When wood, paper, and wax are burned, they appear to lose mass. The decrease in mass that results from these combustion reactions was once attributed to the release of "phlogiston" into the air. For most of the eighteenth century scientists accepted the phlogiston theory. Then, in August 1774, the English chemist and clergyman Joseph Priestley isolated oxygen—which he called "dephlogisticated air"—as a product of the decomposition of mercury(II) oxide, HgO. The French chemist Antoine Lavoisier had noticed that nonmetals like phosphorus actually *gain* mass when they burn in air. He concluded that these nonmetals must combine with something in the air. This substance turned out to be Priestley's dephlogisticated air. Lavoisier named the new element "oxygen" (from the Greek word meaning "to form acid"), because he knew that it is also a constituent of all acids.

Lavoisier igniting a mixture of hydrogen and oxygen gases.

Born in 1743, Lavoisier is generally regarded as the father of modern chemistry. He was noted for his carefully controlled experiments and for the use of quantitative measurements. By carrying out chemical reactions, such as the decomposition of mercury(II) oxide in a closed container, he showed that the total mass of the products equals the total mass of the reactants. In other words, the quantity of matter is not changed by chemical reactions. This observation is the basis of the law of conservation of mass and the principle underlying stoichiometry.

Lavoisier determined the composition of water by igniting a mixture of hydrogen and oxygen gases with an electric spark. He also served on the commission that established the metric system on which SI is based. Unfortunately, his scientific career was cut short by the French Revolution. A member of the nobility, Lavoisier was also a tax collector. For these "crimes," he was sent to the guillotine in 1794.

Stoichiometry

Chapter 3

3.1 Atomic Mass 58
Average Atomic Mass

3.2 Molar Mass of an Element and Avogadro's Number 59

3.3 Molecular Mass 62

3.4 The Mass Spectrometer 64

3.5 Percent Composition of Compounds 65

3.6 Experimental Determination of Empirical Formulas 68
Determination of Molecular Formulas

3.7 Chemical Reactions and Chemical Equations 70
Writing Chemical Equations • Balancing Chemical Equations

3.8 Amounts of Reactants and Products 75

3.9 Limiting Reagents and Yields of Reactions 78
Yields of Reactions

ESSENTIAL CONCEPTS

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

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

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

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

3.1 Atomic Mass

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

Section 3.4 describes a method for determining atomic mass.

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

One atomic mass unit is also called one dalton.

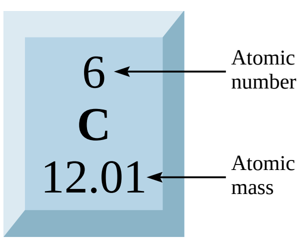
By international agreement, an atom of the carbon isotope (called carbon-12) that has six protons and six neutrons has a mass of exactly 12 ***atomic mass units (amu).*** This carbon-12 atom serves as the standard, so one atomic mass unit is defined as *a mass exactly equal to one-twelfth the mass of one carbon-12 atom:*

$$\text{mass of one carbon-12 atom} = 12 \text{ amu}$$

$$1 \text{ amu} = \frac{\text{mass of one carbon-12 atom}}{12}$$

Experiments have shown that, on average, a hydrogen atom is only 8.400 percent as massive as the standard carbon-12 atom. If we accept the mass of one carbon-12 atom to be exactly 12 amu, then the ***atomic mass*** (that is, *the mass of the atom in atomic mass units*) of hydrogen must be 0.08400×12.00 amu, or 1.008 amu. (Note that atomic mass is also called atomic weight.) Similar calculations show that the atomic mass of oxygen is 16.00 amu and that of iron is 55.85 amu. Thus although we do not know just how much an average iron atom's mass is, we know that it is approximately 56 times as massive as a hydrogen atom.

Average Atomic Mass



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

$$\begin{aligned}\text{average atomic mass of natural carbon} \\ &= (0.9890)(12.00000 \text{ amu}) + (0.0110)(13.00335 \text{ amu}) \\ &= 12.0 \text{ amu}\end{aligned}$$

A more accurate determination gives the atomic mass of carbon as 12.01 amu. Note that in calculations involving percentages, we need to convert percentages to fractions.

For example, 98.90 percent becomes 98.90/100, or 0.9890. Because there are many more carbon-12 atoms than carbon-13 atoms in naturally occurring carbon, the average atomic mass is much closer to 12 amu than 13 amu.

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

Copper.

Example 3.1 Copper, a metal known since ancient times, is used in electrical cables and pennies, among other things. The atomic masses of its two stable isotopes, $^{63}_{29}Cu$ (69.09 percent) and $^{65}_{29}Cu$ (30.91 percent), are 62.93 amu and 64.9278 amu, respectively. Calculate the average atomic mass of copper. The percentages in parentheses denote the relative abundances.

Reasoning and Solution Each isotope contributes to the atomic mass of copper according to its natural abundance. Therefore, the first step is to convert the percentages to fractions. Thus 69.09 percent becomes 0.6909 and 30.91 percent becomes 0.3091. Next we calculate the average atomic mass as follows:

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

Similar problems: 3.9, 3.10.

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

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

3.2 Molar Mass of an Element and Avogadro's Number

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

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

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

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

number (N_A), in honor of the Italian scientist Amedeo Avogadro. The currently accepted value is

$$N_{\text{A}} = 6.0221367 \times 10^{23}$$

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

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

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

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

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

Therefore, we can write the unit factor as

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

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

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

and the unit factor is

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

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

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

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

$$\frac{\text{gram}}{\text{amu}} = \frac{1.993 \times 10^{-23} \text{ g}}{\cancel{1 \text{ carbon-12 atom}}} \times \frac{\cancel{1 \text{ carbon-12 atom}}}{12 \text{ amu}}$$
$$= 1.661 \times 10^{-24} \text{ g/amu}$$

Thus

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

and

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

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

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

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

The molar masses of the elements (in g/mol) are given on the inside front cover of the book.

where X represents the symbol of an element. Figure 3.2 summarizes the relationships between the mass of an element and the number of moles of an element and between moles of an element and the number of atoms of an element. Using the proper unit factors we can convert one quantity to another.

Example 3.2 Zinc (Zn) is a silvery metal that is used in making brass (with copper) and in plating iron to prevent corrosion. How many grams of Zn are in 0.356 mole of Zn?

Reasoning and Solution To convert moles to grams, we need the unit factor

$$\frac{\text{molar mass of Zn}}{1 \text{ mol Zn}} = 1$$

The molar mass of Zn is 65.39 g, so that the mass of Zn in 0.356 mol is

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

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

Comment The mass in 0.356 mole of Zn should be less than the molar mass of Zn.

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

Zinc.

Similar Problem: 3.18.

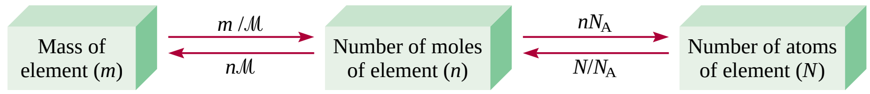
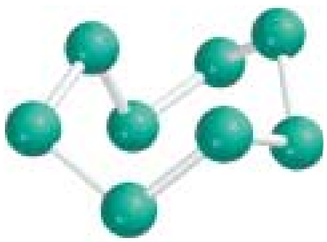


Figure 3.2 *The relationships between mass (in grams) of an element and number of moles of an element, and between numbers of moles of an element and number of atoms of an element. $\mathcal{M}$ is the molar mass (g/mol) of the element and N_A is Avogadro's number.*



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

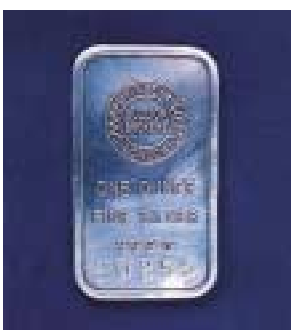
Similar Problem: 3.22.

Example 3.3 Sulfur (S) is a nonmetallic element. Its presence in coal gives rise to the acid rain phenomenon. How many atoms are in 16.3 g of S?

Reasoning and Solution Solving this problem requires two steps. First, we need to find the number of moles of S in 16.3 g of S. Next, we need to calculate the number of S atoms from the known number of moles of S. We can combine the two steps as follows:

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

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



Silver.

Similar Problems: 3.19, 3.20.

Example 3.4 Silver (Ag) is a precious metal used mainly in jewelry. What is the mass (in grams) of one Ag atom?

Reasoning and Solution There are 6.022×10^{23} Ag atoms in 1 mole of Ag and the molar mass of Ag is 107.9 g. Combining these two unit factors, we calculate the mass of a single Ag atom as follows:

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

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

3.3 Molecular Mass

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

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

or

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

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

Example 3.5 Calculate the molecular masses of these compounds: (a) sulfur dioxide (SO_2) and (b) caffeine ($C_8H_{10}N_4O_2$).

Reasoning and Solution To calculate molecular mass, we need to count the number of each type of atom in the molecule and look up its atomic mass in the periodic table (inside front cover).

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

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

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

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

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

SO_2

Similar Problem: 3.26.

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

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

Example 3.6 Methane (CH_4) is the principal component of natural gas. How many moles of CH_4 are present in 6.07 g of CH_4?

Reasoning and Solution This problem is just the opposite of Example 3.2, except that we are dealing with molecules instead of atoms. Therefore, the first step is to calculate the molar mass of CH_4:

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

From the unit factor (1 mol CH_4/16.04 g CH_4) we calculate the number of moles of CH_4 as follows:

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

Comment Because 6.07 g is smaller than the molar mass, the answer is reasonable.

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

Methane gas burning on a cooking range.

Similar Problem: 3.28.

Urea.

Example 3.7 How many hydrogen atoms are present in 25.6 g of urea [$(NH_2)_2CO$], which is used as a fertilizer, in animal feed, and in the manufacture of polymers? The molar mass of urea is 60.06 g.

Reasoning and Solution First we follow the procedure in Example 3.3 to calculate the number of molecules present in 25.6 g of urea. Next we note that there are four hydrogen atoms in every urea molecule. Combining both steps we calculate the total number of hydrogen atoms present

$$25.6\text{ g }\cancel{(NH_2)_2CO} \times \frac{1\text{ mol }\cancel{(NH_2)_2CO}}{60.06\text{ g }\cancel{(NH_2)_2CO}} \times \frac{6.022 \times 10^{23}\text{ }\cancel{\text{molecules }(NH_2)_2CO}}{1\text{ }\cancel{\text{mol }(NH_2)_2CO}}$$

$$\times \frac{4\text{ H atoms}}{1\text{ }\cancel{\text{molecule }(NH_2)_2CO}} = 1.03 \times 10^{24}\text{ H atoms}$$

We could calculate the number of nitrogen, carbon, and oxygen atoms by the same procedure. However, there is a shortcut. Note that the ratio of nitrogen to hydrogen atoms in urea is 2/4, or 1/2, and that of oxygen (and carbon) to hydrogen atoms is 1/4. Therefore, the number of nitrogen atoms in 25.6 g of urea is $(1/2)(1.03 \times 10^{24})$, or 5.15×10^{23} atoms. The number of oxygen atoms (and carbon atoms) is $(1/4)(1.03 \times 10^{24})$, or 2.58×10^{23} atoms.

Similar Problem: 3.30.

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

3.4 The Mass Spectrometer

The most direct and most accurate method for determining atomic and molecular masses is mass spectrometry, which is depicted in Figure 3.3. In a *mass spectrometer,* a gaseous sample is bombarded by a stream of high-energy electrons. Collisions between the electrons and the gaseous atoms (or molecules) produce positive ions by dislodging an electron from each atom or molecule. These positive ions (of mass m and charge e) are accelerated by two oppositely charged plates as they pass through the plates. The emerging ions are deflected into a circular path by a magnet. The radius of the path depends on the charge-to-mass ratio (that is, e/m). Ions of smaller e/m ratio

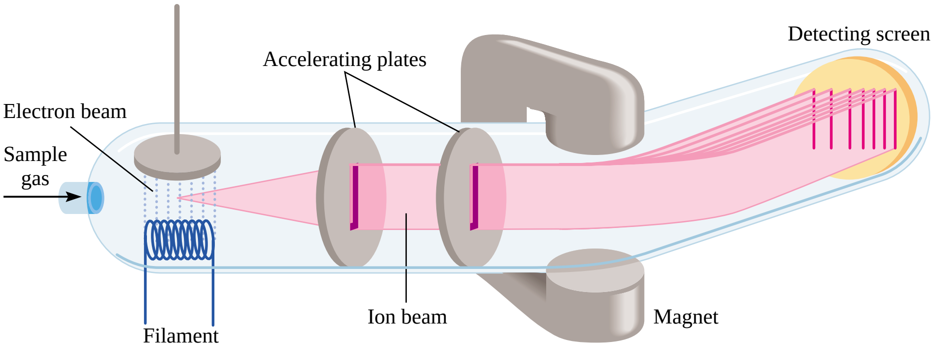


Figure 3.3 *Scnematic diagram of one type of mass spectrometer.*

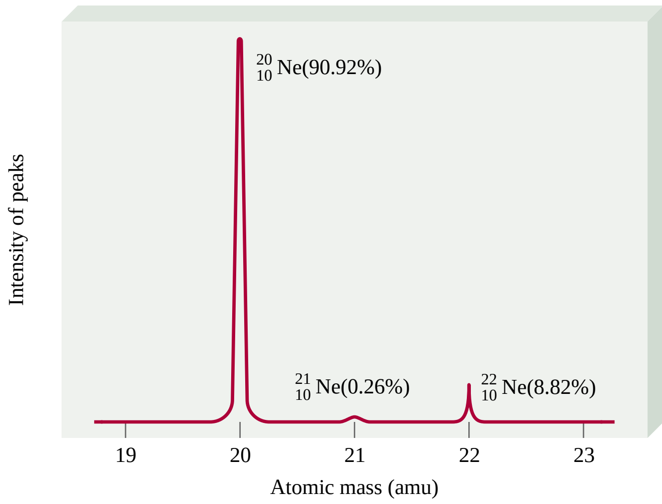


Figure 3.4 *The mass spectrum of the three isotopes of neon.*

trace a wider curve than those having a larger *e*/*m* ratio, so that ions with equal charges but different masses are separated from one another. The mass of each ion (and hence its parent atom or molecule) is determined from the magnitude of its deflection. Eventually the ions arrive at the detector, which registers a current for each type of ion. The amount of current generated is directly proportional to the number of ions, so it enables us to determine the relative abundance of isotopes.

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

3.5 Percent Composition of Compounds

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

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

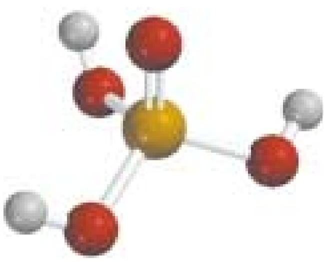
$$\text{percent composition of an element} = \frac{n \times \text{molar mass of element}}{\text{molar mass of compound}} \times 100\% \quad (3.1)$$

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

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

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

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



H_3PO_4

Similar Problem: 3.42.

Example 3.8 Phosphoric acid (H_3PO_4) is a colorless, syrupy liquid used in detergents, fertilizers, and toothpastes, and in carbonated beverages for a "tangy" flavor. Calculate the percent composition by mass of H, P, and O in this compound.

Reasoning and Solution The percent by mass of each element is given by the total mass of the atoms of the element divided by the molar mass of the compound, multiplied by 100 percent. The molar mass of H_3PO_4 is 97.99 g/mol. Therefore, the percent by mass of each of the elements in H_3PO_4 is

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

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

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

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

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

The procedure used in Example 3.8 can be reversed if necessary. Given the percent composition by mass of a compound, we can determine the empirical formula of the compound (Figure 3.5).

Example 3.9 Ascorbic acid (vitamin C) cures scurvy and may help prevent the common cold. It is composed of 40.92 percent carbon (C), 4.58 percent hydrogen (H), and 54.50 percent oxygen (O) by mass. Determine its empirical formula.

Reasoning and Solution To solve a problem of this type, it is convenient to assume that we started with a 100 g of the compound so that each percentage can be directly converted to grams. Therefore, in this sample there will be 40.92 g of C, 4.58 g of H, and 54.50 g of O. Next, we need to calculate the number of moles of each element in the compound. Let n_C, n_H, and n_O be the number of moles of elements present. Using the molar masses of these elements, we write

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

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

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

Thus, we arrive at the formula $C_{3.407}H_{4.54}O_{3.406}$, which gives the identity and the ratios of atoms present. However, because chemical formulas are written with whole numbers, we cannot have 3.407 C atoms, 4.54 H atoms, and 3.406 O atoms. We can make some of the subscripts whole numbers by dividing all the subscripts by the *smallest* subscript (3.406):

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

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

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

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

Comment The molecular formula of ascorbic acid is $C_6H_8O_6$.

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

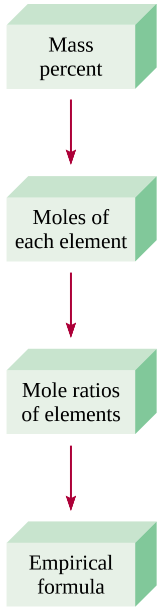
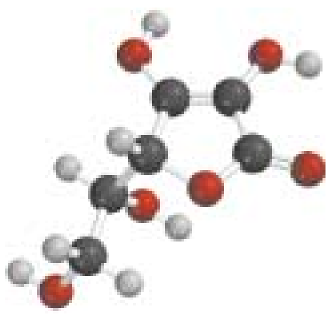


Figure 3.5 *Procedure for calculating the empirical formula of a compound from its percent compositions.*



Ascorbic acid.

Similar Problems: 3.43, 3.44.

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

Chalcopyrite.

Example 3.10 Chalcopyrite ($CuFeS_2$) is a principal ore of copper. Calculate the number of kilograms of Cu in 3.71×10^3 kg of chalcopyrite.

Reasoning and Solution A little thought will convince you that the product of the percent composition by mass of an element in a compound and the mass of the compound should yield the mass of the element in that compound. The molar masses of Cu and $CuFeS_2$ are 63.55 g and 183.5 g, respectively, so the percent composition by mass of Cu is

$$\%\text{Cu} = \frac{63.55\text{ g}}{183.5\text{ g}} \times 100\% = 34.63\%$$

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

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

This calculation can be simplified by combining the above two steps as:

$$\begin{aligned}\text{mass of Cu in CuFeS}_2 &= 3.71 \times 10^3\text{ kg CuFeS}_2 \times \frac{63.55\text{ g Cu}}{183.5\text{ g CuFeS}_2} \\ &= 1.28 \times 10^3\text{ kg Cu}\end{aligned}$$

Similar Problem: 3.50.

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

3.6 Experimental Determination of Empirical Formulas

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

As a specific example let us consider the compound ethanol. When ethanol is burned in an apparatus such as that shown in Figure 3.6, carbon dioxide (CO_2) and water (H_2O) are given off. Because neither carbon nor hydrogen was in the inlet gas, we can conclude that both carbon (C) and hydrogen (H) were present in

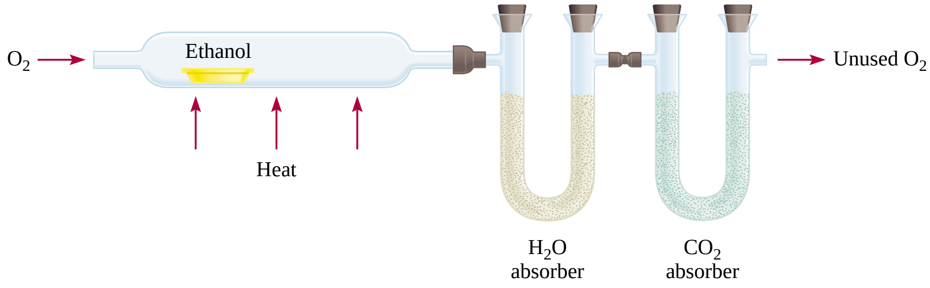


Figure 3.6 *Apparatus for determining the empirical formula of ethanol. The absorbers are substances that can retain water and carbon dioxide, respectively.*

ethanol and that oxygen (O) may also be present. (Molecular oxygen was added in the combustion process, but some of the oxygen may also have come from the original ethanol sample.)

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

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

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

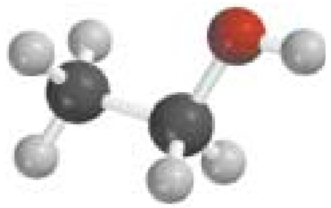
$$\begin{aligned}\text{mass of O} &= \text{mass of sample} - (\text{mass of C} + \text{mass of H})\\ &= 11.5\ \text{g} - (6.00\ \text{g} + 1.51\ \text{g})\\ &= 4.0\ \text{g}\end{aligned}$$

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

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

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

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



The molecular formula of ethanol is the same as its empirical formula.

Determination of Molecular Formulas

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

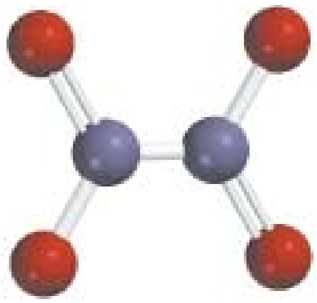
Example 3.11 A sample of a compound of nitrogen (N) and oxygen (O) contains 1.52 g of N and 3.47 g of O. The molar mass of this compound is known to be between 90 g and 95 g. Determine the molecular formula and the accurate molar mass of the compound.

Reasoning and Solution First we need to determine the empirical formula of the compound and then compare its molar mass with the true molar mass of the compound, that is, the experimentally determined molar mass. This comparison will reveal the relationship between the empirical formula and the molecular formula.

Let n_N and n_O be the number of moles of nitrogen and oxygen. Then

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

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


N_2O_4

Thus the formula of the compound is $N_{0.108}O_{0.217}$. We divide the subscripts by the smaller subscript, 0.108. After rounding off, we obtain NO_2 as the empirical formula. The molecular formula will be the same as the empirical formula or some integral multiple of it (for example, two, three, four, or more times the empirical formula). The molar mass of the empirical formula NO_2 is

$$\text{empirical molar mass} = 14.01\ \text{g} + 2(16.00\ \text{g}) = 46.02\ \text{g}$$

Next we determine the number of (NO_2) units present in the molecular formula. This number is found by taking the ratio

$$\frac{\text{molar mass}}{\text{empirical molar mass}} = \frac{95\ \text{g}}{46.02\ \text{g}} = 2.1 \approx 2$$

Therefore the molar mass of the compound is twice the molar mass of the empirical formula. Consequently, there are two NO_2 units in each molecule of the compound, and the molecular formula is $(NO_2)_2$, or N_2O_4. The molar mass of the compound is 2(46.02 g), or 92.04 g, which is between 90 g and 95 g.

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

Similar Problem: 3.54.

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

3.7 Chemical Reactions and Chemical Equations

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

Writing Chemical Equations

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

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

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

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

$$2H_2 + O_2 \longrightarrow 2H_2O \tag{3.3}$$

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

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

We refer to H_2 and O_2 in Equation (3.3) as ***reactants,*** which are *the starting materials in a chemical reaction.* Water is the ***product,*** which is *the substance formed as a result of a chemical reaction.* A chemical equation, then, is just the chemist's shorthand description of a reaction. In a chemical equation the reactants are conventionally written on the left and the products on the right of the arrow:

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

On heating, mercury(II) oxide (HgO) decomposes to form mercury and oxygen.

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

Two hydrogen molecules + One oxygen molecule $\longrightarrow$ Two water molecules

$2H_2 + O_2 \longrightarrow 2H_2O$

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

Table 3.1 | Interpretation of a Chemical Equation

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

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

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

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

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

Balancing Chemical Equations

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

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

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

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

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

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

$$KClO_3 \longrightarrow KCl + O_2$$

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

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

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

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

$$2KClO_3 \longrightarrow 2KCl + 3O_2 \qquad (3.4)$$

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

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

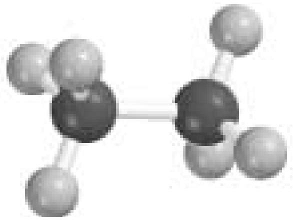
Note that this equation could also be balanced with coefficients that are multiples of 2 (for $KClO_3$), 2 (for KCl), and 3 (for O_2); for example,

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

However, it is common practice to use the *simplest* possible set of whole-number coefficients to balance the equation. Equation (3.4) conforms to this convention.

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

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



C_2H_6

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

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

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

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

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

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

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

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

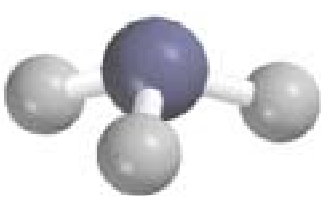
However, we normally prefer to express the coefficients as whole numbers rather than as fractions. Therefore, we multiply the entire equation by 2 to convert $\frac{7}{2}$ to 7:

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

The final tally is

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

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



NH_3

Example 3.12 The first step in the synthesis of nitric acid (HNO_3), an important chemical used in the manufacture of fertilizers, drugs, and explosives, is the reaction between ammonia (NH_3) and oxygen to produce nitric oxide (NO) and water. Write a balanced equation for this reaction.

Reasoning and Solution We follow the procedure describe on p. 00. The unbalanced equation is

$$NH_3 + O_2 \longrightarrow NO + H_2O$$

We see that N appears only once on each side of the equation and in equal number. Therefore, NH_3 and NO must have the same coefficient. To balance H, we place a 2 in front of NH_3 and a 3 in front of H_2O:

$$2NH_3 + O_2 \longrightarrow NO + 3H_2O$$

To balance N, we place a 2 in front of NO:

$$2NH_3 + O_2 \longrightarrow 2NO + 3H_2O$$

There are two O atoms on the left and five O atoms on the right of the arrow. This inequality of O atoms can be eliminated by writing $\frac{5}{2}$ in front of O_2:

$$2NH_3 + \tfrac{5}{2}O_2 \longrightarrow 2NO + 3H_2O$$

As in the case of ethane described earlier, we multiply the entire equation by 2 to convert $\frac{5}{2}$ to 5

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

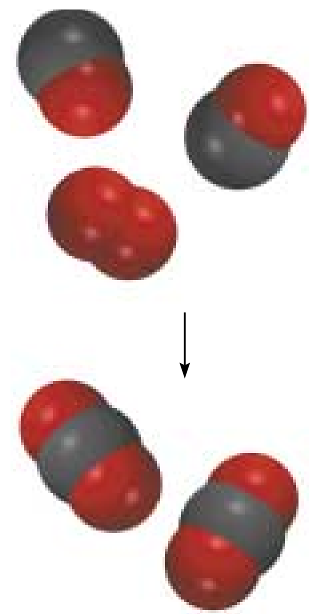
The final tally is

Reactants	Products
N (4)	N (4)
H (12)	H (12)
O (10)	O (10)

Similar Problems: 3.59, 3.60.

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

3.8 Amounts of Reactants and Products



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

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

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

For stoichiometric calculations we would read this equation as "2 moles of carbon monoxide gas combine with 1 mole of oxygen gas to form 2 moles of carbon dioxide gas."

The mole method consists of these steps:

1. Write correct formulas for all reactants and products, and balance the resulting equation.
2. Convert the quantities of some or all given or known substances (usually reactants) into moles.
3. Use the coefficients in the balanced equation to calculate the number of moles of the sought or unknown quantities (usually products) in the problem.
4. Using the calculated numbers of moles and the molar masses, convert the unknown quantities to whatever units are required (typically grams).
5. Check that your answer is reasonable in physical terms.

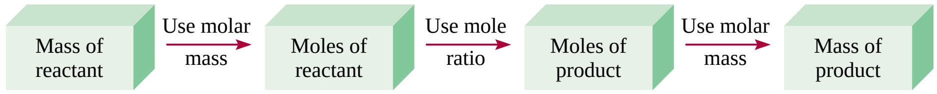


Figure 3.8 *The mole method. First convert the quantity of reactant (in grams or other units) to number of moles. Next, use the mole ratio in the balanced equation to calculate the number of moles of product formed. Finally, convert moles of product to grams of product.*

Step 1 is a prerequisite to any stoichiometric calculation. We must know the identities of the reactants and products, and their mass relationships must not violate the law of conservation of mass (that is, we must have a balanced equation). Step 2 is the critical process of converting grams (or other units) of substances to number of moles. This conversion allows us to analyze the actual reaction in terms of moles only.

To complete step 3, we need the balanced equation furnished by step 1. The key point here is that the coefficients in a balanced equation tell us the ratio in which moles of one substance react with or form moles of another substance. Step 4 is similar to step 2, except that it deals with the quantities sought in the problem. Step 5 is often underestimated but is very important. Figure 3.8 shows the steps involved in stoichiometric calculations.

In stoichiometry we use the symbol $\bumpeq$, which means "stoichiometrically equivalent to" or simply "equivalent to." In the balanced equation for the formation of carbon dioxide, 2 moles of CO react with 1 mole of O_2, so 2 moles of CO are equivalent to 1 mole of O_2:

$$2 \text{ mol CO} \bumpeq 1 \text{ mol } O_2$$

In terms of the factor-label method, we can write the unit factor as

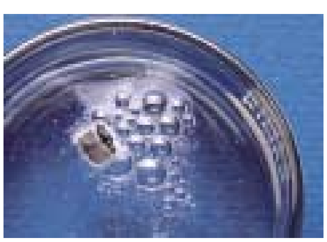
$$\frac{2 \text{ mol CO}}{1 \text{ mol } O_2} = 1 \qquad \text{or} \qquad \frac{1 \text{ mol } O_2}{2 \text{ mol CO}} = 1$$

Similarly, because 2 moles of CO (or 1 mole of O_2) produce 2 moles of CO_2, we can say that 2 moles of CO (or 1 mole of O_2) are equivalent to 2 moles of CO_2:

$$2 \text{ mol CO} \bumpeq 2 \text{ mol } CO_2 \qquad\qquad 1 \text{ mol } O_2 \bumpeq 2 \text{ mol } CO_2$$

so

$$\frac{2 \text{ mol CO}}{2 \text{ mol } CO_2} = 1 \qquad\qquad \frac{1 \text{ mol } O_2}{2 \text{ mol } CO_2} = 1$$



Lithium reacting with water to produce hydrogen gas.

Example 3.13 All alkali metals react with water to produce hydrogen gas and the corresponding alkali metal hydroxide. A typical reaction is that between lithium and water:

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

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

Reasoning and Solution We follow the steps listed on p. 00.

(a)

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

Step 2. No conversion is needed because the amount of the starting material, Li, is given in moles.

Step 3. Because 2 moles of Li produce 1 mole of H_2, or 2 mol Li $\simeq$ 1 mol H_2, we calculate moles of H_2 produced as follows:

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

Step 4. This step is not required.

Step 5. We began with 6.23 moles of Li and produced 3.12 moles of H_2. Because 2 moles of Li produce 1 mole of H_2, 3.12 moles is a reasonable quantity.

(b)

Step 1. The reaction is the same as in (a).

Step 2. The number of moles of Li is given by

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

Step 3. Because 2 moles of Li produce 1 mole of H_2, or 2 mol Li $\simeq$ 1 mol H_2, we calculate the number of moles of H_2 as follows:

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

Step 4. From the molar mass of H_2 (2.016 g), we calculate the mass of H_2 produced:

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

Step 5. Because the molar mass of H_2 is smaller than that of Li and two moles of Li are needed to produce one mole of H_2, we expect the answer to be smaller than 80.57 g.

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

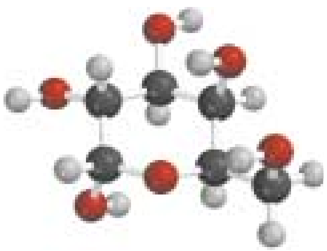
$$2\text{NO}(g) + \text{O}_2(g) \longrightarrow 2\text{NO}_2(g)$$

(a) How many moles of NO_2 are formed by the complete reaction of 0.254 mole of O_2?

(b) How many grams of NO_2 are formed by the complete reaction of 1.44 g of NO?

Similar Problem: 3.72.

After some practice, you may find it convenient to combine steps 2, 3, and 4 in a single equation, as Example 3.14 shows.



$C_6H_{12}O_6$

Example 3.14 The food we eat is degraded, or broken down, in our bodies to provide energy for growth and function. A general overall equation for this very complex process represents the degradation of glucose ($C_6H_{12}O_6$) to carbon dioxide (CO_2) and water (H_2O):

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

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

Reasoning and Solution We follow the steps listed on p. 00.

Step 1. The balanced equation is given.

Steps 2, 3, and 4. From the balanced equation we see that 1 mol $C_6H_{12}O_6 \bumpeq$ 6 mol CO_2. The molar masses of $C_6H_{12}O_6$ and CO_2 are 180.2 g and 44.01 g, respectively. We combine all of these data into one equation:

$$\text{mass of } CO_2 \text{ produced} = 856 \cancel{\text{g } C_6H_{12}O_6} \times \frac{1 \cancel{\text{mol } C_6H_{12}O_6}}{180.2 \cancel{\text{g } C_6H_{12}O_6}} \times \frac{6 \cancel{\text{mol } CO_2}}{1 \cancel{\text{mol } C_6H_{12}O_6}}$$

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

Step 5. Because one mole of $C_6H_{12}O_6$ produces six moles of Co_2 and the molar mass of $C_6H_{12}O_6$ is four times that of CO_2, we expect the mass of CO_2 formed to be greater than 856 g. Therefore, the answer is reasonable.

Similar Problem: 3.75.

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

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

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

3.9 Limiting Reagents and Yields of Reactions

Limiting reagent

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

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

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

NO_2 is a dark brown gas with a choking odor whose color is sometimes visible in polluted air.

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

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

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

and starting with seven moles of O_2, we have

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

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

In stoichiometric calculations, the first step is to decide which reactant is the limiting reagent. After the limiting reagent has been identified, the rest of the problem can be solved as outlined in Section 3.8. Example 3.15 illustrates this approach. We will not include step 5 in the calculations, but you should always examine the reasonableness of *any* chemical calculation.

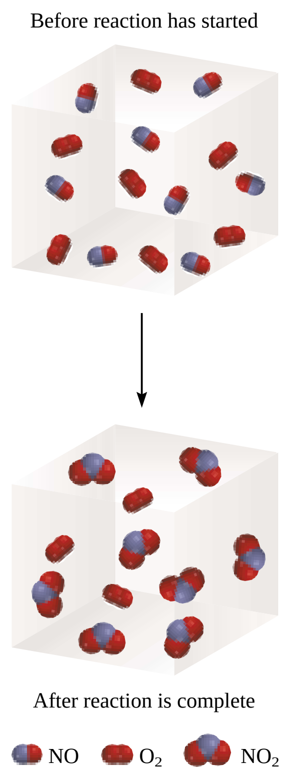


Figure 3.9 *At the start of the reaction, there were eight NO molecules and seven O_2 molecules. At the end, all the NO molecules are gone and only three O_2 molecules are left. Therefore, NO is the limiting reagent and O_2 is the excess reagent. Each molecule can also be treated as one mole of the substance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

Example 3.15 Urea $[(NH_2)_2CO]$ is prepared by reacting ammonia with carbon dioxide:

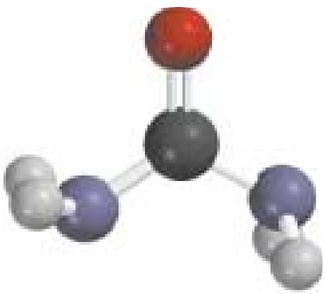
$$2NH_3(g) + CO_2(g) \longrightarrow (NH_2)_2CO(aq) + H_2O(l)$$

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

Reasoning and Solution **(a)** Because we cannot tell by inspection which of the two reactants is the limiting reagent, we have to proceed by first converting their masses into numbers of moles. The molar masses of NH_3 and CO_2 are 17.03 g and 44.01 g, respectively. Thus

$$\begin{aligned}\text{moles of NH}_3 &= 637.2\ \cancel{\text{g NH}_3} \times \frac{1\ \text{mol NH}_3}{17.03\ \cancel{\text{g NH}_3}}\\ &= 37.42\ \text{mol NH}_3\\ \text{moles of CO}_2 &= 1142\ \cancel{\text{g CO}_2} \times \frac{1\ \text{mol CO}_2}{44.01\ \cancel{\text{g CO}_2}}\\ &= 25.95\ \text{mol CO}_2\end{aligned}$$

To determine which of the reactants is the limiting reagent, we first calculate the number of moles of $(NH_2)_2CO$ produced from the given amounts of NH_3 and CO_2.



$(NH_2)_2CO$

In practice, chemists usually choose the more expensive chemical (NH_3 in this case) as the limiting reagent so that all or most of it will be consumed in the reaction.

From the balanced equation, we see that 2 mol NH_3 ≏ 1 mol $(NH_2)_2CO$ and 1 mol CO_2 ≏ 1 mol $(NH_2)_2CO$. Starting with 37.42 moles of NH_3, we write

$$37.42 \cancel{\text{mol NH}_3} \times \frac{1 \text{ mol } (\text{NH}_2)_2\text{CO}}{2 \cancel{\text{mol NH}_3}} = 18.71 \text{ mol } (\text{NH}_2)_2\text{CO}$$

and from 25.95 moles of CO_2,

$$25.95 \cancel{\text{mol CO}_2} \times \frac{1 \text{ mol } (\text{NH}_2)_2\text{CO}}{1 \cancel{\text{mol CO}_2}} = 25.95 \text{ mol } (\text{NH}_2)_2\text{CO}$$

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

(b) The amount of $(NH_2)_2CO$ produced is determined by the amount of limiting reagent present. Thus we write

$$\text{mass of } (\text{NH}_2)_2\text{CO} = 37.42 \cancel{\text{mol NH}_3} \times \frac{1 \cancel{\text{mol (NH}_2)_2\text{CO}}}{2 \cancel{\text{mol NH}_3}} \times \frac{60.06 \text{ g } (\text{NH}_2)_2\text{CO}}{1 \cancel{\text{mol (NH}_2)_2\text{CO}}} = 1124 \text{ g } (\text{NH}_2)_2\text{CO}$$

(c) The number of moles of the excess reagent (CO_2) left is

$$25.95 \text{ mol CO}_2 - \left(37.42 \cancel{\text{mol NH}_3} \times \frac{1 \text{ mol CO}_2}{2 \cancel{\text{mol NH}_3}}\right) = 7.24 \text{ mol CO}_2$$

and

$$\text{mass of CO}_2 \text{ left over} = 7.24 \cancel{\text{mol CO}_2} \times \frac{44.01 \text{ g CO}_2}{1 \cancel{\text{mol CO}_2}} = 319 \text{ g CO}_2$$

Similar Problem: 3.82.

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

$$2\text{Al} + \text{Fe}_2\text{O}_3 \longrightarrow \text{Al}_2\text{O}_3 + 2\text{Fe}$$

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

Yields of Reactions

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

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

$$\%\text{ yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% \qquad (3.5)$$

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

Example 3.16 Titanium is a strong, lightweight, corrosion-resistant metal that is used in rockets, aircraft, jet engines, and bicycle frames. It is prepared by the reaction of titanium(IV) chloride with molten magnesium between 950°C and 1150°C:

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

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

The frame of this bicycle is made of titanium.

Reasoning and Solution We follow the procedure in Example 3.15 to find out which of the two reactants is the limiting agent. This knowledge will enable us to calculate the theoretical yield. The percent yield can then be obtained by applying Equation (3.5).

(a) First we calculate the number of moles of $TiCl_4$ and Mg initially present:

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

$$\text{moles of Mg} = 1.13 \times 10^7\ \cancel{\text{g Mg}} \times \frac{1\text{ mol Mg}}{24.31\ \cancel{\text{g Mg}}} = 4.65 \times 10^5\text{ mol Mg}$$

Next, we must determine which of the two substances is the limiting reagent. From the balanced equation we see that 1 mol $TiCl_4 \Leftrightarrow$ 1 mol Ti and 2 mol Mg $\Leftrightarrow$ 1 mol Ti. Therefore, the amounts of Ti obtained from these two reactants are

$$1.87 \times 10^5\ \cancel{\text{mol TiCl}_4} \times \frac{1\text{ mol Ti}}{1\text{ mol TiCl}_4} = 1.87 \times 10^5\text{ mol Ti}$$

and

$$4.65 \times 10^5\ \cancel{\text{mol Mg}} \times \frac{1\text{ mol Ti}}{2\ \cancel{\text{mol Mg}}} = 2.33 \times 10^5\text{ mol Ti}$$

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

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

(b) To find the percent yield, we write

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

Similar Problems: 3.85, 3.87.

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

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

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

Summary

Atomic masses are measured in atomic mass units (amu), a relative unit based on a value of exactly 12 for the carbon-12 isotope. The atomic mass given for the atoms of a particular element is usually the average of the naturally occurring isotope distribution of that element. The molecular mass of a molecule is the sum of the atomic masses of the atoms in the molecule. Both atomic mass and molecular mass can be accurately determined with a mass spectrometer.

A mole is an Avogadro's number (6.022×10^{23}) of atoms, molecules, or other particles. The molar mass (in grams) of an element or a compound is numerically equal to the mass of the atom, molecule, or formula unit (in amu) and contains an Avogadro's number of atoms (in the case of elements), molecules, or simplest formula units (in the case of ionic compounds).

The percent composition by mass of a compound is the percent by mass of each element present. If we know the percent composition by mass of a compound, we can deduce the empirical formula of the compound and also the molecular formula of the compound if the approximate molar mass is known.

Chemical changes, called chemical reactions, are represented by chemical equations. Substances that undergo change—the reactants—are written on the left and substances formed—the products—appear on the right of the arrow. Chemical equations must be balanced, in accordance with the law of conservation of mass. The number of atoms of each type of element in the reactants and products must be equal.

Stoichiometry is the quantitative study of products and reactants in chemical reactions. Stoichiometric calculations are best done by expressing both the known and unknown quantities in terms of moles and then converting to other units if necessary. A limiting reagent is the reactant that is present in the smallest stoichiometric amount.

It limits the amount of product that can be formed. The amount of product obtained in a reaction (the actual yield) may be less than the maximum possible amount (the theoretical yield). The ratio of the two is expressed as the percent yield.

Key Terms

Actual yield p. 000
Atomic mass p. 000
Atomic mass unit (amu) p. 000
Avogadro's number (N_A) p. 000
Chemical equation p. 000
Chemical reaction p. 000
Excess reagent p. 000
Limiting reagent p. 000
Molar mass ($\mathcal{M}$) p. 000
Mole (mol) p. 000
Molecular mass p. 000
Mole method p. 000
Percent composition p. 000
Percent yield p. 000
Product p. 000
Reactant p. 000
Stoichiometric amount p. 000
Stoichiometry p. 000
Theoretical yield p. 000

Questions and Problems

Atomic Mass and Avogadro's Number

Review Questions

3.1 What is an atomic mass unit?

3.2 What is the mass (in amu) of a carbon-12 atom?

3.3 When we look up the atomic mass of carbon, we find that its value is 12.01 amu rather than 12.00 amu as defined. Why?

3.4 Define the term "mole." What is the unit for mole in calculations? What does the mole have in common with the pair, the dozen, and the gross?

3.5 What does Avogadro's number represent?

3.6 Define molar mass. What are the commonly used units for molar mass?

3.7 Calculate the charge (in coulombs) and mass (in grams) of 1 mole of electrons.

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

Problems

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

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

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

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

3.13 What is the mass in grams of 13.2 amu?

3.14 How many amu are there in 8.4 g?

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

3.16 How many moles of cobalt atoms are there in 6.00×10^9 (6 billion) Co atoms?

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

3.18 How many grams of gold (Au) are there in 15.3 moles of Au?

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

3.20 What is the mass in grams of a single atom of each of these elements? (a) As, (b) Ni.

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

3.22 How many atoms are present in 3.14 g of copper (Cu)?

3.23 Which of these has more atoms: 1.10 g of hydrogen atoms or 14.7 g of chromium atoms?

3.24 Which of these has a greater mass: 2 atoms of lead or 5.1×10^{-23} mole of helium?

Molecular Mass

Problems

3.25 Calculate the molecular mass (in amu) of each of these substances: (a) CH_4, (b) H_2O, (c) H_2O_2, (d) C_6H_6, (e) PCl_5.

3.26 Calculate the molar mass of these substances: (a) S_8, (b) CS_2, (c) $CHCl_3$ (chloroform), (d) $C_6H_8O_6$ (ascorbic acid, or vitamin C).

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

3.28 How many moles of ethane (C_2H_6) are present in 0.334 g of C_2H_6?

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

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

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

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

Mass Spectrometry

Review Questions

3.33 Describe the operation of a mass spectrometer.

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

Problems

3.35 Carbon has two stable isotopes, $^{12}_{6}C$ and $^{13}_{6}C$, and fluorine has only one stable isotope, $^{19}_{9}F$. How many peaks would you observe in the mass spectrum of the positive ion of CF_4^+? Assume no decomposition of the ion into smaller fragments.

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

Percent Composition and Chemical Formulas

Review Questions

3.37 Define percent composition by mass of a compound.

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

3.39 What does the word “empirical” in empirical formula mean?

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

Problems

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

3.42 Sodium, a member of the alkali metal family (Group 1A), is very reactive and thus is never found in nature in its elemental state. It forms ionic compounds with members of the halogen family (Group 7A). Calculate the percent composition by mass of all the elements in each of these compounds: (a) NaF, (b) NaCl, (c) NaBr, (d) NaI.

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

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

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

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

(a) Urea, $(NH_2)_2CO$
(b) Ammonium nitrate, NH_4NO_3
(c) Guanidine, $HNC(NH_2)_2$
(d) Ammonia, NH_3

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

3.48 How many grams of sulfur (S) are needed to combine with 246 g of mercury (Hg) to form HgS?

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

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

3.51 What are the empirical formulas of the compounds with these compositions? (a) 2.1% H, 65.3% O, 32.6% S; (b) 20.2% Al, 79.8% Cl; (c) 40.1% C, 6.6% H, 53.3% O; (d) 18.4% C, 21.5% N, 60.1% K.

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

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

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

Chemical Reactions and Chemical Equations

Review Questions

3.55 Define the following terms: chemical reaction, reactant, product.

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

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

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

Problems

3.59 Balance these equations using the method outlined in Section 3.7:

(a) $C + O_2 \rightarrow CO$
(b) $CO + O_2 \rightarrow CO_2$
(c) $H_2 + Br_2 \rightarrow HBr$
(d) $K + H_2O \rightarrow KOH + H_2$
(e) $Mg + O_2 \rightarrow MgO$
(f) $O_3 \rightarrow O_2$
(g) $H_2O_2 \rightarrow H_2O + O_2$
(h) $N_2 + H_2 \rightarrow NH_3$
(i) $Zn + AgCl \rightarrow ZnCl_2 + Ag$
(j) $S_8 + O_2 \rightarrow SO_2$

3.60 Balance these equations using the method outlined in Section 3.7:

(a) $N_2O_5 \rightarrow N_2O_4 + O_2$
(b) $KNO_3 \rightarrow KNO_2 + O_2$
(c) $NH_4NO_3 \rightarrow N_2O + H_2O$
(d) $NH_4NO_2 \rightarrow N_2 + H_2O$
(e) $NaHCO_3 \rightarrow Na_2CO_3 + H_2O + CO_2$
(f) $P_4O_{10} + H_2O \rightarrow H_3PO_4$
(g) $HCl + CaCO_3 \rightarrow CaCl_2 + H_2O + CO_2$
(h) $Al + H_2SO_4 \rightarrow Al_2(SO_4)_3 + H_2$
(i) $CO_2 + KOH \rightarrow K_2CO_3 + H_2O$
(j) $CH_4 + O_2 \rightarrow CO_2 + H_2O$

Amounts of Reactants and Products

Review Questions

3.61 Define these terms: stoichiometry, stoichiometric amounts, limiting reagent, excess reagent, theoretical yield, actual yield, percent yield.

3.62 On what law is stoichiometry based?

3.63 Describe the basic steps involved in the mole method.

3.64 Why is it essential to use balanced equations in solving stoichiometric problems?

Problems

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

3.72 For many years the recovery of gold (that is, the separation of gold from other materials) involved the treatment of gold by isolation from other substances, using potassium cyanide:

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

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

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

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

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

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

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

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

Limiting Reagents

Review Questions

3.77 Define limiting reagent and excess reagent. What is the significance of the limiting reagent in predicting the amount of the product obtained in a reaction?

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

Problems

3.79 Nitric oxide (NO) reacts instantly with oxygen gas to give nitrogen dioxide (NO_2), a dark-brown gas:

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

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

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

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

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

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

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

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

3.82 Consider the reaction

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

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

Reaction Yield

Review Questions

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

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

Problems

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

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

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

3.86 Nitroglycerin ($C_3H_5N_3O_9$) is a powerful explosive. Its decomposition may be represented by

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

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

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

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

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

3.88 Ethylene (C_2H_4), an important industrial organic chemical, can be prepared by heating hexane (C_6H_{14}) at 800°C:

$$C_6H_{14} \longrightarrow C_2H_4 + \text{other products}$$

If the yield of ethylene production is 42.5 percent, what mass of hexane must be reacted to produce 481 g of ethylene?

Additional Problems

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

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

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

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

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

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

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

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

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

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

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

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

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

3.98 Suppose you are given a cube made of magnesium (Mg) metal of edge length 1.0 cm. (a) Calculate the number of Mg atoms in the cube. (b) Atoms are spherical. Therefore, the Mg atoms in the cube cannot fill all of the available space. If only 74 percent of the space inside the cube is taken up by Mg atoms, calculate the radius in picometers of an Mg atom. (The density of Mg is 1.74 g/cm^3 and the volume of a sphere of radius r is $\frac{4}{3}\pi r^3$.)

3.99 A certain sample of coal contains 1.6 percent sulfur by mass. When the coal is burned, the sulfur is converted to sulfur dioxide. To prevent air pollution, this sulfur dioxide is treated with calcium oxide (CaO) to form calcium sulfite ($CaSO_3$). Calculate the daily mass (in kilograms) of CaO needed by a power plant that uses 6.60×10^6 kg of coal per day.

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

3.101 Octane (C_8H_{18}) is a component of gasoline. Complete combustion of octane yields CO_2 and H_2O. Incomplete combustion produces CO and H_2O, which not only reduces the efficiency of the engine using the fuel but is also toxic. In a certain test run, 1.000 gallon of octane is burned in an engine.

The total mass of CO, CO_2, and H_2O produced is 11.53 kg. Calculate the efficiency of the process; that is, calculate the fraction of octane converted to CO_2. The density of octane is 2.650 kg/gallon.

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

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

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

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

Special Problems

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

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

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

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

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

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

Answers to Practice Exercises

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