 \text{ mol O}_2}{1 \text{ mol C}_3\text{H}_8}
\]

Multiplying the number of moles of C₃H₈ by this factor gives the number of moles of O₂ required:

\[
2.18 \text{ mol C}_3\text{H}_8 \times \frac{5 \text{ mol O}_2}{1 \text{ mol C}_3\text{H}_8} = 10.9 \text{ mol O}_2
\]

Notice that the mole ratio is set up so that the moles of C₃H₈ cancel out, and the units that result are moles of O₂.

Since the original question asked for the mass of oxygen needed to react with 96.1 g of propane, the 10.9 moles of O₂ must be converted to grams. Since the molar mass of O₂ is 32.0 g/mol,

\[
10.9 \text{ mol O}_2 \times \frac{32.0 \text{ g O}_2}{1 \text{ mol O}_2} = 349 \text{ g O}_2
\]

Therefore, 349 g of oxygen are required to burn 96.1 g of propane.

This example can be extended by asking: "What mass of carbon dioxide is produced when 96.1 g of propane are combusted with oxygen?" In this case we must convert between moles of propane and moles of carbon dioxide. This can be accomplished by looking at the balanced equation, which shows that 3 moles of CO₂ are produced for each mole of C₃H₈ reacted. The mole ratio needed to convert from mole of propane to moles of carbon dioxide is

\[
\frac{3 \text{ mol CO}_2}{1 \text{ mol C}_3\text{H}_8}
\]

The conversion is

\[
2.18 \text{ mol C}_3\text{H}_8 \times \frac{3 \text{ mol CO}_2}{1 \text{ mol C}_3\text{H}_8} = 6.54 \text{ mol CO}_2
\]

Then, using the molar mass of CO₂ (44.0 g/mol), we calculate the mass of CO₂ produced:

\[
6.54 \text{ mol CO}_2 \times \frac{44.0 \text{ g CO}_2}{1 \text{ mol CO}_2} = 288 \text{ g CO}_2
\]
We will now summarize the sequence of steps needed to carry out stoichiometric calculations.

\[
\begin{align*}
96.1 \text{ g C}_3\text{H}_8 & \quad \frac{1 \text{ mol C}_3\text{H}_8}{44.1 \text{ g C}_3\text{H}_8} \quad 2.18 \text{ mol C}_3\text{H}_8 & \quad \frac{3 \text{ mol CO}_2}{1 \text{ mol C}_3\text{H}_8} \quad 6.54 \text{ mol CO}_2 \\
& \quad \frac{44.0 \text{ g CO}_2}{1 \text{ mol CO}_2} \quad 288 \text{ g CO}_2
\end{align*}
\]

**Critical Thinking**

Your lab partner has made the observation that you always take the mass of chemicals in lab, but then you use mole ratios to balance the equation. "Why not use the masses in the equation?" your partner asks. What if your lab partner decided to balance equations by using masses as coefficients? Is this even possible? Why or why not?

**Problem-Solving Strategy**

**Calculating Masses of Reactants and Products in Chemical Reactions**

1. Balance the equation for the reaction.
2. Convert the known mass of the reactant or product to moles of that substance.
3. Use the balanced equation to set up the appropriate mole ratios.
4. Use the appropriate mole ratios to calculate the number of moles of the desired reactant or product.
5. Convert from moles back to grams if required by the problem.

\[
\text{Mass of known substance} \xrightarrow{\text{Convert to moles}} \text{Moles of known substance} \xrightarrow{\text{Use mole ratio to convert}} \text{Moles of desired substance} \xrightarrow{\text{Convert to grams}} \text{Mass of desired substance}
\]
Chemical Stoichiometry I

Solid lithium hydroxide is used in space vehicles to remove exhaled carbon dioxide from the living environment by forming solid lithium carbonate and liquid water. What mass of gaseous carbon dioxide can be absorbed by 1.00 kg of lithium hydroxide?

Solution

Where are we going?
To find the mass of \( \text{CO}_2 \) absorbed by 1.00 kg \( \text{LiOH} \)

What do we know?

- Chemical reaction
  
  \[ \text{LiOH}(s) + \text{CO}_2(g) \rightarrow \text{Li}_2\text{CO}_3(s) + \text{H}_2\text{O}(l) \]

- 1.00 kg \( \text{LiOH} \)

What information do we need to find the mass of \( \text{CO}_2 \)?

- Balanced equation for the reaction

How do we get there?

1. What is the balanced equation?

\[ 2\text{LiOH}(s) + \text{CO}_2(g) \rightarrow \text{Li}_2\text{CO}_3(s) + \text{H}_2\text{O}(l) \]

2. What are the moles of \( \text{LiOH} \)?

To find the moles of \( \text{LiOH} \), we need to know the molar mass.

What is the molar mass for \( \text{LiOH} \)?

\[ 6.941 + 16.00 + 1.008 = 23.95 \text{ g/mol} \]

Now we use the molar mass to find the moles of \( \text{LiOH} \):

\[ 1.00 \text{ kg LiOH} \times \frac{1000 \text{ g LiOH}}{1 \text{ kg LiOH}} \times \frac{1 \text{ mol LiOH}}{23.95 \text{ g LiOH}} = 41.8 \text{ mol LiOH} \]

3. What is the mole ratio between \( \text{CO}_2 \) and \( \text{LiOH} \) in the balanced equation?

\[ \frac{1 \text{ mol CO}_2}{2 \text{ mol LiOH}} \]

4. What are the moles of \( \text{CO}_2 \)?

\[ 41.8 \text{ mol LiOH} \times \frac{1 \text{ mol CO}_2}{2 \text{ mol LiOH}} = 20.9 \text{ mol CO}_2 \]

5. What is the mass of \( \text{CO}_2 \) formed from 1.00 kg \( \text{LiOH} \)?

\[ 20.9 \text{ mol CO}_2 \times \frac{44.0 \text{ g CO}_2}{1 \text{ mol CO}_2} = 9.20 \times 10^2 \text{ g CO}_2 \]

Thus 92.0 g of \( \text{CO}_2(g) \) will be absorbed by 1.00 kg of \( \text{LiOH}(s) \).
Chemical Stoichiometry II

Baking soda (NaHCO₃) is often used as an antacid. It neutralizes excess hydrochloric acid secreted by the stomach:

\[ \text{NaHCO}_3(s) + \text{HCl}(aq) \rightarrow \text{NaCl}(aq) + \text{H}_2\text{O}(l) + \text{CO}_2(aq) \]

Milk of magnesia, which is an aqueous suspension of magnesium hydroxide, is also used as an antacid:

\[ \text{Mg(OH)}_2(s) + 2\text{HCl}(aq) \rightarrow 2\text{H}_2\text{O}(l) + \text{MgCl}_2(aq) \]

Which is the more effective antacid per gram, NaHCO₃ or Mg(OH)₂?

Solution

Where are we going?

To compare the acid neutralizing power of NaHCO₃ and Mg(OH)₂ per gram

What do we know?

- Balanced equations for the reactions
- 1.00 g NaHCO₃
- 1.00 g Mg(OH)₂

How do we get there?

For NaHCO₃

1. What is the balanced equation?

\[ \text{NaHCO}_3(s) + \text{HCl}(aq) \rightarrow \text{NaCl}(aq) + \text{H}_2\text{O}(l) + \text{CO}_2(aq) \]

2. What are the moles of NaHCO₃ in 1.00 g?

To find the moles of NaHCO₃, we need to know the molar mass (84.01 g/mol).

\[
\text{1.00 g NaHCO}_3 \times \frac{1 \text{ mol NaHCO}_3}{84.01 \text{ g NaHCO}_3} = 1.19 \times 10^{-2} \text{ mol NaHCO}_3
\]

3. What is the mole ratio between HCl and NaHCO₃ in the balanced equation?

\[
\frac{1 \text{ mol HCl}}{1 \text{ mol NaHCO}_3}
\]

4. What are the moles of HCl?

\[
1.19 \times 10^{-2} \text{ mol NaHCO}_3 \times \frac{1 \text{ mol HCl}}{1 \text{ mol NaHCO}_3} = 1.19 \times 10^{-2} \text{ mol HCl}
\]

Thus 1.00 g of NaHCO₃ will neutralize 1.19 \times 10^{-2} mole of HCl.

For Mg(OH)₂

1. What is the balanced equation?

\[ \text{Mg(OH)}_2(s) + 2\text{HCl}(aq) \rightarrow 2\text{H}_2\text{O}(l) + \text{MgCl}_2(aq) \]

2. What are the moles of Mg(OH)₂ in 1.00 g?

To find the moles of Mg(OH)₂, we need to know the molar mass (58.32 g/mol).

\[
\text{1.00 g Mg(OH)}_2 \times \frac{1 \text{ mol Mg(OH)}_2}{58.32 \text{ g Mg(OH)}_2} = 1.71 \times 10^{-2} \text{ mol Mg(OH)}_2
\]
3. What is the mole ratio between HCl and Mg(OH)_2 in the balanced equation?

\[
\frac{2 \text{ mol HCl}}{1 \text{ mol Mg(OH)}_2}
\]

4. What are the moles of HCl?

\[
1.71 \times 10^{-2} \text{ mol Mg(OH)}_2 \times \frac{2 \text{ mol HCl}}{1 \text{ mol Mg(OH)}_2} = 3.42 \times 10^{-2} \text{ mol HCl}
\]

Thus 1.00 g of Mg(OH)_2 will neutralize \(3.42 \times 10^{-2}\) mole of HCl.

Since 1.00 g NaHCO_3 neutralizes \(1.19 \times 10^{-2}\) mole of HCl and 1.00 g Mg(OH)_2 neutralizes \(3.42 \times 10^{-2}\) mole of HCl, Mg(OH)_2 is the more effective antacid.

Learning Objectives:
LO 3.1, LO 3.3, LO 3.4

3.11 The Concept of Limiting Reactant

Suppose you have a part-time job in a sandwich shop. One very popular sandwich is always made as follows:

2 slices bread + 3 slices meat + 1 slice cheese \(\rightarrow\) sandwich

Assume that you come to work one day and find the following quantities of ingredients:

- 8 slices bread
- 9 slices meat
- 5 slices cheese

How many sandwiches can you make? What will be left over?

To solve this problem, let's see how many sandwiches we can make with each component:

Bread: \(8 \text{ slices bread} \times \frac{1 \text{ sandwich}}{2 \text{ slices bread}} = 4 \text{ sandwiches}\)

Meat: \(9 \text{ slices meat} \times \frac{1 \text{ sandwich}}{3 \text{ slices meat}} = 3 \text{ sandwiches}\)

Cheese: \(5 \text{ slices cheese} \times \frac{1 \text{ sandwich}}{1 \text{ slice cheese}} = 5 \text{ sandwiches}\)

How many sandwiches can you make? The answer is three. When you run out of meat, you must stop making sandwiches. The meat is the limiting ingredient (Fig. 3.9).

What do you have left over? Making three sandwiches requires six pieces of bread. You started with eight slices, so you have two slices of bread left. You also used three pieces of cheese for the three sandwiches, so you have two pieces of cheese left.

In this example, the ingredient present in the largest number (the meat) was actually the component that limited the number of sandwiches you could make. This situation arose because each sandwich required three slices of meat—more than the quantities required of any other ingredient.
When molecules react with each other to form products, considerations very similar to those involved in making sandwiches arise. We can illustrate these ideas with the reaction of \( \text{N}_2(g) \) and \( \text{H}_2(g) \) to form \( \text{NH}_3(g) \):

\[
\text{N}_2(g) + 3\text{H}_2(g) \rightarrow 2\text{NH}_3(g)
\]

Consider the following container of \( \text{N}_2(g) \) and \( \text{H}_2(g) \):
What will this container look like if the reaction between N₂ and H₂ proceeds to completion? To answer this question, you need to remember that each N₂ requires 3 H₂ molecules to form 2 NH₃. To make things clear, we will circle groups of reactants:

\[
\begin{align*}
\text{Before the reaction} & \quad \text{After the reaction} \\
\bigcirc & \quad \bigcirc \\
\bullet & \quad \bullet \\
\bullet & \quad \bullet \\
\bullet & \quad \bullet
\end{align*}
\]

In this case, the mixture of N₂ and H₂ contained just the number of molecules needed to form NH₃ with nothing left over. That is, the ratio of the number of H₂ molecules to N₂ molecules was

\[
\frac{15\text{H}_2}{5\text{N}_2} = \frac{3\text{H}_2}{1\text{N}_2}
\]

This ratio exactly matches the numbers in the balanced equation

\[
3\text{H}_2(g) + \text{N}_2(g) \longrightarrow 2\text{NH}_3(g)
\]

This type of mixture is called a **stoichiometric mixture**—one that contains the relative amounts of reactants that match the numbers in the balanced equation. In this case all reactants will be consumed to form products.

Now consider another container of N₂(g) and H₂(g):

\[
\begin{align*}
\bigcirc & \quad \bigcirc \\
\bullet & \quad \bullet \\
\end{align*}
\]
What will the container look like if the reaction between \( \text{N}_2(g) \) and \( \text{H}_2(g) \) proceeds to completion? Remember that each \( \text{N}_2 \) requires 3 \( \text{H}_2 \). Circling groups of reactants, we have

![Diagram showing before and after reaction of \( \text{N}_2(g) \) and \( \text{H}_2(g) \) forming \( \text{NH}_3(g) \).]

In this case, the hydrogen \((\text{H}_2)\) is limiting. That is, the \( \text{H}_2 \) molecules are used up before all the \( \text{N}_2 \) molecules are consumed. In this situation the amount of hydrogen limits the amount of product (ammonia) that can form—hydrogen is the limiting reactant. Some \( \text{N}_2 \) molecules are left over in this case because the reaction runs out of \( \text{H}_2 \) molecules first. To determine how much product can be formed from a given mixture of reactants, we have to look for the reactant that is limiting—the one that runs out first and thus limits the amount of product that can form. In some cases, the mixture of reactants might be stoichiometric—that is, all reactants run out at the same time. In general, however, you cannot assume that a given mixture of reactants is a stoichiometric mixture, so you must determine whether one of the reactants is limiting. The reactant that runs out first and thus limits the amounts of products that can form is called the limiting reactant.

To this point we have considered examples where the numbers of reactant molecules could be counted. In “real life” you can’t count the molecules directly—you can’t see them, and even if you could, there would be far too many to count. Instead, you must count by weighing. We must therefore explore how to find the limiting reactant, given the masses of the reactants.

### A. Determination of Limiting Reactant Using Reactant Quantities

There are two ways to determine the limiting reactant in a chemical reaction. One involves comparing the moles of reactants to see which runs out first. We will consider this approach here.

In the laboratory or chemical plant, we work with much larger quantities than the few molecules of the preceding example. Therefore, we must learn to deal with limiting reactants using moles. The ideas are exactly the same, except that we are using moles of molecules instead of individual molecules. For example, suppose 25.0 kg of nitrogen and 5.00 kg of hydrogen are mixed and reacted to form ammonia. How do we calculate the mass of ammonia produced when this reaction is run to completion (until one of the reactants is completely consumed)?

As in the preceding example, we must use the balanced equation

\[
\text{N}_2(g) + 3\text{H}_2(g) \rightarrow 2\text{NH}_3(g)
\]
to determine whether nitrogen or hydrogen is the limiting reactant and then to determine the amount of ammonia that is formed. We first calculate the moles of reactants present:

\[
25.0 \text{ kg N}_2 \times \frac{1000 \text{ g N}_2}{1 \text{ kg N}_2} \times \frac{1 \text{ mol N}_2}{28.0 \text{ g N}_2} = 8.93 \times 10^3 \text{ mol N}_2
\]

\[
5.00 \text{ kg H}_2 \times \frac{1000 \text{ g H}_2}{1 \text{ kg H}_2} \times \frac{1 \text{ mol H}_2}{2.016 \text{ g H}_2} = 2.48 \times 10^3 \text{ mol H}_2
\]

Since 1 mole of N\(_2\) reacts with 3 moles of H\(_2\), the number of moles of H\(_2\) that will react exactly with 8.93 \(	imes\) 10\(^3\) moles of N\(_2\) is

\[
8.93 \times 10^3 \text{ mol N}_2 \times \frac{3 \text{ mol H}_2}{1 \text{ mol N}_2} = 2.68 \times 10^3 \text{ mol H}_2
\]

Thus 8.93 \(	imes\) 10\(^3\) moles of N\(_2\) requires 2.68 \(	imes\) 10\(^3\) moles of H\(_2\) to react completely. However, in this case, only 2.48 \(	imes\) 10\(^3\) moles of H\(_2\) are present. This means that the hydrogen will be consumed before the nitrogen. Thus hydrogen is the limiting reactant in this particular situation, and we must use the amount of hydrogen to compute the quantity of ammonia formed:

\[
2.48 \times 10^3 \text{ mol H}_2 \times \frac{2 \text{ mol NH}_3}{3 \text{ mol H}_2} = 1.65 \times 10^3 \text{ mol NH}_3
\]

Converting moles to kilograms gives

\[
1.65 \times 10^3 \text{ mol NH}_3 \times \frac{17.0 \text{ g NH}_3}{1 \text{ mol NH}_3} = 2.80 \times 10^4 \text{ g NH}_3 = 28.0 \text{ kg NH}_3
\]

Note that to determine the limiting reactant, we could have started instead with the given amount of hydrogen and calculated the moles of nitrogen required:

\[
2.48 \times 10^3 \text{ mol H}_2 \times \frac{1 \text{ mol N}_2}{3 \text{ mol H}_2} = 8.27 \times 10^2 \text{ mol N}_2
\]

Thus 2.48 \(	imes\) 10\(^3\) moles of H\(_2\) requires 8.27 \(	imes\) 10\(^2\) moles of N\(_2\). Since 8.93 \(	imes\) 10\(^3\) moles of N\(_2\) are actually present, the nitrogen is in excess. The hydrogen will run out first, and thus again we find that hydrogen limits the amount of ammonia formed.

A related but simpler way to determine which reactant is limiting is to compare the mole ratio of the substances required by the balanced equation with the mole ratio of reactants actually present. For example, in this case the mole ratio of H\(_2\) to N\(_2\) required by the balanced equation is

\[
\frac{3 \text{ mol H}_2}{1 \text{ mol N}_2}
\]

That is,

\[
\frac{\text{mol H}_2}{\text{mol N}_2} \text{ (required)} = \frac{3}{1} = 3
\]

In this experiment we have 2.48 \(	imes\) 10\(^3\) moles of H\(_2\) and 8.93 \(	imes\) 10\(^3\) moles of N\(_2\). Thus the ratio

\[
\frac{\text{mol H}_2}{\text{mol N}_2} \text{ (actual)} = \frac{2.48 \times 10^3}{8.93 \times 10^2} = 2.78
\]

Since 2.78 is less than 3, the actual mole ratio of H\(_2\) to N\(_2\) is too small, and H\(_2\) must be limiting. If the actual H\(_2\) to N\(_2\) mole ratio had been greater than 3, then the H\(_2\) would have been in excess and the N\(_2\) would be limiting.

Always determine which reactant is limiting.
B. Determination of Limiting Reactant Using Quantities of Products Formed

A second method for determining which reactant in a chemical reaction is limiting is to consider the amounts of products that can be formed by completely consuming each reactant. The reactant that produces the smallest amount of product must run out first and thus be limiting. To see how this works, consider again the reaction of 25.0 kg (8.93 \times 10^5 moles) of nitrogen with 5.00 kg (2.48 \times 10^3 moles) of hydrogen.

We will now use these amounts of reactants to determine how much NH₃ would form. Since 1 mol of N₂ forms 2 moles of NH₃, the amount of NH₃ that would be formed if all of the N₂ was used up is calculated as follows:

\[
8.93 \times 10^5 \text{ mol N}_2 \times \frac{2 \text{ mol NH}_3}{1 \text{ mol N}_2} = 1.79 \times 10^6 \text{ mol NH}_3
\]

Next we will calculate how much NH₃ would be formed if the H₂ was completely used up:

\[
2.48 \times 10^3 \text{ mol H}_2 \times \frac{2 \text{ mol NH}_3}{3 \text{ mol H}_2} = 1.65 \times 10^3 \text{ mol NH}_3
\]

Because a smaller amount of NH₃ is produced from the H₂ than from the N₂, the amount of H₂ must be limiting.

Thus because the H₂ is the limiting reactant, the amount of NH₃ that can form is 1.65 \times 10^3 moles. Converting moles to kilograms gives:

\[
1.65 \times 10^3 \text{ mol NH}_3 \times \frac{17 \text{ g NH}_3}{1 \text{ mol NH}_3} = 2.80 \times 10^3 \text{ g NH}_3 = 28.0 \text{ kg NH}_3
\]

---

**Stoichiometry: Limiting Reactant**

Nitrogen gas can be prepared by passing gaseous ammonia over solid copper(II) oxide at high temperatures. The other products of the reaction are solid copper and water vapor. If a sample containing 18.1 g of NH₃ is reacted with 90.4 g of CuO, which is the limiting reactant? How many grams of N₂ will be formed?

**Solution**

*Where are we going?*

To find the limiting reactant
To find the mass of N₂ produced

*What do we know?*

\( \rightarrow \) The chemical reaction

\[ \text{NH}_3(g) + \text{CuO}(s) \rightarrow \text{N}_2(g) + \text{Cu}(s) + \text{H}_2\text{O}(g) \]

\( \rightarrow \) 18.1 g NH₃
\( \rightarrow \) 90.4 g CuO

*What information do we need?*

\( \rightarrow \) Balanced equation for the reaction
\( \rightarrow \) Moles of NH₃
\( \rightarrow \) Moles of CuO

---

Unless otherwise noted, all art on this page is © Cengage Learning 2016.
How do we get there?
To find the limiting reactant

What is the balanced equation?

\[ 2\text{NH}_3(g) + 3\text{CuO(s)} \rightarrow \text{N}_2(g) + 3\text{Cu}(s) + 3\text{H}_2\text{O(g)} \]

What are the moles of NH$_3$ and CuO?
To find the moles, we need to know the molar masses.

\[
\begin{align*}
\text{NH}_3 & : 17.03 \text{ g/mol} \\
\text{CuO} & : 79.55 \text{ g/mol}
\end{align*}
\]

\[
18.1 \text{ g-NH}_3 \times \frac{1 \text{ mol NH}_3}{17.03 \text{ g-NH}_3} = 1.06 \text{ mol NH}_3
\]

\[
90.4 \text{ g-CuO} \times \frac{1 \text{ mol CuO}}{79.55 \text{ g-CuO}} = 1.14 \text{ mol CuO}
\]

A. First we will determine the limiting reactant by comparing the moles of reactants to see which one is consumed first.

What is the mole ratio between NH$_3$ and CuO in the balanced equation?

\[
\frac{3 \text{ mol CuO}}{2 \text{ mol NH}_3}
\]

How many moles of CuO are required to react with 1.06 moles of NH$_3$?

\[
1.06 \text{ mol-NH}_3 \times \frac{3 \text{ mol CuO}}{2 \text{ mol-NH}_3} = 1.59 \text{ mol CuO}
\]

\[ > \text{ Thus 1.59 moles of CuO are required to react with 1.06 moles of NH}_3. \text{ Since only 1.14 moles of CuO are actually present, the amount of CuO is limiting; CuO will run out before NH}_3 \text{ does. We can verify this conclusion by comparing the mole ratio of CuO and NH}_3 \text{ required by the balanced equation:}
\]

\[
\frac{\text{mol CuO}}{\text{mol NH}_3} \text{ (required)} = \frac{3}{2} = 1.5
\]

with the mole ratio actually present:

\[
\frac{\text{mol CuO}}{\text{mol NH}_3} \text{ (actual)} = \frac{1.14}{1.06} = 1.08
\]

\[ > \text{ Since the actual ratio is too small (less than 1.5), CuO is the limiting reactant.} \]

B. Alternatively we can determine the limiting reactant by computing the moles of N$_2$ that would be formed by complete consumption of NH$_3$ and CuO:

\[
1.06 \text{ mol-NH}_3 \times \frac{1 \text{ mol N}_2}{2 \text{ mol-NH}_3} = 0.530 \text{ mol N}_2
\]

\[
1.14 \text{ mol-CuO} \times \frac{1 \text{ mol N}_2}{3 \text{ mol-CuO}} = 0.380 \text{ mol N}_2
\]

As before, we see that the CuO is limiting since it produces the smaller amount of N$_2$.

To find the mass of N$_2$ produced

What are the moles of N$_2$ formed?
Because CuO is the limiting reactant, we must use the amount of CuO to calculate the amount of N$_2$ formed.
What is the mole ratio between \( N_2 \) and \( CuO \) in the balanced equation?

\[
\frac{1 \text{ mol } N_2}{3 \text{ mol } CuO}
\]

What are the moles of \( N_2 \)?

\[
1.14 \text{ mol } CuO \times \frac{1 \text{ mol } N_2}{3 \text{ mol } CuO} = 0.380 \text{ mol } N_2
\]

What mass of \( N_2 \) is produced?

Using the molar mass of \( N_2 \) (28.02 g/mol), we can calculate the mass of \( N_2 \) produced:

\[
\frac{0.380 \text{ mol } N_2 \times 28.02 \text{ g } N_2}{1 \text{ mol } N_2} = 10.6 \text{ g } N_2
\]

See Exercises 3.117 through 3.122

The amount of a product formed when the limiting reactant is completely consumed is called the **theoretical yield** of that product. In Example 3.17, 10.6 g of nitrogen represent the theoretical yield. This is the maximum amount of nitrogen that can be produced from the quantities of reactants used. Actually, the amount of product predicted by the theoretical yield is seldom obtained because of side reactions (other reactions that involve one or more of the reactants or products) and other complications. The **actual yield** of product is often given as a percentage of the theoretical yield. This is called the **percent yield**:

\[
\frac{\text{Actual yield}}{\text{Theoretical yield}} \times 100\% = \text{percent yield}
\]

For example, if the reaction considered in Example 3.17 actually gave 6.63 g of nitrogen instead of the predicted 10.6 g, the percent yield of nitrogen would be

\[
\frac{6.63 \text{ g } N_2}{10.6 \text{ g } N_2} \times 100\% = 62.5\%
\]

**Calculating Percent Yield**

Methanol (CH\(_3\)OH), also called **methyl alcohol**, is the simplest alcohol. It is used as a fuel in race cars and is a potential replacement for gasoline. Methanol can be manufactured by combining gaseous carbon monoxide and hydrogen. Suppose 68.5 kg CO(g) is reacted with 8.60 kg H\(_2\)(g). Calculate the theoretical yield of methanol. If \(3.57 \times 10^4\) g CH\(_3\)OH is actually produced, what is the percent yield of methanol?

**Solution**

**Where are we going?**

To calculate the theoretical yield of methanol

To calculate the percent yield of methanol

**What do we know?**

- The chemical reaction
  
  \[
  \text{H}_2(g) + \text{CO}(g) \rightarrow \text{CH}_3\text{OH}(l)
  \]

- 68.5 kg CO(g)
- 8.60 kg H\(_2\)(g)
- \(3.57 \times 10^4\) g CH\(_3\)OH is produced
What information do we need?
› Balanced equation for the reaction
› Moles of H₂
› Moles of CO
› Which reactant is limiting
› Amount of CH₃OH produced

How do we get there?
To find the limiting reactant

What is the balanced equation?

\[ 2\text{H}_2(\text{g}) + \text{CO}(\text{g}) \rightarrow \text{CH}_3\text{OH}(\ell) \]

What are the moles of H₂ and CO?
To find the moles, we need to know the molar masses.

\[
\begin{align*}
\text{H}_2 & \quad 2.016 \text{ g/mol} \\
\text{CO} & \quad 28.02 \text{ g/mol}
\end{align*}
\]

\[
\begin{align*}
68.5 \text{ kg CO} \times \frac{1000 \text{ g CO}}{1 \text{ kg CO}} \times \frac{1 \text{ mol CO}}{28.02 \text{ g CO}} & = 2.44 \times 10^3 \text{ mol CO} \\
8.60 \text{ kg H}_2 \times \frac{1000 \text{ g H}_2}{1 \text{ kg H}_2} \times \frac{1 \text{ mol H}_2}{2.016 \text{ g H}_2} & = 4.27 \times 10^3 \text{ mol H}_2
\end{align*}
\]

A. Determination of Limiting Reactant Using Reactant Quantities

What is the mole ratio between H₂ and CO in the balanced equation?

\[
\frac{2 \text{ mol H}_2}{1 \text{ mol CO}}
\]

How does the actual mole ratio compare to the stoichiometric ratio?
To determine which reactant is limiting, we compare the mole ratio of H₂ and CO required by the balanced equation

\[
\frac{\text{mol H}_2}{\text{mol CO}} \text{ (required)} = \frac{2}{1} = 2
\]

with the actual mole ratio

\[
\frac{\text{mol H}_2}{\text{mol CO}} \text{ (actual)} = \frac{4.27 \times 10^3}{2.44 \times 10^3} = 1.75
\]

› Since the actual mole ratio of H₂ to CO is smaller than the required ratio, H₂ is limiting.

B. Determination of Limiting Reactant Using Quantities of Products Formed
We can also determine the limiting reactant by calculating the amounts of CH₃OH formed by complete consumption of CO(g) and H₂(g):

\[
\begin{align*}
2.44 \times 10^3 \text{ mol CO} \times \frac{1 \text{ mol CH}_3\text{OH}}{1 \text{ mol CO}} & = 2.44 \times 10^3 \text{ mol CH}_3\text{OH} \\
4.27 \times 10^3 \text{ mol H}_2 \times \frac{1 \text{ mol CH}_3\text{OH}}{2 \text{ mol H}_2} & = 2.14 \times 10^3 \text{ mol CH}_3\text{OH}
\end{align*}
\]

Since complete consumption of the H₂ produces the smaller amount of CH₃OH, the H₂ is the limiting reactant as we determined above.
To calculate the theoretical yield of methanol

**What are the moles of CH₃OH formed?**

We must use the amount of H₂ and the mole ratio between H₂ and CH₃OH to determine the maximum amount of methanol that can be produced:

\[ 4.27 \times 10^3 \text{ mol H}_2 \times \frac{1 \text{ mol CH}_3\text{OH}}{2 \text{ mol H}_2} = 2.14 \times 10^3 \text{ mol CH}_3\text{OH} \]

**What is the theoretical yield of CH₃OH in grams?**

\[ 2.14 \times 10^3 \text{ mol CH}_3\text{OH} \times \frac{32.04 \text{ g CH}_3\text{OH}}{1 \text{ mol CH}_3\text{OH}} = 6.86 \times 10^4 \text{ g CH}_3\text{OH} \]

Thus, from the amount of reactants given, the maximum amount of CH₃OH that can be formed is \( 6.86 \times 10^4 \) g. This is the theoretical yield.

**What is the percent yield of CH₃OH?**

\[ \frac{\text{Actual yield (grams)}}{\text{Theoretical yield (grams)}} \times 100 = \frac{3.57 \times 10^4 \text{ g CH}_3\text{OH}}{6.86 \times 10^4 \text{ g CH}_3\text{OH}} \times 100\% = 52.0\% \]

See Exercises 3.123 and 3.124

---

**Problem-Solving Strategy**

**Solving a Stoichiometry Problem Involving Masses of Reactants and Products**

1. Write and balance the equation for the reaction.
2. Convert the known masses of substances to moles.
3. Determine which reactant is limiting.
4. Using the amount of the limiting reactant and the appropriate mole ratios, compute the number of moles of the desired product.
5. Convert from moles to grams, using the molar mass.

This process is summarized in the diagram below:
For review

Key terms
- chemical stoichiometry
- Stoichiometry
  - Deals with the amounts of substances consumed and/or produced in a chemical reaction.
  - We count atoms by measuring the mass of the sample.
  - To relate mass and the number of atoms, the average atomic mass is required.
- Mole
  - The amount of carbon atoms in exactly 12 g of pure $^{12}$C
  - $6.022 \times 10^{23}$ units of a substance
  - The mass of 1 mole of an element = the atomic mass in grams
- Molar mass
  - Mass (g) of 1 mole of a compound or element
  - Obtained for a compound by finding the sum of the average masses of its constituent atoms
- Percent composition
  - The mass percent of each element in a compound
  - $\text{Mass percent} = \frac{\text{mass of element in 1 mole of substance}}{\text{mass of 1 mole of substance}} \times 100\%$
- Empirical formula
  - The simplest whole-number ratio of the various types of atoms in a compound
  - Can be obtained from the mass percent of elements in a compound
- Molecular formula
  - For molecular substances:
    - The formula of the constituent molecules
    - Always an integer multiple of the empirical formula
  - For ionic substances:
    - The same as the empirical formula
- Chemical reactions
  - Reactants are turned into products.
  - Atoms are neither created nor destroyed.
  - All of the atoms present in the reactants must also be present in the products.
- Characteristics of a chemical equation
  - Represents a chemical reaction
  - Reactants on the left side of the arrow, products on the right side
  - When balanced, gives the relative numbers of reactant and product molecules or ions
Stoichiometry calculations

- Amounts of reactants consumed and products formed can be determined from the balanced chemical equation.
- The limiting reactant is the one consumed first, thus limiting the amount of product that can form.

Yield

- The theoretical yield is the maximum amount that can be produced from a given amount of the limiting reactant.
- The actual yield, the amount of product actually obtained, is always less than the theoretical yield.
- Percent yield = \( \frac{\text{actual yield (g)}}{\text{theoretical yield (g)}} \times 100\% \)

Review questions

Answers to Review Questions can be found on the Student website (accessible from www.cengagebrain.com).

1. Explain the concept of "counting by weighing" using marbles as your example.

2. Atomic masses are relative masses. What does this mean?

3. The atomic mass of boron (B) is given in the periodic table as 10.81, yet no single atom of boron has a mass of 10.81 u. Explain.

4. What three conversion factors and in what order would you use them to convert the mass of a compound into atoms of a particular element in that compound—for example, from 1.00 g aspirin (C₉H₈O₄) to number of hydrogen atoms in the 1.00-g sample?

5. Fig. 3.5 illustrates a schematic diagram of a combustion device used to analyze organic compounds. Given that a certain amount of a compound containing carbon, hydrogen, and oxygen is combusted in this device, explain how the data relating to the mass of CO₂ produced and the mass of H₂O produced can be manipulated to determine the empirical formula.

6. What is the difference between the empirical and molecular formulas of a compound? Can they ever be the same? Explain.

7. Consider the hypothetical reaction between A₂ and AB pictured below.

What is the balanced equation? If 2.50 moles of A₂ are reacted with excess AB, what amount (moles) of product will form? If the mass of AB is 30.0 g and the mass of A₂ are 40.0 g, what is the mass of the product? If 15.0 g of AB is reacted, what mass of A₂ is required to react with all of the AB, and what mass of product is formed?

8. What is a limiting reactant problem? Explain the method you are going to use to solve limiting reactant problems.

9. Consider the following mixture of SO₂(g) and O₂(g).

If SO₂(g) and O₂(g) react to form SO₃(g), draw a representation of the product mixture assuming the reaction goes to completion. What is the limiting reactant in the reaction? If 96.0 g of SO₂ react with 32.0 g O₂, what mass of product will form?

10. Why is the actual yield of a reaction often less than the theoretical yield?