3 Stoichiometry

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Sulfur burning in oxygen to form sulfur dioxide.

Interactive Activity Summary

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Essential Concepts

Atomic Mass and Molar Mass The mass of an atom, which is extremely small, is based on the carbon-12 isotope scale. An atom of the carbon-12 isotope is assigned a mass of exactly 12 atomic mass units (amu). To work with the more convenient scale of grams, chemists use the molar mass. The molar mass of carbon-12 is exactly 12 g and contains an Avogadro's number (6.022×10^{23}) of atoms. The molar masses of other elements are also expressed in grams and contain the same number of atoms. The molar mass of a molecule is the sum of the molar masses of its constituent atoms.

Percent Composition of a Compound The makeup of a compound is most conveniently expressed in terms of its percent composition, which is the percent by mass of each element the compound contains. A knowledge of its chemical formula allows us to calculate the percent composition. Experimental determination of percent composition and the molar mass of a compound enables us to determine its chemical formula.

Writing Chemical Equations An effective way to represent the outcome of a chemical reaction is to write a chemical equation, which uses chemical formulas to describe what happens. A chemical equation must be balanced so that we have the same number and type of atoms for the reactants, the starting materials, and the products, the substances formed at the end of the reaction.

Mass Relationships of a Chemical Reaction A chemical equation enables us to predict the amount of product(s) formed, called the yield, knowing how much reactant(s) was (were) used. This information is of great importance for reactions run on the laboratory or industrial scale. In practice, the actual yield is almost always less than that predicted from the equation because of various complications.

3.1 Atomic Mass

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

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

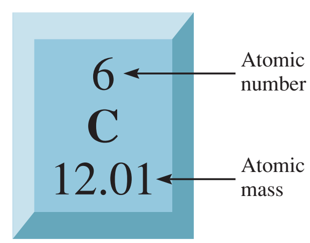
Section 3.4 describes a method for determining atomic mass.

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

One atomic mass unit is also called one dalton.

Average Atomic Mass

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



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

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

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

Copper.

EXAMPLE 3.1

DCM, Worked Examples

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

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

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

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

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

Similar problems: 3.5, 3.6.

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

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

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

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

The adjective formed from the noun "mole" is "molar."

In the SI system the ***mole (mol)*** is *the amount of a substance that contains as many elementary entities (atoms, molecules, or other particles) as there are atoms in exactly 12 g (or 0.012 kg) of the carbon-12 isotope*. The actual number of atoms in 12 g of carbon-12 is determined experimentally. This number is called ***Avogadro's number*** (N_A), in honor of the Italian scientist Amedeo Avogadro. The currently accepted value is

$$N_A = 6.0221367 \times 10^{23}$$

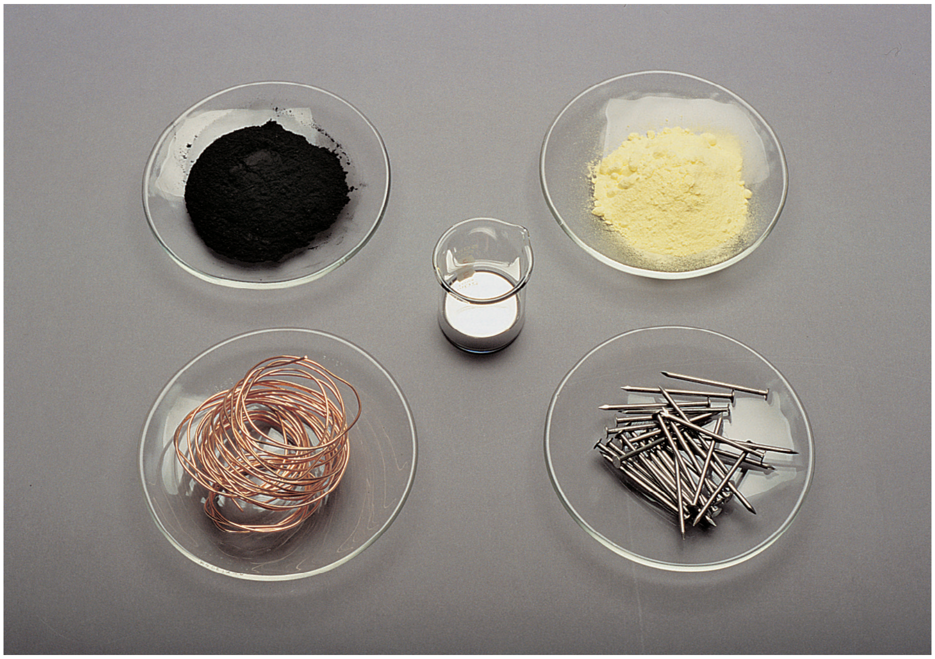

Figure 3.1 One mole each of several common elements. Carbon (black charcoal powder), sulfur (yellow powder), iron (as nails), copper (wires), and mercury (shiny liquid metal).

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

✓ Tip for the Instructor
Emphasize that Avogadro's number is so large because an atom is so small.

We have seen that 1 mole of carbon-12 atoms has a mass of exactly 12 g and contains 6.022×10^{23} atoms. This mass of carbon-12 is its ***molar mass ($\mathcal{M}$),*** defined as *the mass (in grams or kilograms) of 1 mole of units* (such as atoms or molecules) of a substance. Note that the molar mass of carbon-12 (in grams) is numerically equal to its atomic mass in amu. Likewise, the atomic mass of sodium (Na) is 22.99 amu and its molar mass is 22.99 g; the atomic mass of phosphorus is 30.97 amu and its molar mass is 30.97 g; and so on. If we know the atomic mass of an element, we also know its molar mass.

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

Using atomic mass and molar mass, we can calculate the mass in grams of a single carbon-12 atom. From our discussion we know that 1 mole of carbon-12 atoms weighs exactly 12 grams. This enables us to write the equality

✓ Tip for the Instructor
Point out that the masses listed in the periodic table represent the average mass of the atoms in amu's or the average mass of 1 mole of atoms in grams.

$$12.00 \text{ g carbon-12} = 1 \text{ mol carbon-12 atoms}$$

Therefore, we can write the conversion factor as

$$\frac{12.00 \text{ g carbon-12}}{1 \text{ mol carbon-12 atoms}}$$

(Note that we use the unit "mol" to represent "mole" in calculations.) Similarly, because there are 6.022×10^{23} atoms in 1 mole of carbon-12 atoms, we have

$$1 \text{ mol carbon-12 atoms} = 6.022 \times 10^{23} \text{ carbon-12 atoms}$$

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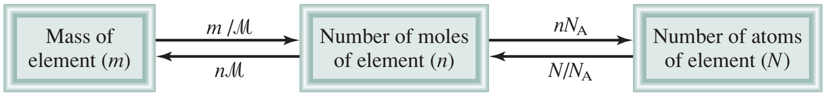


Figure 3.2 The relationships between mass (m in grams) of an element and number of moles of an element (n) and between number of moles of an element and number of atoms (N) of an element. $\mathcal{M}$ is the molar mass (g/mol) of the element and N_A is Avogadro's number.

and the conversion factor is

$$\frac{1 \text{ mol carbon-12 atoms}}{6.022 \times 10^{23} \text{ carbon-12 atoms}}$$

We can now calculate the mass (in grams) of 1 carbon-12 atom as follows:

$$\cancel{1 \text{ carbon-12 atom}} \times \frac{\cancel{1 \text{ mol carbon-12 atoms}}}{6.022 \times 10^{23} \cancel{\text{ carbon-12 atoms}}} \times \frac{12.00 \text{ g carbon-12}}{\cancel{1 \text{ mol carbon-12 atoms}}}$$
$$= 1.993 \times 10^{-23} \text{ g carbon-12}$$

We can use this result to determine the relationship between atomic mass units and grams. Because the mass of every carbon-12 atom is exactly 12 amu, the number of atomic mass units equivalent to 1 gram is

$$\frac{\text{amu}}{\text{gram}} = \frac{1 \cancel{\text{ carbon-12 atom}}}{1.993 \times 10^{-23} \text{ g}} \times \frac{12 \text{ amu}}{1 \cancel{\text{ carbon-12 atom}}}$$
$$= 6.022 \times 10^{23} \text{ amu/g}$$

Thus

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

and

$$1 \text{ amu} = 1.661 \times 10^{-24} \text{ g}$$

This example shows that Avogadro's number can be used to convert from the atomic mass units to mass in grams and vice versa.

The notions of Avogadro's number and molar mass enable us to carry out conversions between mass and moles of atoms and between the number of atoms and mass and to calculate the mass of a single atom. We will employ the following conversion factors in the calculations:

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

where X represents the symbol of an element. Figure 3.2 summarizes the relationships between the mass of an element and the number of moles of an element and between moles of an element and the number of atoms of an element.

Tip for the Instructor
The link between the amount of a substance and number of particles in the substance is moles of substance. 1 mole = 6.022×10^{23} particles.

Zinc.

EXAMPLE 3.2

DCM, Worked Examples

Zinc (Zn) is a silvery metal that is used in making brass (with copper) and in plating iron to prevent corrosion. How many moles of Zn are there in 23.3 g of Zn?

(Continued)

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

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

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

From this equality, we can write the two conversion factors

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

The conversion factor on the left is the correct one. Grams will cancel, leaving unit of mol for the answer. The number of moles of Zn is

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

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

Check Because 23.3 g is less than the molar mass of Zn, we expect the result to be less than 1 mole.

Similar problem: 3.15.

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

EXAMPLE 3.3

DCM, Worked Examples

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

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

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

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

the conversion factor is

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

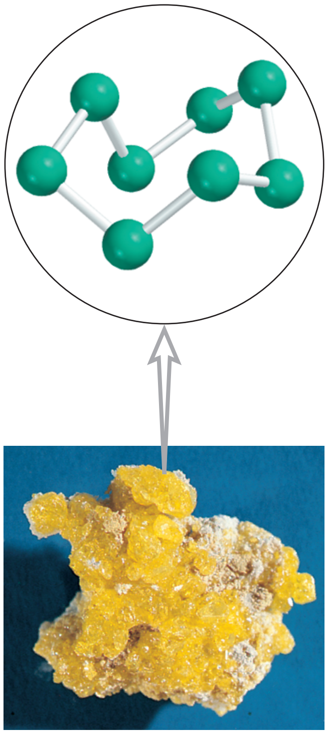
Avogadro's number is the key to the second step. We have

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

and the conversion factors are

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

(Continued)



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

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

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

We can combine these conversions in one step as follows:

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

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

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

Similar problems: 3.20, 3.21.

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

Silver.

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Similar problem: 3.17.

EXAMPLE 3.4

DCM, Worked Examples

Silver (Ag) is a precious metal used mainly in jewelry. What is the mass (in grams) of one Ag atom?

Strategy The question asks for the mass of one Ag atom. How many Ag atoms are in 1 mole of Ag and what is the molar mass of Ag?

Solution Because 1 mole of Ag atom contains 6.022×10^{23} Ag atoms and weighs 107.9 g, we can calculate the mass of one Ag atom as follows:

$$1\ \cancel{\text{Ag atom}} \times \frac{1\ \cancel{\text{mol Ag}}}{6.022 \times 10^{23}\ \cancel{\text{Ag atoms}}} \times \frac{107.9\ \text{g}}{1\ \cancel{\text{mol Ag}}} = 1.792 \times 10^{-22}\ \text{g}$$

Practice Exercise What is the mass (in grams) of one iodine (I) atom?

3.3 Molecular Mass

Interactivity: Molecular Mass
Online Learning Center, Interactives

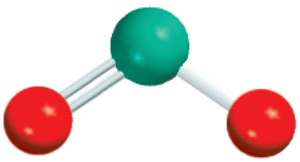
If we know the atomic masses of the component atoms, we can calculate the mass of a molecule. The ***molecular mass*** (sometimes called *molecular weight*) is *the sum of the atomic masses (in amu) in the molecule*. For example, the molecular mass of H_2O is

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

or

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

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



SO_2

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EXAMPLE 3.5

DCM, Worked Examples

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

(Continued)

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

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

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

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

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

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

Similar problems: 3.23, 3.24.

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

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

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

EXAMPLE 3.6

DCM, Worked Examples

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

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

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

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

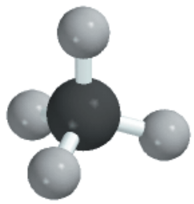
Because

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

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

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

(Continued)



CH_4

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Methane gas burning on a cooking range.

We now write

$$6.07\ \cancel{\text{g CH}_4} \times \frac{1\ \text{mol CH}_4}{16.04\ \cancel{\text{g CH}_4}} = 0.378\ \text{mol CH}_4$$

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

Similar problem: 3.26.

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

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

Urea.

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EXAMPLE 3.7

DCM, Worked Examples

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

Strategy We are asked to solve for atoms of hydrogen in 25.6 g of urea. We cannot convert directly from grams of urea to atoms of hydrogen. What unit do we need to obtain first before we can convert to atoms? How should Avogadro's number be used here? How many atoms of H are in 1 molecule of urea?

Solution To calculate number of H atoms, we first must convert grams of urea to number of molecules of urea. This part is similar to Example 3.3. The molecular formula of urea shows there are four H atoms in one urea molecule. We need three conversion factors: the molar mass of urea, Avogadro's number, and the number of H atoms in 1 molecule of urea. We can combine these three conversions

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

into one calculation,

$$25.6\ \cancel{\text{g (NH}_2)_2\text{CO}} \times \frac{1\ \cancel{\text{mol (NH}_2)_2\text{CO}}}{60.06\ \cancel{\text{g (NH}_2)_2\text{CO}}} \times \frac{6.022 \times 10^{23}\ \cancel{\text{molecules (NH}_2)_2\text{CO}}}{1\ \cancel{\text{mol (NH}_2)_2\text{CO}}}$$
$$\times \frac{4\ \text{H atoms}}{1\ \cancel{\text{molecule (NH}_2)_2\text{CO}}} = 1.03 \times 10^{24}\ \text{H atoms}$$

The preceding method utilizes the ratio of molecules (urea) to atoms (hydrogen). We can also solve the problem by reading the formula as the ratio of moles of urea to moles of hydrogen using the following conversions

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

Try it.

Similar problems: 3.27, 3.28.

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

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

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

For molecules, formula mass and molecular mass refer to the same quantity.

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

and its molar mass is 58.44 g.

Tip for the Instructor
Point out that the combined mass of a Na^+ ion and a Cl^- ion is equal to the combined mass of a Na atom and a Cl atom.

3.4 The Mass Spectrometer

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

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

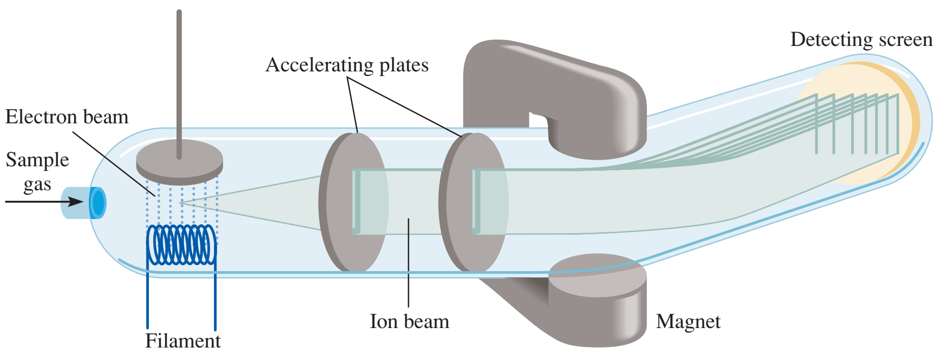

Figure 3.3
Schematic diagram of one type of mass spectrometer.

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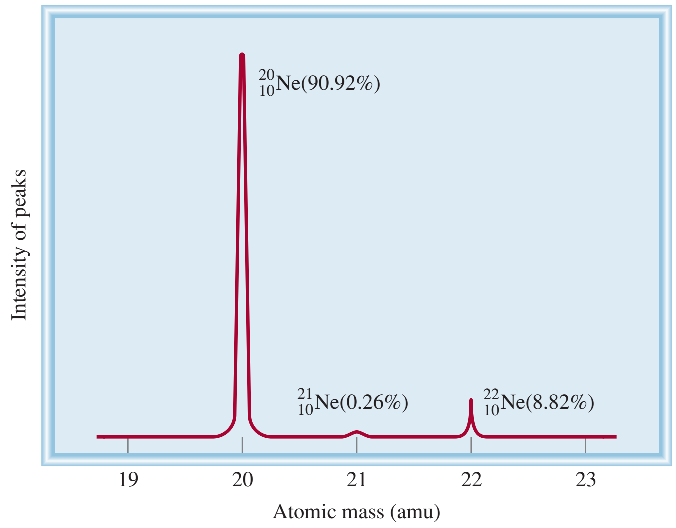

Figure 3.4
The mass spectrum of the three isotopes of neon.
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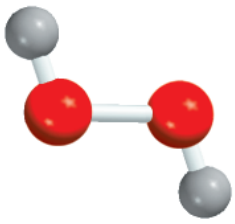
3.5 Percent Composition of Compounds

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

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

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



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

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

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

The sum of the percentages is 5.926 percent + 94.06 percent = 99.99 percent. The small discrepancy from 100 percent is due to the way we rounded off the molar masses of the elements. Note that the empirical formula (HO) would give us the same results.

EXAMPLE 3.8

DCM, Worked Examples

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

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

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

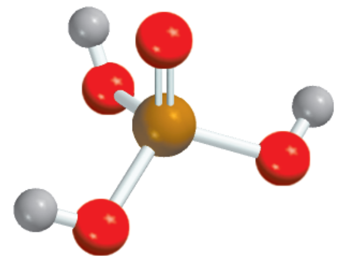
$$\%H = \frac{3(1.008\text{ g})\text{ H}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = 3.086\%$$

$$\%P = \frac{30.97\text{ g P}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = 31.61\%$$

$$\%O = \frac{4(16.00\text{ g})\text{ O}}{97.99\text{ g H}_3\text{PO}_4} \times 100\% = 65.31\%$$

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

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



H_3PO_4

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Similar problem: 3.40.

The procedure used in Example 3.8 can be reversed if necessary. Given the percent composition by mass of a compound, we can determine the empirical formula of the compound (Figure 3.5). Because we are dealing with percentages and the sum of all the percentages is 100 percent, it is convenient to assume that we started with 100 g of a compound, as Example 3.9 shows.

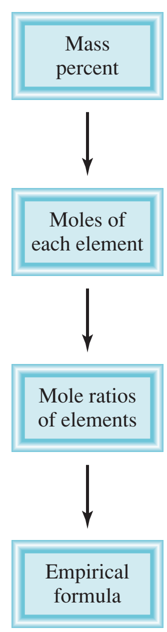

Figure 3.5 Procedure for calculating the empirical formula of a compound from its percent compositions.

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EXAMPLE 3.9

DCM, Worked Examples

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

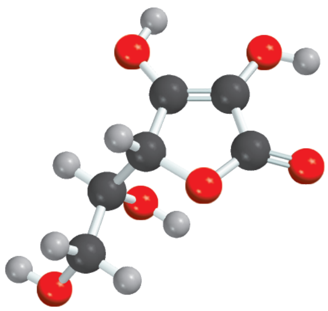
Strategy In a chemical formula, the subscripts represent the ratio of the number of moles of each element that combine to form one mole of the compound. How can we convert from mass percent to moles? If we assume an exactly 100-g sample of the compound, do we know the mass of each element in the compound?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

Solution If we have 100 g of ascorbic acid, then each percentage can be converted directly to grams. In this sample, there will be 40.92 g of C, 4.58 g of H, and 54.50 g of O. Because the subscripts in the formula represent a mole ratio, we need to convert

(Continued)

the grams of each element to moles. The conversion factor needed is the molar mass of each element. Let n represent the number of moles of each element so that

$$n_C = 40.92\ \cancel{\text{g C}} \times \frac{1\ \text{mol C}}{12.01\ \cancel{\text{g C}}} = 3.407\ \text{mol C}$$
$$n_H = 4.58\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.008\ \cancel{\text{g H}}} = 4.54\ \text{mol H}$$
$$n_O = 54.50\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = 3.406\ \text{mol O}$$



The molecular formula of ascorbic acid is $C_6H_8O_6$.

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Thus, we arrive at the formula $C_{3.407}H_{4.54}O_{3.406}$, which gives the identity and the mole ratios of atoms present. However, chemical formulas are written with whole numbers. Try to convert to whole numbers by dividing all the subscripts by the smallest subscript (3.406):

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

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

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

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

Similar problems: 3.49, 3.50.

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

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

Tip for the Instructor
Remind students that the subscripts in a chemical formula can represent either an atom ratio in one molecule or a mole ratio in 1 mole of the compound.

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

Chalcopyrite.

EXAMPLE 3.10

DCM, Worked Examples

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

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

(Continued)

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

$$\%Cu = \frac{\text{molar mass of Cu}}{\text{molar mass of } CuFeS_2} \times 100\%$$
$$= \frac{63.55 \text{ g}}{183.5 \text{ g}} \times 100\% = 34.63\%$$

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

$$\text{mass of Cu in } CuFeS_2 = 0.3463 \times (3.71 \times 10^3 \text{ kg}) = 1.28 \times 10^3 \text{ kg}$$

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

Similar problem: 3.45.

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

3.6 Experimental Determination of Empirical Formulas

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

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

The masses of CO_2 and of H_2O produced can be determined by measuring the increase in mass of the CO_2 and H_2O absorbers, respectively. Suppose that in one experiment the combustion of 11.5 g of ethanol produced 22.0 g of CO_2 and 13.5 g

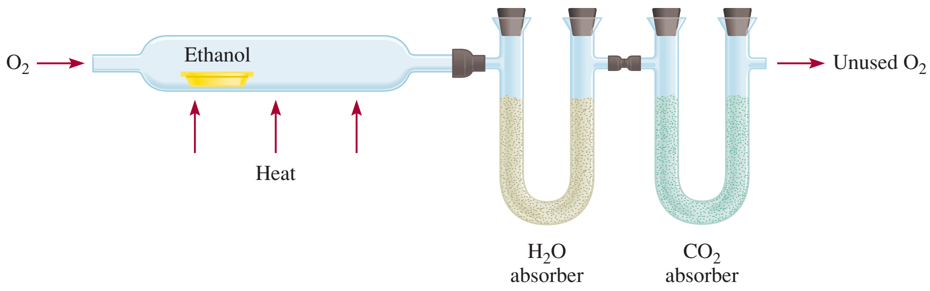

Figure 3.6
Apparatus for determining the empirical formula of ethanol. The absorbers are substances that can retain water and carbon dioxide, respectively.

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of H_2O. We can calculate the mass of carbon and hydrogen in the original 11.5-g sample of ethanol as follows:

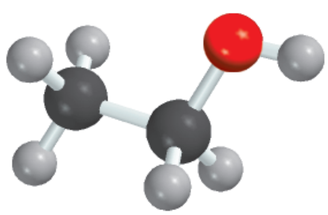
$$\begin{aligned}\text{mass of C} &= 22.0\ \cancel{\text{g CO}_2} \times \frac{1\ \cancel{\text{mol CO}_2}}{44.01\ \cancel{\text{g CO}_2}} \times \frac{1\ \cancel{\text{mol C}}}{1\ \cancel{\text{mol CO}_2}} \times \frac{12.01\ \text{g C}}{1\ \cancel{\text{mol C}}} \\ &= 6.00\ \text{g C} \\ \text{mass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

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

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

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

$$\begin{aligned}\text{moles of C} &= 6.00\ \cancel{\text{g C}} \times \frac{1\ \text{mol C}}{12.01\ \cancel{\text{g C}}} = 0.500\ \text{mol C} \\ \text{moles of H} &= 1.51\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.008\ \cancel{\text{g H}}} = 1.50\ \text{mol H} \\ \text{moles of O} &= 4.0\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = 0.25\ \text{mol O}\end{aligned}$$



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

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

Determination of Molecular Formulas

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

EXAMPLE 3.11

DCM, Worked Examples

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

(Continued)

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

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

$$n_N = 1.52\ \cancel{g\ N} \times \frac{1\ mol\ N}{14.01\ \cancel{g\ N}} = 0.108\ mol\ N$$
$$n_O = 3.47\ \cancel{g\ O} \times \frac{1\ mol\ O}{16.00\ \cancel{g\ O}} = 0.217\ mol\ O$$

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

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

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

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

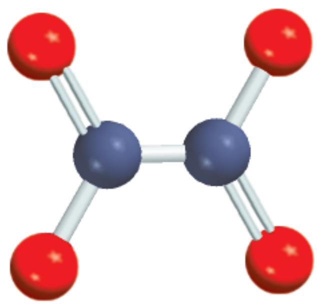
$$\frac{\text{molar mass}}{\text{empirical molar mass}} = \frac{90\ g}{46.01\ g} \approx 2$$

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

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

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

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



N_2O_4

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Similar problems: 3.52, 3.53, 3.54.

3.7 Chemical Reactions and Chemical Equations

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

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

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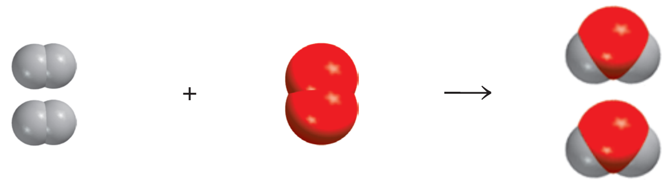

Two hydrogen molecules + One oxygen molecule ⟶ Two water molecules

$2H_2 + O_2 \longrightarrow 2H_2O$

Writing Chemical Equations

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

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

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

Equation (3.2) is not complete, however, because there are twice as many oxygen atoms on the left side of the arrow (two) as on the right side (one). To conform with the law of conservation of mass, there must be the same number of each type of atom on both sides of the arrow; that is, we must have as many atoms after the reaction ends as we did before it started. We can *balance* Equation (3.2) by placing the appropriate coefficient (2 in this case) in front of H_2 and H_2O:

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

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

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

TABLE 3.1 Interpretation of a Chemical Equation

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

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

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

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

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

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

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

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

Balancing Chemical Equations

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

✓ **Tip for the Instructor**
Remind students that balancing chemical equations is based on the law of conservation of mass.

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

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

once on each side of the equation but in unequal numbers of atoms. Balance these elements. Finally, balance elements that appear in two or more formulas on the same side of the equation.

4. Check your balanced equation to be sure that you have the same total number of each type of atoms on both sides of the equation arrow.

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

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

$$KClO_3 \longrightarrow KCl + O_2$$

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

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

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

$$2KClO_3 \longrightarrow 2KCl + 3O_2 \qquad (3.3)$$

Tip for the Instructor
Some students have difficulty counting atoms when balancing equations. Consider $Cu(NO_3)_2$. Emphasize that each subscript in NO_3 must be multiplied by 2. If there is a coefficient, then the atoms also have to be multiplied by this number.

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

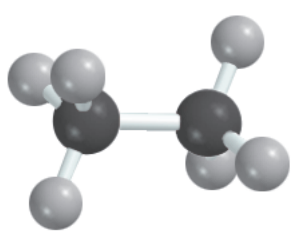
Reactants	Products
K (2)	K (2)
Cl (2)	Cl (2)
O (6)	O (6)

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

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

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

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



C_2H_6

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

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

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

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

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

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

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

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

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

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

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

The final tally is

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

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

EXAMPLE 3.12

DCM, Worked Examples

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

Strategy Remember that the formula of an element or compound cannot be changed when balancing a chemical equation. The equation is balanced by placing the appropriate coefficients in front of the formulas. Follow the procedure described on p. 73.

Solution The unbalanced equation is

$$Al + O_2 \longrightarrow Al_2O_3$$

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

$$2Al + O_2 \longrightarrow Al_2O_3$$

(Continued)

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

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

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

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

or

$$4Al + 3O_2 \longrightarrow 2Al_2O_3$$

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

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

The equation is balanced.

Similar problems: 3.59, 3.60.

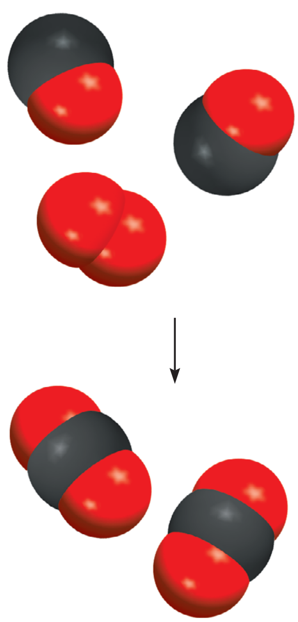
Practice Exercise Balance the equation representing the reaction between iron(III) oxide, Fe_2O_3, and carbon monoxide (CO) to yield iron (Fe) and carbon dioxide (CO_2).

3.8 Amounts of Reactants and Products

Interactivity: The Mole Method
Online Learning Center, Interactives

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

Whether the units given for reactants (or products) are moles, grams, liters (for gases), or some other units, we use moles to calculate the amount of product formed in a reaction. This approach is called the ***mole method,*** which means simply that *the stoichiometric coefficients in a chemical equation can be interpreted as the number of moles of each substance*. For example, the combustion of carbon monoxide in air produces carbon dioxide:



DCM, Art Library

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$

The stoichiometric coefficients show that two molecules of CO react with one molecule of O_2 to form two molecules of CO_2. It follows that the relative numbers of moles are the same as the relative numbers of molecules:

$2CO(g)$	+	$O_2(g)$	$\longrightarrow$	$2CO_2(g)$
2 molecules		1 molecule		2 molecules
$2(6.022 \times 10^{23}$ molecules)		6.022×10^{23} molecules		$2(6.022 \times 10^{23}$ molecules)
2 mol		1 mol		2 mol

Thus this equation can also be read as "2 moles of carbon monoxide gas combine with 1 mole of oxygen gas to form 2 moles of carbon dioxide gas." In stoichiometric calculations, we say that two moles of CO are equivalent to two moles of CO_2, that is,

$$2 \text{ mol CO} \simeq 2 \text{ mol } CO_2$$

where the symbol $\simeq$ means "stoichiometrically equivalent to" or simply "equivalent to." The mole ratio between CO and CO_2 is 2:2 or 1:1, meaning that if 10 moles of CO are reacted, 10 moles of CO_2 will be produced. Likewise, if 0.20 mole of CO is reacted, 0.20 mole of CO_2 will be formed. This relationship enables us to write the conversion factors

$$\frac{2 \text{ mol CO}}{2 \text{ mol } CO_2} \quad \text{and} \quad \frac{2 \text{ mol } CO_2}{2 \text{ mol CO}}$$

Similarly, we have 1 mol $O_2 \simeq 2$ mol CO_2 and 2 mol CO $\simeq$ 1 mol O_2.

Let's consider a simple example in which 4.8 moles of CO react completely with O_2 to form CO_2. To calculate the amount of CO_2 produced in moles, we use the conversion factor that has CO in the denominator and write

$$\begin{aligned} \text{moles of } CO_2 \text{ produced} &= 4.8 \cancel{\text{ mol CO}} \times \frac{1 \text{ mol } CO_2}{1 \cancel{\text{ mol CO}}} \\ &= 4.8 \text{ mol } CO_2 \end{aligned}$$

Now suppose 10.7 g of CO react completely with O_2 to form CO_2. How many grams of CO_2 will be formed? To do this calculation, we note that the link between CO and CO_2 is the mole ratio from the balanced equation. So we need to first convert grams of CO to moles of CO, then to moles of CO_2, and finally to grams of CO_2. The conversion steps are

$$\text{grams of CO} \longrightarrow \text{moles of CO} \longrightarrow \text{moles of } CO_2 \longrightarrow \text{grams of } CO_2$$

First we convert 10.7 g of CO to number of moles of CO, using the molar mass of CO as the conversion factor:

$$\begin{aligned} \text{moles of CO} &= 10.7 \cancel{\text{ g CO}} \times \frac{1 \text{ mol CO}}{28.01 \cancel{\text{ g CO}}} \\ &= 0.382 \text{ mol CO} \end{aligned}$$

Next we calculate the number of moles of CO_2 produced:

$$\begin{aligned} \text{moles of } CO_2 &= 0.382 \cancel{\text{ mol CO}} \times \frac{2 \text{ mol } CO_2}{2 \cancel{\text{ mol CO}}} \\ &= 0.382 \text{ mol } CO_2 \end{aligned}$$

Finally, we calculate the mass of CO_2 produced in grams using the molar mass of CO_2 as the conversion factor:

$$\begin{aligned} \text{grams of } CO_2 &= 0.382 \cancel{\text{ mol } CO_2} \times \frac{44.01 \text{ g } CO_2}{1 \cancel{\text{ mol } CO_2}} \\ &= 16.8 \text{ g } CO_2 \end{aligned}$$

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

$$\begin{aligned} \text{grams of } CO_2 &= 10.7 \cancel{\text{ g CO}} \times \frac{1 \cancel{\text{ mol CO}}}{28.01 \cancel{\text{ g CO}}} \times \frac{1 \cancel{\text{ mol } CO_2}}{1 \cancel{\text{ mol CO}}} \times \frac{44.01 \text{ g } CO_2}{1 \cancel{\text{ mol } CO_2}} \\ &= 16.8 \text{ g } CO_2 \end{aligned}$$

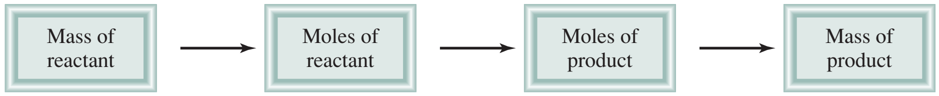


Figure 3.8 The mole method. First convert the quantity of reactant (in grams or other units) to number of moles. Next, use the mole ratio in the balanced equation to calculate the number of moles of product formed. Finally, convert moles of product to grams of product.

Transparency/DCM, Art Library

Similarly, we can calculate the mass of O_2 in grams consumed in this reaction. By using the relationship 2 mol CO $\simeq$ 1 mol O_2, we write

$$\begin{aligned}\text{grams of } O_2 &= 10.7\ \cancel{\text{g CO}} \times \frac{1\ \cancel{\text{mol CO}}}{28.01\ \cancel{\text{g CO}}} \times \frac{1\ \cancel{\text{mol } O_2}}{2\ \cancel{\text{mol CO}}} \times \frac{32.00\text{ g } O_2}{1\ \cancel{\text{mol } O_2}} \\ &= 6.11\text{ g } O_2\end{aligned}$$

Figure 3.8 shows the steps involved in stoichiometric calculations using the mole method.

Lithium reacting with water to produce hydrogen gas.

DCM, Photo Library

Demonstration
Periodicity of alkali metals, Chemistry at Work CD

EXAMPLE 3.13

DCM, Worked Examples

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

$$2\text{Li}(s) + 2\text{H}_2\text{O}(l) \longrightarrow 2\text{LiOH}(aq) + \text{H}_2(g)$$

(a) How many moles of H_2 will be formed by the complete reaction of 6.23 moles of Li with water? (b) How many grams of H_2 will be formed by the complete reaction of 80.57 g of Li with water?

(a) Strategy Looking at the balanced equation, how do we compare the amounts of Li and H_2? We can compare them based on the *mole ratio* from the balanced equation.

Solution Because the balanced equation is given in the problem, the mole ratio between Li and H_2 is known: 2 mole Li $\simeq$ 1 mol H_2. From this relationship, we have two conversion factors:

$$\frac{2\text{ mol Li}}{1\text{ mol H}_2} \quad \text{and} \quad \frac{1\text{ mol H}_2}{2\text{ mol Li}}$$

The conversion factor on the right is the correct one. Moles of Li will cancel, leaving units of "mol H_2" for the answer. We calculate moles of H_2 produced as follows:

$$\text{moles of H}_2 \text{ produced} = 6.23\ \cancel{\text{mol Li}} \times \frac{1\text{ mol H}_2}{2\ \cancel{\text{mol Li}}} = 3.12\text{ mol H}_2$$

Check Does the answer seem reasonable? Should the moles of H_2 produced be half the moles of Li reacted?

(b) Strategy We compare Li and H based on the *mole ratio* in the balanced equation. Before we can determine the moles of H_2 produced, we need to convert to moles of Li. What conversion factor is needed to convert from grams of Li to moles of Li? Another conversion factor is needed to convert moles of H_2 to grams of H_2.

Solution The molar mass of Li will enable us to convert from grams of Li to moles of Li. As in part (a), the balanced equation is given, so the mole ratio between Li and

(Continued)

H_2 is known; that is, 2 mol Li $\simeq$ 1 mol H_2. Finally, the molar mass of H_2 will convert moles of H_2 to grams of H_2. This sequence is summarized as follows:

$$\text{grams of Li} \longrightarrow \text{moles of Li} \longrightarrow \text{moles of H}_2 \longrightarrow \text{grams of H}_2$$

The number of moles of Li in 80.57 g Li is

$$\text{moles of Li} = 80.57\ \cancel{\text{g Li}} \times \frac{1\text{ mol Li}}{6.941\ \cancel{\text{g Li}}} = 11.61\text{ mol Li}$$

Next, we calculate the number of moles of H_2 produced:

$$\text{moles of H}_2 = 11.61\ \cancel{\text{mol Li}} \times \frac{1\text{ mol H}_2}{2\ \cancel{\text{mol Li}}} = 5.805\text{ mol H}_2$$

Finally, the amount of H_2 in grams is given by

$$\text{grams of H}_2 = 5.805\ \cancel{\text{mol H}_2} \times \frac{2.016\text{ g H}_2}{1\ \cancel{\text{mol H}_2}} = 11.70\text{ g H}_2$$

After some practice, you will find it convenient to combine all the steps in a single sequence of conversions:

$$\begin{aligned}\text{grams of H}_2 &= 80.57\ \cancel{\text{g Li}} \times \frac{1\ \cancel{\text{mol Li}}}{6.941\ \cancel{\text{g Li}}} \times \frac{1\ \cancel{\text{mol H}_2}}{2\ \cancel{\text{mol Li}}} \times \frac{2.016\text{ g H}_2}{1\ \cancel{\text{mol H}_2}} \\ &= 11.70\text{ g H}_2\end{aligned}$$

Check Does the answer seem reasonable? Should the mass of H_2 produced be less than the mass of Li reacted? Compare the molar mass of H_2 with that of Li. Also, compare the mole ratio of H_2 and Li in the equation.

Similar problems: 3.65, 3.71.

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

$$2\text{NO}(g) + \text{O}_2(g) \longrightarrow 2\text{NO}_2(g)$$

(a) How many moles of NO_2 are formed by the complete reaction of 0.254 mole of O_2?
(b) How many grams of NO_2 are formed by the complete reaction of 1.44 g of NO?

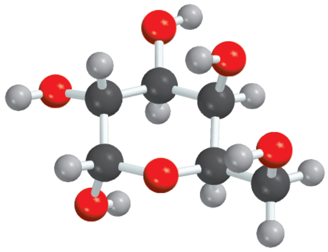
Example 3.14 shows another mass of reactant to mass of product calculation (see Figure 3.8).

EXAMPLE 3.14

DCM, Worked Examples

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

$$\text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \longrightarrow 6\text{CO}_2 + 6\text{H}_2\text{O}$$



$C_6H_{12}O_6$

DCM, Art Library

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

Strategy Looking at the balanced equation, how do we compare the amounts of $C_6H_{12}O_6$ and CO_2? We can compare them based on the *mole ratio* from the balanced

(Continued)

equation. Starting with grams of $C_6H_{12}O_6$, how do we convert to moles of $C_6H_{12}O_6$? Once moles of CO_2 are determined using the mole ratio from the balanced equation, how do we convert to grams of CO_2?

Solution We see from the balanced equation, that 1 mol $C_6H_{12}O_6 \simeq$ 6 mol CO_2. If we can convert grams to moles of $C_6H_{12}O_6$, then we can use the mole ratio to calculate moles of CO_2. Once we have moles of CO_2, we can convert to grams of CO_2. These conversions are summarized next:

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

We combine all of these steps into one equation:

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

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

Similar problem: 3.72.

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

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

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

3.9 Limiting Reagents and Reaction Yield

Animations:
Limiting Reagent
Online Learning Center, Animations
Chemistry Animations Library, Chemical Reactions, Limiting_Reagent

Interactivity:
Limiting Reactant Game
Online Learning Center, Interactives

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

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

Consider the formation of nitrogen dioxide (NO_2) from nitric oxide (NO) and oxygen:

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

Suppose initially we have 8 moles of NO and 7 moles of O_2 (Figure 3.9). One way to determine which of the two reactants is the limiting reagent is to calculate the number of moles of NO_2 obtained based on the initial quantities of NO and O_2. From the preceding definition, we see that only the limiting reagent will yield the smaller amount of the product. Starting with 8 moles of NO, we find the number of moles of NO_2 produced is

$$8\ \cancel{\text{mol NO}} \times \frac{2\ \text{mol NO}_2}{2\ \cancel{\text{mol NO}}} = 8\ \text{mol NO}_2$$

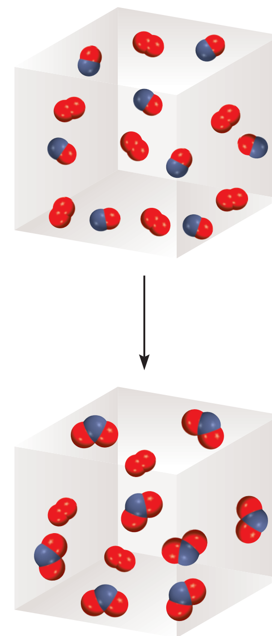
and starting with 7 moles of O_2, the number of moles of NO_2 formed is

$$7\ \cancel{\text{mol O}_2} \times \frac{2\ \text{mol NO}_2}{1\ \cancel{\text{mol O}_2}} = 14\ \text{mol NO}_2$$

Because NO results in a smaller amount of NO_2, it must be the limiting reagent. Therefore, O_2 is the excess reagent.

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

Before reaction has started



After reaction is complete

NO O_2 NO_2

Figure 3.9
At the start of the reaction, there were eight NO molecules and seven O_2 molecules. At the end, all the NO molecules are gone and only three O_2 molecules are left. Therefore, NO is the limiting reagent and O_2 is the excess reagent. Each molecule can also be treated as one mole of the substance in this reaction.

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EXAMPLE 3.15

DCM, Worked Examples

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

$$2NH_3(g) + CO_2(g) \longrightarrow (NH_2)_2CO(aq) + H_2O(l)$$

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

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

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

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

Combining these conversions in one step, we write

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

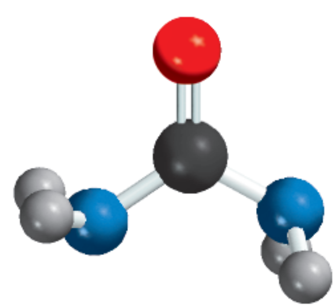
Second, for 1142 g of CO_2, the conversions are

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

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

$$\begin{aligned}\text{moles of (NH}_2)_2\text{CO} &= 1142\ \cancel{\text{g CO}_2} \times \frac{1\ \cancel{\text{mol CO}_2}}{44.01\ \cancel{\text{g CO}_2}} \times \frac{1\ \text{mol (NH}_2)_2\text{CO}}{1\ \cancel{\text{mol CO}_2}}\\ &= 25.95\ \text{mol (NH}_2)_2\text{CO}\end{aligned}$$

(Continued)



$(NH_2)_2CO$

DCM, Art Library

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

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

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

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

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

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

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

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

so that

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

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

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

Similar problem: 3.86.

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

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

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

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

Reaction Yield

✓ Tip for the Instructor
Remind students that the theoretical yield is the yield that they calculate using the balanced equation. The actual yield is the yield obtained by carrying out the reaction.

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

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

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

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

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

EXAMPLE 3.16

DCM, Worked Examples

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

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

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

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

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

$$\text{grams of } TiCl_4 \longrightarrow \text{moles of } TiCl_4 \longrightarrow \text{moles of Ti}$$

so that

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

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

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

(Continued)

The frame of this bicycle is made of titanium.

and we write

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

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

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

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

Solution The percent yield is given by

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

Check Should the percent yield be less than 100 percent?

Similar problems: 3.89, 3.90.

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

$$5Ca + V_2O_5 \longrightarrow 5CaO + 2V$$

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

Summary of Facts and Concepts

1. Atomic masses are measured in atomic mass units (amu), a relative unit based on a value of exactly 12 for the C-12 isotope. The atomic mass given for the atoms of a particular element is the average of the naturally occurring isotope distribution of that element. The molecular mass of a molecule is the sum of the atomic masses of the atoms in the molecule. Both atomic mass and molecular mass can be accurately determined with a mass spectrometer.
2. A mole is Avogadro's number (6.022×10^{23}) of atoms, molecules, or other particles. The molar mass (in grams) of an element or a compound is numerically equal to its mass in atomic mass units (amu) and contains Avogadro's number of atoms (in the case of elements), molecules (in the case of molecular substances), or simplest formula units (in the case of ionic compounds).
3. The percent composition by mass of a compound is the percent by mass of each element present. If we know the percent composition by mass of a compound, we can deduce the empirical formula of the compound and also the molecular formula of the compound if the approximate molar mass is known.
4. Chemical changes, called chemical reactions, are represented by chemical equations. Substances that undergo change—the reactants—are written on the left and the substances formed—the products—appear to the right of the arrow. Chemical equations must be balanced, in accordance with the law of conservation of mass. The number of atoms of each element in the reactants must equal the number in the products.

5. Stoichiometry is the quantitative study of products and reactants in chemical reactions. Stoichiometric calculations are best done by expressing both the known and unknown quantities in terms of moles and then converting to other units if necessary. A limiting reagent is the reactant that is present in the smallest stoichiometric amount. It limits the amount of product that can be formed. The amount of product obtained in a reaction (the actual yield) may be less than the maximum possible amount (the theoretical yield). The ratio of the two multiplied by 100 percent is expressed as the percent yield.

Key Words

Actual yield, p. 82
Atomic mass, p. 57
Atomic mass unit (amu), p. 57
Avogadro's number (N_A), p. 58
Chemical equation, p. 71
Chemical reaction, p. 71
Excess reagent, p. 80
Limiting reagent, p. 80
Molar mass ($\mathcal{M}$), p. 59
Mole (mol), p. 58
Mole method, p. 76
Molecular mass, p. 62
Percent composition by mass, p. 66
Percent yield, p. 83
Product, p. 73
Reactant, p. 73
Stoichiometric amount, p. 80
Stoichiometry, p. 76
Theoretical yield, p. 82

Questions and Problems

Atomic Mass

Review Questions

3.1 What is an atomic mass unit? Why is it necessary to introduce such a unit?

3.2 What is the mass (in amu) of a carbon-12 atom? Why is the atomic mass of carbon listed as 12.01 amu in the table on the inside front cover of this book?

3.3 Explain clearly what is meant by the statement "The atomic mass of gold is 197.0 amu."

3.4 What information would you need to calculate the average atomic mass of an element?

Problems

••3.5 The atomic masses of $^{35}_{17}Cl$ (75.53 percent) and $^{37}_{17}Cl$ (24.47 percent) are 34.968 amu and 36.956 amu, respectively. Calculate the average atomic mass of chlorine. The percentages in parentheses denote the relative abundances.

••**3.6** The atomic masses of $^{6}_{3}Li$ and $^{7}_{3}Li$ are 6.0151 amu and 7.0160 amu, respectively. Calculate the natural abundances of these two isotopes. The average atomic mass of Li is 6.941 amu.

•3.7 What is the mass in grams of 13.2 amu?

•**3.8** How many amu are there in 8.4 g?

Avogadro's Number and Molar Mass

Review Questions

3.9 Define the term "mole." What is the unit for mole in calculations? What does the mole have in common with the pair, the dozen, and the gross? What does Avogadro's number represent?

3.10 What is the molar mass of an atom? What are the commonly used units for molar mass?

Problems

•••3.11 Earth's population is about 6.5 billion. Suppose that every person on Earth participates in a process of counting identical particles at the rate of two particles per second. How many years would it take to count 6.0×10^{23} particles? Assume that there are 365 days in a year.

•••**3.12** The thickness of a piece of paper is 0.0036 in. Suppose a certain book has an Avogadro's number of pages; calculate the thickness of the book in light-years. (*Hint:* See Problem 1.38 for the definition of light-year.)

••3.13 How many atoms are there in 5.10 moles of sulfur (S)?

•**3.14** How many moles of cobalt (Co) atoms are there in 6.00×10^{9} (6 billion) Co atoms?

•3.15 How many moles of calcium (Ca) atoms are in 77.4 g of Ca?

•**3.16** How many grams of gold (Au) are there in 15.3 moles of Au?

••3.17 What is the mass in grams of a single atom of each of the following elements? (a) Hg, (b) Ne.

••**3.18** What is the mass in grams of a single atom of each of the following elements? (a) As, (b) Ni.

••3.19 What is the mass in grams of 1.00×10^{12} lead (Pb) atoms?

••**3.20** How many atoms are present in 3.14 g of copper (Cu)?

••3.21 Which of the following has more atoms: 1.10 g of hydrogen atoms or 14.7 g of chromium atoms?

••**3.22** Which of the following has a greater mass: 2 atoms of lead or 5.1×10^{-23} mole of helium?

Molecular Mass

Problems

•3.23 Calculate the molecular mass or formula mass (in amu) of each of the following substances: (a) CH_4, (b) NO_2, (c) SO_3, (d) C_6H_6, (e) NaI, (f) K_2SO_4, (g) $Ca_3(PO_4)_2$.

•**3.24** Calculate the molar mass of the following substances: (a) Li_2CO_3, (b) CS_2, (c) $CHCl_3$ (chloroform), (d) $C_6H_8O_6$ (ascorbic acid, or vitamin C), (e) KNO_3, (f) Mg_3N_2.

•3.25 Calculate the molar mass of a compound if 0.372 mole of it has a mass of 152 g.

••**3.26** How many molecules of ethane (C_2H_6) are present in 0.334 g of C_2H_6?

••3.27 Calculate the number of C, H, and O atoms in 1.50 g of glucose ($C_6H_{12}O_6$), a sugar.

••**3.28** Urea [$(NH_2)_2CO$] is used for fertilizer and many other things. Calculate the number of N, C, O, and H atoms in 1.68×10^4 g of urea.

••3.29 Pheromones are a special type of compound secreted by the females of many insect species to attract the males for mating. One pheromone has the molecular formula $C_{19}H_{38}O$. Normally, the amount of this pheromone secreted by a female insect is about 1.0×10^{-12} g. How many molecules are there in this quantity?

••**3.30** The density of water is 1.00 g/mL at 4°C. How many water molecules are present in 2.56 mL of water at this temperature?

Mass Spectrometry

Review Questions

3.31 Describe the operation of a mass spectrometer.

3.32 Describe how you would determine the isotopic abundance of an element from its mass spectrum.

Problems

••3.33 Carbon has two stable isotopes, $^{12}_{6}C$ and $^{13}_{6}C$, and fluorine has only one stable isotope, $^{19}_{9}F$. How many peaks would you observe in the mass spectrum of the positive ion of CF_4^+? Assume that the ion does not break up into smaller fragments.

•••**3.34** Hydrogen has two stable isotopes, $^{1}_{1}H$ and $^{2}_{1}H$, and sulfur has four stable isotopes, $^{32}_{16}S$, $^{33}_{16}S$, $^{34}_{16}S$, and $^{36}_{16}S$. How many peaks would you observe in the mass spectrum of the positive ion of hydrogen sulfide, H_2S^+? Assume no decomposition of the ion into smaller fragments.

Percent Composition and Chemical Formulas

Review Questions

3.35 Use ammonia (NH_3) to explain what is meant by the percent composition by mass of a compound.

3.36 Describe how the knowledge of the percent composition by mass of an unknown compound can help us identify the compound.

3.37 What does the word "empirical" in empirical formula mean?

3.38 If we know the empirical formula of a compound, what additional information do we need to determine its molecular formula?

Problems

••3.39 Tin (Sn) exists in Earth's crust as SnO_2. Calculate the percent composition by mass of Sn and O in SnO_2.

••**3.40** For many years chloroform ($CHCl_3$) was used as an inhalation anesthetic in spite of the fact that it is also a toxic substance that may cause severe liver, kidney, and heart damage. Calculate the percent composition by mass of this compound.

••3.41 Cinnamic alcohol is used mainly in perfumery, particularly in soaps and cosmetics. Its molecular formula is $C_9H_{10}O$. (a) Calculate the percent composition by mass of C, H, and O in cinnamic alcohol. (b) How many molecules of cinnamic alcohol are contained in a sample of mass 0.469 g?

••**3.42** All of the substances listed below are fertilizers that contribute nitrogen to the soil. Which of these is the richest source of nitrogen on a mass percentage basis?

(a) Urea, $(NH_2)_2CO$

(b) Ammonium nitrate, NH_4NO_3

(c) Guanidine, $HNC(NH_2)_2$

(d) Ammonia, NH_3

••3.43 Allicin is the compound responsible for the characteristic smell of garlic. An analysis of the compound gives the following percent composition by mass: C: 44.4 percent; H: 6.21 percent; S: 39.5 percent; O: 9.86 percent. Calculate its empirical formula. What is its molecular formula given that its molar mass is about 162 g?

••**3.44** Peroxyacylnitrate (PAN) is one of the components of smog. It is a compound of C, H, N, and O. Determine the percent composition of oxygen and the empirical formula from the following percent composition by mass: 19.8 percent C, 2.50 percent H, 11.6 percent N.

Biological: 3.29, 3.40, 3.72, 3.103, 3.104. Conceptual: 3.33, 3.34, 3.63, 3.64, 3.81, 3.82, 3.94.

What is its molecular formula given that its molar mass is about 120 g?

••3.45 The formula for rust can be represented by Fe_2O_3. How many moles of Fe are present in 24.6 g of the compound?

••**3.46** How many grams of sulfur (S) are needed to react completely with 246 g of mercury (Hg) to form HgS?

••3.47 Calculate the mass in grams of iodine (I_2) that will react completely with 20.4 g of aluminum (Al) to form aluminum iodide (AlI_3).

••**3.48** Tin(II) fluoride (SnF_2) is often added to toothpaste as an ingredient to prevent tooth decay. What is the mass of F in grams in 24.6 g of the compound?

••3.49 What are the empirical formulas of the compounds with the following compositions? (a) 2.1 percent H, 65.3 percent O, 32.6 percent S, (b) 20.2 percent Al, 79.8 percent Cl.

••**3.50** What are the empirical formulas of the compounds with the following compositions? (a) 40.1 percent C, 6.6 percent H, 53.3 percent O, (b) 18.4 percent C, 21.5 percent N, 60.1 percent K.

•3.51 The anticaking agent added to Morton salt is calcium silicate, $CaSiO_3$. This compound can absorb up to 2.5 times its mass of water and still remains a free-flowing powder. Calculate the percent composition of $CaSiO_3$.

••**3.52** The empirical formula of a compound is CH. If the molar mass of this compound is about 78 g, what is its molecular formula?

•3.53 The molar mass of caffeine is 194.19 g. Is the molecular formula of caffeine $C_4H_5N_2O$ or $C_8H_{10}N_4O_2$?

••**3.54** Monosodium glutamate (MSG), a food-flavor enhancer, has been blamed for "Chinese restaurant syndrome," the symptoms of which are headaches and chest pains. MSG has the following composition by mass: 35.51 percent C, 4.77 percent H, 37.85 percent O, 8.29 percent N, and 13.60 percent Na. What is its molecular formula if its molar mass is about 169 g?

Chemical Reactions and Chemical Equations

Review Questions

3.55 Use the formation of water from hydrogen and oxygen to explain the following terms: chemical reaction, reactant, product.

3.56 What is the difference between a chemical reaction and a chemical equation?

3.57 Why must a chemical equation be balanced? What law is obeyed by a balanced chemical equation?

3.58 Write the symbols used to represent gas, liquid, solid, and the aqueous phase in chemical equations.

Problems

••3.59 Balance the following equations using the method outlined in Section 3.7:

(a) $C + O_2 \longrightarrow CO$
(b) $CO + O_2 \longrightarrow CO_2$
(c) $H_2 + Br_2 \longrightarrow HBr$
(d) $K + H_2O \longrightarrow KOH + H_2$
(e) $Mg + O_2 \longrightarrow MgO$
(f) $O_3 \longrightarrow O_2$
(g) $H_2O_2 \longrightarrow H_2O + O_2$
(h) $N_2 + H_2 \longrightarrow NH_3$
(i) $Zn + AgCl \longrightarrow ZnCl_2 + Ag$
(j) $S_8 + O_2 \longrightarrow SO_2$
(k) $NaOH + H_2SO_4 \longrightarrow Na_2SO_4 + H_2O$
(l) $Cl_2 + NaI \longrightarrow NaCl + I_2$
(m) $KOH + H_3PO_4 \longrightarrow K_3PO_4 + H_2O$
(n) $CH_4 + Br_2 \longrightarrow CBr_4 + HBr$

••**3.60** Balance the following equations using the method outlined in Section 3.7:

(a) $N_2O_5 \longrightarrow N_2O_4 + O_2$
(b) $KNO_3 \longrightarrow KNO_2 + O_2$
(c) $NH_4NO_3 \longrightarrow N_2O + H_2O$
(d) $NH_4NO_2 \longrightarrow N_2 + H_2O$
(e) $NaHCO_3 \longrightarrow Na_2CO_3 + H_2O + CO_2$
(f) $P_4O_{10} + H_2O \longrightarrow H_3PO_4$
(g) $HCl + CaCO_3 \longrightarrow CaCl_2 + H_2O + CO_2$
(h) $Al + H_2SO_4 \longrightarrow Al_2(SO_4)_3 + H_2$
(i) $CO_2 + KOH \longrightarrow K_2CO_3 + H_2O$
(j) $CH_4 + O_2 \longrightarrow CO_2 + H_2O$
(k) $Be_2C + H_2O \longrightarrow Be(OH)_2 + CH_4$
(l) $Cu + HNO_3 \longrightarrow Cu(NO_3)_2 + NO + H_2O$
(m) $S + HNO_3 \longrightarrow H_2SO_4 + NO_2 + H_2O$
(n) $NH_3 + CuO \longrightarrow Cu + N_2 + H_2O$

Amounts of Reactants and Products

Review Questions

3.61 On what law is stoichiometry based? Why is it essential to use balanced equations in solving stoichiometric problems?

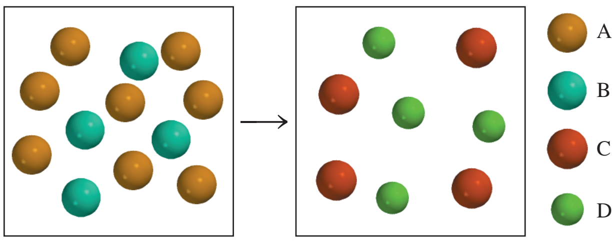
3.62 Describe the steps involved in the mole method.

Problems

•3.63 Which of the following equations best represents the reaction shown in the diagram on p. 88?

(a) $8A + 4B \longrightarrow C + D$

(b) $4A + 8B \longrightarrow 4C + 4D$
(c) $2A + B \longrightarrow C + D$
(d) $4A + 2B \longrightarrow 4C + 4D$
(e) $2A + 4B \longrightarrow C + D$



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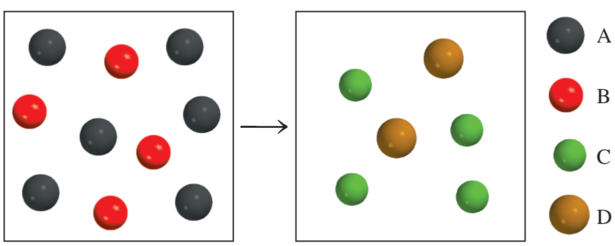
•**3.64** Which of the following equations best represents the reaction shown in the diagram?

(a) $A + B \longrightarrow C + D$
(b) $6A + 4B \longrightarrow C + D$
(c) $A + 2B \longrightarrow 2C + D$
(d) $3A + 2B \longrightarrow 2C + D$
(e) $3A + 2B \longrightarrow 4C + 2D$



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•3.65 Consider the combustion of carbon monoxide (CO) in oxygen gas

$$2CO(g) + O_2(g) \longrightarrow 2CO_2(g)$$

Starting with 3.60 moles of CO, calculate the number of moles of CO_2 produced if there is enough oxygen gas to react with all of the CO.

•**3.66** Silicon tetrachloride ($SiCl_4$) can be prepared by heating Si in chlorine gas:

$$Si(s) + 2Cl_2(g) \longrightarrow SiCl_4(l)$$

In one reaction, 0.507 mole of $SiCl_4$ is produced. How many moles of molecular chlorine were used in the reaction?

•3.67 Ammonia is a principal nitrogen fertilizer. It is prepared by the reaction between hydrogen and nitrogen.

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

In a particular reaction, 6.0 moles of NH_3 were produced. How many moles of H_2 and how many moles of N_2 were reacted to produce this amount of NH_3?

•**3.68** Consider the combustion of butane (C_4H_{10}):

$$2C_4H_{10}(g) + 13O_2(g) \longrightarrow 8CO_2(g) + 10H_2O(l)$$

In a particular reaction, 5.0 moles of C_4H_{10} are reacted with an excess of O_2. Calculate the number of moles of CO_2 formed.

••3.69 The annual production of sulfur dioxide from burning coal and fossil fuels, auto exhaust, and other sources is about 26 million tons. The equation for the reaction is

$$S(s) + O_2(g) \longrightarrow SO_2(g)$$

How much sulfur (in tons), present in the original materials, would result in that quantity of SO_2?

••**3.70** When baking soda (sodium bicarbonate or sodium hydrogen carbonate, $NaHCO_3$) is heated, it releases carbon dioxide gas, which is responsible for the rising of cookies, donuts, and bread. (a) Write a balanced equation for the decomposition of the compound (one of the products is Na_2CO_3). (b) Calculate the mass of $NaHCO_3$ required to produce 20.5 g of CO_2.

••3.71 When potassium cyanide (KCN) reacts with acids, a deadly poisonous gas, hydrogen cyanide (HCN), is given off. Here is the equation:

$$KCN(aq) + HCl(aq) \longrightarrow KCl(aq) + HCN(g)$$

If a sample of 0.140 g of KCN is treated with an excess of HCl, calculate the amount of HCN formed, in grams.

•**3.72** Fermentation is a complex chemical process of wine making in which glucose is converted into ethanol and carbon dioxide:

$$\underset{\text{glucose}}{C_6H_{12}O_6} \longrightarrow \underset{\text{ethanol}}{2C_2H_5OH} + 2CO_2$$

Starting with 500.4 g of glucose, what is the maximum amount of ethanol in grams and in liters that can be obtained by this process? (Density of ethanol = 0.789 g/mL.)

•••3.73 Each copper(II) sulfate unit is associated with five water molecules in crystalline copper(II) sulfate pentahydrate ($CuSO_4 \cdot 5H_2O$). When this compound is heated in air above 100°C, it loses the water molecules and also its blue color:

$$CuSO_4 \cdot 5H_2O \longrightarrow CuSO_4 + 5H_2O$$

If 9.60 g of $CuSO_4$ are left after heating 15.01 g of the blue compound, calculate the number of moles of H_2O originally present in the compound.

••**3.74** For many years the recovery of gold—that is, the separation of gold from other materials—involved the use of potassium cyanide:

$$4Au + 8KCN + O_2 + 2H_2O \longrightarrow 4KAu(CN)_2 + 4KOH$$

What is the minimum amount of KCN in moles needed to extract 29.0 g (about an ounce) of gold?

Industrial: 3.28, 3.41, 3.42, 3.51, 3.67, 3.89, 3.91, 3.95, 3.102, 3.111, 3.115.

••3.75 Limestone ($CaCO_3$) is decomposed by heating to quicklime (CaO) and carbon dioxide. Calculate how many grams of quicklime can be produced from 1.0 kg of limestone.

••**3.76** Nitrous oxide (N_2O) is also called "laughing gas." It can be prepared by the thermal decomposition of ammonium nitrate (NH_4NO_3). The other product is H_2O. (a) Write a balanced equation for this reaction. (b) How many grams of N_2O are formed if 0.46 mole of NH_4NO_3 is used in the reaction?

••3.77 The fertilizer ammonium sulfate [$(NH_4)_2SO_4$] is prepared by the reaction between ammonia (NH_3) and sulfuric acid:

$$2NH_3(g) + H_2SO_4(aq) \longrightarrow (NH_4)_2SO_4(aq)$$

How many kilograms of NH_3 are needed to produce 1.00×10^5 kg of $(NH_4)_2SO_4$?

••**3.78** A common laboratory preparation of oxygen gas is the thermal decomposition of potassium chlorate ($KClO_3$). Assuming complete decomposition, calculate the number of grams of O_2 gas that can be obtained from 46.0 g of $KClO_3$. (The products are KCl and O_2.)

Limiting Reagents

Review Questions

3.79 Define limiting reagent and excess reagent. What is the significance of the limiting reagent in predicting the amount of the product obtained in a reaction? Can there be a limiting reagent if only one reactant is present?

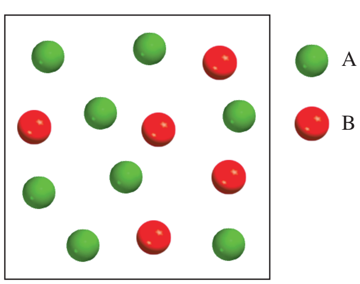
3.80 Give an everyday example that illustrates the limiting reagent concept.

Problems

••3.81 Consider the reaction

$$2A + B \longrightarrow C$$

(a) In the diagram here that represents the reaction, which reactant, A or B, is the limiting reagent? (b) Assuming complete reaction, draw a molecular-model representation of the amounts of reactants and products left after the reaction. The atomic arrangement in C is ABA.



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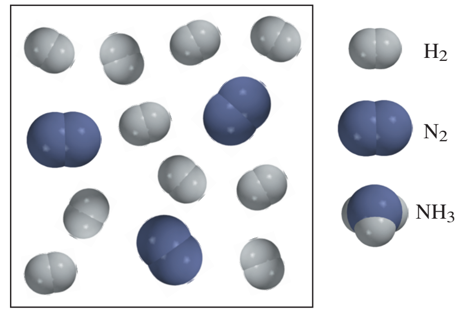
••**3.82** Consider the reaction

$$N_2 + 3H_2 \longrightarrow 2NH_3$$

Assuming each model represents one mole of the substance, show the number of moles of the product and the excess reagent left after the complete reaction.



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••3.83 Nitric oxide (NO) reacts with oxygen gas to form nitrogen dioxide (NO_2), a dark-brown gas:

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

In one experiment 0.886 mole of NO is mixed with 0.503 mole of O_2. Calculate which of the two reactants is the limiting reagent. Calculate also the number of moles of NO_2 produced.

•••**3.84** The depletion of ozone (O_3) in the stratosphere has been a matter of great concern among scientists in recent years. It is believed that ozone can react with nitric oxide (NO) that is discharged from the high-altitude jet plane, the SST. The reaction is

$$O_3 + NO \longrightarrow O_2 + NO_2$$

If 0.740 g of O_3 reacts with 0.670 g of NO, how many grams of NO_2 will be produced? Which compound is the limiting reagent? Calculate the number of moles of the excess reagent remaining at the end of the reaction.

••3.85 Propane (C_3H_8) is a component of natural gas and is used in domestic cooking and heating. (a) Balance the following equation representing the combustion of propane in air:

$$C_3H_8 + O_2 \longrightarrow CO_2 + H_2O$$

(b) How many grams of carbon dioxide can be produced by burning 3.65 moles of propane? Assume that oxygen is the excess reagent in this reaction.

•••**3.86** Consider the reaction

$$MnO_2 + 4HCl \longrightarrow MnCl_2 + Cl_2 + 2H_2O$$

If 0.86 mole of MnO_2 and 48.2 g of HCl react, which reagent will be used up first? How many grams of Cl_2 will be produced?

Reaction Yield

Review Questions

3.87 Why is the theoretical yield of a reaction determined only by the amount of the limiting reagent?

3.88 Why is the actual yield of a reaction almost always smaller than the theoretical yield?

Problems

••3.89 Hydrogen fluoride is used in the manufacture of Freons (which destroy ozone in the stratosphere) and in the production of aluminum metal. It is prepared by the reaction

$$CaF_2 + H_2SO_4 \longrightarrow CaSO_4 + 2HF$$

In one process 6.00 kg of CaF_2 are treated with an excess of H_2SO_4 and yield 2.86 kg of HF. Calculate the percent yield of HF.

••**3.90** Nitroglycerin ($C_3H_5N_3O_9$) is a powerful explosive. Its decomposition can be represented by

$$4C_3H_5N_3O_9 \longrightarrow 6N_2 + 12CO_2 + 10H_2O + O_2$$

This reaction generates a large amount of heat and many gaseous products. It is the sudden formation of these gases, together with their rapid expansion, that produces the explosion. (a) What is the maximum amount of O_2 in grams that can be obtained from 2.00×10^2 g of nitroglycerin? (b) Calculate the percent yield in this reaction if the amount of O_2 generated is found to be 6.55 g.

••3.91 Titanium(IV) oxide (TiO_2) is a white substance produced by the action of sulfuric acid on the mineral ilmenite ($FeTiO_3$):

$$FeTiO_3 + H_2SO_4 \longrightarrow TiO_2 + FeSO_4 + H_2O$$

Its opaque and nontoxic properties make it suitable as a pigment in plastics and paints. In one process 8.00×10^3 kg of $FeTiO_3$ yielded 3.67×10^3 kg of TiO_2. What is the percent yield of the reaction?

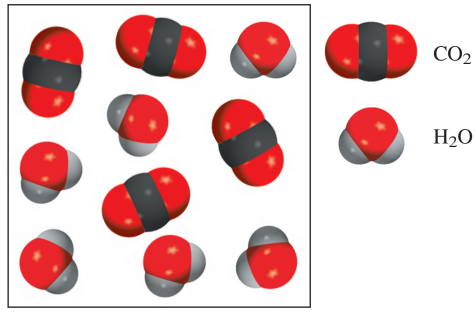
••**3.92** When heated, lithium reacts with nitrogen to form lithium nitride:

$$6Li(s) + N_2(g) \longrightarrow 2Li_3N(s)$$

What is the theoretical yield of Li_3N in grams when 12.3 g of Li are heated with 33.6 g of N_2? If the actual yield of Li_3N is 5.89 g, what is the percent yield of the reaction?

Additional Problems

•••3.93 The following diagram represents the products (CO_2 and H_2O) formed after the combustion of a hydrocarbon (a compound containing only C and H atoms). Write an equation for the reaction. (*Hint:* The molar mass of the hydrocarbon is about 30 g.)



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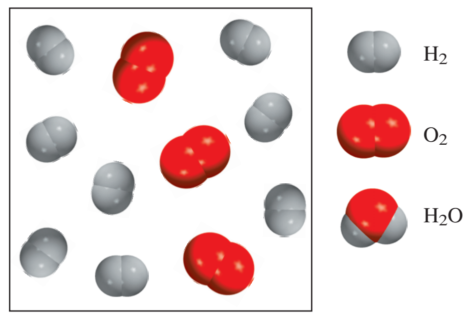
••**3.94** Consider the reaction of hydrogen gas with oxygen gas:

$$2H_2(g) + O_2(g) \longrightarrow 2H_2O(g)$$



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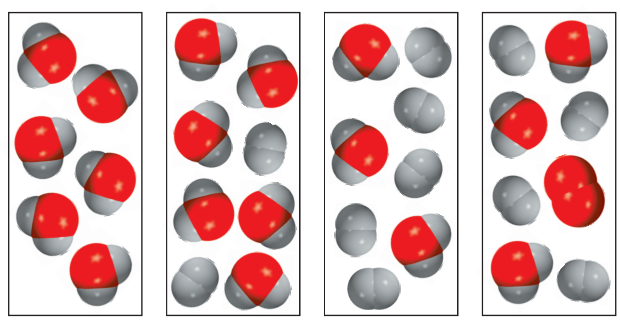
Assuming complete reaction, which of the diagrams shown below represents the amounts of reactants and products left after the reaction?



(a) (b) (c) (d)

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•••3.95 Industrially, nitric acid is produced by the Ostwald process represented by the following equations:

$$4NH_3(g) + 5O_2(g) \longrightarrow 4NO(g) + 6H_2O(l)$$
$$2NO(g) + O_2(g) \longrightarrow 2NO_2(g)$$
$$2NO_2(g) + H_2O(l) \longrightarrow HNO_3(aq) + HNO_2(aq)$$

What mass of NH_3 (in g) must be used to produce 1.00 ton of HNO_3 by the above procedure, assuming an 80 percent yield in each step? (1 ton = 2000 lb; 1 lb = 453.6 g.)

•••**3.96** A sample of a compound of Cl and O reacts with an excess of H_2 to give 0.233 g of HCl and 0.403 g of H_2O. Determine the empirical formula of the compound.

•••3.97 The atomic mass of element X is 33.42 amu. A 27.22-g sample of X combines with 84.10 g of another element Y to form a compound XY. Calculate the atomic mass of Y.

•••**3.98** The aluminum sulfate hydrate $[Al_2(SO_4)_3 \cdot xH_2O]$ contains 8.20 percent Al by mass. Calculate x, that is, the number of water molecules associated with each $Al_2(SO_4)_3$ unit.

••3.99 An iron bar weighed 664 g. After the bar had been standing in moist air for a month, exactly one-eighth of the iron turned to rust (Fe_2O_3). Calculate the final mass of the iron bar and rust.

•••**3.100** A certain metal oxide has the formula MO, where M denotes the metal. A 39.46-g sample of the compound is strongly heated in an atmosphere of hydrogen to remove oxygen as water molecules. At the end, 31.70 g of the metal is left over. If O has an atomic mass of 16.00 amu, calculate the atomic mass of M and identify the element.

•••3.101 An impure sample of zinc (Zn) is treated with an excess of sulfuric acid (H_2SO_4) to form zinc sulfate ($ZnSO_4$) and molecular hydrogen (H_2). (a) Write a balanced equation for the reaction. (b) If 0.0764 g of H_2 is obtained from 3.86 g of the sample, calculate the percent purity of the sample. (c) What assumptions must you make in (b)?

•••**3.102** One of the reactions that occurs in a blast furnace, where iron ore is converted to cast iron, is

$$Fe_2O_3 + 3CO \longrightarrow 2Fe + 3CO_2$$

Suppose that 1.64×10^3 kg of Fe are obtained from a 2.62×10^3-kg sample of Fe_2O_3. Assuming that the reaction goes to completion, what is the percent purity of Fe_2O_3 in the original sample?

•••3.103 Carbon dioxide (CO_2) is the gas that is mainly responsible for global warming (the greenhouse effect). The burning of fossil fuels is a major cause of the increased concentration of CO_2 in the atmosphere. Carbon dioxide is also the end product of metabolism (see Example 3.14). Using glucose as an example of food, calculate the annual human production of CO_2 in grams, assuming that each person consumes 5.0×10^2 g of glucose per day. The world's population is 6.5 billion, and there are 365 days in a year.

••**3.104** Carbohydrates are compounds containing carbon, hydrogen, and oxygen in which the hydrogen to oxygen ratio is 2:1. A certain carbohydrate contains 40.0 percent carbon by mass. Calculate the empirical and molecular formulas of the compound if the approximate molar mass is 178 g.

••3.105 Heating 2.40 g of the oxide of metal X (molar mass of X = 55.9 g/mol) in carbon monoxide (CO) yields the pure metal and carbon dioxide. The mass of the metal product is 1.68 g. From the data given, show that the simplest formula of the oxide is X_2O_3 and write a balanced equation for the reaction.

••**3.106** A compound X contains 63.3 percent manganese (Mn) and 36.7 percent O by mass. When X is heated, oxygen gas is evolved and a new compound Y containing 72.0 percent Mn and 28.0 percent O is formed. (a) Determine the empirical formulas of X and Y. (b) Write a balanced equation for the conversion of X to Y.

•••3.107 A sample containing NaCl, Na_2SO_4, and $NaNO_3$ gives the following elemental analysis: Na: 32.08 percent; O: 36.01 percent; Cl: 19.51 percent. Calculate the mass percent of each compound in the sample.

•••**3.108** When 0.273 g of Mg is heated strongly in a nitrogen (N_2) atmosphere, a chemical reaction occurs. The product of the reaction weighs 0.378 g. Calculate the empirical formula of the compound containing Mg and N. Name the compound.

•••3.109 A mixture of methane (CH_4) and ethane (C_2H_6) of mass 13.43 g is completely burned in oxygen. If the total mass of CO_2 and H_2O produced is 64.84 g, calculate the fraction of CH_4 in the mixture.

•••**3.110** The following is a crude but effective method for estimating the *order of magnitude* of Avogadro's number using stearic acid ($C_{18}H_{36}O_2$). When stearic acid is added to water, its molecules collect at the surface and form a monolayer; that is, the layer is only one molecule thick. The cross-sectional area of each stearic acid molecule has been measured to be 0.21 nm^2. In one experiment it is found that 1.4×10^{-4} g of stearic acid is needed to form a monolayer over water in a dish of diameter 20 cm. Based on these measurements, what is Avogadro's number? (The area of a circle of radius r is πr^2.)

•••3.111 Octane (C_8H_{18}) is a component of gasoline. Complete combustion of octane yields H_2O and CO_2. Incomplete combustion produces H_2O and CO, which not only reduces the efficiency of the engine using the fuel but is also toxic. In a certain test run, 1.000 gallon of octane is burned in an engine. The total mass of CO, CO_2, and H_2O produced is 11.53 kg. Calculate the efficiency of the process; that is, calculate the fraction of octane converted to CO_2. The density of octane is 2.650 kg/gallon.

••**3.112** A reaction having a 90 percent yield may be considered a successful experiment. However, in the synthesis of complex molecules such as chlorophyll and many anticancer drugs, a chemist often has to carry out multiple-step synthesis. What is the overall percent yield for such a synthesis, assuming it is a 30-step reaction with a 90 percent yield at each step?

•••3.113 A mixture of $CuSO_4 \cdot 5H_2O$ and $MgSO_4 \cdot 7H_2O$ is heated until all the water is lost. If 5.020 g of the mixture gives 2.988 g of the anhydrous salts, what is the percent by mass of $CuSO_4 \cdot 5H_2O$ in the mixture?

Special Problems

3.114 (a) A research chemist used a mass spectrometer to study the two isotopes of an element. Over time, she recorded a number of mass spectra of these isotopes. On analysis, she noticed that the ratio of the taller peak (the more abundant isotope) to the shorter peak (the less abundant isotope) gradually increased with time. Assuming that the mass spectrometer was functioning normally, what do you think was causing this change?

(b) Mass spectrometry can be used to identify the formulas of molecules having small molecular masses. To illustrate this point, identify the molecule which most likely accounts for the observation of a peak in a mass spectrum at: 16 amu, 17 amu, 18 amu, and 64 amu.

(c) Note that there are (among others) two likely molecules that would give rise to a peak at 44 amu, namely, C_3H_8 and CO_2. In such cases, a chemist might try to look for other peaks generated when some of the molecules break apart in the spectrometer. For example, if a chemist sees a peak at 44 amu and also one at 15 amu, which molecule is producing the 44-amu peak? Why?

(d) Using the following precise atomic masses: ^{1}H(1.00797 amu), ^{12}C(12.00000 amu), and ^{16}O(15.99491 amu), how precisely must the masses of C_3H_8 and CO_2 be measured to distinguish between them?

(e) Every year millions of dollars' worth of gold is stolen. In most cases the gold is melted down and shipped abroad. This way the gold retains its value while losing all means of identification. Gold is a highly unreactive metal that exists in nature in the uncombined form. During the mineralization of gold, that is, the formation of gold nuggets from microscopic gold particles, various elements such as cadmium (Cd), lead (Pb), and zinc (Zn) are incorporated into the nuggets. The amounts and types of the impurities or trace elements in gold vary according to the location where it was mined. Based on this knowledge, describe how you would identify the source of a piece of gold suspected of being stolen from Fort Knox, the federal gold depository.

3.115 Potash is any potassium mineral that is used for its potassium content. Most of the potash produced in the United States goes into fertilizer. The major sources of potash are potassium chloride (KCl) and potassium sulfate (K_2SO_4). Potash production is often reported as the potassium oxide (K_2O) equivalent or the amount of K_2O that could be made from a given mineral. (a) If KCl costs \$0.055 per kg, for what price (dollar per kg) must K_2SO_4 be sold in order to supply the same amount of potassium on a per dollar basis? (b) What mass (in kg) of K_2O contains the same number of moles of K atoms as 1.00 kg of KCl?

Answers to Practice Exercises

3.1 10.81 amu. **3.2** 2.57×10^3 g. **3.3** 8.49×10^{21} K atoms. **3.4** 2.107×10^{-22} g. **3.5** 32.04 amu. **3.6** 1.66 moles. **3.7** 5.81×10^{24} H atoms. **3.8** H: 2.055%; S: 32.69%; O: 65.25%. **3.9** $KMnO_4$ (potassium permanganate). **3.10** 196 g. **3.11** B_2H_6. **3.12** $Fe_2O_3 + 3CO \longrightarrow 2Fe + 3CO_2$. **3.13** (a) 0.508 mole, (b) 2.21 g. **3.14** 235 g. **3.15** (a) 234 g, (b) 234 g. **3.16** (a) 863 g, (b) 93.0%.