THE MOLE: RELATING THE MICROSCOPIC WORLD OF ATOMS TO LABORATORY MEASUREMENTS

3

The rich and famous often fly to exotic vacation spots using private airplanes such as this. Even now you may be dreaming about your upcoming vacation after the final exam. Here, the plane is prepared for takeoff with the necessary mass (weight) of aviation fuel to reach the planned destination with some excess to spare. Professionals use complex calculations that include the mole concept described in this chapter to determine the mass of fuel needed to transport vacationers safely to their next destination. *(Alice M. Prescott/Unicorn Stock Photos)*

CHAPTER OUTLINE

THIS CHAPTER IN CONTEXT In Chapters 1 and 2 we reviewed the basics of the mathematics and language of chemistry. In this chapter we combine the material from Chapters 1 and 2 to learn the fundamentals of chemical calculations. These calculations are important for success in laboratory work in this course. You will also find this chapter to be important for future courses in organic chemistry, biochemistry, and almost any other advanced laboratory course in the sciences.

Our chemical calculations are called **stoichiometry** (stoy-kee-AH-meh-tree), which loosely translates as "the measure of the elements." Stoichiometry involves converting chemical formulas and equations that represent individual atoms, molecules, and formula units to the laboratory scale that uses milligrams, grams, and even kilograms of these substances. To do this we introduce the *mole concept.* The mole concept allows the chemist to scale up from the atomic and molecular level to the laboratory scale much as the baker in Figure 3.1 scales up the amount of ingredients

FIG. 3.1 **Manufacture on small and large scales.** Making a single gingerbread man requires 10 currants for eyes and buttons, 1/10 of a cup of spiced cookie dough, and a teaspoon of glacé icing. To manufacture gingerbread men by the million, you will have to order raw materials by the ton. To scale up the recipe, you will need to know the masses of raw materials required to manufacture some fixed number of gingerbread men.

from a single gingerbread man to a mass-production scale. Chemical conversions are similar in nature to the gingerbread man example but of course they answer different questions. Some of these questions are

How many grams of product can be made if we react *x* grams of *A* and *y* grams of *B*?

How can we be sure to get the most product from an expensive reactant?

If a reaction has a 70% yield, how many grams of reactants are needed to produce the amount of product needed?

How many grams of each reactant are needed so that there will be no reactants left over (i.e., no waste)?

Our stoichiometric calculations are almost always factor-label conversions from one set of units to another as we saw in Chapter 1. To be successful at factor-label calculations we need two things, a knowledge of the equalities that can be made into conversion factors and a logical sequence of steps to apply the conversion factors to our problem. Figure 3.6 at the end of this chapter organizes the equalities and sequence of steps in a simple flowchart. As you read this chapter, you might want to look at Figure 3.6 to see how all the parts fit together neatly.

3.1 The Mole Conveniently Links Mass to Number of Atoms or Molecules

We can tell from the fundamental measurements of the mass of the proton, neutron, and electron that even the largest of the atoms must have extremely small masses and correspondingly small sizes. Any sample of matter that is observable by the naked eye must have very large numbers of atoms or molecules. The methods of calculation developed in Chapter 1 and the mole concept allow us to count by weighing and then use that information to solve some very interesting problems.

Counting by weighing is familiar to everyone even if you are not aware of it. A pound of chocolate chips counts out the needed number of chocolate chips for your cookies. A quarter pound of rice counts out the correct number of rice grains to accompany your meal. Weighing a bag of dimes, knowing that each dime weighs 2.27 grams, will allow you to calculate the number of coins. Similarly, the mass of a chemical substance can be used to determine the number of atoms or molecules in the sample. This last conversion is possible because of the mole concept.

The SI unit for the *amount of substance* is the mole

The **mole** (abbreviated as mol) is the SI unit for the amount of substance. The amount of substance does not refer to the mass or volume of your sample but it does refer to the number of atoms, molecules, or formula units, etc., in your sample. **One mole is defined**

Mole is a Latin word with several meanings, including: a shapeless mass; a large number; or trouble or difficulty.

as the number of atoms in exactly 12 grams of ^{12}C atoms. Based on this definition and the fact that the average atomic masses in the periodic table are relative values, we can deduce that we will have a mole of any element if we weigh an amount equal to the atomic mass in gram units (this is often called the **gram atomic mass**). For example, the atomic mass of sodium is 22.99 u, so one mole of sodium has a mass of 22.99 g and contains as many atoms as there are in a 12.00 g sample of carbon-12.

TOOLS

One mole of any element is equal to the atomic mass with gram units

$$1 \text{ mole of element } X = \text{gram atomic mass of } X$$

Figure 3.2 is a photo showing one mole of some common elements: iron, mercury, copper, and sulfur.

The mole concept also applies to compounds

Many chemists use the terms *molecular weight* and *atomic weight* for molecular mass and atomic mass.

Molecules and ionic compounds discussed in Chapter 2 have definite formulas. For molecular compounds and elements, adding the atomic masses of all atoms in the formula results in the **molecular mass** (**molecular weight**). The gram molecular mass of a molecular substance (a mass in grams numerically equal to the molecular mass) is also equal to one mole.

$$1 \text{ mole of molecule } X = \text{gram molecular mass of } X$$

For example, a molecule of H_2O consists of 2 atoms of H (with a total mass of 2×1.00 u $= 2.00$ u) and one atom of O (with a mass of 16.00 u) for a total of 18.00 u. Therefore, the molecular mass of H_2O is 18.00 u. The gram molecular mass of H_2O is 18.00 g, so 1 mol H_2O = 18.00 g H_2O.

TOOLS

***Molecular mass** or **formula mass** is the sum of the masses of all atoms in a chemical formula*

Similarly, the **formula mass** of an ionic compound is the sum of the masses of all the atoms in the formula of an ionic compound.

$$1 \text{ mole of ionic compound } X = \text{gram formula mass of } X$$

For example, the ionic compound calcium chloride, $CaCl_2$, has a formula mass that is the sum of the atomic masses of one calcium atom and two chlorine atoms. One calcium atom has an atomic mass of 40.08 u. Two chlorine atoms each with an atomic mass of 35.45 u have a total mass of 70.90 u. Adding these together gives us 110.98 u for the formula mass of $CaCl_2$. Therefore, 1 mol $CaCl_2$ has a mass of 110.98 g. There is a distinct similarity between all three equations above. To simplify discussions we will often use the following relationship between moles and mass unless one of the other, equivalent, definitions provides more clarity.

TOOLS

***Molar mass** is the mass in grams of one mole of any substance*

$$1 \text{ mole of } X = \text{gram molar mass of } X$$

The gram **molar mass** is simply the mass of one mole of the substance under consideration. Figure 3.3 depicts one mole of four different compounds.

FIG. 3.2 **Moles of elements.** Each sample of these elements contains the same number of atoms. *(Michael Watson.)*

FIG. 3.3 **Moles of compounds.** One mole of four different compounds: water, sodium chloride, copper sulfate pentahydrate, and sodium chromate. Each sample contains the identical number of formula units or molecules. *(Michael Watson.)*

Convert mass to moles and moles to mass using molar masses

At this point we recognize the above relationships or equalities as the necessary information for doing conversion problems similar to those in Chapter 1. Now, however, the problems will be couched in chemical terms. We will also use all of the principles in Section 1.6 to end up with the maximum, and correct, number of significant figures in our answers. To do this we will need to round our atomic or molar masses to at least one more significant figure than the data given in the example.

The term *molar mass* has been coined as a general term to cover all items previously called atomic masses, atomic weights, molecular masses, molecular weights, formula masses, and formula weights.

EXAMPLE 3.1
Converting from Grams to Moles

How many moles of sulfur are there in a 23.5 g sample of sulfur?

ANALYSIS: We see that the problem starts with a certain mass of sulfur and asks us to convert it to moles. This uses the tool we just described that equates moles and grams of an element. The equality shows that there is a one-step conversion possible using 1 mol S = 32.06 g S.

SOLUTION: Let's begin by expressing the question in the form of an equation.

$$\underset{\text{start}}{23.5\text{ g S}} = \underset{\text{end}}{?\text{ mol S}}$$

Now use the equality to cancel the grams of sulfur as shown below.

$$23.5\ \cancel{\text{g S}} \times \left(\frac{1\text{ mol S}}{32.06\ \cancel{\text{g S}}}\right) = 0.733\text{ mol S}$$

IS THE ANSWER REASONABLE? First review the math to be sure that the units cancel properly, and they do. Second, round off all numbers to one significant figure and calculate an estimated answer. This gives 20/30 = 2/3, and our answer is not very different (very different is a factor of 10 or more) from 2/3. We are justified in being confident in our answer.

Solving a stoichiometry problem is much like giving directions to get from your house to your college. You need to know both the starting and ending points. Setting up the problem in this way gives you those reference points. The factor-label ratios get us from one to the other.

EXAMPLE 3.2
Converting from Moles to Grams

We need 0.254 mol of iron(III) chloride for a certain experiment. How many grams do we need to weigh?

ANALYSIS: The formula for iron(III) chloride is $FeCl_3$. As in the last example we need the tool for the conversion between mass and moles. We write the equality as

$$1\text{ mol FeCl}_3 = \text{gram molar mass FeCl}_3$$

This tells us we need the gram molar mass of $FeCl_3$ that is the sum of the gram atomic masses of one iron atom and three chlorine atoms.

$$\text{gram molar mass} = 55.85\text{ g Fe mol}^{-1} + (3 \times 35.45\text{ g Cl mol}^{-1}) = 162.20\text{ g FeCl}_3\text{ mol}^{-1}$$

The equality can be written as 1 mol $FeCl_3$ = 162.20 g $FeCl_3$.

SOLUTION: The problem starts with

$$0.254\text{ mol FeCl}_3 = ?\text{ g FeCl}_3$$

Use the factor label to perform the conversion:

$$0.254\ \cancel{\text{mol FeCl}_3}\left(\frac{162.20\text{ g FeCl}_3}{1\ \cancel{\text{mol FeCl}_3}}\right) = 41.2\text{ g FeCl}_3$$

IS THE ANSWER REASONABLE? First we verify that the units cancel properly, and they do. Next we do an approximate calculation. If we round 0.254 to 0.25 and 162.20 to 160, the arithmetic becomes 0.25 × 160 = 40, which gives a result that is very close to the calculated value. We also could have estimated the answer by rounding to one significant figure, which gives 0.3 × 200 = 60, and still have concluded that the math was correct. Remember, this is just an estimate, but it tells us our more precise answer is correct.

Practice Exercise 1: How many moles of aluminum are there in a 3.47 gram sheet of aluminum foil used to wrap your sandwich for lunch today? (Hint: Recall the tool that relates the mass of an element to moles of that element.)

Practice Exercise 2: Your laboratory balance can weigh samples to three decimal places. If the uncertainty in your weighing is ± 0.002 g, what is the uncertainty in moles if the sample being weighed is pure silicon?

The number of particles in a mole is called Avogadro's number

Avogadro's number was named for Amedeo Avogadro (1776–1856), an Italian scientist who was one of the pioneers of stoichiometry.

TOOLS

Avogadro's number

The definition of the mole refers to a number equal to the number of atoms in exactly 12 g of ^{12}C. Just what is that number? After much experimentation the scientific community agrees that the value, to four significant figures, is 6.022×10^{23}. In honor of Amedeo Avogadro, this value has been named **Avogadro's number.** Now we can write a very important relationship between the atomic scale and the laboratory scale as

$$1 \text{ mole of } X = 6.022 \times 10^{23} \text{ units of } X$$

Avogadro's number is a link between moles of substance and elementary units of substance in a stoichiometry problem. If a problem does not mention atoms or molecules at all, you don't need to use Avogadro's number in the calculation!

The units of our chemicals can be atoms, molecules, formula units, etc.

We use Avogadro's number to relate the macroscopic and microscopic worlds

The relationships developed above allow us to connect the laboratory scale with the atomic scale using our standard factor-label calculations as shown in the next two examples.

EXAMPLE 3.3
Converting from the Laboratory Scale to the Atomic Scale

How many atoms of copper are there in a piece of pure copper wire that weighs 14.3 grams?

ANALYSIS: Here we do not have any tool that directly converts grams of copper to atoms of copper. However, we do have one tool that relates mass to moles (the atomic mass of copper) and another tool that relates moles to atoms (Avogadro's number). We need to start with the grams of copper and use the appropriate conversion factors derived from these tools in sequence.

$$\text{grams copper} \longrightarrow \text{moles copper} \longrightarrow \text{atoms copper}$$

SOLUTION: We start by mathematically stating the problem:

$$14.3 \text{ g Cu} = ? \text{ atoms Cu}$$

The first step will be to convert grams of copper to moles of copper. The atomic mass gives us

$$1 \text{ mol Cu} = 63.546 \text{ g Cu}$$

Estimates are done without calculators. For exponential numbers the numerical part of the calculation is separated from the exponents. The numerical part, to one significant figure, is usually easy to evaluate. The exponent is easier since it involves simple addition and subtraction.

This will allow us to construct a conversion factor to take us from grams to moles. To go from moles of copper to the number of copper atoms, we need Avogadro's number, which gives the relationship

$$1 \text{ mol Cu} = 6.02 \times 10^{23} \text{ atom Cu}$$

This will provide a conversion factor to take us from moles to atoms.

To assemble the solution, we begin with the given amount of copper (14.3 g) and apply conversion factors that eliminate units we don't want and take us to the units of the answer. This could be done in two steps or in one complete step as shown here. Note how the units cancel.

$$14.3 \cancel{\text{g Cu}} \times \left(\frac{1 \cancel{\text{mol Cu}}}{63.546 \cancel{\text{g Cu}}}\right) \times \left(\frac{6.022 \times 10^{23} \text{ atoms Cu}}{1 \cancel{\text{mol Cu}}}\right) = 1.35 \times 10^{23} \text{ atoms Cu}$$

Also notice that the first factor converts grams of copper to moles of copper and the second takes us from moles of copper to atoms of copper.

IS THE ANSWER REASONABLE? The most common mistake students make in this kind of calculation is using Avogadro's number incorrectly, or not using it at all. Think about the answer for a moment. We know copper atoms are very small, so in 14.3 g Cu there will be an enormous number of atoms. Our answer is a very large number, so it appears to be reasonable.

EXAMPLE 3.4
Calculating the Mass of a Molecule

What is the mass in grams of one molecule of carbon tetrachloride?

ANALYSIS: Using the nomenclature tools of Chapter 2, the formula of the molecule in question is CCl_4. In this problem we're asked to express the mass of a single CCl_4 molecule (composed of just 5 atoms) in a laboratory sized unit, grams. This tells us we need to use Avogadro's number, which is a tool that relates molecules to moles. Then we can use the molecular mass as a tool to relate moles to grams.

SOLUTION: Let's begin by expressing the question in the form of an equation.

$$1 \text{ molecule } CCl_4 = ?\text{ g } CCl_4$$

Avogadro's number lets us write

$$1 \text{ mol } CCl_4 = 6.02 \times 10^{23} \text{ molecules } CCl_4$$

This allows us to calculate the number of moles of CCl_4

$$1 \cancel{\text{molecule } CCl_4} \times \left(\frac{1 \text{ mol } CCl_4}{6.02 \times 10^{23} \cancel{\text{molecules } CCl_4}} \right) = 1.661 \times 10^{-24} \text{ mol } CCl_4$$

To find grams, we need the molecular mass of CCl_4, which is 153.823. Therefore, 1 mol CCl_4 = 153.823 g CCl_4. Now we can calculate grams of CCl_4.

$$1.661 \times 10^{-24} \cancel{\text{mol } CCl_4} \times \left(\frac{153.823 \text{ g } CCl_4}{1 \cancel{\text{mol } CCl_4}} \right) = 2.56 \times 10^{-22} \text{ g } CCl_4$$

In stepwise calculations such as this we normally keep at least one extra significant figure until the final result is determined. The calculated mass of one molecule of CCl_4 is 2.56×10^{-22} g.

IS THE ANSWER REASONABLE? We expect a single molecule to have a very small mass. Our answer is a very small number, so it appears to be reasonable.

Practice Exercise 3: Would you be able to use a balance capable of weighing to the nearest 0.001 g to weigh 5.64×10^{18} formula units of calcium nitrate? [Hint: What is the mass of this amount of $Ca(NO_3)_2$?]

Practice Exercise 4: If the uncertainty in weighing a sample in the lab is ±0.002 g, what is this uncertainty in terms of molecules of sucrose, $C_{12}H_{22}O_{11}$?

3.2 CHEMICAL FORMULAS RELATE AMOUNTS OF SUBSTANCES IN A COMPOUND

Consider the chemical formula for water, H_2O:

- One molecule of water contains 2 H atoms and 1 O atom.
- Two molecules of water contain 4 H atoms and 2 O atoms.
- A dozen molecules of water contain 2 dozen H atoms and 1 dozen O atoms.
- A mole of molecules of water contains 2 moles of H atoms and 1 mole of O atoms.

Whether we're dealing with atoms, dozens of atoms, or moles of atoms, the chemical formula tells us that the ratio of H atoms to O atoms is always 2 to 1. In addition we can write the following **Stoichiometric equivalencies** concerning the water molecule:

$$1 \text{ mol } H_2O \Leftrightarrow 2 \text{ mol H} \qquad 1 \text{ mol } H_2O \Leftrightarrow 1 \text{ mol O} \qquad 1 \text{ mol O} \Leftrightarrow 2 \text{ mol H}$$

We recall that the symbol $\Leftrightarrow$ means "is chemically equivalent to" and it is treated mathematically as an equal sign (see page 26 in Chapter 1).

TOOLS

Subscripts tell us the number of atoms in a formula

Within chemical compounds, moles of atoms always combine in the same ratio as the individual atoms themselves.

This fact lets us prepare mole-to-mole conversion factors involving elements in compounds as we need them. For example, in the formula P_4O_{10}, the subscripts mean that there are 4 moles of P for every 10 moles of O in this compound. We can relate P and O within the compound using the following conversion factors.

$$4 \text{ mol P} \Leftrightarrow 10 \text{ mol O} \qquad \text{from which we write} \qquad \frac{4 \text{ mol P}}{10 \text{ mol O}} \quad \text{or} \quad \frac{10 \text{ mol O}}{4 \text{ mol P}}$$

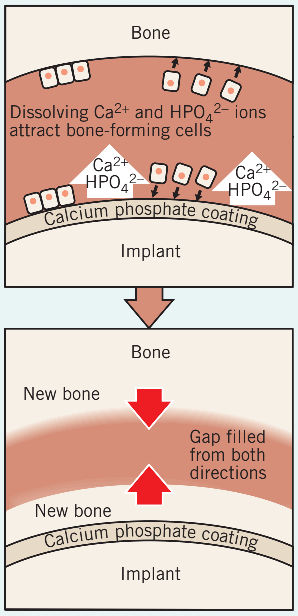
The formula P_4O_{10} also implies other equivalencies, each with its two associated conversion factors.

$$1 \text{ mol } P_4O_{10} \Leftrightarrow 4 \text{ mol P} \qquad \text{or} \qquad \frac{1 \text{ mol } P_4O_{10}}{4 \text{ mol P}} \quad \text{and} \quad \frac{4 \text{ mol P}}{1 \text{ mol } P_4O_{10}}$$

$$1 \text{ mol } P_4O_{10} \Leftrightarrow 10 \text{ mol O} \qquad \text{or} \qquad \frac{1 \text{ mol } P_4O_{10}}{10 \text{ mol O}} \quad \text{and} \quad \frac{10 \text{ mol O}}{1 \text{ mol } P_4O_{10}}$$

EXAMPLE 3.5
Calculating Amount of a Compound by Analyzing One Element

Calcium phosphate is widely found in nature in the form of natural minerals. It is also found in bones and some kidney stones. In many instances if we determine one element in a compound we can find out how much of the compound is present. In one case a sample is found to contain 0.864 mole of phosphorus. How many moles of $Ca_3(PO_4)_2$ will that represent?



Some surfaces on bone implants are coated with calcium phosphate to permit bone to actually bond to the surface.

ANALYSIS: We need to use the mole ratio tool that gives the relationships between the compound's formula and the individual elements in that formula. Specifically we need to use the equivalence 2 mol P $\Leftrightarrow$ 1 mol $Ca_3(PO_4)_2$ to construct the conversion factor needed to convert moles of P into moles of $Ca_3(PO_4)_2$.

SOLUTION: The initial question is written as an equation:

$$0.864 \text{ mol P} = ? \text{ mol } Ca_3(PO_4)_2$$

Seeing that mol P must cancel and mol $Ca_3(PO_4)_2$ must remain, the correct conversion factor must be 1 mol $Ca_3(PO_4)_2$/2 mol P and we solve the equation as

$$0.864 \cancel{\text{mol P}} \left(\frac{1 \text{ mol } Ca_3(PO_4)_2}{2 \cancel{\text{mol P}}}\right) = 0.432 \text{ mol } Ca_3(PO_4)_2$$

IS THE ANSWER REASONABLE? For a quick check, you can round 0.864 to 1 and divide by 2 to get 0.5. There is little difference between our estimate, 0.5, and the calculated answer, 0.432.

Whenever a problem asks you to convert an amount of one substance into an amount of a different substance, the most important conversion factor in the problem is usually a mole-to-mole relationship between the two substances.

Practice Exercise 5: Aluminum sulfate is analyzed and it is determined that the sample contains 0.0774 mole of sulfate ions. How many moles of aluminum does the sample contain? (Hint: Construct the correct formula for aluminum sulfate, then use the tool in this section.)

Practice Exercise 6: How many moles of nitrogen atoms are combined with 8.60 mol of oxygen atoms in dinitrogen pentoxide, N_2O_5?

One common use of stoichiometry in the lab occurs when we must relate the masses of two raw materials that are needed to make a compound. These calculations are summarized by the following sequence of steps to convert the mass of compound *A* to the mass of compound *B*.

$$\text{mass of } A \longrightarrow \text{moles of } A \longrightarrow \text{moles of } B \longrightarrow \text{mass of } B$$

TOOLS
Sequence of steps for mass-to-mass conversions

In the following example we see how this is applied.

EXAMPLE 3.6
Calculating Amounts of One Element from Amounts of Another in a Compound

Chlorophyll a, the green pigment in leaves, has the formula $C_{55}H_{72}MgN_4O_5$. If 0.0011 g of Mg is available to a plant cell for chlorophyll a synthesis, how many grams of carbon will be required to completely use up the magnesium?

ANALYSIS: Let's begin, as usual, by restating the problem as follows.

$$0.0011 \text{ g Mg} \Leftrightarrow ?\text{ g C} \qquad \text{(for chlorophyll a only)}$$

A mole-to-mole ratio is the tool to use in problems that convert the moles of one substance into the moles of another. The formula of chlorophyll a, $C_{55}H_{72}MgN_4O_5$, relates Mg to C within the compound. We use the formula's subscripts as the tool we need to establish the relationship between moles of Mg and moles of C.

$$1 \text{ mol Mg} \Leftrightarrow 55 \text{ mol C}$$

We know we'll need to use this relationship to solve the problem. Let's drop it into the middle of our calculation sequence:

$$0.0011 \text{ g Mg} \longrightarrow \text{mol Mg} \xrightarrow{\boxed{1 \text{ mol Mg} \Leftrightarrow 55 \text{ mol C}}} \text{mol C} \longrightarrow ?\text{ g C}$$

By placing this tool between our given information (0.0011 g Mg) and our desired units (g C) sequence, we've cut a difficult problem into two simpler ones. All we have to do now to complete the conversion of units is relate grams of Mg to moles of Mg, and moles of C to grams of C. The atomic mass of C links moles of C to grams of C, and the atomic mass of Mg links moles of Mg to grams of Mg. Rounding them to three significant figures, we can write

$$1 \text{ mol Mg} = 24.3 \text{ g Mg}$$
$$1 \text{ mol C} = 12.0 \text{ g C}$$

Our complete sequence for the problem is

$$0.0011 \text{ g Mg} \xrightarrow{\boxed{1 \text{ mol Mg} = 24.31 \text{ g Mg}}} \text{mol Mg} \xrightarrow{\boxed{1 \text{ mol Mg} \Leftrightarrow 55 \text{ mol C}}} \text{mol C} \xrightarrow{\boxed{1 \text{ mol C} = 12.0 \text{ g C}}} \text{g C}$$

SOLUTION: We now set up the solution by forming conversion factors so the units cancel:

$$0.0011 \cancel{\text{g Mg}} \times \left(\frac{1 \cancel{\text{mol Mg}}}{24.3 \cancel{\text{g Mg}}}\right) \times \left(\frac{55 \cancel{\text{mol C}}}{1 \cancel{\text{mol Mg}}}\right) \times \left(\frac{12.0 \text{ g C}}{1 \cancel{\text{mol C}}}\right) = 0.030 \text{ g C}$$

A plant cell must supply 0.030 g C for every 0.0011 g Mg to completely use up the magnesium in the synthesis of chlorophyll a.

IS THE ANSWER REASONABLE? After checking that our units cancel properly, a quick estimate of the answer can be made by rounding all numbers to one significant figure. One way to do this results in the following expression (without units):

$$\frac{0.001 \times 1 \times 50 \times 10}{20 \times 1 \times 1} = \frac{0.5}{20} = \frac{0.05}{2} = 0.025$$

This value is close to the answer we got and gives us confidence that it is correct. (Note that if we rounded the 55 up to 60 our estimate would have been 0.030, which would still confirm our conclusion.)

Our answer was 0.030 g C from 0.0011 g Mg, so the mass of carbon we obtained is about 30 times the mass of the magnesium we started with. This seems reasonable because there are 55 times as many C atoms as Mg but a Mg atom weighs twice as much as a carbon atom.

Practice Exercise 7: How many grams of iron are needed to combine with 25.6 g of O to make Fe_2O_3? (Hint: Determine the mole ratios that the formula provides.)

Practice Exercise 8: An important iron ore called hematite contains iron(III) oxide. How many grams of iron are in a 15.0 g sample of hematite?

Practice Exercise 9: How many grams of iron will combine with 12.0 g of oxygen to form iron(III) oxide? Hematite, mentioned above, is often highly polished and used as a semiprecious gemstone.

3.3 Chemical formulas can be determined from experimental mass measurements

In pharmaceutical research, chemists often synthesize entirely new compounds, or isolate new compounds from plant and animal tissues. They must then determine the formula and structure of the new compound. This is usually accomplished using mass spectroscopy, which gives an experimental value for the molecular mass. The compound can also be decomposed chemically to find the masses of elements within a given amount of compound. Let's see how experimental mass measurements can be used to determine a compound's formula.

Percentage composition describes the relative masses of the elements in a compound

The usual form for describing the relative masses of the elements in a compound is a list of *percentages by mass* called the compound's **percentage composition.** The **percentage by mass** of an element is the number of grams of the element present in 100 g of the compound. In general, a percentage by mass is found by using the following equation.

TOOLS
Percentage composition

$$\%\text{ by mass of element} = \frac{\text{mass of element}}{\text{mass of whole sample}} \times 100\% \qquad (3.1)$$

EXAMPLE 3.7
Calculating a Percentage Composition from Chemical Analysis

A sample of a liquid with a mass of 8.657 g was decomposed into its elements and gave 5.217 g of carbon, 0.9620 g of hydrogen, and 2.478 g of oxygen. What is the percentage composition of this compound?

ANALYSIS: We must use the tool expressed in Equation 3.1 and apply it to each element. The "mass of whole sample" here is 8.657 g, so we take each element in turn and perform the calculations.

SOLUTION:

$$\text{For C:} \quad \frac{5.217 \text{ g C}}{8.657 \text{ g sample}} \times 100\% = 60.26\% \text{ C}$$

$$\text{For H:} \quad \frac{0.9620 \text{ g H}}{8.657 \text{ g sample}} \times 100\% = 11.11\% \text{ H}$$

$$\text{For O:} \quad \frac{2.478 \text{ g O}}{8.657 \text{ g sample}} \times 100\% = \underline{28.62\% \text{ O}}$$

$$\text{Sum of percentages:} \quad 99.99\%$$

One of the useful things about a percentage composition is that it tells us the mass of each of the elements in 100 g of the substance. For example, the results in this problem tell us that in 100.00 g of the liquid there are 60.26 g of carbon, 11.11 g of hydrogen, and 28.62 g of oxygen.

IS THE ANSWER REASONABLE? The "check" is that the percentages must add up to 100%, allowing for small differences caused by rounding. We can also check the individual results by rounding all the numbers to one significant figure to estimate the results. For example, the percentage C would be estimated as $5/9 \times 100$, which is a little over 50% and agrees with our answer.

Practice Exercise 10: An organic compound weighing 0.6672 g is decomposed giving 0.3481 g carbon and 0.0870 g hydrogen. What are the percentages of hydrogen and carbon in this compound? Is it likely that this compound contains another element? (Hint: Recall the tool concerning the conservation of mass.)

Practice Exercise 11: From 0.5462 g of a compound there was isolated 0.2012 g of nitrogen and 0.3450 g of oxygen. What is the percentage composition of this compound? Are any other elements present?

Experimental percentage compositions can help identify an unknown compound

Elements can combine in many different ways. Nitrogen and oxygen, for example, form all of the following compounds: N_2O, NO, NO_2, N_2O_3, N_2O_4, and N_2O_5. To identify an unknown sample of a compound of nitrogen and oxygen, one might compare the percentage composition found by experiment with the calculated, or theoretical, percentages for each possible formula. Which formula, for example, fits the percentage composition calculated in Practice Exercise 11? A strategy for matching empirical formulas with mass percentages is outlined in the following example.

EXAMPLE 3.8
Calculating a Theoretical Percentage Composition from a Chemical Formula

Do the mass percentages of 25.94% N and 74.06% O match the formula N_2O_5?

ANALYSIS: To calculate the theoretical percentages by mass of N and O in N_2O_5, we need the masses of N and O in a specific sample of N_2O_5. *If we choose 1 mol of the given compound to be this sample, calculating the percentages will be simple using the tool in Equation 3.1.*

SOLUTION: We know that 1 mol of N_2O_5 must contain 2 mol N and 5 mol O. The corresponding number of grams of N and O are found as follows.

$$2\text{ N:} \quad 2 \cancel{\text{mol N}} \times \frac{14.01 \text{ g N}}{1 \cancel{\text{mol N}}} = 28.02 \text{ g N}$$

$$5\text{ O:} \quad 5 \cancel{\text{mol O}} \times \frac{16.00 \text{ g O}}{1 \cancel{\text{mol O}}} = \underline{80.00 \text{ g O}}$$

$$1 \text{ mol } N_2O_5 = 108.02 \text{ g } N_2O_5$$

Now we can calculate the percentages.

$$\text{For \% N:} \quad \frac{28.02 \text{ g N}}{108.02 \text{ g sample}} \times 100\% = 25.94\% \text{ N in } N_2O_5$$

$$\text{For \% O:} \quad \frac{80.00 \text{ g O}}{108.02 \text{ g sample}} \times 100\% = 74.06\% \text{ O in } N_2O_5$$

Thus the experimental values do match the theoretical percentages for the formula N_2O_5.

IS THE ANSWER REASONABLE? We can easily check our math. Since the denominator in each fraction is close to 100, the numerator is a simple estimate of the percentage. For nitrogen the numerator of 28 compares well to our 25.94% answer to satisfy us that the calculation was done correctly.

Practice Exercise 12: Calculate the theoretical percentage composition of N_2O_4. (Hint: Recall the definition of percentage composition.)

Practice Exercise 13: Calculate the theoretical percentage compositions for N_2O, NO, NO_2, N_2O_3, N_2O_4, and N_2O_5. Which of these compounds produced the data in Practice Exercise 11?

An empirical formula can be determined from the masses of the different elements in a sample of a compound

The compound that forms when phosphorus burns in oxygen consists of molecules with the formula P_4O_{10}. When a formula gives the composition of one *molecule*, it is called a **molecular formula.** Notice, however, that both the subscripts 4 and 10 are divisible by 2, so the *smallest* numbers that tell us the *ratio* of P to O are 2 and 5. We can write a simpler (but less informative) formula that expresses this ratio, P_2O_5. This is called the **empirical formula** because it can be obtained from an experimental analysis of the compound.

TOOLS
Empirical formula

The empirical formula expresses the simplest whole number ratio of the atoms of each element in a compound.

We already know that the ratio of atoms in a compound is the same as a ratio of the moles of those atoms in the compound. We will determine the simplest ratio of moles from experimental data. The experimental data we need is any information that allows us to determine the moles of each element in the compound. We will investigate three types of data that can be used to determine empirical formulas. They are (a) masses of the elements, (b) percentage composition, and (c) combustion data. In all three, the goal is to obtain the simplest ratio of moles of each element in the formula.

The next four examples illustrate how we can calculate empirical formulas. We will then look at what additional data are required to obtain a compound's molecular formula.

EXAMPLE 3.9
Calculating an Empirical Formula from Mass Data

A 2.57 g sample of a compound composed of only tin and chlorine was found to contain 1.17 g of tin. What is the compound's empirical formula?

ANALYSIS: The subscripts in an empirical formula give the relative number of moles of elements in a compound. If we can find the *mole* ratio of Sn to Cl, we will have the empirical formula. The first step, therefore, is to convert the numbers of grams of Sn and Cl to the numbers of moles of Sn and Cl using the tool that relates mass to moles. Then we convert these numbers into their simplest *whole-number* ratio.

The problem did not give the mass of chlorine in the 2.57 g sample. But there are only two elements present in the compound, tin and chlorine. We know the mass of the tin, and we know the total mass of compound. The law of conservation of mass, one of our tools from the previous chapter, requires that the mass of Cl is the difference between 2.57 g of compound and 1.17 g of Sn.

SOLUTION: First, we find the mass of Cl in 2.57 g of compound:

$$\text{Mass of Cl} = 2.57 \text{ g compound} - 1.17 \text{ g Sn} = 1.40 \text{ g Cl}$$

Now we use the atomic masses to convert the mass data for tin and chlorine into moles.

$$1.17 \cancel{\text{g Sn}} \times \frac{1 \text{ mol Sn}}{118.71 \cancel{\text{g Sn}}} = 0.00986 \text{ mol Sn}$$

$$1.40 \cancel{\text{g Cl}} \times \frac{1 \text{ mol Cl}}{35.45 \cancel{\text{g Cl}}} = 0.0395 \text{ mol Cl}$$

We could now write a formula: $Sn_{0.00986}Cl_{0.0395}$, which does express the mole ratio, but subscripts also represent atom ratios and need to be integers. To convert the decimal subscripts to integers we begin by dividing each by the smallest number in the set. *This is always the way to begin the search for whole-number subscripts; pick the smallest number of the set as the divisor.* It's guaranteed to make at least one subscript a whole number, namely, 1. Here, we divide both numbers by 0.00986.

$$Sn_{\frac{0.00986}{0.00986}}Cl_{\frac{0.0395}{0.00986}} = Sn_{1.00}Cl_{4.01}$$

We may round 4.01 to 4, because even if the third significant digit is uncertain, we do know the second significant digit, the zero, with certainty; so the empirical formula is $SnCl_4$.

IS THE ANSWER REASONABLE? If $SnCl_4$ is the right formula, one mole of the compound contains 118.7 grams of tin and 142 grams of chlorine, or a little more chlorine than tin. The statement of the problem also gives us slightly more chlorine than tin. You should also recall from Chapter 2 that tin forms either the Sn^{2+} or the Sn^{4+} ion and that chlorine forms only the Cl^- ion. Therefore either $SnCl_2$ or $SnCl_4$ are reasonable compounds and one of them was our answer.

We cannot forget that we now have a storehouse of reasonable chemical formulas that were developed in Chapter 2.

Practice Exercise 14: A 1.525 g sample of a compound between nitrogen and oxygen contains 0.712 g of nitrogen. Calculate its empirical formula. (Hint: How many grams of oxygen are there?)

Practice Exercise 15: A 1.525 g sample of a compound between sulfur and oxygen was prepared by burning 0.7625 g of sulfur in air and collecting the product. What is the empirical formula for the compound formed?

Sometimes our strategy of using the lowest common divisor does not give whole numbers. Let's see how to handle such a situation.

EXAMPLE 3.10

Calculating an Empirical Formula from Mass Composition

One of the compounds of iron and oxygen, "black iron oxide," occurs naturally in the mineral magnetite. When a 2.448 g sample was analyzed it was found to have 1.771 g of Fe. Calculate the empirical formula of this compound.

ANALYSIS: To calculate the empirical formula, we need to know the masses of both iron and oxygen, but we've only been given the mass of iron. We use the law of conservation of mass as a tool (page 36) to calculate the mass of oxygen. Next we will use our tools for converting masses to moles, recalling that one mole of an element is equal to its atomic mass in gram units.

The mineral magnetite, like any magnet, is able to affect the orientation of a compass needle. *(Paul Silverman/Fundamental Photographs.)*

Then we'll write a trial formula and see whether we can adjust the subscripts to their smallest whole numbers by the strategy learned in Example 3.9.

SOLUTION: The mass of O is, as we said, found by difference.

$$2.448 \text{ g compound} - 1.771 \text{ g Fe} = 0.677 \text{ g O}$$

The moles of Fe and O in the sample can now be calculated.

$$1.771 \cancel{\text{g Fe}} \times \frac{1 \text{ mol Fe}}{55.845 \cancel{\text{g Fe}}} = 0.03171 \text{ mol Fe}$$

$$0.677 \cancel{\text{g O}} \times \frac{1 \text{ mol O}}{16.00 \cancel{\text{g O}}} = 0.0423 \text{ mol O}$$

These results let us write the formula as $Fe_{0.03171}O_{0.0423}$.

Our first effort to change the ratio of 0.03171 to 0.0423 into whole numbers is to divide both by the smaller, 0.03171.

$$Fe_{\frac{0.03171}{0.03171}}O_{\frac{0.0423}{0.03171}} = Fe_{1.000}O_{1.33}$$

This time we cannot round 1.33 to 1.0. The subscript for oxygen has three significant figures, so we can be sure that the digits 1.3 in 1.33 are known with certainty. Therefore the subscript for O, 1.33, is much too far from a whole number to round off and retain the required precision. In a *mole* sense, the ratio of 1 to 1.33 is correct; we just need a way to restate this ratio in whole numbers. Let's look at a simple strategy that will give us whole-number subscripts.

TOOLS Techniques for finding whole-number subscripts for empirical formulas

Trial and error is an easy way to obtain integer subscripts. We try multiplying the subscripts by 2, then 3, 4, 5, 6, and so on. The lowest multiplier that results in integer subscripts is the correct one to use. For example, let's multiply each subscript in $Fe_{1.000}\,O_{1.33}$ by a whole number, 2. *Since we multiply all subscripts by 2 we do not change the ratio*; it changes only the size of the numbers used to state it.

$$Fe_{(1.000 \times 2)}O_{(1.33 \times 2)} = Fe_{2.000}O_{2.66}$$

This didn't work either; 2.66 is also too far from a whole number (based on the allowed precision) to be rounded off. Let's try using 3 instead of 2 *on the original ratio of 1.000 to 1.33.*

$$Fe_{(1.000 \times 3)}O_{(1.33 \times 3)} = Fe_{3.000}O_{3.99}$$

We are now justified in rounding; 3.99 is acceptably close to 4. The empirical formula of the oxide of iron is Fe_3O_4. A different method is noted in the margin, where Table 3.1 shows us which whole number multiplier should be used to convert a decimal that cannot be rounded to a whole number.

TABLE 3.1

Decimal Numbers and Their Rational Fractions

Decimal	Fraction[a]
0.20	1/5
0.25	1/4
0.33	1/3
0.40	2/5
0.50	1/2
0.60	3/5
0.66	2/3
0.75	3/4
0.80	4/5

[a]Use the denominator of the fraction as a multiplier to create whole-number subscripts in empirical formulas.

IS THE ANSWER REASONABLE? First, the fact that our calculation gives whole number subscripts is a good indicator that we've solved the problem correctly. Second, another way to check our answer is to estimate the percentage of iron from the given data and from our result. The given data are 1.771 g Fe and 2.448 g of sample and the percentage iron is estimated as

$$\frac{1.771 \text{ g}}{2.448 \text{ g}} \times 100 \approx \frac{\mathbf{1.8\ g}}{\mathbf{2.4\ g}} \times \mathbf{100} = \frac{3}{4} \times 100 = \text{approximately } 75\%$$

In one mole of the compound Fe_3O_4, the mass of iron is $3 \times 55.8 = 167.4$ and the molar mass is 231.4. The percentage of iron is estimated as

$$\frac{167.4 \text{ g}}{231.4 \text{ g}} \times 100 \approx \frac{170 \text{ g}}{230 \text{ g}} \times 100 = \frac{\mathbf{1.7\ g}}{\mathbf{2.3\ g}} \times \mathbf{100} = \text{approximately } 75\%$$

We don't have to do any calculations because we can see that mathematical expressions from both calculations are almost the same, and the answers will be very close to each other. Let's compare the bold term from each equation,

$$\frac{1.8\text{ g}}{2.4\text{ g}} \times 100 \approx \frac{1.7\text{ g}}{2.3\text{ g}} \times 100$$

We are able to conclude that our percentages of iron are the same and our empirical formula is reasonable.

Practice Exercise 16: When aluminum is produced on an industrial scale 5.68 tons of aluminum and 5.04 tons of oxygen are obtained. What is the empirical formula of the compound used to produce aluminum? (Hint: 1 ton = 2000 lb and 1 lb = 454 g.)

Practice Exercise 17: A 2.012 g sample of a compound of nitrogen and oxygen has 0.522 g of nitrogen. Calculate its empirical formula.

Empirical formulas can be determined from mass percentages

Only rarely is it possible to obtain the masses of every element in a compound by the use of just one weighed sample. Two or more analyses carried out on different samples are often needed. For example, suppose an analyst is given a compound known to consist exclusively of calcium, chlorine, and oxygen. The mass of calcium in one weighed sample and the mass of chlorine in another sample would be determined in separate experiments. Then the mass data for calcium and chlorine would be converted to percentages by mass *so that the data from different samples relate to the same sample size, namely, 100 g of the compound.* The percentage of oxygen would be calculated by difference because % Ca + % Cl + % O = 100%. Each mass percentage represents a certain number of grams of the element, which is next converted into the corresponding number of moles of the element. The mole proportions are converted to whole numbers in the way we just studied, giving us the subscripts for the empirical formula. Let's see how this works.

TOOLS

Percentage composition helps to correlate results from different experiments

EXAMPLE 3.11

Calculating an Empirical Formula from Percentage Composition

A white powder used in paints, enamels, and ceramics has the following percentage composition: Ba, 69.6%; C, 6.09%; and O, 24.3%. What is its empirical formula? What is the name of this compound?

ANALYSIS: Consider having 100 grams of this compound. The percentages of the elements given in the problem are numerically the same as the masses of these elements in our 100 g sample. We see a general principle that by assuming a 100 g sample, all percent signs can be changed to gram units. Now that we have the masses of the elements we can use the procedures and tools used in Examples 3.9 and 3.10.

SOLUTION: Assuming a 100 g sample of the compound we quickly convert 69.6% Ba to 69.6 g Ba, 6.09% C to 6.09 g C, and 24.3% O to 24.3 g O. Now we convert these to moles.

$$\text{Ba:}\quad 69.6\ \cancel{\text{g Ba}} \times \frac{1\text{ mol Ba}}{137.33\ \cancel{\text{g Ba}}} = 0.507\text{ mol Ba}$$

$$\text{C:}\quad 6.09\ \cancel{\text{g C}} \times \frac{1\text{ mol C}}{12.01\ \cancel{\text{g C}}} = 0.507\text{ mol C}$$

$$\text{O:}\quad 24.3\ \cancel{\text{g O}} \times \frac{1\text{ mol O}}{16.00\ \cancel{\text{g O}}} = 1.52\text{ mol O}$$

Our preliminary empirical formula is then

$$Ba_{0.507}C_{0.507}O_{1.52}$$

We next divide each subscript by the smallest, 0.507.

$$Ba_{\frac{0.507}{0.507}}C_{\frac{0.507}{0.507}}O_{\frac{1.52}{0.507}} = Ba_{1.00}C_{1.00}O_{3.00}$$

The subscripts are whole numbers, so the empirical formula is $BaCO_3$, representing barium carbonate.

IS THE ANSWER REASONABLE? The fact that our calculations led to whole number subscripts is a strong clue that the answer is correct. In addition, our knowledge of ionic compounds and the polyatomic carbonate ion from Chapter 2 tell us that the barium ion is Ba^{2+} and the carbonate ion is CO_3^{2-}; $BaCO_3$ is a reasonable formula.

Practice Exercise 18: A white solid used to whiten paper has the following percentage composition: Na, 32.4%; S, 22.6%. The unanalyzed element is oxygen. What is the compound's empirical formula? (Hint: What law allows you to calculate the % oxygen?)

Practice Exercise 19: Cinnamon gets some of its flavor from cinnamaldehyde that is 81.79% C, 6.10% H, and the rest oxygen. Determine the empirical formula for this compound.

Percentage composition is important since it allowed us to determine the amount of three substances using only two experiments. This in itself is a considerable saving in time and effort. Additionally, it is often difficult to analyze a sample for certain elements, oxygen for example, and using percentage measurements helps avoid this problem.

Empirical formulas can be determined from indirect analyses

In practice, a compound is seldom broken down completely to its *elements* in a quantitative analysis. Instead, the compound is changed into other *compounds*. The reactions separate the elements by capturing each one entirely (quantitatively) in a *separate* compound *whose formula is known*.

In the following example, we illustrate the indirect analysis of a compound made entirely of carbon, hydrogen, and oxygen. Such compounds burn completely in pure oxygen—it is called a *combustion reaction*—and the sole products are carbon dioxide and water. (This particular kind of indirect analysis is sometimes called a *combustion analysis*.) The complete combustion of methyl alcohol (CH_3OH), for example, occurs according to the following equation.

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

Organic compounds react with a stream of pure oxygen to give CO_2 and H_2O. The flowing gases pass through a preweighed tube of $CaSO_4$ to absorb the water and then through a tube of NaOH deposited on a binder to absorb the carbon dioxide. The increase in mass of the $CaSO_4$ and NaOH tubes represents the mass of water and CO_2, respectively.

The carbon dioxide and water can be separated and are individually weighed. Notice that all of the carbon atoms in the original compound end up among the CO_2 molecules, and all of the hydrogen atoms are in H_2O molecules. In this way at least two of the original elements, C and H, are quantitatively measured.

We will calculate the mass of carbon in the CO_2 collected, which equals the mass of carbon in the original sample. Similarly, we will calculate the mass of hydrogen in the H_2O collected, which equals the mass of hydrogen in the original sample. When added together, the mass of C and mass of H are less than the total mass of the sample because part of the sample is composed of oxygen. The law of conservation of mass allows us to subtract the sum of the C and H masses from the original sample mass to obtain the mass of oxygen in the sample of the compound.

EXAMPLE 3.12
Empirical Formula from Indirect Analysis

A 0.5438 g sample of a liquid consisting of only C, H, and O was burned in pure oxygen, and 1.039 g of CO_2 and 0.6369 g of H_2O were obtained. What is the empirical formula of the compound?

ANALYSIS: There are two parts to this problem. First we need to calculate the mass of the elements, C and H, by determining the number of grams of C in the CO_2 and the number of grams of H in the H_2O. (This kind of calculation was illustrated in Example 3.6 and uses the tools that tell us how to create conversion factors from grams to moles and from moles of one substance to moles of another.) These values represent the number of grams of C and H in the original sample. Adding them together and subtracting the sum from the mass of the original sample will give us the mass of oxygen in the sample.

In the second half of the solution, we use the masses of C, H, and O to calculate the empirical formula as in Example 3.9.

SOLUTION: First we find the number of grams of C in the CO_2 and of H in the H_2O. We use the normal conversion sequence from grams of compound, to moles of compound, to moles of element, and then to grams of element as shown in the next two equations.

$$1.039\ \cancel{\text{g CO}_2} \times \frac{1\ \cancel{\text{mol CO}_2}}{44.009\ \cancel{\text{g CO}_2}} \times \frac{1\ \cancel{\text{mol C}}}{1\ \cancel{\text{mol CO}_2}} \times \frac{12.011\ \text{g C}}{1\ \cancel{\text{mol C}}} = 0.2836\ \text{g C}$$

$$0.6369\ \cancel{\text{g H}_2\text{O}} \times \frac{1\ \cancel{\text{mol H}_2\text{O}}}{18.015\ \cancel{\text{g H}_2\text{O}}} \times \frac{2\ \cancel{\text{mol H}}}{1\ \cancel{\text{mol H}_2\text{O}}} \times \frac{1.0079\ \text{g H}}{1\ \cancel{\text{mol H}}} = 0.07125\ \text{g H}$$

The total mass of C and H is therefore the sum of these two quantities.

$$\text{Total mass of C and H} = 0.2836\ \text{g C} + 0.07125\ \text{g H} = 0.3548\ \text{g}$$

The difference between this total and the 0.5438 g in the original sample is the mass of oxygen (the only other element).

$$\text{Mass of O} = 0.5438\ \text{g} - 0.3548\ \text{g} = 0.1890\ \text{g O}$$

Now we can convert the masses of the elements to an empirical formula.

$$\text{For C:}\quad 0.2836\ \cancel{\text{g C}} \times \frac{1\ \text{mol C}}{12.011\ \cancel{\text{g C}}} = 0.02361\ \text{mol C}$$

$$\text{For H:}\quad 0.07125\ \cancel{\text{g H}} \times \frac{1\ \text{mol H}}{1.0079\ \cancel{\text{g H}}} = 0.07068\ \text{mol H}$$

$$\text{For O:}\quad 0.1890\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{15.999\ \cancel{\text{g O}}} = 0.01181\ \text{mol O}$$

Our preliminary empirical formula is thus $C_{0.02361}H_{0.07068}O_{0.01181}$. We divide all of these subscripts by the smallest number, 0.01181.

$$C_{\frac{0.02361}{0.01181}}H_{\frac{0.07068}{0.01181}}O_{\frac{0.01181}{0.01181}} = C_{1.998}H_{5.985}O_1$$

The results are acceptably close to integers to say that the empirical formula is C_2H_6O.

IS THE ANSWER REASONABLE? Our checks on problems need to be quick and efficient. In previous examples we have been able to use our knowledge of ionic compounds to see if formulas are reasonable. In the future, with some knowledge of organic chemistry you will know that the formula C_2H_6O is reasonable. Beyond that, the fact that we obtained whole number subscripts after all these calculations is also a good indicator that we've solved the problem correctly.

Practice Exercise 20: A sample containing only sulfur and carbon is completely burned in air. The analysis produced 0.640 g SO_2 and 0.220 g of CO_2. What is the empirical formula? (Hint: Use the tools for relating grams of a compound to grams of an element.)

Practice Exercise 21: The combustion of a 5.048 g sample of a compound of C, H, and O gave 7.406 g CO_2 and 3.027 g H_2O. Calculate the empirical formula of the compound.

As we said earlier, more than one sample of a substance must be analyzed whenever more than one reaction is necessary to separate the elements. This is also true in indirect analyses. For example, if a compound contains C, H, N, and O, combustion converts the C and H to CO_2 and H_2O, which are separated by special techniques and weighed. The mass of C in the CO_2 sample and the mass of H in the H_2O sample are then calculated in the usual way. A second reaction with a different sample of the compound can be used to obtain the nitrogen, either as N_2 or as NH_3. Because different size samples are used, the masses of C and H from one sample and the mass of N from another cannot be used to calculate the empirical formula. So we convert the masses of the elements found in their respective samples into percentages of the element by mass in the compound. We add up the percentages, subtract from 100 to get the percentage of O, and then calculate the empirical formula from the percentage composition as described earlier.

Molecular formulas are determined from empirical formulas and molecular masses

The empirical formula is the accepted formula unit for ionic compounds. For molecular compounds, however, chemists prefer *molecular* formulas because they give the number of atoms of each type in a molecule.

Sometimes an empirical formula and a molecular formula are the same. Two examples are H_2O and NH_3. Usually, however, the subscripts of a molecular formula are whole-number multiples of those in the empirical formula. The subscripts of the molecular formula P_4O_{10}, for example, are each two times those in the empirical formula, P_2O_5, as you saw earlier. The molecular mass of P_4O_{10} is likewise two times the formula mass of P_2O_5. This observation provides us with a way to find out the molecular formula for a compound provided we have a way of determining experimentally the molecular mass of the compound. If the experimental molecular mass *equals* the calculated empirical formula mass, the empirical formula itself is also a molecular formula. Otherwise, the experimental molecular mass will be some whole-number multiple of the value calculated from the empirical formula. Whatever the whole number is, it's a common multiplier for the subscripts of the empirical formula.

Molecular masses can sometimes be obtained using mass spectroscopy, discussed in Chapter 1. Other methods will be discussed in Chapters 10, 11, and 12.

EXAMPLE 3.13
Determining a Molecular Formula from an Empirical Formula and a Molecular Mass

Styrene, the raw material for polystyrene foam plastics, has an empirical formula of CH. Its molecular mass is 104 g mol^{-1}. What is its molecular formula?

ANALYSIS: The molecular mass of styrene, 104 g mol^{-1}, is some simple multiple of the formula mass of the empirical formula, CH. When we compute that multiple it will tell us how many CH units make up the styrene molecule. We can compute this multiple by dividing the molecular mass by the empirical formula mass.

SOLUTION: For the empirical formula, CH, the formula mass is

$$12.01 + 1.008 = 13.02$$

To find how many CH units weighing 13.02 are in a mass of 104, we divide.

$$\frac{104}{13.02} = 7.99$$

Rounding this to 8, we see that 104 is 8 times larger than 13.02, so the correct molecular formula of styrene must have subscripts 8 times those in CH. Styrene, therefore, is C_8H_8.

IS THE ANSWER REASONABLE? The molecular mass of C_8H_8 is approximately $(8 \times 12) + (8 \times 1) = 104$ g mol^{-1}, which is consistent with the molecular mass we started with.

Practice Exercise 22: After determining that the empirical formulas of two different compounds were CH_2Cl and CHCl a student mixed up the data for the molecular masses. However, the student knew that one compound had a molecular mass of 100 and the other had a molecular mass of 289 g mol^{-1}. What are the likely molecular formulas of the two compounds? (Hint: Recall the relationship between the molecular and empirical formula.)

Practice Exercise 23: The empirical formula of hydrazine is NH_2, and its molecular mass is 32.0 g mol^{-1}. What is its molecular formula?

3.4 CHEMICAL EQUATIONS LINK AMOUNTS OF SUBSTANCES IN A REACTION

Balancing an equation involves adjusting coefficients

We learned in Chapter 2 that a *chemical equation* is a shorthand, quantitative description of a chemical reaction. An equation is *balanced* when all atoms present among the reactants are also somewhere among the products. As we learned, coefficients, the numbers in front of formulas, are multiplier numbers for their respective formulas, and the values of the coefficients determine whether an equation is balanced.

Always approach the balancing of an equation as a two-step process.

Step 1. *Write the unbalanced "equation."* Organize the formulas in the pattern of an equation with plus signs and an arrow. Use *correct* formulas. (You learned to write many of them in Chapter 2, but until we have studied more chemistry, you will usually be given formulas.)

Step 2. *Adjust the coefficients to get equal numbers of each kind of atom on both sides of the arrow.* When doing step 2, make no changes in the formulas, either in the atomic symbols or their subscripts. If you do, the equation will involve different substances from those intended. You may still be able to balance it, but the equation will not be for the reaction you want.

We'll begin with simple equations that can be balanced easily by inspection. An example is the reaction of zinc metal with hydrochloric acid (margin photo). First, we need the correct formulas, and this time we'll include the physical states because they are different. The reactants are zinc, Zn(*s*), and hydrochloric acid, an aqueous solution of the gas hydrogen chloride, HCl, symbolized as HCl(*aq*). We also need formulas for the products. Zn changes to a water-soluble compound, zinc chloride, $ZnCl_2(aq)$, and hydrogen gas, $H_2(g)$, bubbles out as the other product. (Recall that hydrogen occurs naturally as a *diatomic molecule*, not as an atom.)

Zinc metal reacts with hydrochloric acid. *(Richard Megna/Fundamental Photographs.)*

Step 1. Write an unbalanced equation.

$$\mathrm{Zn}(s) + \mathrm{HCl}(aq) \longrightarrow \mathrm{ZnCl_2}(aq) + \mathrm{H_2}(g) \qquad \text{(unbalanced)}$$

Step 2. Adjust the coefficients to get equal numbers of each kind of atom on both sides of the arrow.

There is no simple set of rules for adjusting coefficients. Experience is the greatest help, and experience has taught chemists that the following guidelines often get to the solution most directly when they are applied in the order given.

TOOLS

Guidelines for balancing chemical equations

Some Guidelines for Balancing Equations

1. Balance elements other than H and O first.
2. Elements should be balanced last (e.g., Zn and H_2 in our example).
3. Balance as a group those polyatomic ions that appear unchanged on both sides of the arrow.

Using the guidelines given here, we'll look at Cl first in our example. Because there are two Cl to the right of the arrow but only one to the left, we put a 2 in front of the HCl on the left side. The result is

$$\mathrm{Zn}(s) + 2\mathrm{HCl}(aq) \longrightarrow \mathrm{ZnCl_2}(aq) + \mathrm{H_2}(g)$$

We then balance the hydrogen and zinc and find that no additional coefficient changes are needed. Everything is now balanced. On each side we find 1 Zn, 2 H, and 2 Cl. One complication is that an infinite number of *balanced* equations can be written for any given reaction! We might, for example, have adjusted the coefficients so that our equation came out as follows.

$$2\mathrm{Zn}(s) + 4\mathrm{HCl}(aq) \longrightarrow 2\mathrm{ZnCl_2}(aq) + 2\mathrm{H_2}(g)$$

This equation is also correctly balanced. For simplicity, we prefer the *smallest* whole-number coefficients when writing balanced equations.

EXAMPLE 3.14

Writing a Balanced Equation

Sodium hydroxide and phosphoric acid, H_3PO_4, react as aqueous solutions to give sodium phosphate and water. The sodium phosphate remains in solution. Write the balanced equation for this reaction.

ANALYSIS: First, we need to write an unbalanced equation that includes the reactant formulas on the left-hand side and the product formulas on the right. We are given the formula only for phosphoric acid. We need to use the tools in Chapter 2 to determine that sodium hydroxide is NaOH, water is H_2O, and sodium phosphate has a formula of Na_3PO_4. Next we write the unbalanced equation placing all the reactants to the left of the arrow and all products to the right. Finally we use the procedures suggested in the tool for balancing equations to adjust stoichiometric coefficients (*never change subscripts!*) until there are the same number of each type of atom on the left and right sides of the equation.

SOLUTION: We include the designation (*aq*) for all substances dissolved in water (except H_2O itself; we'll usually not give it any designation when it is in its liquid state).

$$\mathrm{NaOH}(aq) + \mathrm{H_3PO_4}(aq) \longrightarrow \mathrm{Na_3PO_4}(aq) + \mathrm{H_2O} \qquad \text{(unbalanced)}$$

There are several things not in balance, but our guidelines suggest that we work with Na first rather than with O, H, or PO_4. There are 3 Na on the right side, so we put a 3 in front of NaOH on the left, as a trial.

$$3\mathrm{NaOH}(aq) + \mathrm{H_3PO_4}(aq) \longrightarrow \mathrm{Na_3PO_4}(aq) + \mathrm{H_2O} \qquad \text{(unbalanced)}$$

Now the Na are in balance. The unit of PO_4 is balanced also. Not counting the PO_4, we have on the left 3 O and 3 H in 3NaOH plus 3 H in H_3PO_4, for a net of 3 O and 6 H on the left. On the right, in H_2O, we have 1 O and 2 H. The ratio of 3 O to 6 H on the left is equivalent to the ratio of 1 O to 2 H on the right, so we write the multiplier (coefficient) 3 in front of H_2O.

$$3NaOH(aq) + H_3PO_4(aq) \longrightarrow Na_3PO_4(aq) + 3H_2O \qquad \text{(balanced)}$$

We now have a balanced equation.

IS THE ANSWER REASONABLE? On each side we have 3 Na, 1 PO_4, 6 H, and 3 O besides those in PO_4, and since the coefficients for $H_3PO_4(aq)$ and $Na_3PO_4(aq)$ are 1 our coefficients cannot be reduced to smaller whole numbers.

Practice Exercise 24: Write the balanced chemical equation that describes what happens when a solution containing aluminum chloride is mixed with a solution containing sodium phosphate and the product of the reaction is solid aluminum phosphate and a solution of sodium chloride. (Hint: Write the correct formulas based on information in Chapter 2.)

Practice Exercise 25: When aqueous solutions of calcium chloride, $CaCl_2$, and potassium phosphate, K_3PO_4, are mixed, a reaction occurs in which solid calcium phosphate, $Ca_3(PO_4)_2$, separates from the solution. The other product is $KCl(aq)$. Write the balanced equation.

The strategy of balancing whole units of polyatomic ions, like PO_4, as a group is extremely useful. Using this method we have less atom counting to do and balancing equations is often easier.

Coefficients in a balanced equation provide mole-to-mole ratios among reactants and products

So far we have focused on relationships between elements within a single compound. We have seen that the essential conversion factor between substances within a compound is the mole-to-mole ratio obtained from the compound's formula. In this section, we'll see that the same techniques can be used to relate substances involved in a chemical reaction. The critical link between substances involved in a reaction is a mole-to-mole ratio obtained from the coefficients in the chemical equation that describes the reaction.

To see how chemical equations can be used to obtain mole-to-mole relationships, consider the equation that describes the burning of octane (C_8H_{18}) in oxygen (O_2) to give carbon dioxide and steam:

The chemical equation gives relative amounts of molecules of each type that participate in the reaction. It does *not* mean that 2 octane molecules actually collide with 25 O_2 molecules. The reaction occurs in many steps, which the chemical equation does not show.

$$2C_8H_{18}(l) + 25O_2(g) \longrightarrow 16CO_2(g) + 18H_2O(g)$$

This equation can be interpreted on a *microscopic* (molecular) scale as follows:

For every two molecules of liquid octane that react with twenty-five molecules of oxygen gas, sixteen molecules of carbon dioxide gas and eighteen molecules of steam are produced.

This statement immediately suggests many equivalence relationships that can be used to build conversion factors in stoichiometry problems:

$$2 \text{ molecules } C_8H_{18} \Leftrightarrow 25 \text{ molecules } O_2$$
$$2 \text{ molecules } C_8H_{18} \Leftrightarrow 16 \text{ molecules } CO_2$$
$$2 \text{ molecules } C_8H_{18} \Leftrightarrow 18 \text{ molecules } H_2O$$
$$25 \text{ molecules } O_2 \Leftrightarrow 16 \text{ molecules } CO_2$$
$$25 \text{ molecules } O_2 \Leftrightarrow 18 \text{ molecules } H_2O$$
$$16 \text{ molecules } CO_2 \Leftrightarrow 18 \text{ molecules } H_2O$$

Any of these microscopic relationships can be scaled up to the macroscopic level by multiplying both sides of the equivalency by Avogadro's number, which effectively allows us to replace "molecules" with "moles" or "mol":

TOOLS
Equivalencies deduced from a balanced chemical equation

$$2 \text{ mol } C_8H_{18} \Leftrightarrow 25 \text{ mol } O_2$$
$$2 \text{ mol } C_8H_{18} \Leftrightarrow 16 \text{ mol } CO_2$$
$$2 \text{ mol } C_8H_{18} \Leftrightarrow 18 \text{ mol } H_2O$$
$$25 \text{ mol } O_2 \Leftrightarrow 16 \text{ mol } CO_2$$
$$25 \text{ mol } O_2 \Leftrightarrow 18 \text{ mol } H_2O$$
$$16 \text{ mol } CO_2 \Leftrightarrow 18 \text{ mol } H_2O$$

We can interpret the equation on a macroscopic (mole) scale as follows:

Two moles of liquid octane react with twenty-five moles of oxygen gas to produce sixteen moles of carbon dioxide gas and eighteen moles of steam.

To use these equivalencies in a stoichiometry problem, the equation must be **balanced.** That means that every atom found in the reactants must also be found somewhere in the products. You must always check to see whether this is so for a given equation before you can use the coefficients in the equation to build equivalencies and conversion factors.

First, let's see how mole-to-mole relationships obtained from a balanced chemical equation can be used to convert moles of one substance to moles of another when both substances are involved in a chemical reaction.

EXAMPLE 3.15
Stoichiometry of Chemical Reactions

How many moles of sodium phosphate can be made from 0.240 mol of sodium hydroxide by the following unbalanced reaction?

$$NaOH(aq) + H_3PO_4(aq) \longrightarrow Na_3PO_4(aq) + H_2O$$

ANALYSIS: The question asks us to relate amounts of two different substances. *A mole-to-mole relationship is the tool that defines the relationship between two different substances in a stoichiometry problem.* The balanced equation is the tool to use because it gives the coefficients we need. We are given an unbalanced equation and need to balance this equation to use this tool.

$$3NaOH(aq) + H_3PO_4(aq) \longrightarrow Na_3PO_4(aq) + 3H_2O$$

From the coefficients, we now know that

$$3 \text{ mol NaOH} \Leftrightarrow 1 \text{ mol } Na_3PO_4$$

This enables us to prepare the conversion factor that we need.

SOLUTION: We write the question in equation form as

$$0.240 \text{ mol NaOH} \Leftrightarrow ? \text{ mol } Na_3PO_4$$

and convert 0.240 mol NaOH to the numbers of moles of Na_3PO_4 equivalent to it in the reaction as follows.

$$0.240 \cancel{\text{mol NaOH}} \times \frac{1 \text{ mol } Na_3PO_4}{3 \cancel{\text{mol NaOH}}} = 0.0800 \text{ mol } Na_3PO_4$$

Thus we can make 0.0800 mol Na_3PO_4 from 0.240 mol NaOH.

IS THE ANSWER REASONABLE? The equation tells us that 3 mol NaOH $\Leftrightarrow$ 1 mol Na_3PO_4, so the actual number of moles of Na_3PO_4 (0.0800 mol) should be one-third the actual number of moles of NaOH (0.240 mol), and it is. We can also check that the units cancel correctly.

Practice Exercise 26: In the reaction $2SO_2(g) + O_2(g) \longrightarrow 2SO_3(g)$ how many moles of O_2 are needed to produce 6.76 moles of SO_3? (Hint: Write the equivalence that relates O_2 to SO_3.)

Practice Exercise 27: How many moles of sulfuric acid, H_2SO_4, are needed to react with 0.366 mol of NaOH by the following reaction?

$$2NaOH(aq) + H_2SO_4(aq) \longrightarrow Na_2SO_4(aq) + 2H_2O$$

Mole-to-mole ratios link masses of different substances in chemical reactions

The most common stoichiometric calculation the chemist does is to relate grams of one substance with grams of another in a chemical reaction. For example, glucose ($C_6H_{12}O_6$) is one of the body's primary energy sources. The body combines glucose and oxygen to give carbon dioxide and water. The balanced equation for the overall reaction is

$$C_6H_{12}O_6(aq) + 6O_2(aq) \longrightarrow 6CO_2(aq) + 6H_2O(l)$$

How many grams of oxygen must the body take in to completely process 1.00 g of glucose? The problem can be expressed as

$$1.00 \text{ g } C_6H_{12}O_6 \Leftrightarrow ? \text{ g } O_2$$

The first thing we should notice about this problem is that we're relating *two different substances* in a reaction. The equivalence that relates the substances is the mole-to-mole relationship between glucose and O_2 given by the chemical equation. In this case, the equation tells us that

$$1 \text{ mol } C_6H_{12}O_6 \Leftrightarrow 6 \text{ mol } O_2$$

If we insert that mole-to-mole conversion between our starting point (1.00 g $C_6H_{12}O_6$) and the desired quantity (g O_2) we have cut the problem into three simple steps:

$$\boxed{1 \text{ mol } C_6H_{12}O_6 \Leftrightarrow 6 \text{ mol } O_2}$$

$$1.00 \text{ g } C_6H_{12}O_6 \longrightarrow \text{mol } C_6H_{12}O_6 \longrightarrow \text{mol } O_2 \longrightarrow \text{g } O_2$$

TOOLS

Sequence of steps for mass-to-mass calculations using balanced chemical equations

We convert grams of $C_6H_{12}O_6$ to moles of $C_6H_{12}O_6$ (using the molecular mass of $C_6H_{12}O_6$). We then convert mol $C_6H_{12}O_6$ to mol O_2 using the equivalence relationship from the balanced equation. Finally, we convert mol O_2 into g O_2 using the molecular mass of O_2.

Figure 3.4 outlines this flow for *any* stoichiometry problem that relates reactant or product masses. If we know the *balanced equation* for a reaction and the *mass* of any reactant or product, we can calculate the required or expected mass of *any* other substance in the equation. Example 3.16 shows how it works.

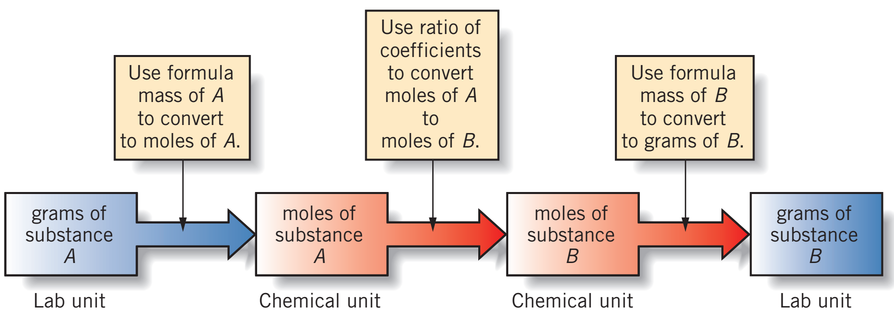


FIG. 3.4 The sequence of calculations for solving stoichiometry problems. This sequence applies to all calculations that start with the mass of one substance (*A*) and require the mass of a second substance (*B*) as the answer.

EXAMPLE 3.16
Stoichiometric Mass Calculations

Portland cement is a mixture of the oxides of calcium, aluminum, and silicon. The raw material for its calcium oxide is calcium carbonate, which occurs as the chief component of a natural rock, limestone. When calcium carbonate is strongly heated it decomposes. One product, carbon dioxide, is driven off to leave the desired calcium oxide as the only other product.

A chemistry student is to prepare 1.50×10^2 g of calcium oxide in order to test a particular "recipe" for Portland cement. How many grams of calcium carbonate should be used, assuming that all will be converted?

ANALYSIS: We begin by obtaining a balanced chemical reaction. From the nomenclature tools we find that calcium carbonate is $CaCO_3$. Using the tools from Chapter 2, the formulas for carbon dioxide and calcium oxide are CO_2 and CaO, respectively. Our balanced equation must be

$$\mathrm{CaCO_3}(s) \xrightarrow{\text{heat}} \mathrm{CaO}(s) + \mathrm{CO_2}(g)$$

Special reaction conditions are often indicated with words or symbols above the arrow. In this reaction temperatures above 2000 °C are needed and this is indicated with the word, *heat*, above the arrow.

Now we can state the problem in mathematical form as

$$1.50 \times 10^2 \text{ g CaO} \Leftrightarrow \text{? g CaCO}_3$$

In problems that convert an amount of one substance to amount of a different substance in a chemical reaction, the tool we use is a mole-to-mole conversion factor. From the balanced chemical equation, we have

$$1 \text{ mol CaO} \Leftrightarrow 1 \text{ mol CaCO}_3$$

In our road map, this is the central conversion between CaO and $CaCO_3$ as shown below.

$$\boxed{1 \text{ mol CaO} \Leftrightarrow 1 \text{ mol CaCO}_3}$$

$$1.50 \times 10^2 \text{ g CaO} \longrightarrow \text{mol CaO} \longrightarrow \text{mol CaCO}_3 \longrightarrow \text{g CaCO}_3$$

For the complete calculation we must convert g CaO to mol CaO. *The equality tool relating mass and moles uses the molar mass:*

$$56.08 \text{ g CaO} = 1 \text{ mol CaO}$$

Next, the mole ratio tool converts moles of CaO to moles of $CaCO_3$. Finally, we must also convert mol $CaCO_3$ to g $CaCO_3$. Again, the tool defining the equality between mass and moles uses the molar mass:

$$100.09 \text{ g CaCO}_3 = 1 \text{ mol CaCO}_3$$

Putting this all together, our overall strategy will be as follows.

$$\boxed{1 \text{ mol CaO} \Leftrightarrow 1 \text{ mol CaCO}_3}$$

$$1.50 \times 10^2 \text{ g CaO} \longrightarrow \text{mol CaO} \longrightarrow \text{mol CaCO}_3 \longrightarrow \text{g CaCO}_3$$

$$\boxed{56.08 \text{ g CaO} = 1 \text{ mol CaO}} \qquad \boxed{1 \text{ mol CaCO}_3 = 100.09 \text{ g CaCO}_3}$$

SOLUTION: We assemble conversion factors so the units cancel correctly:

$$1.50 \times 10^2 \cancel{\text{g CaO}} \times \left(\frac{1 \cancel{\text{mol CaO}}}{56.08 \cancel{\text{g CaO}}}\right) \times \left(\frac{1 \cancel{\text{mol CaCO}_3}}{1 \cancel{\text{mol CaO}}}\right) \times \left(\frac{100.09 \text{ g CaCO}_3}{1 \cancel{\text{mol CaCO}_3}}\right)$$
$$= 268 \text{ g CaCO}_3$$

Notice how the calculation flows from grams of CaO to moles of CaO, then to moles of $CaCO_3$ (using the equation), and finally to grams of $CaCO_3$. We cannot emphasize too much that *the key step in all calculations of reaction stoichiometry is the use of the balanced equation.*

IS THE ANSWER REASONABLE? In a mass-to-mass calculation like this the first check is the magnitude of the answer compared to the starting mass. In the majority of reactions the calculated mass is not less than 1/5 of the starting mass nor is it larger than five times the starting mass. Our result is reasonable on this criterion. We can make a more detailed check by first making sure that the units cancel properly. We can also round all numbers to one or two significant figures and estimate the answer. We would estimate $\frac{150 \times 100}{50} = 300$ and this value is close to our answer of 268, giving us confidence in the calculation. Alternately we may round the denominator to 60 instead of 50 to get an equally good estimate of 250.

EXAMPLE 3.17
Stoichiometric Mass Calculations

The thermite reaction is one of the most spectacular reactions of aluminum with iron(III) oxide by which metallic iron and aluminum oxide are made. So much heat is generated that the iron forms in the liquid state (Figure 3.5).

A certain welding operation requires at least 86.0 g of iron each time a weld is made. What is the minimum mass, in grams, of iron(III) oxide that must be used for each weld? Also calculate how many grams of aluminum are needed.

FIG. 3.5 **The thermite reaction.** Pictured here is a device for making white-hot iron by the reaction of aluminum with iron oxide and letting the molten iron run down into a mold between the ends of two steel railroad rails. The rails are thereby welded together. *(Courtesy Orgo-Thermit.)*

ANALYSIS: First we need to write a balanced chemical equation. From the information given and our nomenclature tools (Chapter 2) we determine that Al and Fe_2O_3 are the reactants and that Fe and Al_2O_3 are the products. The equation is written and then balanced to obtain

$$2\text{Al}(s) + \text{Fe}_2\text{O}_3(s) \longrightarrow \text{Al}_2\text{O}_3(s) + 2\text{Fe}(l)$$

Now, we state the problem in mathematical form:

$$86.0 \text{ g Fe} \Leftrightarrow ? \text{ g Fe}_2\text{O}_3$$

Remember that all problems in reaction stoichiometry must be solved at the mole level because an equation's coefficients disclose *mole* ratios, not mass ratios. So we use our tool that relates mass to moles to convert the number of grams of Fe to moles. Then we can use the tool that gives us the mole-to-mole relationship indicated by the coefficients in the balanced equation,

$$1 \text{ mol Fe}_2\text{O}_3 \Leftrightarrow 2 \text{ mol Fe}$$

to see how many *moles* of Fe_2O_3 are needed. Finally we use our tools to convert this answer into grams of Fe_2O_3. The other calculations follow the same pattern.

SOLUTION: We'll set up the first calculation as a chain; the steps are summarized below the conversion factors.

$$\underset{\text{grams Fe}}{86.0\ \cancel{\text{g Fe}}} \times \underset{\text{moles Fe}}{\frac{1\ \cancel{\text{mol Fe}}}{55.85\ \cancel{\text{g Fe}}}} \times \underset{\text{moles Fe}_2\text{O}_3}{\frac{1\ \cancel{\text{mol Fe}_2\text{O}_3}}{2\ \cancel{\text{mol Fe}}}} \times \underset{\text{grams Fe}_2\text{O}_3}{\frac{159.70 \text{ g Fe}_2\text{O}_3}{1\ \cancel{\text{mol Fe}_2\text{O}_3}}} = 123 \text{ g Fe}_2\text{O}_3$$

$$\text{grams Fe} \rightarrow \text{moles Fe} \rightarrow \text{moles Fe}_2\text{O}_3 \rightarrow \text{grams Fe}_2\text{O}_3$$

A minimum of 123 g of Fe_2O_3 is required to make 86.0 g of Fe.

Next, we calculate the number of grams of Al needed, but we know that we must first find the number of *moles* of Al required. Only from this can the grams of Al be calculated. The relevant mole-to-mole relationship, again using the balanced equation, is

$$2 \text{ mol Al} \Leftrightarrow 2 \text{ mol Fe}$$

▫ We could simplify the mole ratio to 1 mol Al ⇔ 1 mol Fe. Leaving the 2-to-2 ratio maintains the relationship with the balanced equation coefficients.

Employing another chain calculation to find the mass of Al needed to make 86.0 g of Fe, we have (using 26.98 as the atomic mass of Al)

$$86.0\ \cancel{\text{g Fe}} \times \frac{1\ \cancel{\text{mol Fe}}}{55.85\ \cancel{\text{g Fe}}} \times \frac{2\ \cancel{\text{mol Al}}}{2\ \cancel{\text{mol Fe}}} \times \frac{26.98 \text{ g Al}}{1\ \cancel{\text{mol Al}}} = 41.5 \text{ g Al}$$

$$\text{grams Fe} \rightarrow \text{moles Fe} \rightarrow \text{moles Al} \rightarrow \text{grams Al}$$

ARE THE ANSWERS REASONABLE? The estimate that our answers in a mass-to-mass calculation should be within 1/5 to 5 times the initial mass is true for both Al and Fe_2O_3. Rounding the numbers to one or two significant figures and estimating the answer (after rechecking that the units cancel properly) results in

$$\frac{90 \times 160}{60 \times 2} = 120 \text{ g } Fe_2O_3 \qquad \text{and} \qquad \frac{90 \times 30}{60} = 45 \text{ g Al}$$

Both estimates are close to our calculated values and give us confidence that we calculated correctly.

Practice Exercise 28: Using the information in Example 3.17 calculate the mass of Al_2O_3 formed under the conditions specified. (Hint: Recall the law of conservation of mass.)

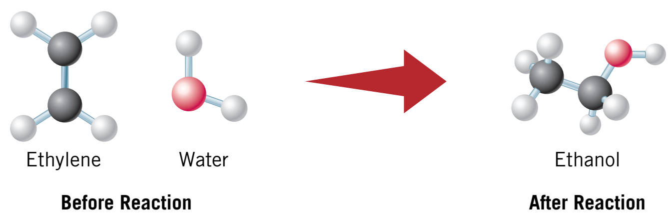
Practice Exercise 29: How many grams of carbon dioxide are also produced by the reaction described in Example 3.16?

3.5 The reactant in shortest supply limits the amount of product that can form

We've seen that balanced chemical equations can tell us how to mix reactants together in just the right proportions to get a certain amount of product. For example, ethanol, C_2H_5OH, is prepared industrially as follows:

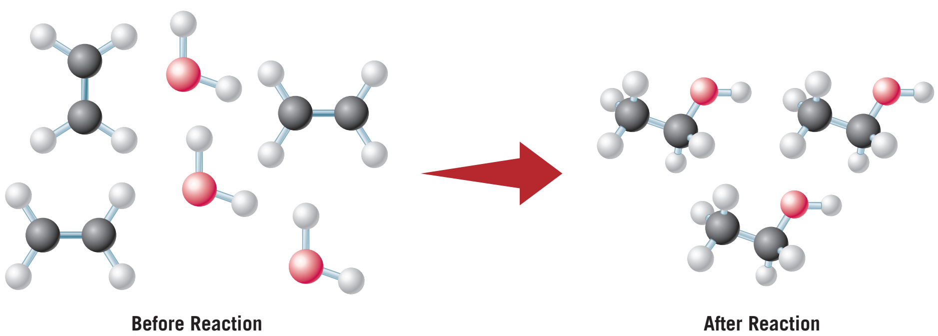
$$\underset{\text{ethylene}}{C_2H_4} + H_2O \longrightarrow \underset{\text{ethanol}}{C_2H_5OH}$$

The equation tells us that one mole of ethylene will react with one mole of water to give one mole of ethanol. We can also interpret the equation on a molecular level: Every molecule of ethylene that reacts requires one molecule of water to produce one molecule of ethanol:

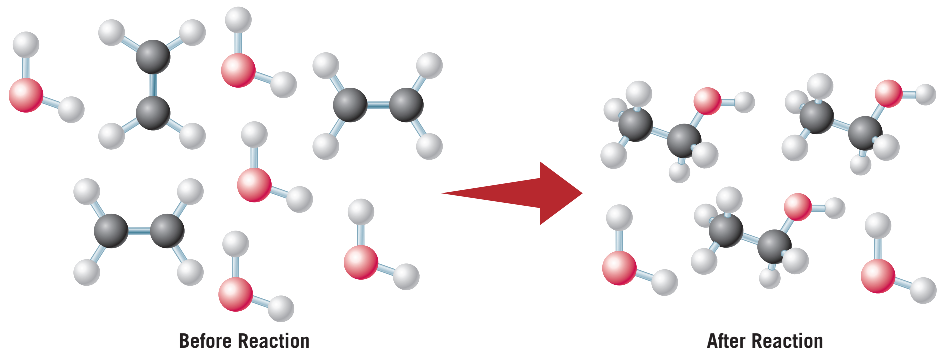


Notice that in both the "before" and "after" views of the reaction, the numbers of carbon, hydrogen, and oxygen atoms are the same.

If we have three molecules of ethylene reacting with three molecules of water, then three ethanol molecules are produced:



What happens if we mix 3 molecules of ethylene with 5 molecules of water? The ethylene will be completely used up before all the water is, and the product will contain two unreacted water molecules:



We don't have enough ethylene to use up all the water. The excess water remains after the reaction stops. This situation can be a problem in the manufacture of chemicals because not only do we waste one of our reactants (water, in this case), but we also obtain a product that is contaminated with unused reactant.

In this reaction mixture, ethylene is called the **limiting reactant** because it limits the amount of product (ethanol) that forms. The water is called an **excess reactant,** because we have more of it than is needed to completely consume all the ethylene.

TOOLS *Limiting reactants*

To predict the amount of product we'll actually obtain in a reaction, we need to know which of the reactants is the limiting reactant. In the last example above, we saw that we needed only 3 H_2O molecules to react with 3 C_2H_4 molecules, but we had 5 H_2O molecules, so H_2O is present in excess and C_2H_4 is the limiting reactant. We could also have reasoned that 5 molecules of H_2O would require 5 molecules of C_2H_4, and since we have only 3 molecules of C_2H_4, it must be the limiting reactant.

Once we have identified the limiting reactant, it is possible to compute the amount of product that will actually form, and the amount of excess reactant that will be left over after the reaction stops. We must use the amount of the limiting reactant given in the problem for these calculations.

Example 3.18 shows how to solve a typical limiting reactant problem when the amounts of the reactants are given in mass units.

EXAMPLE 3.18
Limiting Reactant Calculation

Gold(III) hydroxide is used for electroplating gold onto other metals. It can be made by the following reaction.

$$2KAuCl_4(aq) + 3Na_2CO_3(aq) + 3H_2O \longrightarrow 2Au(OH)_3(aq) + 6\,NaCl(aq) + 2KCl(aq) + 3CO_2(g)$$

To prepare a fresh supply of $Au(OH)_3$, a chemist at an electroplating plant has mixed 20.00 g of $KAuCl_4$ with 25.00 g of Na_2CO_3 (both dissolved in a large excess of water). What is the maximum number of grams of $Au(OH)_3$ that can form?

ANALYSIS: The clue that tells us this is a limiting reactant question is that *the quantities of two reactants are given*. Once we determine which reactant limits the product, we use its mass in our calculation. We will need to use a combination of our stoichiometry tools to solve this problem.

To find the limiting reactant, we arbitrarily pick one of the reactants ($KAuCl_4$ or Na_2CO_3) and calculate whether it would all be used up. If so, we've found the limiting reactant. If not, the other reactant limits. (We were told that water is in excess, so we know that it does not limit the reaction.)

SOLUTION: We will show, in the two boxes below, the calculations needed to determine which is the limiting reactant. In solving a limiting reactant problem you will need to do only one of these calculations.

We start with $KAuCl_4$ as the reactant to work with and calculate how many grams of Na_2CO_3 *should* be provided to react with 20.00 g of $KAuCl_4$. The formula masses are 377.88 for $KAuCl_4$ and 105.99 for Na_2CO_3. We'll set up a chain calculation using the following mole- to-mole relationship.

$$2 \text{ mol } KAuCl_4 \Leftrightarrow 3 \text{ mol } Na_2CO_3$$

$$\text{grams } KAuCl_4 \rightarrow \text{moles } KAuCl_4 \rightarrow \text{moles } Na_2CO_3 \rightarrow \text{grams } Na_2CO_3$$

$$20.00 \cancel{\text{ g } KAuCl_4} \times \frac{1 \cancel{\text{ mol } KAuCl_4}}{377.88 \cancel{\text{ g } KAuCl_4}} \times \frac{3 \cancel{\text{ mol } Na_2CO_3}}{2 \cancel{\text{ mol } KAuCl_4}} \times \frac{105.99 \text{ g } Na_2CO_3}{1 \cancel{\text{ mol } Na_2CO_3}}$$
$$= 8.415 \text{ g } Na_2CO_3$$

We find that 20.00 g of $KAuCl_4$ needs 8.415 g of Na_2CO_3. The 25.00 g of Na_2CO_3 taken is therefore more than enough to let the $KAuCl_4$ react completely. The Na_2CO_3 is the excess reactant, so **$KAuCl_4$ is the limiting reactant.**

We start with Na_2CO_3 as the reactant to work with and calculate how many grams of $KAuCl_4$ *should* be provided to react with 25.00 g of Na_2CO_3. The formula masses are 377.88 for $KAuCl_4$ and 105.99 for Na_2CO_3. We'll set up a chain calculation using the following mole-to-mole relationship.

$$3 \text{ mol } Na_2CO_3 \Leftrightarrow 2 \text{ mol } KAuCl_4$$

$$\text{grams } Na_2CO_3 \rightarrow \text{moles } Na_2CO_3 \rightarrow \text{moles } KAuCl_4 \rightarrow \text{grams } KAuCl_4$$

$$25.00 \cancel{\text{ g } Na_2CO_3} \times \frac{1 \cancel{\text{ mol } Na_2CO_3}}{105.99 \cancel{\text{ g } Na_2CO_3}} \times \frac{2 \cancel{\text{ mol } KAuCl_4}}{3 \cancel{\text{ mol } Na_2CO_3}} \times \frac{377.88 \text{ g } KAuCl_4}{1 \cancel{\text{ mol } KAuCl_4}}$$
$$= 59.42 \text{ g } KAuCl_4$$

We find that 25.00 g Na_2CO_3 would require much more $KAuCl_4$ than provided, so we conclude that **$KAuCl_4$ is the limiting reactant.**

After determining which reactant is the limiting reactant, return to the statement of the problem and use the amount of the limiting reactant stated in the problem to perform further calculations.

The result from either calculation above is sufficient to designate $KAuCl_4$ as the limiting reactant. From here on, we have a routine calculation converting the mass of the limiting reactant, $KAuCl_4$, to mass of product, $Au(OH)_3$. We know from the equation's coefficients that

$$1 \text{ mol } KAuCl_4 \Leftrightarrow 1 \text{ mol } Au(OH)_3$$

Using this, and the conversion factors constructed from the formula masses, we set up the following chain calculation.

$$\text{grams } KAuCl_4 \rightarrow \text{moles } KAuCl_4 \rightarrow \text{moles } Au(OH)_3 \rightarrow \text{grams } Au(OH)_3$$

$$20.00 \cancel{\text{ g } KAuCl_4} \times \left(\frac{1 \cancel{\text{ mol } KAuCl_4}}{377.88 \cancel{\text{ g } KAuCl_4}}\right) \times \left(\frac{1 \cancel{\text{ mol } Au(OH)_3}}{1 \cancel{\text{ mol } KAuCl_4}}\right) \times \left(\frac{247.99 \text{ g } Au(OH)_3}{1 \cancel{\text{ mol } Au(OH)_3}}\right)$$
$$= 13.13 \text{ g } Au(OH)_3$$

Thus from 20.00 g of $KAuCl_4$ we can make a maximum of 13.13 g of $Au(OH)_3$.

In this synthesis, some of the initial 25.00 g of Na_2CO_3 is left over. Since one of our calculations showed that 20.00 g of $KAuCl_4$ requires only 8.415 g of Na_2CO_3 out of 25.00 g Na_2CO_3, the difference, (25.00 g − 8.415 g) = 16.58 g of Na_2CO_3, remains unreacted. It is possible that the chemist used an excess to ensure that every last bit of the very expensive $KAuCl_4$ would be changed to $Au(OH)_3$.

IS THE ANSWER REASONABLE? First, the resulting mass is within the range of 1/5 to 5 times the starting mass and is not unreasonable. Again, we check that our units cancel properly and then we estimate the answer as $\frac{20 \times 250}{400} = 12.5$ g $Au(OH)_3$. That estimate is close to our answer, which assures us the calculation was done correctly.

Practice Exercise 30: A Kipp generator is an old device for making carbon dioxide as needed. It consists of an enclosed flask that contains limestone, $CaCO_3$, and has a valve to add hydrochloric acid, $HCl(aq)$, as needed. The reaction between the limestone and hydrochloric acid produces carbon dioxide as shown in the reaction

$$CaCO_3(s) + 2HCl(aq) \longrightarrow CO_2(g) + CaCl_2(aq) + H_2O$$

How many grams of CO_2 can be made by reacting 125 g of $CaCO_3$ with 125 g of HCl? How many grams of which reactant are left over? (Hint: Find the limiting reactant.)

Practice Exercise 31: In an industrial process for making nitric acid, the first step is the reaction of ammonia with oxygen at high temperature in the presence of a platinum gauze. Nitrogen monoxide forms as follows.

$$4NH_3 + 5O_2 \longrightarrow 4NO + 6H_2O$$

How many grams of nitrogen monoxide can form if a mixture initially contains 30.00 g of NH_3 and 40.00 g of O_2?

3.6 The Predicted Amount of Product Is Not Always Obtained Experimentally

In most experiments designed for chemical synthesis, the amount of a product actually isolated falls short of the calculated maximum amount. Losses occur for several reasons. Some are mechanical, such as materials sticking to glassware. In some reactions, losses occur by the evaporation of a volatile product. In others, a product is a solid that separates from the solution as it forms because it is largely insoluble. The solid is removed by filtration. What stays in solution, although relatively small, contributes to some loss of product.

One of the common causes of obtaining less than the stoichiometric amount of a product is the occurrence of a **competing reaction** (or **side reaction**). It produces a **by-product,** a substance made by a reaction that competes with the **main reaction.** The synthesis of phosphorus trichloride, for example, gives some phosphorus pentachloride as well, because PCl_3 can react further with Cl_2.

$$\text{Main reaction:} \quad 2P(s) + 3Cl_2(g) \longrightarrow 2PCl_3(l)$$

$$\text{Competing reaction:} \quad PCl_3(l) + Cl_2(g) \longrightarrow PCl_5(s)$$

The competition is between newly formed PCl_3 and still unreacted phosphorus for still unchanged chlorine.

The **actual yield** of desired product is simply how much is isolated, stated in mass units or moles. The **theoretical yield** of the product is what must be obtained if no losses occur. When less than the theoretical yield of product is obtained, chemists generally calculate the *percentage yield* of product to describe how well the preparation went. The **percentage yield** is the actual yield calculated as a percentage of the theoretical yield.

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

TOOLS *Theoretical, actual, and percentage yields*

Both the actual and theoretical yields must be in the same units, of course.

It is important to realize that the actual yield is an experimentally determined quantity. It cannot be calculated. The theoretical yield is always a calculated quantity based on a chemical equation and the amounts of the reactants available.

Let's now work an example that combines the determination of the limiting reactant with a calculation of percentage yield.

EXAMPLE 3.19
Calculating a Percentage Yield

A chemist set up a synthesis of phosphorus trichloride by mixing 12.0 g of phosphorus with 35.0 g of chlorine gas and obtained 42.4 g of liquid phosphorus trichloride. Calculate the percentage yield of this compound.

ANALYSIS: We start by determining the formulas for the reactants and products and then balancing the chemical equation. Phosphorus is represented as P(*s*), chlorine gas is $Cl_2(g)$, and the product is $PCl_3(l)$. The balanced equation is

$$2\text{P}(s) + 3\text{Cl}_2(g) \longrightarrow 2\text{PCl}_3(l)$$

Now we notice that the masses of *both* reactants are given, so this must be a limiting reactant problem. The first step is to figure out which reactant, P or Cl_2, is the limiting reactant, because we must base all calculations on the limiting reactant. Our basic tools to use are the mass-to-moles relationship and the mole ratio expressed by the balanced equation.

SOLUTION: In any limiting reactant problem, we can arbitrarily pick one reactant and do a calculation to see whether it can be entirely used up. We'll choose phosphorus and see whether there is enough to react with 35.0 g of chlorine. The following calculation gives us the answer.

$$12.0\ \cancel{\text{g P}} \times \frac{1\ \cancel{\text{mol P}}}{30.97\ \cancel{\text{g P}}} \times \frac{3\ \cancel{\text{mol Cl}_2}}{2\ \cancel{\text{mol P}}} \times \frac{70.90\ \text{g Cl}_2}{1\ \cancel{\text{mol Cl}_2}} = 41.2\ \text{g Cl}_2$$

Thus, with 35.0 g of Cl_2 provided but 41.2 g of Cl_2 needed, there is not enough Cl_2 to react with all 12.0 g of P. The Cl_2 will be all used up before the P is used up, so Cl_2 is the limiting reactant. We therefore base the calculation of the theoretical yield of PCl_3 on Cl_2. (Be careful to use the 35.0 g of Cl_2 given in the problem, *not* the 41.2 g calculated while we determined the limiting reactant.)

To find the *theoretical yield* of PCl_3, we calculate how many grams of PCl_3 could be made from 35.0 g of Cl_2 if everything went perfectly according to the equation given.

$$35.0\ \cancel{\text{g Cl}_2} \times \frac{1\ \cancel{\text{mol Cl}_2}}{70.90\ \cancel{\text{g Cl}_2}} \times \frac{2\ \cancel{\text{mol PCl}_3}}{3\ \cancel{\text{mol Cl}_2}} \times \frac{137.32\ \text{g PCl}_3}{1\ \cancel{\text{mol PCl}_3}} = 45.2\ \text{g PCl}_3$$

$$\text{grams Cl} \rightarrow \text{moles Cl}_2 \rightarrow \text{moles PCl}_3 \rightarrow \text{grams PCl}_3$$

The actual yield was 42.4 g of PCl_3, not 45.2 g, so the percentage yield is calculated as follows.

$$\text{Percentage yield} = \frac{42.4\ \text{g PCl}_3}{45.2\ \text{g PCl}_3} \times 100\% = 93.8\%$$

Thus 93.8% of the theoretical yield of PCl_3 was obtained.

IS THE ANSWER REASONABLE? The obvious check is that the calculated or theoretical yield can never be *less* than the actual yield. Second, our answer is within the range of 1/5 to 5 times the starting amount. Finally an estimated answer, after checking that all units cancel properly, is $\frac{35 \times 2 \times 140}{70 \times 3} \approx 50$ g PCl_3, which is close to the 45.2 g we calculated.

Practice Exercise 32: In the synthesis of aspirin we react salicylic acid with acetic anhydride. The balanced chemical equation is

$$\underset{\text{salicylic acid}}{2HOOCC_6H_4OH} + \underset{\text{acetic anhydride}}{C_4H_6O_3} \longrightarrow \underset{\text{acetyl salicylic acid}}{2HOOCC_6H_4O_2C_2H_3} + \underset{\text{water}}{H_2O}$$

If we mix together 28.2 grams of salicylic acid with 15.6 grams of acetic anhydride in this reaction we obtain 30.7 grams of aspirin. What are the theoretical and percentage yields of our experiment? (Hint: What is the limiting reactant?)

Practice Exercise 33: Ethanol, C_2H_5OH, can be converted to acetic acid (the acid in vinegar), $HC_2H_3O_2$, by the action of sodium dichromate in aqueous sulfuric acid according to the following equation.

$$3C_2H_5OH(aq) + 2Na_2Cr_2O_7(aq) + 8H_2SO_4(aq) \longrightarrow 3HC_2H_3O_2(aq) + 2Cr_2(SO_4)_3(aq) + 2Na_2SO_4(aq) + 11H_2O$$

In one experiment, 24.0 g of C_2H_5OH, 90.0 g of $Na_2Cr_2O_7$, and an excess of sulfuric acid were mixed, and 26.6 g of acetic acid ($HC_2H_3O_2$) was isolated. Calculate the theoretical and percentage yields of $HC_2H_3O_2$.

SUMMARY

Mole Concept and Formula Mass or Molecular Mass. In the SI definition, one mole of any substance is an amount with the same number, **Avogadro's number** (6.022×10^{23}), of atoms, molecules, or formula units as there are atoms in 12 g (exactly) of carbon-12. For monatomic elements, the **atomic mass** in grams is one mole of that element. The sum of the atomic masses of all of the atoms appearing in a chemical formula gives the **formula mass** or the **molecular mass.**

Molar Mass. This is a general term for the mass in grams numerically equal to the atomic mass, molecular mass, or formula mass. Like an atomic mass, a formula mass, or a molecular mass, the **molar mass** is a tool for grams-to-moles or moles-to-grams conversions.

Chemical Formulas. The actual composition of a molecule is given by its **molecular formula.** An **empirical formula** gives the ratio of atoms, but in the smallest whole numbers, and it is generally the *only* formula we write for ionic compounds. In the case of a molecular compound, the molecular mass is a small whole-number multiple of the empirical formula mass.

Empirical Formulas. An empirical formula may be experimentally determined if there is some way to determine the small whole-number ratio of the atoms in the substance. This calculation can be done if we know the mass or percentage of each element in the compound.

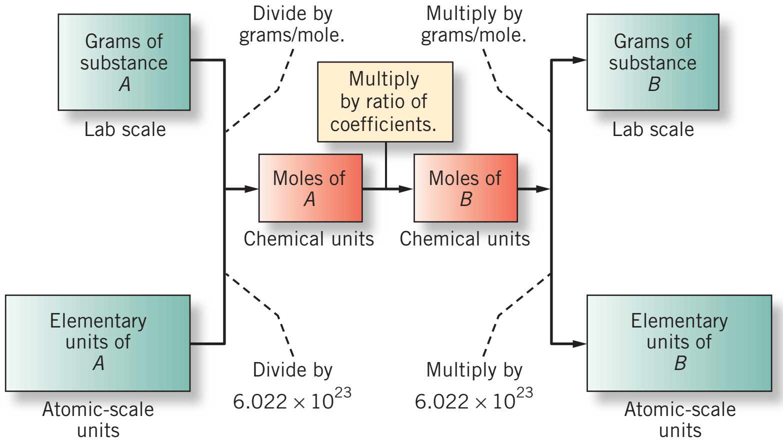
Formula Stoichiometry. A chemical formula is a tool for stoichiometric calculations, because its subscripts tell us the mole ratios in which the various elements are combined.

Balanced Equations and Reaction Stoichiometry. A balanced equation is a tool for reaction stoichiometry because its coefficients disclose the stoichiometric equivalencies. When balancing an equation, only the coefficients can be adjusted, never the subscripts. All problems of reaction stoichiometry must be solved by first converting to moles.

Yields of Products. A reactant taken in a quantity less than required by another reactant, as determined by the reaction's stoichiometry, is called the **limiting reactant.** The **theoretical yield** of a product can be no more than permitted by the limiting reactant. Sometimes **competing reactions** (side reactions) producing by-products reduce the **actual yield.** The ratio of the actual to the theoretical yields, expressed as a percentage, is the **percentage yield.**

Stoichiometric Calculations. These are generally problems where units are converted. The sequence of steps typically used in stoichiometric calculations is shown in Figure 3.6. Conversion factors in this sequence are found in the molar mass, Avogadro's number, the chemical formula, or the balanced chemical reaction.

FIG. 3.6 **Stoichiometry pathways.** This summarizes all of the possible stoichiometric calculations encountered in this chapter. The boxes represent either grams, moles, or elementary units (atoms, molecules, formula units, or ions). Problems will give starting information representing one of the boxes. The question asked will tell you where to end. Perform conversions as noted in the instructions between each box.



TOOLS FOR PROBLEM SOLVING

In this chapter you learned to apply the following concepts as tools in solving problems. Study each one carefully so that you know what each is used for. When faced with solving a problem, recall what each tool does and consider whether it will be helpful in finding a solution. This will aid you in selecting the tools you need. In this chapter we see that many of the tools from Chapters 1 and 2 must be used with the new tools from this chapter.

Atomic mass *(page 88)* Atomic masses are used to form a conversion factor to calculate mass from moles of an element, or moles from the mass of an element.

$$\text{Gram atomic mass of } X = 1 \text{ mole } X$$

Formula mass, molecular mass *(page 88)* The formula mass or molecular mass is used to form a conversion factor to calculate mass from moles of a compound, or moles from the mass of a compound.

$$\text{Gram molecular mass of } X = 1 \text{ mole } X$$

$$\text{Gram formula mass of } X = 1 \text{ mole } X$$

Molar mass *(page 88)* This is a general term encompassing atomic, molecular, and formula masses. All are the sum of the masses of the elements in the chemical formula.

$$\text{Gram molar mass of } X = 1 \text{ mole of } X$$

Avogadro's number *(page 90)* This relates macroscopic lab-sized quantities (e.g., moles) to numbers of individual atomic-sized particles such as atoms, molecules, or ions.

$$1 \text{ mole } X = 6.022 \times 10^{23} \text{ particles of } X$$

Chemical formula, subscripts *(page 92)* Subscripts in a formula establish atom ratios and mole ratios between the elements in the substance.

Conversion sequence *(page 93)* This is the logical sequence of steps required for a mass-to-mass conversion problem using a chemical formula; also see Figure 3.6.

Percentage composition *(page 94 and 99)* The percentage composition is used to represent the composition of a compound and can be the basis for computing the empirical formula. Comparing experimental and theoretical percentage compositions can help establish the identity of a compound. Percentage composition also helps correlate information from different experiments.

$$\text{Percentage of } X = \frac{\text{mass of } X \text{ in the sample}}{\text{mass of the entire sample}} \times 100\%$$

Determination of an empirical formula *(page 96)* The simplest ratio of elements in a molecule or in the formula for an ionic compound can be calculated when the mass of each element of a compound is experimentally determined.

Methods for finding integer subscripts *(page 98)* Dividing all molar amounts by the smallest value often normalizes subscripts to integers. If decimals remain, multiplication by a small whole number can result in integer subscripts.

Guidelines for balancing chemical equations *(page 104)* Balancing equations means setting coefficients so that equal numbers of each atom will be reactants as well as products. A logical sequence for balancing equations by inspection is presented.

Equivalencies obtained from balanced equations *(page 106)* Balanced chemical equations give us relationships between all reactants and products that can be used in factor-label calculations.

Sequence of conversions using balanced equations *(page 107)* As with chemical formulas, a logical sequence of conversions allows calculation of amounts of all components of a chemical reaction. See Figure 3.6.

Limiting reactant calculations *(page 111)* When the amounts of at least two reactants are known, solution of problems requires identifying the limiting reactant. All calculations must be based only on the amount of the limiting reactant available.

Theoretical, actual, and percentage yields *(page 113)* The theoretical yield is calculated from the limiting reactant. The actual yield must be determined by experiment, and the percentage yield relates the magnitude of the actual yield to the percentage yield.

$$\text{Percentage yield} = \frac{\text{actual mass by experiment}}{\text{theoretical mass by calculation}} \times 100\%$$

QUESTIONS, PROBLEMS, AND EXERCISES

Answers to problems whose numbers are printed in color are given in Appendix B. More challenging problems are marked with asterisks. ILW = Interactive Learningware solution is available at www.wiley.com/college/brady. OH = an Office Hours video is available for this problem.

REVIEW QUESTIONS

Mole Concept

3.1 How would you estimate the number of atoms in a gram of iron, using the mass in grams of an atomic mass unit?

3.2 What is the definition of the mole?

3.3 Why are moles used when all stoichiometry problems could be done using only the mass in grams of an atomic mass unit?

3.4 Which contains more molecules: 2.5 mol of H_2O or 2.5 mol of H_2?

Chemical Formulas

3.5 How many moles of iron atoms are in one mole of Fe_2O_3? How many iron atoms are in one mole of Fe_2O_3?

3.6 Write all the mole-to-mole conversion factors that can be written based on the following chemical formulas.
(a) SO_2 (b) As_2O_3 (c) K_2SO_4 (d) Na_2HPO_4

3.7 Write all the mole-to-mole conversion factors that can be written based on the following chemical formulas.
(a) Mn_3O_4 (b) Sb_2S_5 (c) $(NH_4)_2SO_4$ (d) Hg_2Cl_2

3.8 What information is required to convert grams of a substance into moles of that same substance?

3.9 Why is the expression "1.0 mol of oxygen" ambiguous? Why doesn't a similar ambiguity exist in the expression "64 g of oxygen?"

3.10 The atomic mass of aluminum is 26.98. What specific conversion factors does this value make available for relating a mass of aluminum (in grams) and a quantity of aluminum given in moles?

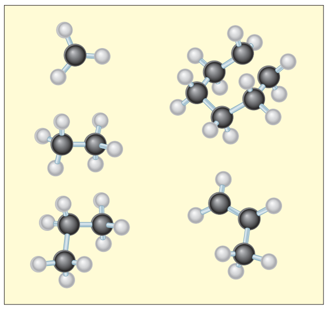
Empirical Formulas

3.11 In general, what fundamental information, obtained from experimental measurements, is required to calculate the empirical formula of a compound?

3.12 Why is the changing of subscripts not allowed when balancing a chemical equation?

3.13 Under what circumstances can we change, or assign, subscripts in a chemical formula?

3.14 How many distinct empirical formulas are shown by the following models for compounds formed between elements *A* and *B*? Explain. (Element *A* is represented by a black sphere and element *B* by a light gray sphere.)



Avogadro's Number

3.15 How would Avogadro's number change if the atomic mass unit were to be redefined as 2×10^{-27} kg, exactly?

3.16 What information is required to convert grams of a substance into molecules of that same substance?

Stoichiometry with Balanced Equations

3.17 When given the *unbalanced* equation

$$\mathrm{Na}(s) + \mathrm{Cl_2}(g) \longrightarrow \mathrm{NaCl}(s)$$

and asked to balance it, student *A* wrote

$$\mathrm{Na}(s) + \mathrm{Cl_2}(g) \longrightarrow \mathrm{NaCl_2}(s)$$

and student *B* wrote

$$2\mathrm{Na}(s) + \mathrm{Cl_2}(g) \longrightarrow 2\mathrm{NaCl}(s)$$

Both equations are balanced, but which student is correct? Explain why the other student's answer is incorrect.

3.18 Give a step-by-step procedure for estimating the number grams of *A* required to completely react with 10 moles of *B,* given the following information:

A and *B* react to form A_5B_2.
A has a molecular mass of 100.0.
B has a molecular mass of 200.0.
There are 6.022×10^{23} molecules of *A* in a mole of *A*.

Which of these pieces of information weren't needed?

3.19 If two substances react completely in a 1-to-1 ratio *both* by mass and by moles, what must be true about these substances?

3.20 What information is required to determine how many grams of sulfur would react with a gram of arsenic?

3.21 A mixture of 0.020 mol of Mg and 0.020 mol of Cl_2 reacted completely to form $MgCl_2$ according to the equation

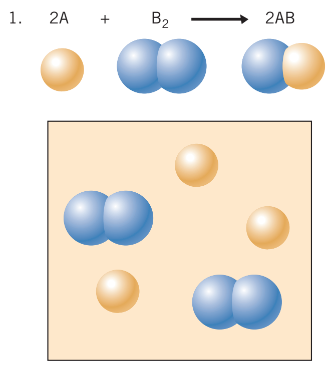
$$\mathrm{Mg} + \mathrm{Cl_2} \longrightarrow \mathrm{MgCl_2}$$

What information describes the *stoichiometry* of this reaction? What information gives the *scale* of the reaction?

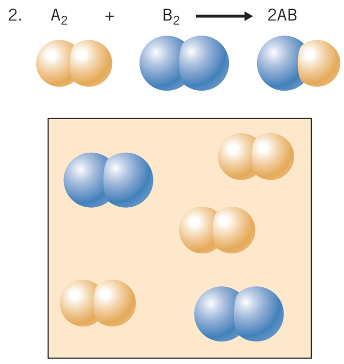
3.22 In a report to a supervisor, a chemist described an experiment in the following way: "0.0800 mol of H_2O_2 decomposed into 0.0800 mol of H_2O and 0.0400 mol of O_2." Express the chemistry and stoichiometry of this reaction by a conventional chemical equation.

3.23 On April 16, 1947, in Texas City, Texas, two cargo ships, the *Grandcamp* and the *High Flier,* were each loaded with approximately 2000 tons of ammonium nitrate fertilizer. The *Grandcamp* caught fire and exploded, followed by the *High Flier*. Over 600 people were killed and one-third of the city was destroyed. Considering a much smaller mass, how would you calculate the number of N_2 molecules that could be produced after the explosion of 1.00 kg of NH_4NO_3?

3.24 Molecules containing *A* and *B* react to form *AB* as shown at the top of the next column. Based on the equations and the contents of the boxes labeled "Initial," sketch for each reaction the molecular models of what is present after the reaction is over. (In both cases, the species *B* exists as B_2. In reaction 1, *A* is monatomic; in reaction 2, *A* exists as diatomic molecules A_2.)



Initial



Initial

REVIEW PROBLEMS

The Mole Concept and Stoichiometric Equivalencies

3.25 In what smallest whole-number ratio must N and O atoms combine to make dinitrogen tetroxide, N_2O_4? What is the mole ratio of the elements in this compound?

3.26 In what atom ratio are the elements present in methane, CH_4 (the chief component of natural gas)? In what mole ratio are the atoms of the elements present in this compound?

3.27 How many moles of tantalum atoms correspond to 1.56×10^{21} atoms of tantalum?

3.28 How many moles of iodine molecules correspond to 1.80×10^{24} molecules of I_2?

3.29 Sucrose (table sugar) has the formula $C_{12}H_{22}O_{11}$. In this compound, what is the
(a) atom ratio of C to H?
(b) mole ratio of C to O?
(c) atom ratio of H to O?
(d) mole ratio of H to O?

3.30 Nail polish remover is sometimes the volatile liquid ethyl acetate, $CH_3COOC_2H_5$. In this compound, what is the
(a) atom ratio of C to O?
(b) mole ratio of C to O?
(c) atom ratio of C to H?
(d) mole ratio of C to H?

3.31 How many moles of Bi atoms are needed to combine with 1.58 mol of O atoms to make bismuth oxide, Bi_2O_3?

3.32 How many moles of vanadium atoms, V, are needed to combine with 0.565 mol of O atoms to make vanadium pentoxide, V_2O_5?

3.33 How many moles of Cr are in 2.16 mol of Cr_2O_3?

3.34 How many moles of O atoms are in 4.25 mol of calcium carbonate, $CaCO_3$, the chief constituent of seashells?

3.35 Aluminum sulfate, $Al_2(SO_4)_3$, is a compound used in sewage treatment plants.
(a) Construct a pair of conversion factors that relate moles of aluminum to moles of sulfur for this compound.
(b) Construct a pair of conversion factors that relate moles of sulfur to moles of $Al_2(SO_4)_3$.
(c) How many moles of Al are in a sample of this compound if the sample also contains 0.900 mol S?
(d) How many moles of S are in 1.16 mol $Al_2(SO_4)_3$?

3.36 Magnetite is a magnetic iron ore. Its formula is Fe_3O_4.
(a) Construct a pair of conversion factors that relate moles of Fe to moles of Fe_3O_4.
(b) Construct a pair of conversion factors that relate moles of Fe to moles of O in Fe_3O_4.
(c) How many moles of Fe are in 2.75 mol of Fe_3O_4?
(d) If this compound could be prepared from Fe_2O_3 and O_2, how many moles of Fe_2O_3 would be needed to prepare 4.50 mol Fe_3O_4?

3.37 How many moles of H_2 and N_2 can be formed by the decomposition of 0.145 mol of ammonia, NH_3?

3.38 How many moles of S are needed to combine with 0.225 mol Al to give Al_2S_3?

ILW **3.39** How many moles of UF_6 would have to be decomposed to provide enough fluorine to prepare 1.25 mol of CF_4? (Assume sufficient carbon is available.)

3.40 How many moles of Fe_3O_4 are required to supply enough iron to prepare 0.260 mol Fe_2O_3? (Assume sufficient oxygen is available.)

3.41 How many atoms of carbon are combined with 4.13 moles of hydrogen in a sample of the compound propane, C_3H_8? (Propane is used as the fuel in gas barbecues.)

3.42 How many atoms of hydrogen are found in 2.31 mol of propane, C_3H_8?

3.43 What is the total number of C, H, and O atoms in 0.260 moles of glucose, $C_6H_{12}O_6$?

3.44 What is the total number of N, H, and O atoms in 0.356 mol of ammonium nitrate, NH_4NO_3, an important fertilizer?

Measuring Moles of Elements and Compounds

3.45 How many atoms are in 6.00 g of carbon-12?

OH **3.46** How many atoms are in 1.50 mol of carbon-12? How many grams does this much carbon-12 weigh?

3.47 Determine the mass in grams of each of the following:
(a) 1.35 mol Fe (b) 24.5 mol O (c) 0.876 mol Ca

3.48 Determine the mass in grams of each of the following:
(a) 0.546 mol S (b) 3.29 mol N (c) 8.11 mol Al

3.49 What is the mass, in grams, of 2×10^{12} atoms of potassium?

3.50 What is the mass, in grams, of 4×10^{17} atoms of sodium?

3.51 How many moles of nickel are in 17.7 g of Ni?

3.52 How many moles of chromium are in 85.7 g of Cr?

3.53 Calculate the formula mass of each of the following to the maximum number of significant figures possible using the periodic table inside the front cover.
(a) $NaHCO_3$ (d) potassium dichromate
(b) $(NH_4)_2CO_3$ (e) aluminum sulfate
(c) $CuSO_4 \cdot 5H_2O$

3.54 Calculate the formula mass of each of the following to the maximum number of significant figures possible using the periodic table inside the front cover.
(a) calcium nitrate (d) $Fe_4[Fe(CN)_6]_3$
(b) $Pb(C_2H_5)_4$ (e) magnesium phosphate
(c) $Na_2SO_4 \cdot 10H_2O$

3.55 Calculate the mass in grams of the following.
(a) 1.25 mol $Ca_3(PO_4)_2$
(b) 0.625 mmol iron(III) nitrate
(c) 0.600 μmol C_4H_{10}
(d) 1.45 mol ammonium carbonate

3.56 What is the mass in grams of the following?
(a) 0.754 mol zinc chloride
(b) 0.194 μmol potassium chlorate
(c) 0.322 mmol $POCl_3$
(d) 4.31×10^{-3} mol $(NH_4)_2HPO_4$

3.57 Calculate the number of moles of each compound in the following samples.
(a) 21.5 g calcium carbonate
(b) 1.56 ng NH_3
(c) 16.8 g strontium nitrate
(d) 6.98 μg Na_2CrO_4

3.58 Calculate the number of moles of each compound in the following samples.
(a) 9.36 g calcium hydroxide
(b) 38.2 kg lead(II)sulfate
(c) 4.29 g H_2O_2
(d) 4.65 mg $NaAuCl_4$

ILW **3.59** One sample of CaC_2 contains 0.150 mol of carbon. How many moles and how many grams of calcium are also in the sample? [Calcium carbide, CaC_2, was once used to make signal flares for ships. Water dripped onto CaC_2 reacts to give acetylene (C_2H_2), which burns brightly.]

OH **3.60** How many moles of iodine are in 0.500 mol of $Ca(IO_3)_2$? How many grams of calcium iodate are needed to supply this much iodine? [Iodized salt contains a trace amount of calcium iodate, $Ca(IO_3)_2$, to help prevent a thyroid condition called goiter.]

3.61 How many moles of nitrogen, N, are in 0.650 mol of ammonium carbonate? How many grams of this compound supply this much nitrogen?

3.62 How many moles of nitrogen, N, are in 0.556 mol of ammonium nitrate? How many grams of this compound supply this much nitrogen?

3.63 How many kilograms of a fertilizer made of pure $(NH_4)_2CO_3$ would be required to supply 1.00 kilogram of nitrogen to the soil?

3.64 How many kilograms of a fertilizer made of pure P_2O_5 would be required to supply 1.00 kilogram of phosphorus to the soil?

Percentage Composition

3.65 Calculate the percentage composition by mass for each of the following:
(a) sodium dihydrogenphosphate
(b) $NH_4H_2PO_4$
(c) $(CH_3)_2CO$
(d) calcium sulfate dihydrate
(e) $CaSO_4{\cdot}2H_2O$

3.66 Calculate the percentage composition by mass of each of the following:
(a) $(CH_3)_2N_2H_2$
(b) $CaCO_3$
(c) iron(III) nitrate
(d) C_3H_8
(e) aluminum sulfate

3.67 Which has a higher percentage of oxygen: morphine ($C_{17}H_{19}NO_3$) or heroin ($C_{21}H_{23}NO_5$)?

3.68 Which has a higher percentage of nitrogen: carbamazepine ($C_{15}H_{12}N_2O$) or carbetapentane ($C_{20}H_{31}NO_3$)?

3.69 Freon is a trade name for a group of gaseous compounds once used as propellants in aerosol cans. Which has a higher percentage of chlorine: Freon-12 (CCl_2F_2) or Freon-141b ($C_2H_3Cl_2F$)?

3.70 Which has a higher percentage of fluorine: Freon-12 (CCl_2F_2) or Freon 113 ($C_2Cl_3F_3$)?

OH **3.71** It was found that 2.35 g of a compound of phosphorus and chlorine contained 0.539 g of phosphorus. What are the percentages by mass of phosphorus and chlorine in this compound?

3.72 An analysis revealed that 5.67 g of a compound of nitrogen and oxygen contained 1.47 g of nitrogen. What are the percentages by mass of nitrogen and oxygen in this compound?

3.73 Phencyclidine ("angel dust") is $C_{17}H_{25}N$. A sample suspected of being this illicit drug was found to have a percentage composition of 84.71% C, 10.42% H, and 5.61% N. Do these data acceptably match the theoretical data for phencyclidine?

3.74 The hallucinogenic drug LSD has the molecular formula $C_{20}H_{25}N_3O$. One suspected sample contained 74.07% C, 7.95% H, and 9.99% N.
(a) What is the percentage O in the sample?
(b) Are these data consistent for LSD?

3.75 How many grams of O are combined with 7.14×10^{21} atoms of N in the compound dinitrogen pentoxide?

3.76 How many grams of C are combined with 4.25×10^{23} atoms of H in the compound C_5H_{12}?

Empirical Formulas

3.77 Write empirical formulas for the following compounds.
(a) S_2Cl_2 (b) $C_6H_{12}O_6$ (c) NH_3 (d) As_2O_6 (e) H_2O_2

3.78 What are the empirical formulas of the following compounds?
(a) $C_2H_4(OH)_2$
(b) $H_2S_2O_8$
(c) C_4H_{10}
(d) B_2H_6
(e) C_2H_5OH

3.79 Quantitative analysis of a sample of sodium pertechnetate with a mass of 0.896 g found 0.111 g of sodium and 0.477 g of technetium. The remainder was oxygen. Calculate the empirical formula of sodium pertechnetate. (Radioactive sodium pertechnetate is used as a brain-scanning agent in medicine.)

3.80 A sample of Freon was found to contain 0.423 g C, 2.50 g Cl, and 1.34 g F. What is the empirical formula of this compound?

3.81 A dry-cleaning fluid composed of only carbon and chlorine was found to be composed of 14.5% C and 85.5% Cl (by mass). What is the empirical formula of this compound?

3.82 One compound of mercury with a formula mass of 519 g mol^{-1} contains 77.26% Hg, 9.25% C, and 1.17% H (with the balance being O). Calculate the empirical and molecular formulas.

3.83 Cinnamic acid, a compound related to the flavor component of cinnamon, is 72.96% carbon, 5.40% hydrogen, and the rest is oxygen. What is the empirical formula of this acid?

3.84 Vanillin, a compound used as a flavoring agent in food products, has the following percentage composition: 63.2% C, 5.26% H, and 31.6% O. What is the empirical formula of vanillin?

ILW **3.85** When 0.684 g of an organic compound containing only carbon, hydrogen, and oxygen was burned in oxygen, 1.312 g CO_2 and 0.805 g H_2O were obtained. What is the empirical formula of the compound?

3.86 Methyl ethyl ketone (often abbreviated MEK) is a powerful solvent with many commercial uses. A sample of this compound (which contains only C, H, and O) weighing 0.822 g was burned in oxygen to give 2.01 g CO_2 and 0.827 g H_2O. What is the empirical formula for MEK?

3.87 When 6.853 mg of a sex hormone was burned in a combustion analysis, 19.73 mg of CO_2 and 6.391 mg of H_2O were obtained. What is the empirical formula of the compound?

3.88 When a sample of a compound in the vitamin D family was burned in a combustion analysis, 5.983 mg of the compound gave 18.490 mg of CO_2 and 6.232 mg of H_2O. What is the empirical formula of the compound?

Molecular Formulas

3.89 The following are empirical formulas and the masses per mole for three compounds. What are their molecular formulas?
(a) NaS_2O_3; 270.4 g/mol
(b) C_3H_2Cl; 147.0 g/mol
(c) C_2HCl; 181.4 g/mol

3.90 The following are empirical formulas and the masses per mole for three compounds. What are their molecular formulas?
(a) Na_2SiO_3; 732.6 g/mol
(b) $NaPO_3$; 305.9 g/mol
(c) CH_3O; 62.1 g/mol

3.91 The compound described in Problem 3.87 was found to have a molecular mass of 290. What is its molecular formula?

3.92 The compound described in Problem 3.88 was found to have a molecular mass of 399 g mol^{-1}. What is the molecular formula of this compound?

ILW **3.93** A sample of a compound of mercury and bromine with a mass of 0.389 g was found to contain 0.111 g bromine. Its molecular mass was found to be 561 g mol^{-1}. What are its empirical and molecular formulas?

3.94 A 0.6662 g sample of "antimonal saffron" was found to contain 0.4017 g of antimony. The remainder was sulfur. The formula mass of this compound is 404 g mol^{-1}. What are the empirical and molecular formulas of this pigment? (This compound is a red pigment used in painting.)

3.95 A sample of a compound of C, H, N, and O, with a mass of 0.6216 g was found to contain 0.1735 g C, 0.01455 g H, and 0.2024 g N. Its formula mass is 129 g mol^{-1}. Calculate its empirical and molecular formulas.

3.96 Strychnine, a deadly poison, has a formula mass of 334 g mol^{-1} and a percentage composition of 75.42% C, 6.63% H, 8.38% N, and the balance oxygen. Calculate the empirical and molecular formulas of strychnine.

Balancing Chemical Equations

3.97 How many moles of hydrogen are part of the expression "$2Ba(OH)_2 \cdot 8H_2O$," taken from a balanced equation?

3.98 How many moles of oxygen are part of the expression "$3Ca_3(PO_4)_2$," taken from a balanced equation?

OH **3.99** Write the equation that expresses in acceptable chemical shorthand the following statement: "Iron can be made to react with molecular oxygen to give iron(III) oxide."

3.100 The conversion of one air pollutant, nitrogen monoxide, produced in vehicle engines, into another, nitrogen dioxide, occurs when nitrogen monoxide reacts with molecular oxygen in the air. Write the balanced equation for this reaction.

3.101 Balance the following equations.
(a) Calcium hydroxide reacts with hydrogen chloride to form calcium chloride and water.
(b) Silver nitrate and calcium chloride react to form calcium nitrate and silver chloride.
(c) Lead nitrate reacts with sodium sulfate to form lead sulfate and sodium nitrate.
(d) Iron(III) oxide and carbon react to form iron and carbon dioxide.
(e) Butane reacts with oxygen to form carbon dioxide and water.

3.102 Balance the following equations.
(a) $SO_2 + O_2 \longrightarrow SO_3$
(b) $NaHCO_3 + H_2SO_4 \longrightarrow Na_2SO_4 + H_2O + CO_2$
(c) $P_4O_{10} + H_2O \longrightarrow H_3PO_4$
(d) $Fe_2O_3 + H_2 \longrightarrow Fe + H_2O$
(e) $Al + H_2SO_4 \longrightarrow Al_2(SO_4)_3 + H_2$

3.103 Balance the following equations.
(a) $Mg(OH)_2 + HBr \longrightarrow MgBr_2 + H_2O$
(b) $HCl + Ca(OH)_2 \longrightarrow CaCl_2 + H_2O$
(c) $Al_2O_3 + H_2SO_4 \longrightarrow Al_2(SO_4)_3 + H_2O$
(d) $KHCO_3 + H_3PO_4 \longrightarrow K_2HPO_4 + H_2O + CO_2$
(e) $C_9H_{20} + O_2 \longrightarrow CO_2 + H_2O$

3.104 Balance the following equations.
(a) $CaO + HNO_3 \longrightarrow Ca(NO_3)_2 + H_2O$
(b) $Na_2CO_3 + Mg(NO_3)_2 \longrightarrow MgCO_3 + NaNO_3$
(c) $(NH_4)_3PO_4 + NaOH \longrightarrow Na_3PO_4 + NH_3 + H_2O$
(d) $LiHCO_3 + H_2SO_4 \longrightarrow Li_2SO_4 + H_2O + CO_2$
(e) $C_4H_{10}O + O_2 \longrightarrow CO_2 + H_2O$

3.105 Chemical reactions can be used to change the charge of ions. Fe^{3+} is converted to Fe^{2+} when iron(III) chloride reacts with tin(II) chloride to make iron(II) chloride and tin(IV) chloride. Write and balance the equation that represents this reaction.

3.106 A precipitation reaction is one where soluble reactants form an insoluble product. A common precipitation reaction involves the reaction of the soluble salt aluminum chloride with soluble silver nitrate to form the insoluble silver chloride and soluble aluminum nitrate. Write and balance the equation for this reaction along with the appropriate states indicated in parentheses.

Stoichiometry Based on Chemical Equations

3.107 Chlorine is used by textile manufacturers to bleach cloth. Excess chlorine is destroyed by its reaction with sodium thiosulfate, $Na_2S_2O_3$, as follows.

$$Na_2S_2O_3(aq) + 4Cl_2(g) + 5H_2O \longrightarrow 2NaHSO_4(aq) + 8HCl(aq)$$

(a) How many moles of $Na_2S_2O_3$ are needed to react with 0.12 mol of Cl_2?
(b) How many moles of HCl can form from 0.12 mol of Cl_2?
(c) How many moles of H_2O are required for the reaction of 0.12 mol of Cl_2?
(d) How many moles of H_2O react if 0.24 mol HCl is formed?

3.108 The octane in gasoline burns according to the following equation.

$$2C_8H_{18} + 25O_2 \longrightarrow 16CO_2 + 18H_2O$$

(a) How many moles of O_2 are needed to react fully with 6 mol of octane?
(b) How many moles of CO_2 can form from 0.5 mol of octane?
(c) How many moles of water are produced by the combustion of 8 mol of octane?
(d) If this reaction is used to synthesize 6.00 mol of CO_2, how many moles of oxygen are needed? How many moles of octane?

3.109 The following reaction is used to extract gold from pretreated gold ore:

$$2Au(CN)_2^-(aq) + Zn(s) \longrightarrow 2Au(s) + Zn(CN)_4^{2-}(aq)$$

(a) How many grams of Zn are needed to react with 0.11 mol of $Au(CN)_2^-$?
(b) How many grams of Au can form from 0.11 mol of $Au(CN)_2^-$?
(c) How many grams of $Au(CN)_2^-$ are required for the reaction of 0.11 mol of Zn?

OH **3.110** Propane burns according to the following equation.

$$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$$

(a) How many grams of O_2 are needed to react fully with 3 mol of propane?
(b) How many grams of CO_2 can form from 0.1 mol of propane?
(c) How many grams of water are produced by the combustion of 4 mol of propane?

3.111 The incandescent white of a fireworks display is caused by the reaction of phosphorus with O_2 to give P_4O_{10}.
(a) Write the balanced chemical equation for the reaction.
(b) How many grams of O_2 are needed to combine with 6.85 g of P?
(c) How many grams of P_4O_{10} can be made from 8.00 g of O_2?
(d) How many grams of P are needed to make 7.46 g of P_4O_{10}?

3.112 The combustion of butane, C_4H_{10}, produces carbon dioxide and water. When one sample of C_4H_{10} was burned, 4.46 g of water was formed.
(a) Write the balanced chemical equation for the reaction.
(b) How many grams of butane were burned?
(c) How many grams of O_2 were consumed?
(d) How many grams of CO_2 were formed?

ILW **3.113** In *dilute* nitric acid, HNO_3, copper metal dissolves according to the following equation.

$$3Cu(s) + 8HNO_3(aq) \longrightarrow 3Cu(NO_3)_2(aq) + 2NO(g) + 4H_2O$$

How many grams of HNO_3 are needed to dissolve 11.45 g of Cu according to this equation?

3.114 The reaction of hydrazine, N_2H_4, with hydrogen peroxide, H_2O_2, has been used in rocket engines. One way these compounds react is described by the equation

$$N_2H_4 + 7H_2O_2 \longrightarrow 2HNO_3 + 8H_2O$$

According to this equation, how many grams of H_2O_2 are needed to react completely with 852 g of N_2H_4?

3.115 Oxygen gas can be produced in the laboratory by decomposition of hydrogen peroxide (H_2O_2):

$$2H_2O_2(aq) \longrightarrow 2H_2O + O_2(g)$$

How many kilograms of O_2 can be produced from 1.0 kg of H_2O_2?

3.116 Oxygen gas can be produced in the laboratory by decomposition of potassium chlorate ($KClO_3$):

$$2KClO_3(s) \longrightarrow 2KCl(s) + 3O_2(g)$$

How many kilograms of O_2 can be produced from 1.0 kg of $KClO_3$?

Limiting Reactant Calculations

3.117 The reaction of powdered aluminum and iron(III) oxide,

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

produces so much heat the iron that forms is molten. Because of this, railroads use the reaction to provide molten steel to weld steel rails together when laying track. Suppose that in one batch of reactants 4.20 mol of Al was mixed with 1.75 mol of Fe_2O_3.
(a) Which reactant, if either, was the limiting reactant?
(b) Calculate the number of grams of iron that can be formed from this mixture of reactants.

3.118 Ethanol (C_2H_5OH) is synthesized for industrial use by the following reaction, carried out at very high pressure:

$$C_2H_4(g) + H_2O(g) \longrightarrow C_2H_5OH(l)$$

What is the maximum amount of ethanol that can be produced when 1.0 kg of ethylene (C_2H_4) and 0.010 kg of steam are placed into the reaction vessel?

ILW **3.119** Silver nitrate, $AgNO_3$, reacts with iron(III) chloride, $FeCl_3$, to give silver chloride, AgCl, and iron(III) nitrate, $Fe(NO_3)_3$. A solution containing 18.0 g of $AgNO_3$ was mixed with a solution containing 32.4 g of $FeCl_3$. How many grams of which reactant remains after the reaction is over?

3.120 Chlorine dioxide, ClO_2, has been used as a disinfectant in air-conditioning systems. It reacts with water according to the equation

$$6ClO_2 + 3H_2O \longrightarrow 5HClO_3 + HCl$$

If 142.0 g of ClO_2 is mixed with 38.0 g of H_2O, how many grams of which reactant remain if the reaction is complete?

3.121 Some of the acid in acid rain is produced by the following reaction:

$$3NO_2(g) + H_2O(l) \longrightarrow 2HNO_3(aq) + NO(g)$$

If a falling raindrop weighing 0.050 g comes into contact with 1.0 mg of $NO_2(g)$, how much HNO_3 can be produced?

3.122 Phosphorus pentachloride reacts with water to give phosphoric acid and hydrogen chloride according to the following equation.

$$PCl_5 + 4H_2O \longrightarrow H_3PO_4 + 5HCl$$

In one experiment, 0.360 mol of PCl_5 was slowly added to 2.88 mol of water.
(a) Which reactant, if either, was the limiting reactant?
(b) How many grams of HCl were formed in the reaction?

Theoretical Yield and Percentage Yield

3.123 Barium sulfate, $BaSO_4$, is made by the following reaction.

$$Ba(NO_3)_2(aq) + Na_2SO_4(aq) \longrightarrow BaSO_4(s) + 2NaNO_3(aq)$$

An experiment was begun with 75.00 g of $Ba(NO_3)_2$ and an excess of Na_2SO_4. After collecting and drying the product, 64.45 g of $BaSO_4$ was obtained. Calculate the theoretical yield and percentage yield of $BaSO_4$.

3.124 The Solvay process for the manufacture of sodium carbonate begins by passing ammonia and carbon dioxide through a solution of sodium chloride to make sodium bicarbonate and ammonium chloride. The equation for the overall reaction is

$$H_2O + NaCl + NH_3 + CO_2 \longrightarrow NH_4Cl + NaHCO_3$$

In the next step, sodium bicarbonate is heated to give sodium carbonate and two gases, carbon dioxide and steam.

$$2NaHCO_3 \longrightarrow Na_2CO_3 + CO_2 + H_2O$$

What is the theoretical yield of sodium carbonate, expressed in grams, if 120 g NaCl was used in the first reaction? If 85.4 g of Na_2CO_3 was obtained, what was the percentage yield?

ILW **3.125** Aluminum sulfate can be made by the following reaction.

$$2AlCl_3(aq) + 3H_2SO_4(aq) \longrightarrow Al_2(SO_4)_3(aq) + 6HCl(aq)$$

It is quite soluble in water, so to isolate it the solution has to be evaporated to dryness. This drives off the volatile HCl, but the residual solid has to be heated to a little over 200 °C to drive off all of the water. In one experiment, 25.0 g of $AlCl_3$ was mixed with 30.0 g of H_2SO_4. Eventually, 28.46 g of pure $Al_2(SO_4)_3$ was isolated. Calculate the percentage yield.

3.126 The combustion of methyl alcohol in an abundant excess of oxygen follows the equation

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

When 6.40 g of CH_3OH was mixed with 10.2 g of O_2 and ignited, 6.12 g of CO_2 was obtained. What was the percentage yield of CO_2?

*3.127 The potassium salt of benzoic acid, potassium benzoate ($KC_7H_5O_2$), can be made by the action of potassium permanganate on toluene (C_7H_8) as follows.

$$C_7H_8 + 2KMnO_4 \longrightarrow KC_7H_5O_2 + 2MnO_2 + KOH + H_2O$$

If the yield of potassium benzoate cannot realistically be expected to be more than 71%, what is the minimum number of grams of toluene needed to produce 11.5 g of potassium benzoate?

*3.128 Manganese trifluoride, MnF_3, can be prepared by the following reaction. OH

$$2MnI_2(s) + 13F_2(g) \longrightarrow 2MnF_3(s) + 4IF_5(l)$$

If the percentage yield of MnF_3 is always approximately 56%, how many grams of MnF_3 can be expected if 10.0 grams of each reactant is used in an experiment?

ADDITIONAL EXERCISES

3.129 Mercury is an environmental pollutant because it can be converted by certain bacteria into the very poisonous substance methyl mercury, $(CH_3)_2Hg$. This compound ends up in the food chain and accumulates in the tissues of aquatic organisms, particularly fish, which renders them unsafe to eat. It is estimated that in the United States 263 tons of mercury are released into the atmosphere each year. If only 1.0 percent of this mercury is changed to $(CH_3)_2Hg$, how many pounds of this compound are formed annually?

*3.130 Lead compounds are often highly colored and are toxic to mold, mildew, and bacteria, properties that in the past were useful for paints used before 1960. Today we know lead is very hazardous and it is not used in paint; however, old paint is still a problem. If a certain lead-based paint contains 14.5% $PbCr_2O_7$ and 73% of the paint evaporates as it dries, what mass of lead will be in a paint chip that weighs 0.15 g?

3.131 A superconductor is a substance that is able to conduct electricity without resistance, a property that is very desirable in the construction of large electromagnets. Metals have this property if cooled to temperatures a few degrees above absolute zero, but this requires the use of expensive liquid helium (boiling point 4 K). Scientists have discovered materials that become superconductors at higher temperatures, but they are ceramics. Their brittle nature has so far prevented them from being made into long wires. A recently discovered compound of magnesium and boron, which consists of 52.9% Mg and 47.1% B, shows special promise as a high-temperature superconductor because it is inexpensive to make and can be fabricated into wire relatively easily. What is the formula of the compound?

*3.132 A 0.1246 g sample of a compound of chromium and chlorine was dissolved in water. All of the chloride ion was then captured by silver ion in the form of AgCl. A mass of 0.3383 g of AgCl was obtained. Calculate the empirical formula of the compound of Cr and Cl.

*3.133 A compound of Ca, C, N, and S was subjected to quantitative analysis and formula mass determination, and the following data were obtained. A 0.250 g sample was mixed with Na_2CO_3 to convert all of the Ca to 0.160 g of $CaCO_3$. A 0.115 g sample of the compound was carried through a series of reactions until all of its S was changed to 0.344 g of $BaSO_4$. A 0.712 g sample was processed to liberate all of its N as NH_3, and 0.155 g NH_3 was obtained. The formula mass was found to be 156. Determine the empirical and molecular formulas of the compound.

3.134 Ammonium nitrate will detonate if ignited in the presence of certain impurities. The equation for this reaction at a high temperature is

$$2NH_4NO_3(s) \xrightarrow{>300\ °C} 2N_2(g) + O_2(g) + 4H_2O(g)$$

Notice that all of the products are gases and so must occupy a vastly greater volume than the solid reactant.

(a) How many moles of *all* gases are produced from 1 mol of NH_4NO_3?

(b) If 1.00 ton of NH_4NO_3 exploded according to this equation, how many moles of *all* gases would be produced? (1 ton = 2000 lb.)

3.135 A lawn fertilizer is rated as 6.00% nitrogen, meaning 6.00 g of N in 100 g of fertilizer. The nitrogen is present in the form of urea, $(NH_2)_2CO$. How many grams of urea are present in 100 g of the fertilizer to supply the rated amount of nitrogen?

*3.136 Nitrogen is the “active ingredient” in many quick acting fertilizers. You are operating a farm of 1500 acres to produce soybeans. Which of the following fertilizers will you choose as the most economical for your farm? (a) NH_4NO_3 at $625 for 25 kg, (b) $(NH_4)_2HPO_4$ at $55 for 1 kg, (c) urea, CH_4ON_2, at $60 for 5 kg, (d) ammonia, NH_3, at $128 for 50 kg

3.137 Based solely on the amount of available carbon, how many grams of sodium oxalate, $Na_2C_2O_4$, could be obtained from 125 g of C_6H_6? (Assume that no loss of carbon occurs in any of the reactions needed to produce the $Na_2C_2O_4$.)

3.138 According to NASA, the space shuttle’s external fuel tank for the main propulsion system carries 1,361,936 lb of liquid oxygen and 227,641 lb of liquid hydrogen. During takeoff, these chemicals are consumed as they react to form water. If the reaction is continued until all of one reactant is gone, how many pounds of which reactant are left over?

*3.139 For a research project, a student decided to test the effect of the lead(II) ion (Pb^{2+}) on the ability of salmon eggs to hatch. This ion was obtainable from the water-soluble salt, lead(II) nitrate, $Pb(NO_3)_2$, which the student decided to make by the following reaction. (The desired product was to be isolated by the slow evaporation of the water.)

$$PbO(s) + 2HNO_3(aq) \longrightarrow Pb(NO_3)_2(aq) + H_2O$$

Losses of product for various reasons were anticipated, and a yield of 86.0% was expected. In order to have 5.00 g of product at this yield, how many grams of PbO should be taken? (Assume that sufficient nitric acid, HNO_3, would be used.)

3.140 Chlorine atoms cause chain reactions in the stratosphere that destroy ozone that protects the earth’s surface from ultraviolet radiation. The chlorine atoms come from chlorofluorocarbons, compounds that contain carbon, fluorine, and chlorine, which were used for many years as refrigerants. One of these compounds is Freon-12, CF_2Cl_2. If a sample contains 1.0×10^{-9} g of Cl, how many grams of F should be present if all of the F and Cl atoms in the sample came from CF_2Cl_2 molecules?

*3.141 Lime, CaO, can be produced in two steps shown in the equations below. If the percentage yield of the first step is 83.5% and the percentage yield of the second step is 71.4%, what is the expected overall percentage yield for producing CaO from $CaCl_2$?

$$CaCl_2(aq) + CO_2(g) + H_2O \longrightarrow CaCO_3(s) + 2HCl(aq)$$

$$CaCO_3(s) \xrightarrow{\text{heat}} CaO + H_2O$$

EXERCISES IN CRITICAL THINKING

3.142 A newspaper story describing the local celebration of Mole Day on October 23 (selected for Avogadro's number, 6.022×10^{23}) attempted to give the readers a sense of the size of the number by stating that a mole of M&Ms would be equal to 18 tractor trailers full. Assuming that an M&M occupies a volume of about $0.5\ cm^3$, calculate the dimensions of a cube required to hold one mole of M&Ms. Would 18 tractor trailers be sufficient?

3.143 Suppose you had one mole of pennies and that you were going to spend 500 million dollars each and every second until you spent your entire fortune. How many years would it take you to spend all this cash? (Assume 1 year = 365 days.)

3.144 Using the above two exercises as examples, devise a creative way to demonstrate the size of the mole, or Avogadro's number.

3.145 List the different ways in which a chemist could use the information used to determine empirical formulas.

3.146 Calculate the percentage carbon in $C_{20}H_{42}$ and $C_{21}H_{44}$. If you were to burn one gram of each compound and quantitatively collect the carbon dioxide and water produced, would you be able to discern the difference between these two compounds with the equipment in your laboratory? In your evaluation consider the difference in masses expected from each sample and the number of decimal places your balance must read to. Also, list, in order of importance, all factors that can create error in this experiment.