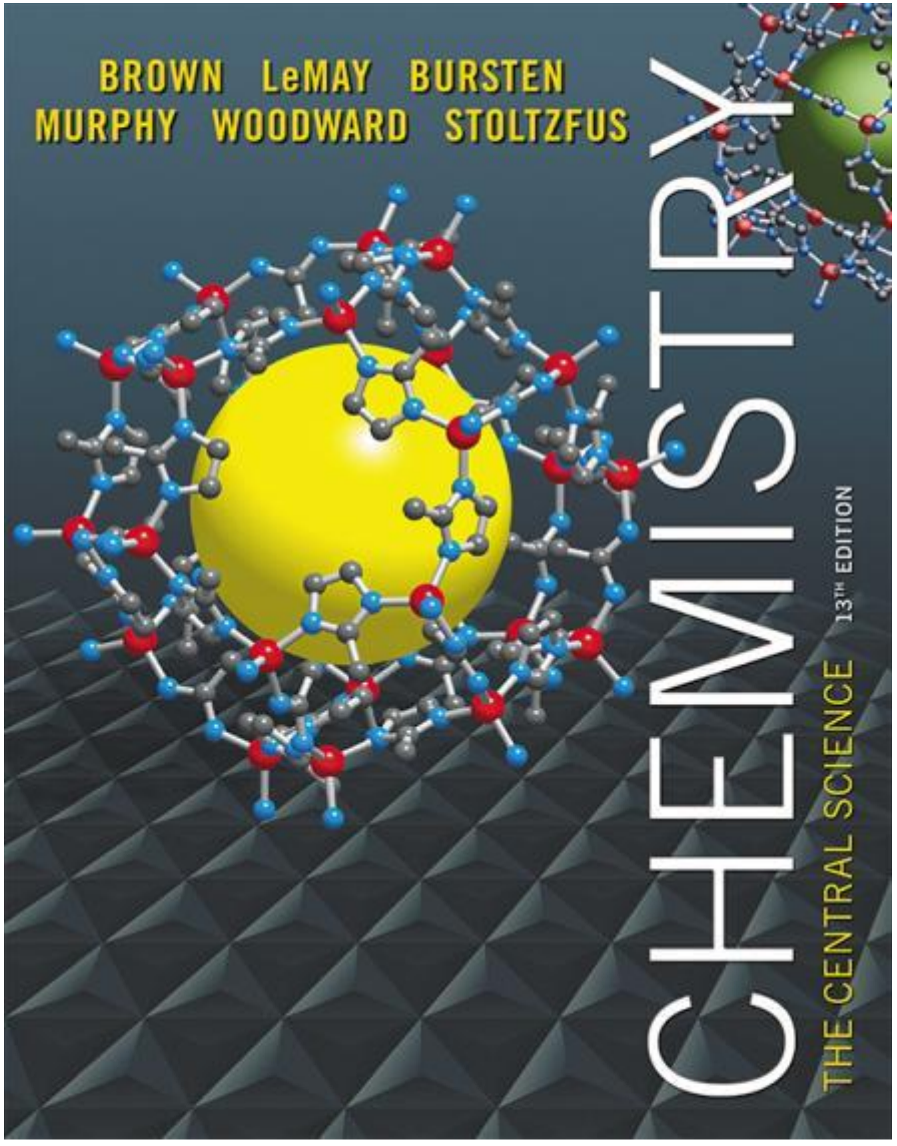

Lecture Presentation

Chapter 3

Chemical Reactions and Reaction Stoichiometry

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Hamden, CT

Stoichiometry

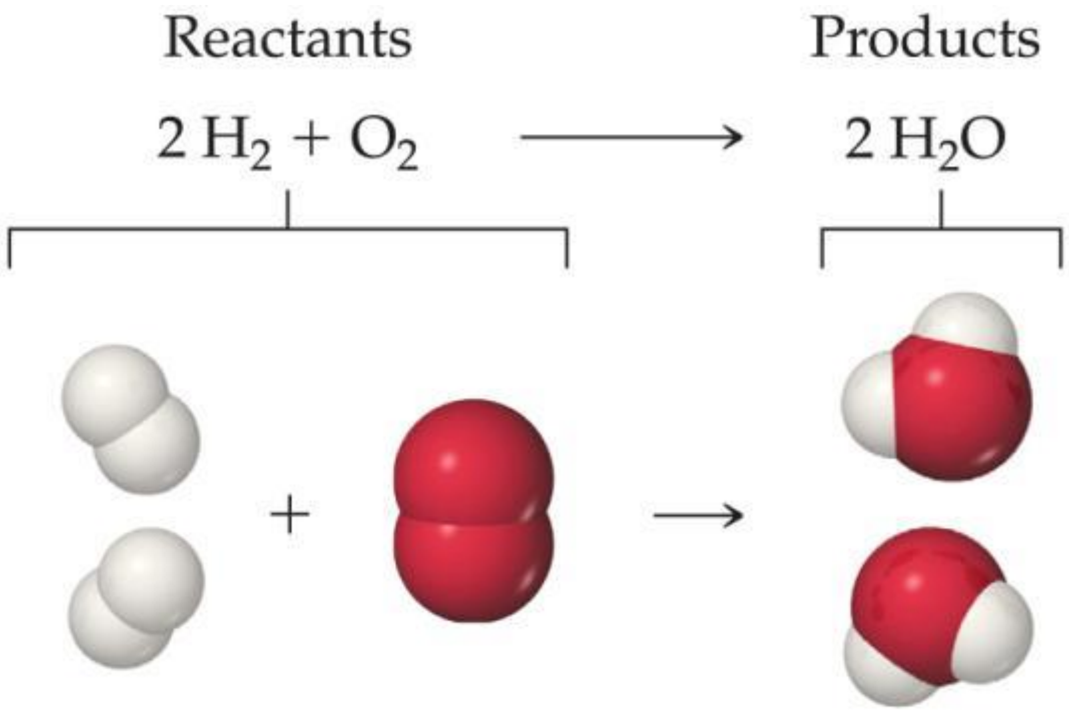
- The study of the mass relationships in chemistry
- Based on the Law of Conservation of Mass (Antoine Lavoisier, 1789)

"We may lay it down as an incontestable axiom that, in all the operations of art and nature, nothing is created; an equal amount of matter exists both before and after the experiment. Upon this principle, the whole art of performing chemical experiments depends."

—Antoine Lavoisier

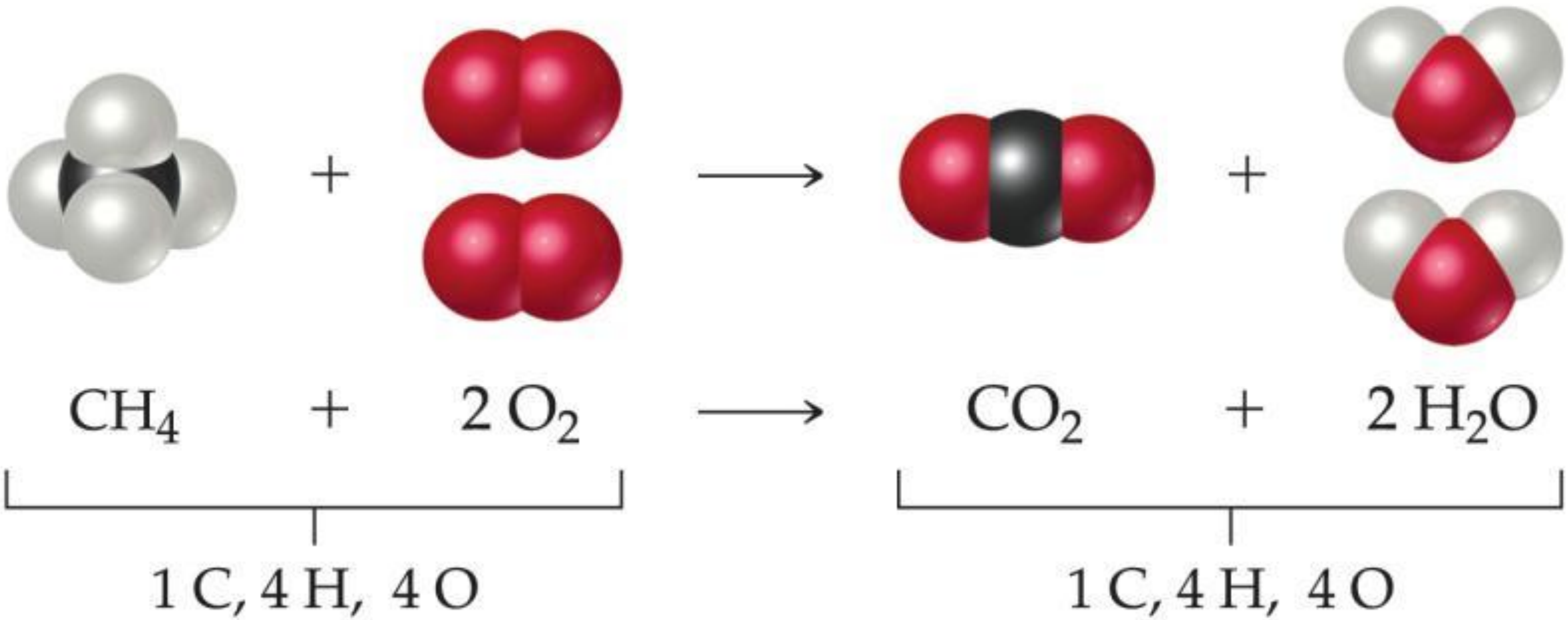
Chemical Equations

Chemical equations are concise representations of chemical reactions.



What Is in a Chemical Equation?

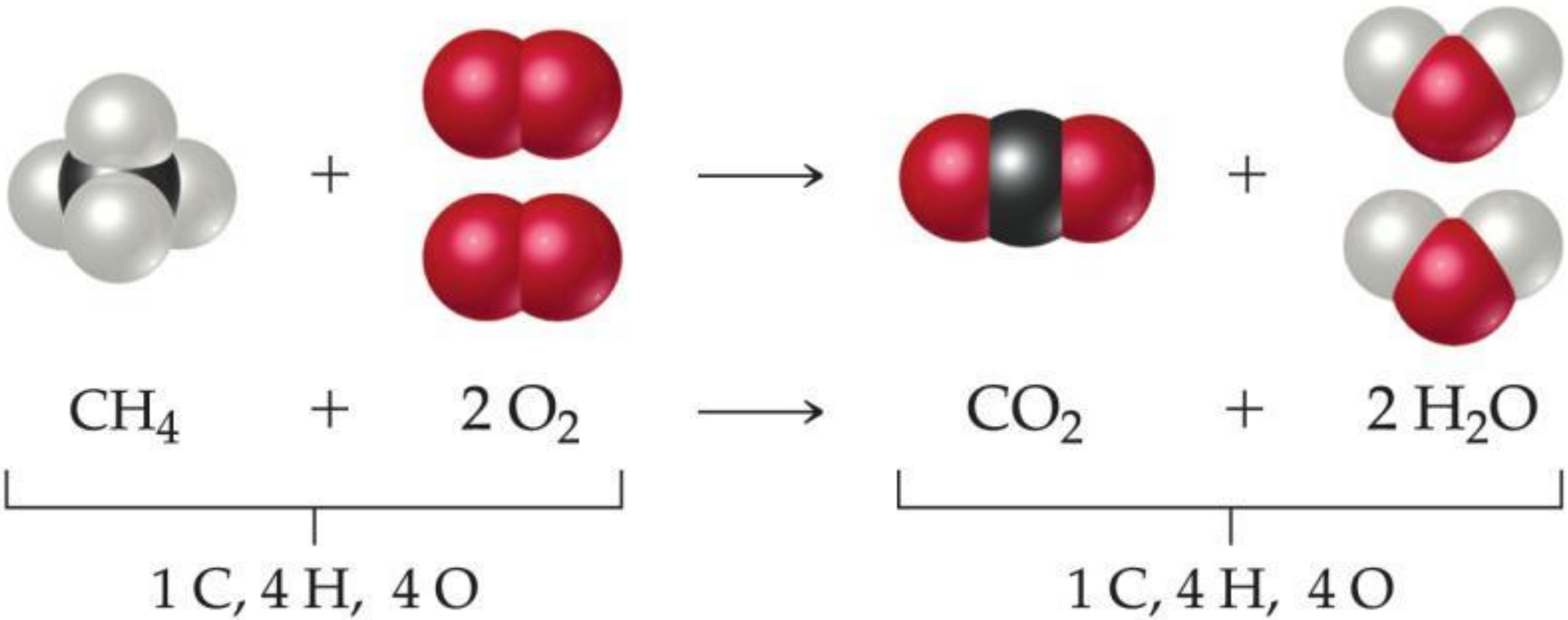
$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



Reactants appear on the left side of the equation.

What Is in a Chemical Equation?

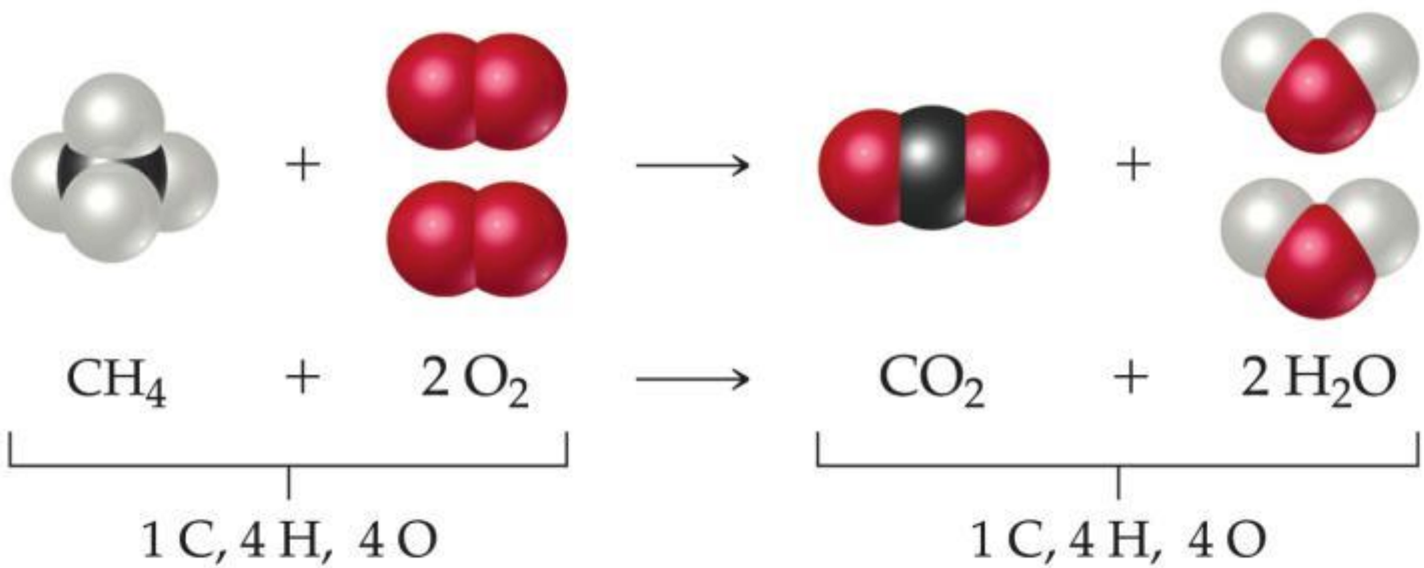
$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



Products appear on the right side of the equation.

What Is in a Chemical Equation?

$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



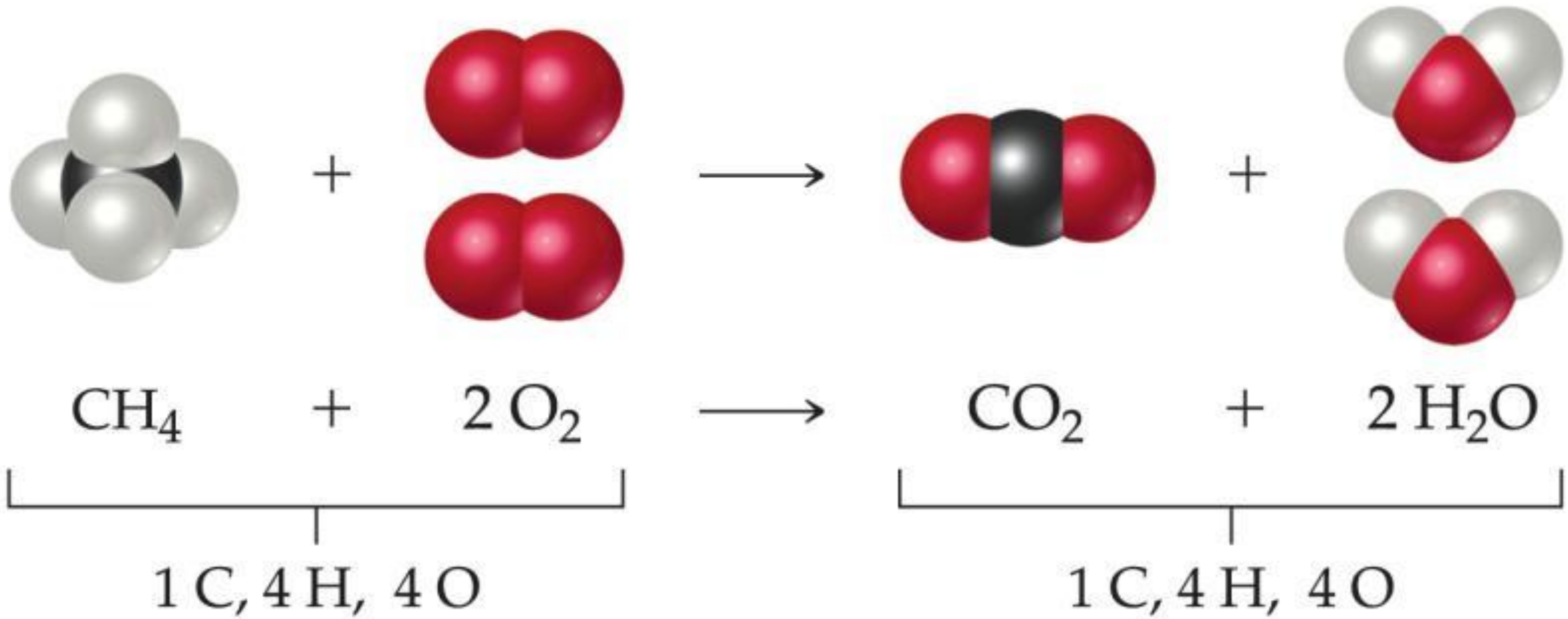
The **states** of the reactants and products are written in parentheses to the right of each compound.

(g) = gas; (l) = liquid; (s) = solid;

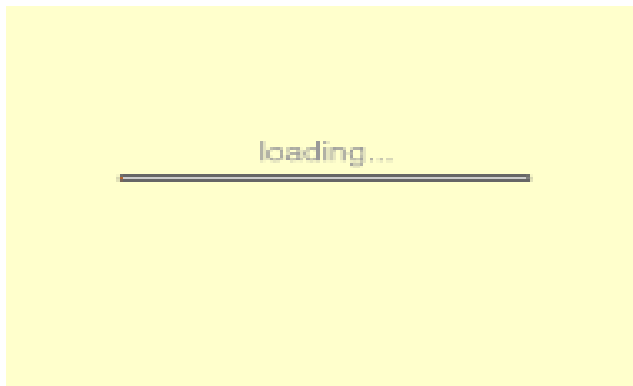
(aq) = in aqueous solution

What Is in a Chemical Equation?

$$CH_4(g) + 2O_2(g) \longrightarrow CO_2(g) + 2H_2O(g)$$



Coefficients are inserted to balance the equation to follow the law of conservation of mass.



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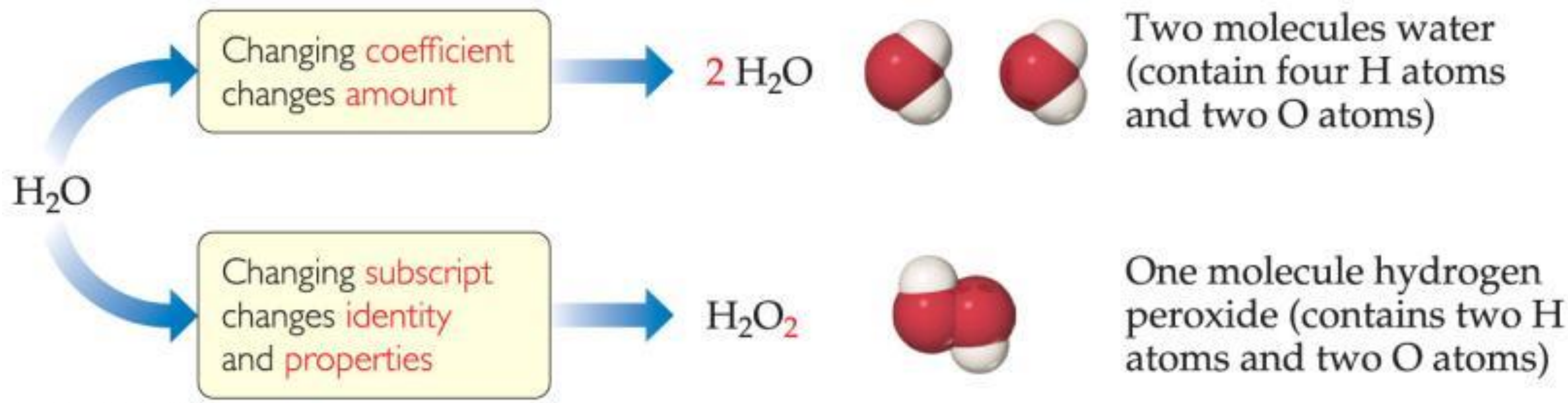
Stoichiometry

Why Do We Add Coefficients Instead of Changing Subscripts to Balance?



- Hydrogen and oxygen can make water OR hydrogen peroxide:
  - $2\ H_2(g) + O_2(g) \rightarrow 2\ H_2O(l)$
  - $H_2(g) + O_2(g) \rightarrow H_2O_2(l)$

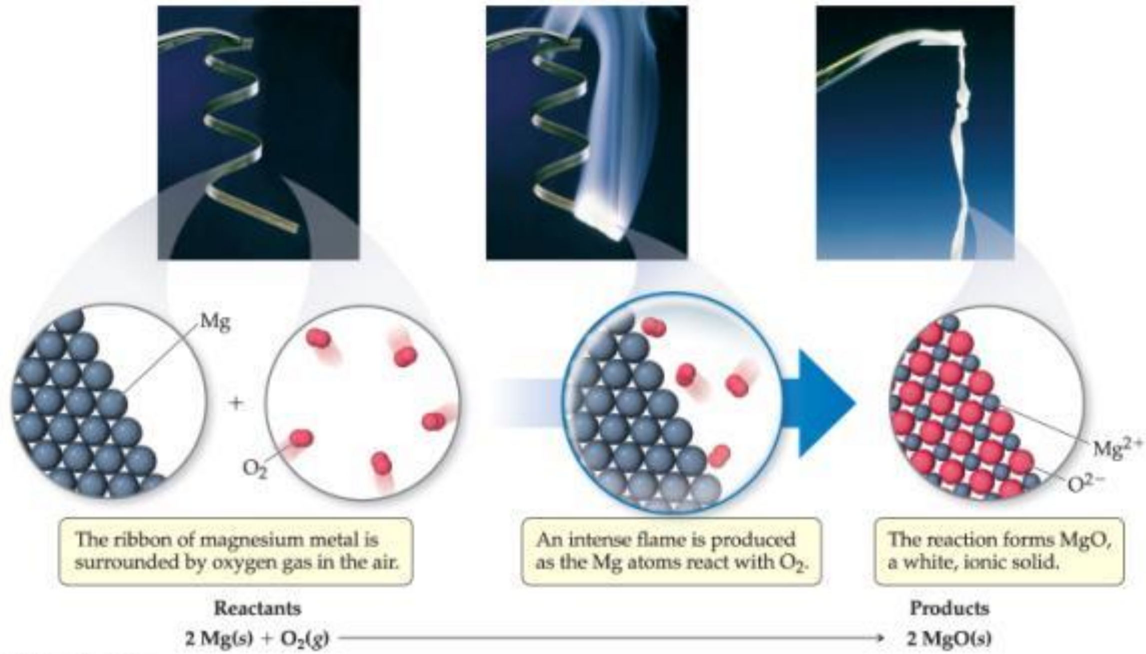
Stoichiometry

Three Types of Reactions

- Combination reactions
- Decomposition reactions
- Combustion reactions

Recognizing a pattern of reactivity for a class of substances gives you a broader understanding than merely memorizing a large number of unrelated reactions.

Combination Reactions



In **combination reactions** two or more substances react to form one product.

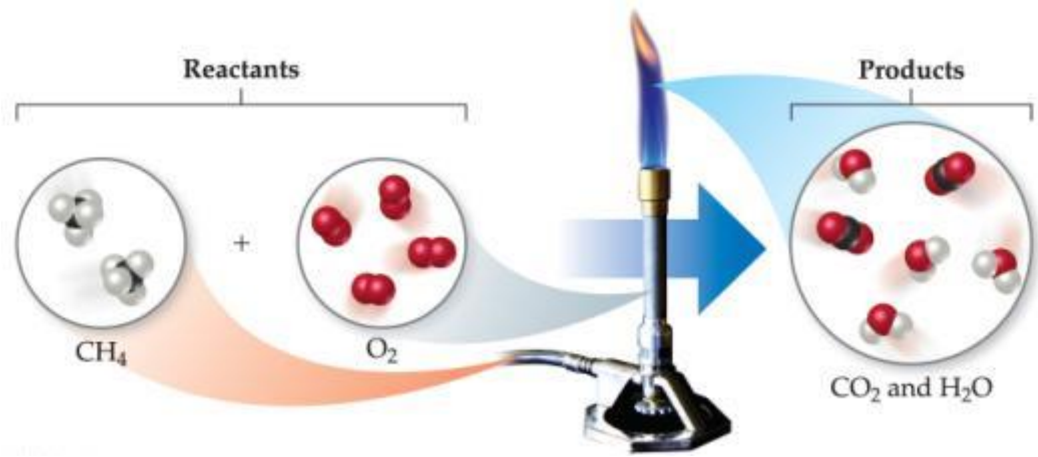
- Examples:
  - $2\ Mg(s) + O_2(g) \longrightarrow 2\ MgO(s)$
  - $N_2(g) + 3\ H_2(g) \longrightarrow 2\ NH_3(g)$
  - $C_3H_6(g) + Br_2(l) \longrightarrow C_3H_6Br_2(l)$

Decomposition Reactions

In a **decomposition reaction** one substance breaks down into two or more substances.

- Examples:
  - $CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$
  - $2\ KClO_3(s) \longrightarrow 2\ KCl(s) + O_2(g)$
  - $2\ NaN_3(s) \longrightarrow 2\ Na(s) + 3\ N_2(g)$

Combustion Reactions



- **Combustion reactions** are generally rapid reactions that produce a flame.
- **Combustion reactions** most often involve oxygen in the air as a reactant.

- Examples:
  - $CH_4(g) + 2\ O_2(g) \longrightarrow CO_2(g) + 2\ H_2O(g)$
  - $C_3H_8(g) + 5\ O_2(g) \longrightarrow 3\ CO_2(g) + 4\ H_2O(g)$

Formula Weight (FW)

- A **formula weight** is the sum of the atomic weights for the atoms in a chemical formula.
- This is the quantitative significance of a formula.
- The formula weight of calcium chloride, $CaCl_2$, would be

$$\begin{array}{r} \text{Ca: } 1(40.08\text{ amu}) \\ \underline{+\text{ Cl: } 2(35.453\text{ amu})} \\ 110.99\text{ amu} \end{array}$$

Molecular Weight (MW)

- A **molecular weight** is the sum of the atomic weights of the atoms in a molecule.
- For the molecule ethane, C_2H_6, the molecular weight would be

$$\begin{array}{rr} \text{C:} & 2(12.011\ \text{amu}) \\ +\ \text{H:} & 6(1.00794\ \text{amu}) \\ \hline & 30.070\ \text{amu} \end{array}$$

Ionic Compounds and Formulas

- Remember, ionic compounds exist with a three-dimensional order of ions. There is no simple group of atoms to call a molecule.
- As such, ionic compounds use empirical formulas and formula weights (not molecular weights).

Percent Composition

One can find the percentage of the mass of a compound that comes from each of the elements in the compound by using this equation:

$$\% \text{ Element} = \frac{(\text{number of atoms})(\text{atomic weight})}{(\text{FW of the compound})} \times 100$$

Percent Composition

So the percentage of carbon in ethane is

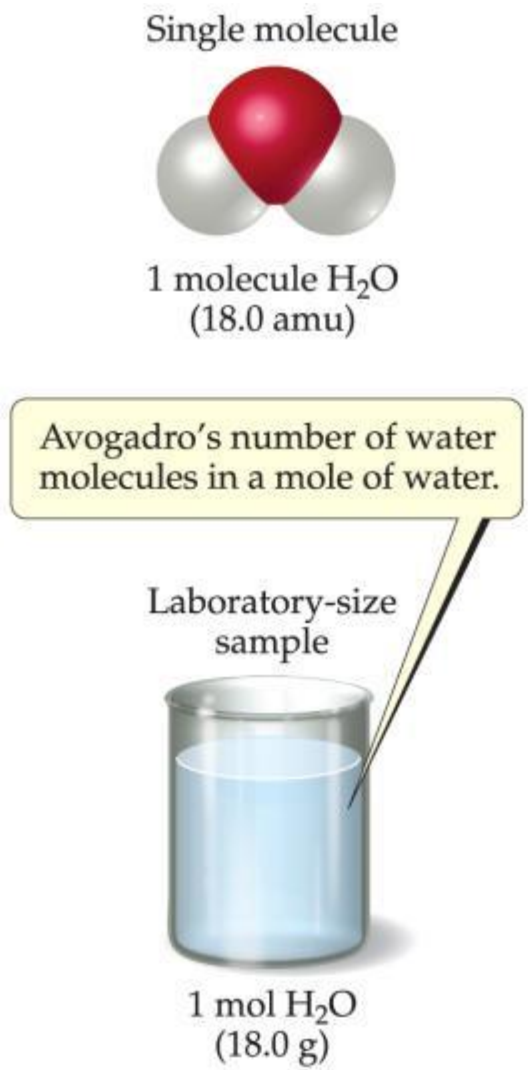
$$\%C = \frac{(2)(12.011\ \text{amu})}{(30.070\ \text{amu})}$$

$$= \frac{24.022\ \text{amu}}{30.070\ \text{amu}} \times 100$$

$$= 79.887\%$$

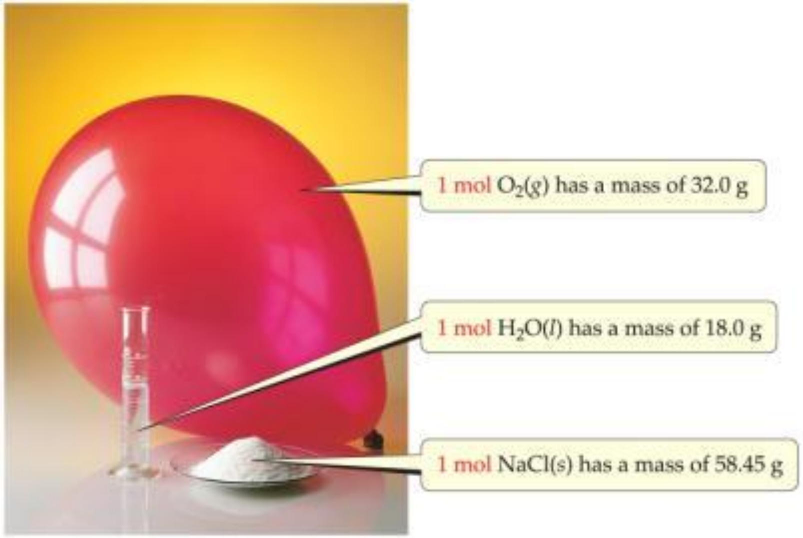
Avogadro's Number

- In a lab, we cannot work with individual molecules. They are too small.
- 6.02 × 10^{23} atoms or molecules is an amount that brings us to lab size. It is ONE MOLE.
- One mole of ^{12}C has a mass of 12.000 g.



Molar Mass

- A **molar mass** is the mass of 1 mol of a substance (i.e., g/mol).
- The molar mass of an element is the atomic weight for the element from the periodic table. If it is diatomic, it is twice that atomic weight.
- The formula weight (in amu's) will be the same number as the molar mass (in g/mol).



Using Moles

Moles provide a bridge from the molecular scale to the real-world scale.

Mole Relationships

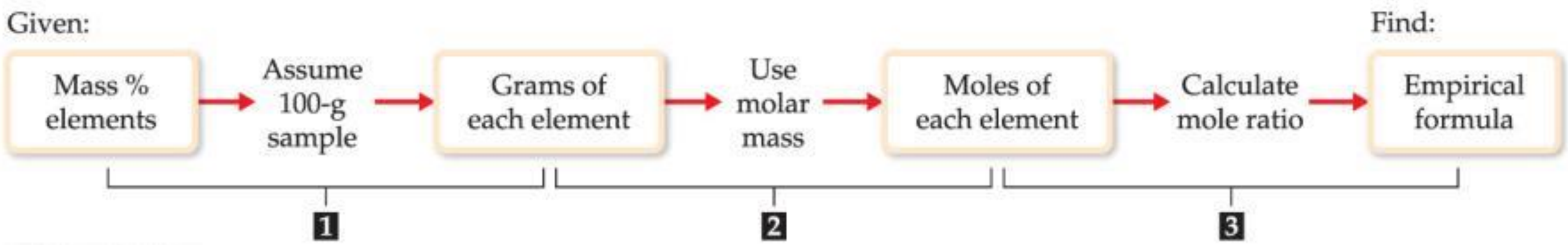
Table 3.2 Mole Relationships

Name of Substance	Formula	Formula Weight (amu)	Molar Mass (g/mol)	Number and Kind of Particles in One Mole
Atomic nitrogen	N	14.0	14.0	6.02×10^{23} N atoms
Molecular nitrogen	N_2	28.0	28.0	$\begin{cases} 6.02 \times 10^{23}\ N_2 \text{ molecules} \\ 2(6.02 \times 10^{23})\ N \text{ atoms} \end{cases}$
Silver	Ag	107.9	107.9	6.02×10^{23} Ag atoms
Silver ions	Ag^+	107.9[a]	107.9	6.02×10^{23} Ag^+ ions
Barium chloride	$BaCl_2$	208.2	208.2	$\begin{cases} 6.02 \times 10^{23}\ BaCl_2 \text{ formula units} \\ 6.02 \times 10^{23}\ Ba^{2+} \text{ ions} \\ 2(6.02 \times 10^{23})\ Cl^- \text{ ions} \end{cases}$

[a]Recall that the mass of an electron is more than 1800 times smaller than the masses of the proton and the neutron; thus, ions and atoms have essentially the same mass.

- One mole of atoms, ions, or molecules contains Avogadro's number of those particles.
- One mole of molecules or formula units contains Avogadro's number times the number of atoms or ions of each element in the compound.

Determining Empirical Formulas



One can determine the empirical formula from the percent composition by following these three steps.

Determining Empirical Formulas—an Example

The compound *para*-aminobenzoic acid (you may have seen it listed as PABA on your bottle of sunscreen) is composed of carbon (61.31%), hydrogen (5.14%), nitrogen (10.21%), and oxygen (23.33%). Find the empirical formula of PABA.

Determining Empirical Formulas—an Example

Assuming 100.00 g of *para*-aminobenzoic acid,

$$\text{C:} \quad 61.31\text{ g} \times \frac{1\text{ mol}}{12.01\text{ g}} = 5.105\text{ mol C}$$

$$\text{H:} \quad 5.14\text{ g} \times \frac{1\text{ mol}}{1.01\text{ g}} = 5.09\text{ mol H}$$

$$\text{N:} \quad 10.21\text{ g} \times \frac{1\text{ mol}}{14.01\text{ g}} = 0.7288\text{ mol N}$$

$$\text{O:} \quad 23.33\text{ g} \times \frac{1\text{ mol}}{16.00\text{ g}} = 1.456\text{ mol O}$$

Determining Empirical Formulas—an Example

Calculate the mole ratio by dividing by the smallest number of moles:

$$\text{C:} \quad \frac{5.105\ \text{mol}}{0.7288\ \text{mol}} = 7.005 \approx 7$$

$$\text{H:} \quad \frac{5.09\ \text{mol}}{0.7288\ \text{mol}} = 6.984 \approx 7$$

$$\text{N:} \quad \frac{0.7288\ \text{mol}}{0.7288\ \text{mol}} = 1.000$$

$$\text{O:} \quad \frac{1.458\ \text{mol}}{0.7288\ \text{mol}} = 2.001 \approx 2$$

Determining Empirical Formulas—an Example

These are the subscripts for the empirical formula:

$C_7H_7NO_2$

Determining a Molecular Formula

- Remember, the number of atoms in a molecular formula is a multiple of the number of atoms in an empirical formula.
- If we find the empirical formula and know a molar mass (molecular weight) for the compound, we can find the molecular formula.

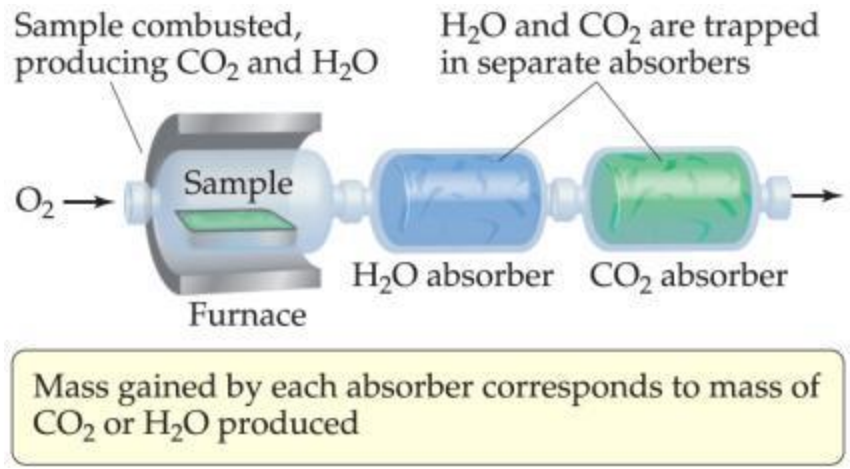
Determining a Molecular Formula—an Example

- The empirical formula of a compound was found to be CH. It has a molar mass of 78 g/mol. What is its molecular formula?
- Solution:

Whole-number multiple = 78/13 = 6

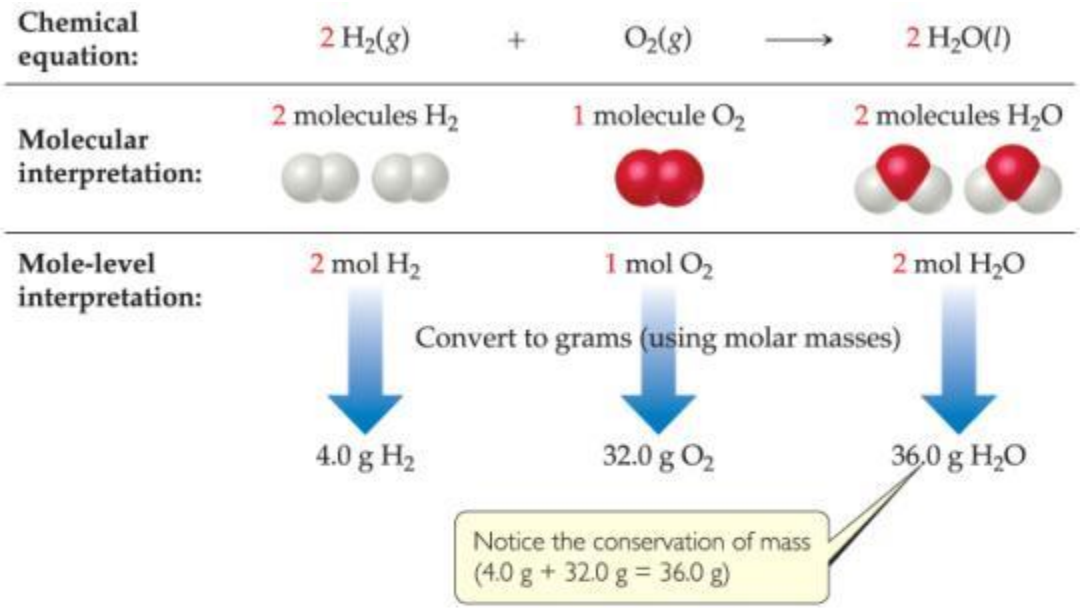
The molecular formula is C_6H_6.

Combustion Analysis



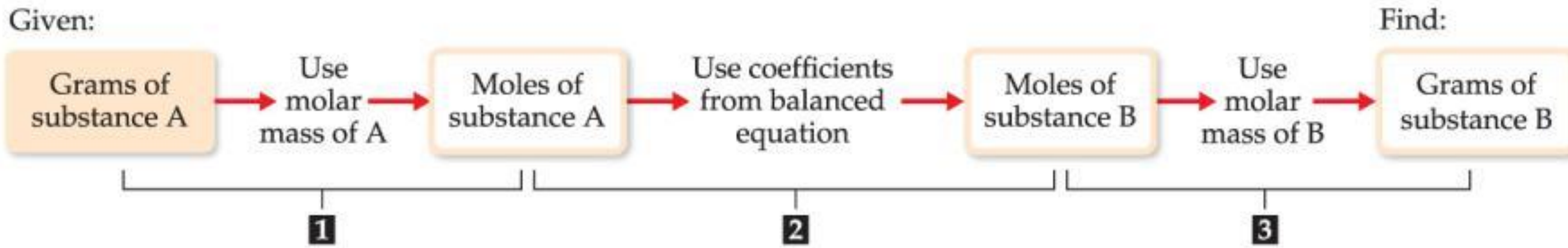
- Compounds containing C, H, and O are routinely analyzed through combustion in a chamber like the one shown in Figure 3.14.
  - C is determined from the mass of CO_2 produced.
  - H is determined from the mass of H_2O produced.
  - O is determined by the difference after C and H have been determined.

Quantitative Relationships



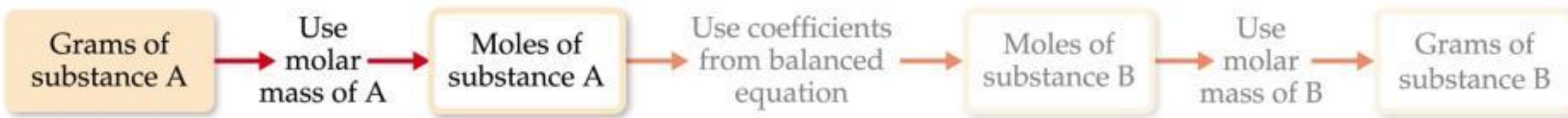
- The coefficients in the balanced equation show
  - relative numbers of *molecules* of reactants and products.
  - relative numbers of *moles* of reactants and products, which can be converted to *mass*.

Stoichiometric Calculations



We have already seen in this chapter how to convert from grams to moles or moles to grams. The NEW calculation is how to compare two DIFFERENT materials, using the MOLE RATIO from the balanced equation!

An Example of a Stoichiometric Calculation



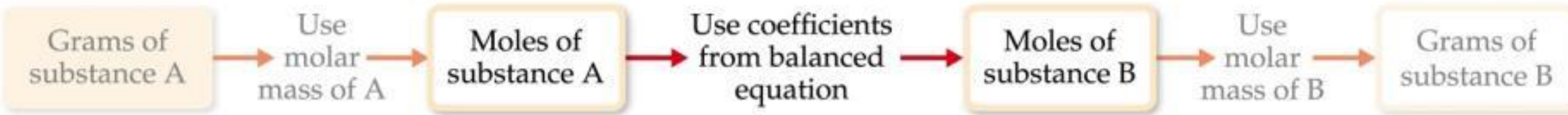
$$\text{Moles } C_6H_{12}O_6 = (1.00\ \cancel{g\ C_6H_{12}O_6})\left(\frac{1\ \text{mol}\ C_6H_{12}O_6}{180.0\ \cancel{g\ C_6H_{12}O_6}}\right)$$

- How many grams of water can be produced from 1.00 g of glucose?

$$C_6H_{12}O_6(s) + 6\ O_2(g) \rightarrow 6\ CO_2(g) + 6\ H_2O(l)$$

- There is 1.00 g of glucose to start.
- The first step is to convert it to moles.

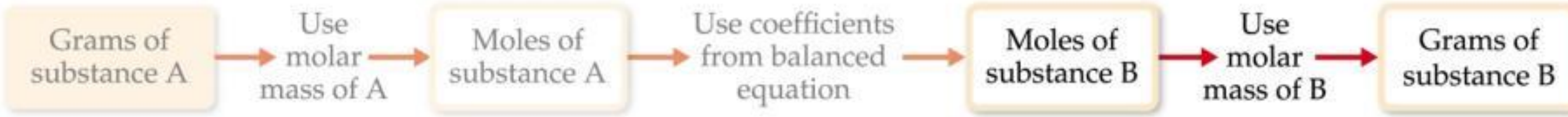
An Example of a Stoichiometric Calculation



$$\text{Moles } H_2O = (1.00 \text{ g } \cancel{C_6H_{12}O_6})\left(\frac{1 \text{ mol } \cancel{C_6H_{12}O_6}}{180.0 \text{ g } \cancel{C_6H_{12}O_6}}\right)\left(\frac{6 \text{ mol } H_2O}{1 \text{ mol } \cancel{C_6H_{12}O_6}}\right)$$

- The NEW calculation is to convert moles of one substance in the equation to moles of another substance.
- The MOLE RATIO comes from the balanced equation.

An Example of a Stoichiometric Calculation



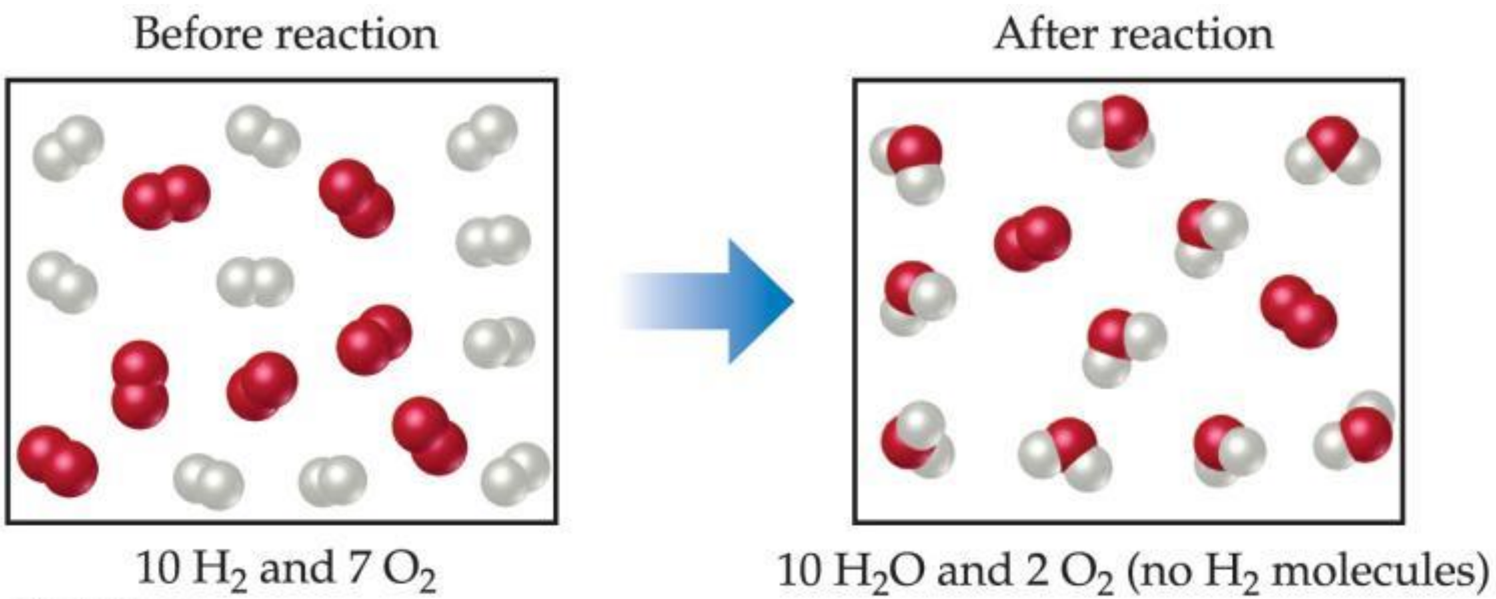
$$\text{Grams } H_2O = (1.00 \text{ g } \cancel{C_6H_{12}O_6})\left(\frac{1 \text{ } \cancel{\text{mol } C_6H_{12}O_6}}{180.0 \text{ g } \cancel{C_6H_{12}O_6}}\right)\left(\frac{6 \text{ } \cancel{\text{mol } H_2O}}{1 \text{ } \cancel{\text{mol } C_6H_{12}O_6}}\right)\left(\frac{18.0 \text{ g } H_2O}{1 \text{ } \cancel{\text{mol } H_2O}}\right)$$

$$= 0.600 \text{ g } H_2O$$

- There is 1.00 g of glucose to start.
- The first step is to convert it to moles.

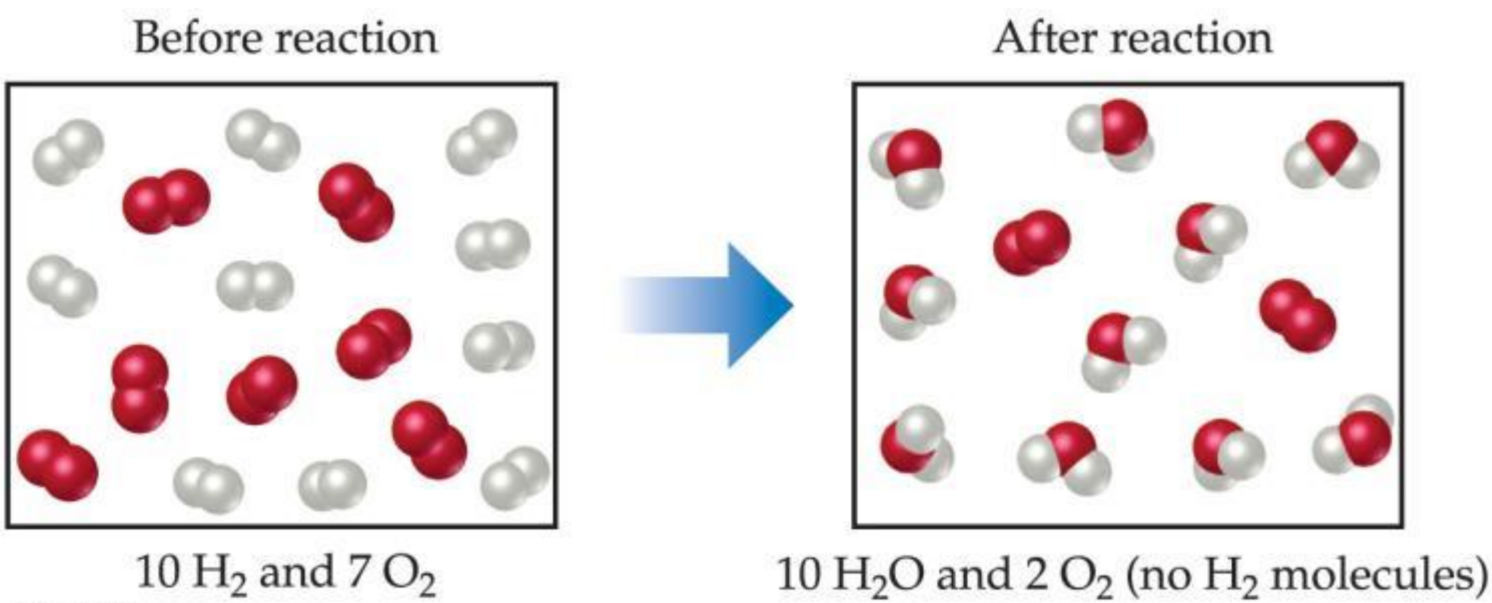
Limiting Reactants

- The **limiting reactant** is the reactant present in the smallest stoichiometric amount.
  – In other words, it's the reactant you'll run out of first (in this case, the H_2).



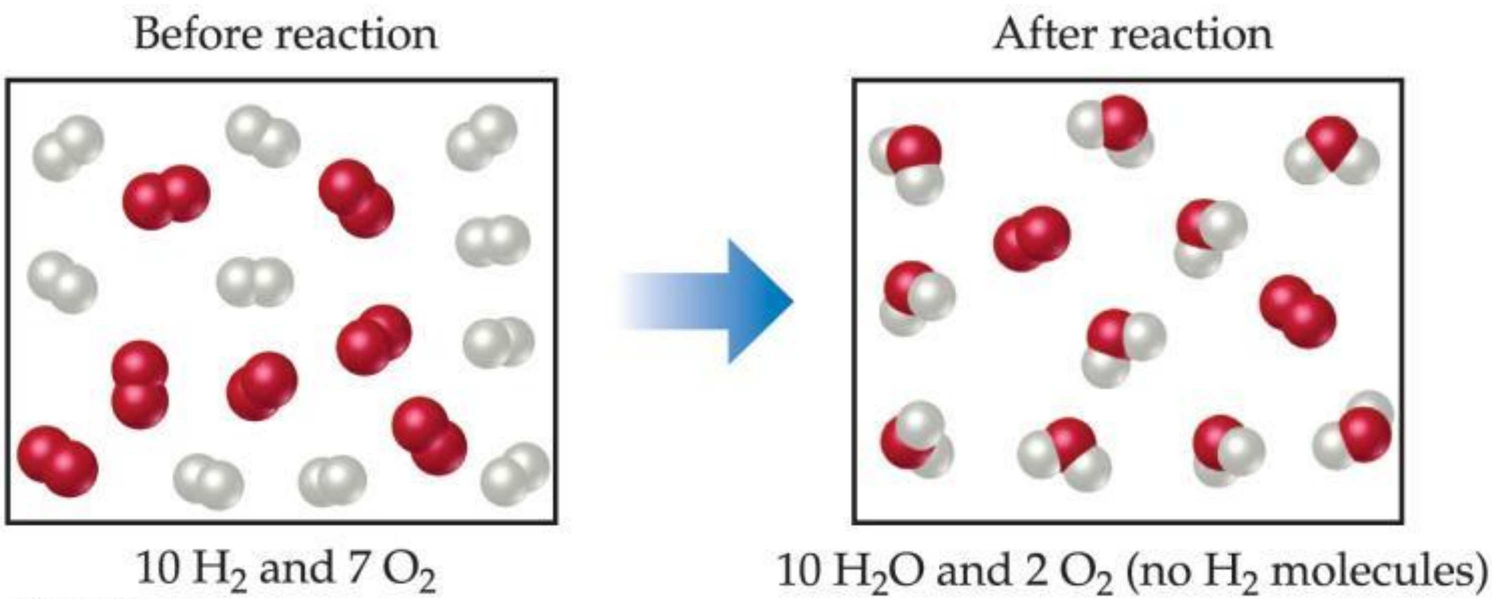
Limiting Reactants

In the example below, the O_2 would be the **excess reagent**.



Limiting Reactants

- The **limiting reactant** is used in all stoichiometry calculations to determine amounts of products and amounts of any other reactant(s) used in a reaction.



Theoretical Yield

- The **theoretical yield** is the maximum amount of product that can be made.
  - In other words, it's the amount of product possible as calculated through the stoichiometry problem.
- This is different from the **actual yield**, which is the amount one actually produces and measures.

Percent Yield

One finds the **percent yield** by comparing the amount actually obtained (actual yield) to the amount it was possible to make (theoretical yield):

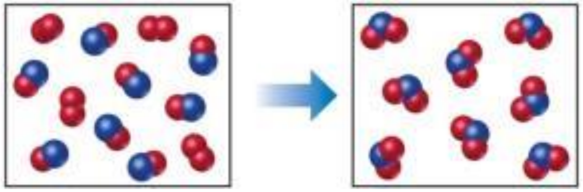
$$\text{Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

Operational Skills

- Calculating the formula weight from a formula.
- Calculating the mass of an atom or molecule.
- Converting moles of substance to grams and vice versa.
- Calculating the number of molecules in a given mass.
- Calculating the percentage composition from the formula.
- Calculating the mass of an element in a given mass of compound.
- Calculating the percentages C and H by combustion.
- Determining the empirical formula from percentage composition.
- Determining the true molecular formula.
- Relating quantities in a chemical equation.
- Calculating with a limiting reagent.

Sample Exercise 3.1 Interpreting and Balancing Chemical Equations

The following diagram represents a chemical reaction in which the red spheres are oxygen atoms and the blue spheres are nitrogen atoms. **(a)** Write the chemical formulas for the reactants and products. **(b)** Write a balanced equation for the reaction. **(c)** Is the diagram consistent with the law of conservation of mass?



Solution

(a) The left box, which represents reactants, contains two kinds of molecules, those composed of two oxygen atoms (O_2) and those composed of one nitrogen atom and one oxygen atom (NO). The right box, which represents products, contains only one kind of molecule, which is composed of one nitrogen atom and two oxygen atoms (NO_2).

(b) The unbalanced chemical equation is $O_2 + NO \rightarrow NO_2$ (unbalanced)

An inventory of atoms on each side of the equation shows that there are one N and three O on the left side of the arrow and one N and two O on the right. To balance O we must increase the number of O atoms on the right while keeping the coefficients for NO and NO_2 equal. Sometimes a trial-and-error approach is required; we need to go back and forth several times from one side of an equation to the other, changing coefficients first on one side of the equation and then the other until it is balanced. In our present case, let's start by increasing the number of O atoms on the right side of the equation by placing the coefficient 2 in front of NO_2:

$$O_2 + NO \rightarrow 2\ NO_2 \text{ (unbalanced)}$$

Sample Exercise 3.1 Interpreting and Balancing Chemical Equations

Continued

Now the equation gives two N atoms and four O atoms on the right, so we go back to the left side. Placing the coefficient 2 in front of NO balances both N and O:

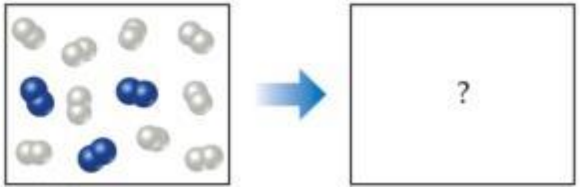
$$\underbrace{O_2 + 2\,NO}_{2\,N,\,4\,O} \longrightarrow \underbrace{2\,NO_2}_{2\,N,\,4\,O} \quad \text{(balanced)}$$

(c) The reactants box contains four O_2 and eight NO. Thus, the molecular ratio is one O_2 for each two NO, as required by the balanced equation. The products box contains eight NO_2, which means the number of NO_2 product molecules equals the number of NO reactant molecules, as the balanced equation requires.

There are eight N atoms in the eight NO molecules in the reactants box. There are also $4 \times 2 = 8$ O atoms in the O_2 molecules and 8 O atoms in the NO molecules, giving a total of 16 O atoms. In the products box, we find eight NO_2 molecules, which contain eight N atoms and $8 \times 2 = 16$ O atoms. Because there are equal numbers of N and O atoms in the two boxes, the drawing is consistent with the law of conservation of mass.

Practice Exercise 1

In the following diagram, the white spheres represent hydrogen atoms and the blue spheres represent nitrogen atoms.



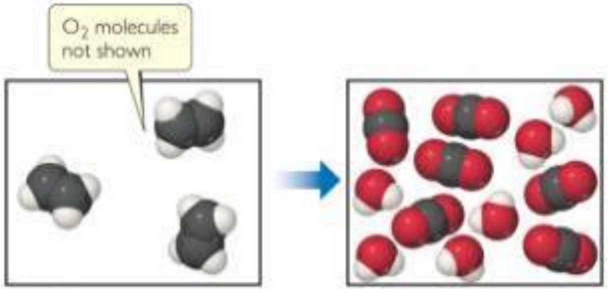
Sample Exercise 3.1 Interpreting and Balancing Chemical Equations

Continued

The two reactants combine to form a single product, ammonia, NH_3, which is not shown. Write a balanced chemical equation for the reaction. Based on the equation and the contents of the left (reactants) box, find how many NH_3 molecules should be shown in the right (products) box. **(a)** 2, **(b)** 3, **(c)** 4, **(d)** 6, **(e)** 9.

Practice Exercise 2

In the following diagram, the white spheres represent hydrogen atoms, the black spheres carbon atoms, and the red spheres oxygen atoms.



In this reaction, there are two reactants, ethylene, C_2H_2, which is shown, and oxygen, O_2, which is not shown, and two products, CO_2 and H_2O, both of which are shown. **(a)** Write a balanced chemical equation for the reaction. **(b)** Determine the number of O_2 molecules that should be shown in the left (reactants) box.

Sample Exercise 3.2 Balancing Chemical Equations

Balance the equation

$$Na(s) + H_2O\,(l) \rightarrow NaOH(aq) + H_2(g)$$

Solution

Begin by counting each kind of atom on the two sides of the arrow. There are one Na, one O, and two H on the left side, and one Na, one O, and three H on the right. The Na and O atoms are balanced, but the number of H atoms is not. To increase the number of H atoms on the left, let's try placing the coefficient 2 in front of H_2O:

$$Na(s) + 2H_2O\,(l) \rightarrow NaOH(aq) + H_2(g)$$

Although beginning this way does not balance H, it does increase the number of reactant H atoms, which we need to do. (Also, adding the coefficient 2 on H_2O unbalances O, but we will take care of that after we balance H.) Now that we have 2 H_2O on the left, we balance H by putting the coefficient 2 in front of NaOH:

$$Na(s) + 2H_2O\,(l) \rightarrow 2\,NaOH(aq) + H_2(g)$$

Balancing H in this way brings O into balance, but now Na is unbalanced, with one Na on the left and two on the right. To rebalance Na, we put the coefficient 2 in front of the reactant:

$$2\,Na(s) + 2H_2O\,(l) \rightarrow 2\,NaOH(aq) + H_2(g)$$

We now have two Na atoms, four H atoms, and two O atoms on each side. The equation is balanced.

Sample Exercise 3.2 Balancing Chemical Equations

Continued

Comment Notice that we moved back and forth, placing a coefficient in front of H_2O, then NaOH, and finally Na. In balancing equations, we often find ourselves following this pattern of moving back and forth from one side of the arrow to the other, placing coefficients first in front of a formula on one side and then in front of a formula on the other side until the equation is balanced. You can always tell if you have balanced your equation correctly by checking that the number of atoms of each element is the same on the two sides of the arrow, and that you've chosen the smallest set of coefficients that balances the equation.

Practice Exercise 1

The unbalanced equation for the reaction between methane and bromine is

$$\_\_CH_4(g) + \_\_\ Br_2(l) \rightarrow \_\_\ CBr_4(s) + \_\_\ HBr(g)$$

Once this equation is balanced what is the value of the coefficient in front of bromine Br_2?
(**a**) 1, (**b**) 2, (**c**) 3, (**d**) 4, (**e**) 6.

Practice Exercise 2

Balance these equations by providing the missing coefficients:
(**a**) $\_\_\ Fe(s) + \_\_\ O_2(g) \rightarrow \_\_Fe_2O_3(s)$
(**b**) $\_\_\ Al(s) + \_\_\ HCl(aq) \rightarrow \_\_\ AlCl_3(aq) + \_\_\ H_2(g)$
(**c**) $\_\_\ CaCO_3(s) + \_\_\ HCl(aq) \rightarrow \_\_\ CaCl_2(aq) + \_\_\ CO_2(g) + \_\_\ H_2O(l)$

Sample Exercise 3.3 Writing Balanced Equations for Combination and Decomposition Reactions

Write a balanced equation for **(a)** the combination reaction between lithium metal and fluorine gas and **(b)** the decomposition reaction that occurs when solid barium carbonate is heated (two products form, a solid and a gas).

Solution

(a) With the exception of mercury, all metals are solids at room temperature. Fluorine occurs as a diatomic molecule. Thus, the reactants are Li(*s*) and $F_2(g)$. The product will be composed of a metal and a nonmetal, so we expect it to be an ionic solid. Lithium ions have a 1+ charge, Li^+, whereas fluoride ions have a 1− charge, F^-. Thus, the chemical formula for the product is LiF. The balanced chemical equation is

$$2\,Li(s) + F_2(g) \rightarrow 2\,LiF(s)$$

(b) The chemical formula for barium carbonate is $BaCO_3$. As mentioned, many metal carbonates decompose to metal oxides and carbon dioxide when heated. In Equation 3.7, for example, $CaCO_3$ decomposes to form CaO and CO_2. Thus, we expect $BaCO_3$ to decompose to BaO and CO_2. Barium and calcium are both in group 2A in the periodic table, which further suggests they react in the same way:

$$BaCO_3(s) \rightarrow BaO(s) + CO_2(g)$$

Practice Exercise 1

Which of the following reactions is the balanced equation that represents the decomposition reaction that occurs when silver (I) oxide is heated? **(a)** $AgO(s) \rightarrow Ag(s) + O(g)$; **(b)** $2\,AgO(s) \rightarrow 2\,Ag(s) + O_2(g)$; **(c)** $Ag_2O(s) \rightarrow 2\,Ag(s) + O2(g)$; **(d)** $Ag_2O(s) \rightarrow 4\,Ag(s) + O_2(g)$; **(e)** $Ag_2O(s) \rightarrow 4\,Ag(s) + O_2(g)$;

Sample Exercise 3.3 Writing Balanced Equations for Combination and Decomposition Reactions

Continued

Practice Exercise 2

Write a balanced equation for **(a)** solid mercury (II) sulfide decomposing into its component elements when heated and **(b)** aluminum metal combining with oxygen in the air.

Sample Exercise 3.4 Writing Balanced Equations for Combustion Reactions

Write the balanced equation for the reaction that occurs when methanol, $CH_3OH(l)$, is burned in air.

Solution

When any compound containing C, H, and O is combusted, it reacts with the $O_2(g)$ in air to produce $CO_2(g)$ and $H_2O(g)$. Thus, the unbalanced equation is

$$2\ CH_3OH(l) + O_2(g) \rightarrow CO_2(g) + H_2O(g)$$

The C atoms are balanced, one on each side of the arrow. Because CH_3OH has four H atoms, we place the coefficient 2 in front of H_2O to balance the H atoms:

$$CH_3OH(l) + O_2(g) \rightarrow CO_2(g) + 2\ H_2O(g)$$

Adding this coefficient balances H but gives four O atoms in the products. Because there are only three O atoms in the reactants, we are not finished. We can place the coefficient $\frac{3}{2}$ in front of O_2 to give four O atoms in the reactants ($\frac{3}{2} \times 2 = 3$ O atoms in $\frac{3}{2} O_2$):

$$CH_3OH(l) + \tfrac{3}{2} O_2(g) \longrightarrow CO_2(g) + 2\ H_2O(g)$$

Sample Exercise 3.4 Writing Balanced Equations for Combustion Reactions

Continued

Although this equation is balanced, it is not in its most conventional form because it contains a fractional coefficient. However, multiplying through by 2 removes the fraction and keeps the equation balanced:

$$2\ CH_3OH(l) + 3O_2(g) \rightarrow 2\ CO_2(g) + 4\ H_2O(g)$$

Practice Exercise 1

Write the balanced equation for the reaction that occurs when ethylene glycol, $C_2H_4(OH)_2$, burns in air.

(a) $C_2H_4(OH)_2(l) + 5/2\ O_2(g) \rightarrow 2\ CO_2(g) + 3\ H_2O(g)$
(b) $2\ C_2H_4(OH)_2(l) + 5\ O_2(g) \rightarrow 4\ CO_2(g) + 6\ H_2O(g)$
(c) $C_2H_4(OH)_2(l) + 3\ O_2(g) \rightarrow 2\ CO_2(g) + 3\ H_2O(g)$
(d) $C_2H_4(OH)_2(l) + 5\ O_2(g) \rightarrow 2\ CO_2(g) + 3\ H_2O(g)$
(e) $4\ C_2H_4(OH)_2(l) + 10\ O_2(g) \rightarrow 8\ CO_2(g) + 12\ H_2O(g)$

Practice Exercise 2

Write the balanced equation for the reaction that occurs when ethanol, $C_2H_5OH(l)$, burns in air.

Sample Exercise 3.5 Calculating Formula Weights

Calculate the formula weight of (**a**) sucrose, $C_{12}H_{22}O_{11}$ (table sugar); and (**b**) calcium nitrate, $Ca(NO_3)_2$

Solution

(a) By adding the atomic weights of the atoms in sucrose, we find the formula weight to be 342.0 amu:

$$\begin{aligned} 12\text{ C atoms} &= 12(12.0\text{ amu}) = 144.0\text{ amu} \\ 22\text{ H atoms} &= 22(1.0\text{ amu}) = 22.0\text{ amu} \\ 11\text{ O atoms} &= 11(16.0\text{ amu}) = \underline{176.0\text{ amu}} \\ & \qquad\qquad\qquad\quad\; 342.0\text{ amu} \end{aligned}$$

(b) If a chemical formula has parentheses, the subscript outside the parentheses is a multiplier for all atoms inside. Thus, for $Ca(NO_3)_2$ we have

$$\begin{aligned} 1\text{ Ca atom} &= 1(40.1\text{ amu}) = 40.1\text{ amu} \\ 2\text{ N atoms} &= 2(14.0\text{ amu}) = 28.0\text{ amu} \\ 6\text{ O atoms} &= 6(16.0\text{ amu}) = \underline{96.0\text{ amu}} \\ & \qquad\qquad\qquad\quad\; 164.1\text{ amu} \end{aligned}$$

Practice Exercise 1

Which of the following is the correct formula weight for calcium phosphate? **(a)** 310.2 amu, **(b)** 135.1 amu, **(c)** 182.2 amu, **(d)** 278.2 amu, **(e)** 175.1 amu.

Sample Exercise 3.5 Calculating Formula Weights

Continued

Practice Exercise 2

Calculate the formula weight of **(a)** $Al(OH)_3$, **(b)** CH_3OH, and **(c)** TaON.

Sample Exercise 3.6 Calculating Percentage Composition

Calculate the percentage of carbon, hydrogen, and oxygen (by mass) in $C_{12}H_{22}O_{11}$.

Solution

Let's examine this question using the problem-solving steps in the accompanying "Strategies in Chemistry: Problem Solving" essay.

Analyze We are given a chemical formula and asked to calculate the percentage by mass of each element.

Plan We use Equation 3.10, obtaining our atomic weights from a periodic table. We know the denominator in Equation 3.10, the formula weight of $C_{12}H_{22}O_{11}$, from Sample Exercise 3.5. We must use that value in three calculations, one for each element.

Solve

$$\%C = \frac{(12)(12.0\ \text{amu})}{342.0\ \text{amu}} \times 100\% = 42.1\%$$

$$\%H = \frac{(22)(1.0\ \text{amu})}{342.0\ \text{amu}} \times 100\% = 6.4\%$$

$$\%O = \frac{(11)(16.0\ \text{amu})}{342.0\ \text{amu}} \times 100\% = 51.5\%$$

Check Our calculated percentages must add up to 100%, which they do. We could have used more significant figures for our atomic weights, giving more significant figures for our percentage composition, but we have adhered to our suggested guideline of rounding atomic weights to one digit beyond the decimal point.

Sample Exercise 3.6 Calculating Percentage Composition

Continued

Practice Exercise 1

What is the percentage of nitrogen, by mass, in calcium nitrate? **(a)** 8.54%, **(b)** 17.1%, **(c)** 13.7%, **(d)** 24.4%, **(e)** 82.9%.

Practice Exercise 2

Calculate the percentage of potassium, by mass, in K_2PtCl_6.

Sample Exercise 3.7 Estimating Numbers of Atoms

Without using a calculator, arrange these samples in order of increasing numbers of carbon atoms: 12 g ^{12}C, 1 mol C_2H_2, 9 × 10^{23} molecules of CO_2.

Solution

Analyze We are given amounts of three substances expressed in grams, moles, and number of molecules and asked to arrange the samples in order of increasing numbers of C atoms.

Plan To determine the number of C atoms in each sample, we must convert 12 g ^{12}C, 1 mol C_2H_2, and 9 × 10^{23} molecules CO_2 to numbers of C atoms. To make these conversions, we use the definition of mole and Avogadro's number.

Solve One mole is defined as the amount of matter that contains as many units of the matter as there are C atoms in exactly 12 g of ^{12}C. Thus, 12 g of ^{12}C contains 1 mol of C atoms = 6.02 × 10^{23} C atoms. One mol of C_2H_2 contains 6.02 × 10^{23} C_2H_2 molecules. Because there are two C atoms in each molecule, this sample contains 12.04 × 10^{23} C atoms. Because each CO_2 molecule contains one C atom, the CO_2 sample contains 9 × 10^{23} C atoms. Hence, the order is 12 g ^{12}C (6 × 10^{23} C atoms) $<$ 9 × 10^{23} CO_2 molecules (9 × 10^{23} C atoms) $<$ 1 mol C_2H_2 (12 × 10^{23} C atoms).

Check We can check our results by comparing numbers of moles of C atoms in the samples because the number of moles is proportional to the number of atoms. Thus, 12 g of ^{12}C is 1 mol C, 1 mol of C_2H_2 contains 2 mol C, and 9 × 10^{23} molecules of CO_2 contain 1.5 mol C, giving the same order as stated previously.

Sample Exercise 3.7 Estimating Numbers of Atoms

Continued

Practice Exercise 1

Determine which of the following samples contains the fewest sodium atoms? (**a**) 1 mol sodium oxide, (**b**) 45 g sodium fluoride, (**c**) 50 g sodium chloride, (**d**) 1 mol sodium nitrate?

Practice Exercise 2

Without using a calculator, arrange these samples in order of increasing numbers of O atoms: 1 mol H_2O, 1 mol CO_2, 3×10^{23} molecules of O_3.

Sample Exercise 3.8 Converting Moles to Number of Atoms

Calculate the number of H atoms in 0.350 mol of $C_6H_{12}O_6$.

Solution

Analyze We are given the amount of a substance (0.350 mol) and its chemical formula $C_6H_{12}O_6$. The unknown is the number of H atoms in the sample.

Plan Avogadro's number provides the conversion factor between number of moles of $C_6H_{12}O_6$ and number of molecules of $C_6H_{12}O_6$: 1 mol $C_6H_{12}O_6$ = 6.02×10^{23} molecules of $C_6H_{12}O_6$. Once we know the number of molecules of $C_6H_{12}O_6$, we can use the chemical formula, which tells us that each molecule of $C_6H_{12}O_6$ contains 12 H atoms. Thus, we convert moles of $C_6H_{12}O_6$ to molecules of $C_6H_{12}O_6$ and then determine the number of atoms of H from the number of molecules of $C_6H_{12}O_6$:

$$\text{Moles } C_6H_{12}O_6 \rightarrow \text{molecules } C_6H_{12}O_6 \rightarrow \text{atoms H}$$

Solve

$$\begin{aligned}\text{H atoms} &= (0.350\ \cancel{\text{mol } C_6H_{12}O_6})\left(\frac{6.02 \times 10^{23}\ \cancel{\text{molecules } C_6H_{12}O_6}}{1\ \cancel{\text{mol } C_6H_{12}O_6}}\right)\left(\frac{12\ \text{H atoms}}{1\ \cancel{\text{molecule } C_6H_{12}O_6}}\right)\\ &= 2.53 \times 10^{24}\ \text{H atoms}\end{aligned}$$

Sample Exercise 3.8 Converting Moles to Number of Atoms

Continued

Check We can do a ballpark calculation, figuring that $0.35(6 \times 10^{23})$ is about 2×10^{23} molecules of $C_6H_{12}O_6$. We know that each one of these molecules contains 12 H atoms. $12(2 \times 10^{23})$ gives $24 \times 10^{23} = 2.4 \times 10^{24}$ H atoms, which is close to our result. Because we were asked for the number of H atoms, the units of our answer are correct. We check, too, for significant figures. The given data had three significant figures, as does our answer.

Practice Exercise 1

How many sulfur atoms are in **(a)** 0.45 mol $BaSO_4$ and **(b)** 1.10 mol of aluminum sulfide?

Practice Exercise 2

How many oxygen atoms are in **(a)** 0.25 mol $Ca(NO_3)_2$ and **(b)** 1.50 mol of sodium carbonate?

Sample Exercise 3.9 Calculating Molar Mass

What is the molar mass of glucose, $C_6H_{12}O_6$?

Solution

Analyze We are given a chemical formula and asked to determine its molar mass.

Plan Because the molar mass of any substance is numerically equal to its formula weight, we first determine the formula weight of glucose by adding the atomic weights of its component atoms. The formula weight will have units of amu, whereas the molar mass has units of grams per mole (g/mol).

Solve Our first step is to determine the formula weight of glucose:

$$\begin{aligned} 6\text{ C atoms} &= 6(12.0\text{ amu}) = 72.0\text{ amu} \\ 12\text{ H atoms} &= 12(1.0\text{ amu}) = 12.0\text{ amu} \\ 6\text{ O atoms} &= 6(16.0\text{ amu}) = \underline{96.0\text{ amu}} \\ & \qquad\qquad\qquad\quad 180.0\text{ amu} \end{aligned}$$

Because glucose has a formula weight of 180.0 amu, 1 mol of this substance (6.02×10^{23} molecules) has a mass of 180.0 g. In other words, $C_6H_{12}O_6$ has a molar mass of 180.0 g/mol.

Check A molar mass below 250 seems reasonable based on the earlier examples we have encountered, and grams per mole is the appropriate unit for the molar mass.

Sample Exercise 3.9 Calculating Molar Mass

Continued

Practice Exercise 1

A sample of an ionic compound containing iron and chlorine is analyzed and found to have a molar mass of 126.8 g/mol. What is the charge of the iron in this compound? (**a**) 1+, (**b**) 2+, (**c**) 3+, (**d**) 4+.

Practice Exercise 2

Calculate the molar mass of $Ca(NO_3)_2$.

Sample Exercise 3.10 Converting Grams to Moles

Calculate the number of moles of glucose ($C_6H_{12}O_6$) in 5.380 g of $C_6H_{12}O_6$.

Solution

Analyze We are given the number of grams of a substance and its chemical formula and asked to calculate the number of moles.

Plan The molar mass of a substance provides the factor for converting grams to moles. The molar mass of $C_6H_{12}O_6$ is 180.0 g/mol (Sample Exercise 3.9).

Solve Using 1 mol $C_6H_{12}O_6$ = 180.0 g $C_6H_{12}O_6$ to write the appropriate conversion factor, we have

$$\text{Moles } C_6H_{12}O_6 = (5.380\ \cancel{\text{g } C_6H_{12}O_6})\left(\frac{1 \text{ mol } C_6H_{12}O_6}{180.0\ \cancel{\text{g } C_6H_{12}O_6}}\right) = 0.02989 \text{ mol } C_6H_{12}O_6$$

Check Because 5.380 g is less than the molar mass, an answer less than 1 mol is reasonable. The unit mol is appropriate. The original data had four significant figures, so our answer has four significant figures.

Practice Exercise 1

How many moles of sodium bicarbonate ($NaHCO_3$) are in 508 g of $NaHCO_3$?

Sample Exercise 3.10 Converting Grams to Moles

Continued

Practice Exercise 2

How many moles of water are in 1.00 L of water, whose density is 1.00 g/mL?

Sample Exercise 3.11 Converting Moles to Grams

Calculate the mass, in grams, of 0.433 mol of calcium nitrate.

Solution

Analyze We are given the number of moles and the name of a substance and asked to calculate the number of grams in the substance.

Plan To convert moles to grams, we need the molar mass, which we can calculate using the chemical formula and atomic weights.

Solve Because the calcium ion is Ca^{2+} and the nitrate ion is NO3^{-}, the chemical formula for calcium nitrate is $Ca(NO_3)_2$. Adding the atomic weights of the elements in the compound gives a formula weight of 164.1 amu. Using 1 mol $Ca(NO_3)_2$ = 164.1 g $Ca(NO_3)_2$ to write the appropriate conversion factor, we have

$$\text{Grams } Ca(NO_3)_2 = (0.433\ \cancel{\text{mol } Ca(NO_3)_2})\left(\frac{164.1\text{ g } Ca(NO_3)_2}{1\ \cancel{\text{mol } Ca(NO_3)_2}}\right) = 71.1\text{ g } Ca(NO_3)_2$$

Check The number of moles is less than 1, so the number of grams must be less than the molar mass, 164.1 g. Using rounded numbers to estimate, we have 0.5 × 150 = 75 g, which means the magnitude of our answer is reasonable. Both the units (g) and the number of significant figures (3) are correct.

Sample Exercise 3.11 Converting Moles to Grams

Continued

Practice Exercise 1

What is the mass, in grams, of **(a)** 6.33 mol of $NaHCO_3$ and **(b)** 3.0×10^{-5} mol of sulfuric acid?

Practice Exercise 2

What is the mass, in grams, of **(a)** 0.50 mol of diamond (C) and **(b)** 0.155 mol of ammonium chloride?

Sample Exercise 3.12 Calculating Numbers of Molecules and Atoms from Mass

(a) How many glucose molecules are in 5.23 g of $C_6H_{12}O_6$?
(b) How many oxygen atoms are in this sample?

Solution

Analyze We are given the number of grams and the chemical formula of a substance and asked to calculate **(a)** the number of molecules and **(b)** the number of O atoms in the substance.

Plan (a) The strategy for determining the number of molecules in a given quantity of a substance is summarized in Figure 3.12. We must convert 5.23 g to moles of $C_6H_{12}O_6$ and then convert moles to molecules of $C_6H_{12}O_6$. The first conversion uses the molar mass of $C_6H_{12}O_6$, 180.0 g, and the second conversion uses Avogadro's number.

Solve Molecules $C_6H1_2O_6$

$$= (5.23\ \cancel{\text{g } C_6H_{12}O_6})\left(\frac{1\ \cancel{\text{mol } C_6H_{12}O_6}}{180.0\ \cancel{\text{g } C_6H_{12}O_6}}\right)\left(\frac{6.02 \times 10^{23} \text{ molecules } C_6H_{12}O_6}{1\ \cancel{\text{mol } C_6H_{12}O_6}}\right)$$

$$= 1.75 \times 10^{22} \text{ molecules } C_6H_{12}O_6$$

Check Because the mass we began with is less than a mole, there should be fewer than 6.02×10^{23} molecules in the sample, which means the magnitude of our answer is reasonable. A ballpark estimate of the answer comes reasonably close to the answer we derived in this exercise: $5/200 = 2.5 \times 10^{-2}$ mol; $(2.5 \times 10^{-2})(6 \times 10^{23}) = 15 \times 10^{21} = 1.5 \times 10^{22}$ molecules. The units (molecules) and the number of significant figures (three) are appropriate.

Sample Exercise 3.12 Calculating Numbers of Molecules and Atoms from Mass

Continued

Plan (b) To determine the number of O atoms, we use the fact that there are six O atoms in each $C_6H_{12}O_6$ molecule. Thus, multiplying the number of molecules we calculated in **(a)** by the factor (6 atoms O/1 molecule $C_6H_{12}O_6$) gives the number of O atoms.

Solve

$$\text{Atoms O} = (1.75 \times 10^{22}\ \cancel{\text{molecules } C_6H_{12}O_6})\left(\frac{6 \text{ atoms O}}{\cancel{\text{molecule } C_6H_{12}O_6}}\right)$$
$$= 1.05 \times 10^{23} \text{ atoms O}$$

Check The answer is six times as large as the answer to part **(a)**, exactly what it should be. The number of significant figures (three) and the units (atoms O) are correct.

Practice Exercise 1

How many chlorine atoms are in 12.2 g of CCl_4? **(a)** 4.77×10^{22}, **(b)** 7.34×10^{24}, **(c)** 1.91×10^{23}, **(d)** 2.07×10^{23}.

Practice Exercise 2

(a) How many nitric acid molecules are in 4.20 g of HNO_3?

(b) How many O atoms are in this sample?

Sample Exercise 3.13 Calculating an Empirical Formula

Ascorbic acid (vitamin C) contains 40.92% C, 4.58% H, and 54.50% O by mass. What is the empirical formula of ascorbic acid?

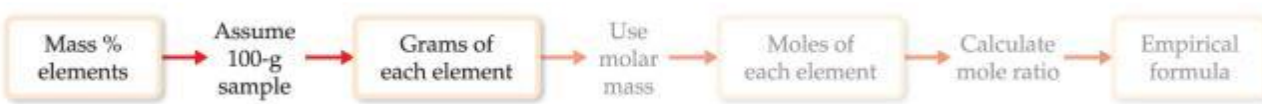
Solution

Analyze We are to determine the empirical formula of a compound from the mass percentages of its elements.

Plan The strategy for determining the empirical formula involves the three steps given in Figure 3.13.

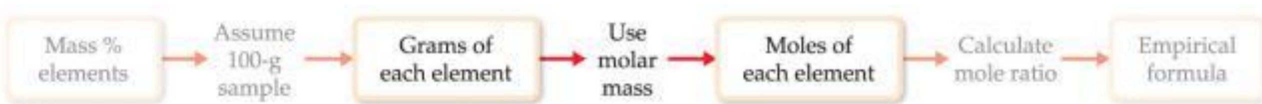
Solve

(1) For simplicity we assume we have exactly 100 g of material, although any other mass could also be used.



In 100.00 g of ascorbic acid we have 40.92 g C, 4.58 g H, and 54.50 g O.

(2) Next we calculate the number of moles of each element. We use atomic masses with four significant figures to match the precision of our experimental masses.



Sample Exercise 3.13 Calculating an Empirical Formula

Continued

$$\text{Moles C} = (40.92\ \cancel{\text{g C}})\left(\frac{1\ \text{mol C}}{12.01\ \cancel{\text{g C}}}\right) = 3.407\ \text{mol C}$$

$$\text{Moles H} = (4.58\ \cancel{\text{g H}})\left(\frac{1\ \text{mol C}}{1.008\ \cancel{\text{g H}}}\right) = 4.54\ \text{mol H}$$

$$\text{Moles O} = (54.50\ \cancel{\text{g O}})\left(\frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}}\right) = 3.406\ \text{mol O}$$

(3) We determine the simplest whole-number ratio of moles by dividing each number of moles by the smallest number of moles.

Mass % elements → Assume 100-g sample → Grams of each element → Use molar mass → **Moles of each element** → **Calculate mole ratio** → **Empirical formula**

$$\text{C:}\frac{3.407}{3.406} = 1.000 \quad \text{H:}\frac{4.54}{3.406} = 1.33 \quad \text{O:}\frac{3.406}{3.406} = 1.000$$

The ratio for H is too far from 1 to attribute the difference to experimental error; in fact, it is quite close to $1\frac{1}{3}$. This suggests we should multiply the ratios by 3 to obtain whole numbers:

$$C : H : O = (3 \times 1 : 3 \times 1.33 : 3 \times 1) = (3 : 4 : 3)$$

Thus, the empirical formula is $C_3H_4O_3$.

Sample Exercise 3.13 Calculating an Empirical Formula

Continued

Check It is reassuring that the subscripts are moderate-size whole numbers. Also, calculating the percentage composition of $C_3H_4O_3$ gives values very close to the original percentages.

Practice Exercise 1

A 2.144-g sample of phosgene, a compound used as a chemical warfare agent during World War I, contains 0.260 g of carbon, 0.347 g of oxygen, and 1.537 g of chlorine. What is the empirical formula of this substance? **(a)** CO_2Cl_6, **(b)** $COCl_2$, **(c)** $C_{0.022}O_{0.022}Cl_{0.044}$, **(d)** C_2OCl_2

Practice Exercise 2

A 5.325-g sample of methyl benzoate, a compound used in the manufacture of perfumes, contains 3.758 g of carbon, 0.316 g of hydrogen, and 1.251 g of oxygen. What is the empirical formula of this substance?

Sample Exercise 3.14 Determining a Molecular Formula

Mesitylene, a hydrocarbon found in crude oil, has an empirical formula of C_3H_4 and an experimentally determined molecular weight of 121 amu. What is its molecular formula?

Solution

Analyze We are given an empirical formula and a molecular weight of a compound and asked to determine its molecular formula.

Plan The subscripts in a compound's molecular formula are whole-number multiples of the subscripts in its empirical formula. We find the appropriate multiple by using Equation 3.11.

Solve The formula weight of the empirical formula C_3H_4 is

$$3(12.0 \text{ amu}) + 4(1.0 \text{ amu}) = 40.0 \text{ amu}$$

Next, we use this value in Equation 3.11:

$$\text{Whole-number multiple} = \frac{\text{molecular weight}}{\text{empirical formula weight}} = \frac{121}{40.0} = 3.03$$

Only whole-number ratios make physical sense because molecules contain whole atoms. The 3.03 in this case could result from a small experimental error in the molecular weight. We therefore multiply each subscript in the empirical formula by 3 to give the molecular formula: C_9H_{12}.

Check We can have confidence in the result because dividing molecular weight by empirical formula weight yields nearly a whole number.

Sample Exercise 3.14 Determining a Molecular Formula

Continued

Practice Exercise 1

Cyclohexane, a commonly used organic solvent, is 85.6% C and 14.4% H by mass with a molar mass of 84.2 g/mol. What is its molecular formula? **(a)** C_6H, **(b)** CH_2, **(c)** C_5H_{24}, **(d)** C_6H_{12}, **(e)** C_4H_8.

Practice Exercise 2

Ethylene glycol, used in automobile antifreeze, is 38.7% C, 9.7% H, and 51.6% O by mass. Its molar mass is 62.1 g/mol. **(a)** What is the empirical formula of ethylene glycol? **(b)** What is its molecular formula?

Sample Exercise 3.15 Determining an Empirical Formula by Combustion Analysis

Isopropyl alcohol, sold as rubbing alcohol, is composed of C, H, and O. Combustion of 0.255 g of isopropyl alcohol produces 0.561 g of CO_2 and 0.306 g of H_2O. Determine the empirical formula of isopropyl alcohol.

Solution

Analyze We are told that isopropyl alcohol contains C, H, and O atoms and are given the quantities of CO_2 and H_2O produced when a given quantity of the alcohol is combusted. We must determine the empirical formula for isopropyl alcohol, a task that requires us to calculate the number of moles of C, H, and O in the sample.

Plan We can use the mole concept to calculate grams of C in the CO_2 and grams of H in the H_2O—the masses of C and H in the alcohol before combustion. The mass of O in the compound equals the mass of the original sample minus the sum of the C and H masses. Once we have the C, H, and O masses, we can proceed as in Sample Exercise 3.13.

Solve Because all of the carbon in the sample is converted to CO_2, we can use dimensional analysis and the following steps to calculate the mass C in the sample.

Mass CO_2 produced → Molar mass CO_2 44.0 g/mol → Moles CO_2 produced → 1 C atom per CO_2 molecule → Moles of C original sample → Molar mass C 12.0 g/mol → Mass C in original sample

Using the values given in this example, the mass of C is

$$\text{Grams C} = (0.561\ \text{g}\ \cancel{CO_2})\left(\frac{1\ \cancel{\text{mol}\ CO_2}}{44.0\ \cancel{\text{g}\ CO_2}}\right)\left(\frac{1\ \cancel{\text{mol}}\ \text{C}}{1\ \cancel{\text{mol}\ CO_2}}\right)\left(\frac{12.0\ \text{g C}}{1\ \cancel{\text{mol C}}}\right)$$

$$= 0.153\ \text{g C}$$

Sample Exercise 3.15 Determining an Empirical Formula by Combustion Analysis

Continued

Because all of the hydrogen in the sample is converted to H_2O, we can use dimensional analysis and the following steps to calculate the mass H in the sample. We use three significant figures for the atomic mass of H to match the significant figures in the mass of H_2O produced.

Mass H_2O produced $\xrightarrow{\text{Molar mass } H_2O \text{ 18.0 g/mol}}$ Moles H_2O produced $\xrightarrow{\text{2 H atoms per } H_2O \text{ molecule}}$ Moles H in original sample $\xrightarrow{\text{Molar mass H 1.01 g/mol}}$ Mass H in original sample

Using the values given in this example, the mass of H is

$$\text{Grams H} = (0.306\ \cancel{\text{g } H_2O})\left(\frac{1\ \cancel{\text{mol } H_2O}}{18.0\ \cancel{\text{g } H_2O}}\right)\left(\frac{2\ \cancel{\text{mol H}}}{1\ \cancel{\text{mol } H_2O}}\right)\left(\frac{1.01\text{ g H}}{1\ \cancel{\text{mol H}}}\right)$$

$$= 0.0343\text{ g H}$$

The mass of the sample, 0.255 g, is the sum of the masses of C, H, and O. Thus, the O mass is

$$\text{Mass of O} = \text{mass of sample} - (\text{mass of C} + \text{mass of H})$$

$$= 0.255\text{ g} - (0.153\text{ g} + 0.0343\text{ g}) = 0.068\text{ g O}$$

The number of moles of C, H, and O in the sample is therefore

$$\text{Moles C} = (0.153\ \cancel{\text{g C}})\left(\frac{1\text{ mol C}}{12.0\ \cancel{\text{g C}}}\right) = 0.0128\text{ mol C}$$

$$\text{Moles H} = (0.0343\ \cancel{\text{g H}})\left(\frac{1\text{ mol H}}{1.01\ \cancel{\text{g H}}}\right) = 0.0340\text{ mol H}$$

$$\text{Moles O} = (0.068\ \cancel{\text{g O}})\left(\frac{1\text{ mol O}}{16.0\ \cancel{\text{g O}}}\right) = 0.0043\text{ mol O}$$

Sample Exercise 3.15 Determining an Empirical Formula by Combustion Analysis

Continued

To find the empirical formula, we must compare the relative number of moles of each element in the sample, as illustrated in Sample Exercise 3.13.

$$\text{C:}\frac{0.0128}{0.0043} = 3.0 \quad \text{H:}\frac{0.0340}{0.0043} = 7.9 \quad \text{O:}\frac{0.0043}{0.0043} = 1.0$$

The first two numbers are very close to the whole numbers 3 and 8, giving the empirical formula C_3H_8O.

Practice Exercise 1

The compound dioxane, which is used as a solvent in various industrial processes, is composed of C, H, and O atoms. Combustion of a 2.203-g sample of this compound produces 4.401 g CO_2 and 1.802 g H_2O. A separate experiment shows that it has a molar mass of 88.1 g/mol. Which of the following is the correct molecular formula for dioxane? **(a)** C_2H_4O, **(b)** $C_4H_4O_2$, **(c)** CH_2, **(d)** $C_4H_8O_2$.

Practice Exercise 2

(a) Caproic acid, responsible for the odor of dirty socks, is composed of C, H, and O atoms. Combustion of a 0.225-g sample of this compound produces 0.512 g CO_2 and 0.209 g H_2O. What is the empirical formula of caproic acid? **(b)** Caproic acid has a molar mass of 116 g/mol. What is its molecular formula?

Sample Exercise 3.16 Calculating Amounts of Reactants and Products

Determine how many grams of water are produced in the oxidation of 1.00 g of glucose, $C_6H_{12}O_6$:

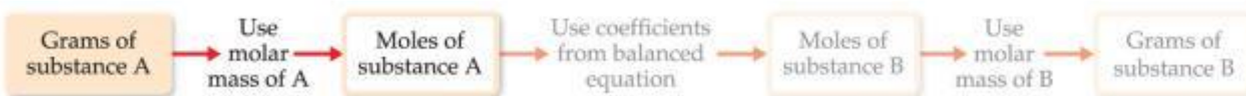
$$C_6H_{12}O_6(s) + 6\ O_2(g) \rightarrow 6\ CO_2(g) + 6\ H_2O(l)$$

Solution

Analyze We are given the mass of a reactant and must determine the mass of a product in the given reaction.

Plan We follow the general strategy outlined in Figure 3.16:
(1) Convert grams of $C_6H_{12}O_6$ to moles using the molar mass of $C_6H_{12}O_6$.
(2) Convert moles of $C_6H_{12}O_6$ to moles of H_2O using the stoichiometric relationship 1 mol $C_6H_{12}O_6 \simeq$ 6 mol H_2O.
(3) Convert moles of H_2O to grams using the molar mass of H_2O.

Solve
(1) First we convert grams of $C_6H_{12}O_6$ to moles using the molar mass of $C_6H_{12}O_6$.

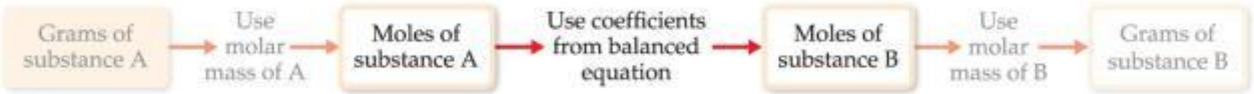


$$\text{Moles } C_6H_{12}O_6 = (1.00\ \cancel{g\ C_6H_{12}O_6})\left(\frac{1\ mol\ C_6H_{12}O_6}{180.0\ \cancel{g\ C_6H_{12}O_6}}\right)$$

(2) Next we convert moles of $C_6H_{12}O_6$ to moles of H_2O using the stoichiometric relationship
1 mol $C_6H_{12}O_6 \simeq$ 6 mol H_2O.

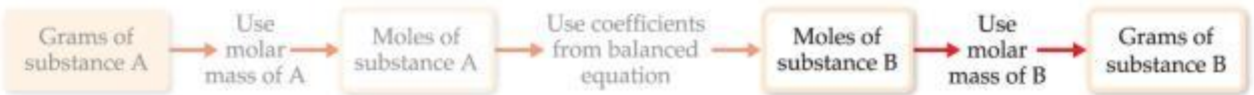
Sample Exercise 3.16 Calculating Amounts of Reactants and Products

Continued



$$\text{Moles } H_2O = (1.00\ \text{g}\ \cancel{C_6H_{12}O_6})\left(\frac{1\ \text{mol}\ \cancel{C_6H_{12}O_6}}{180.0\ \text{g}\ \cancel{C_6H_{12}O_6}}\right)\left(\frac{6\ \text{mol}\ H_2O}{1\ \cancel{\text{mol}\ C_6H_{12}O_6}}\right)$$

(3) Finally, we convert moles of H_2O to grams using the molar mass of H_2O.



$$\text{Grams } H_2O = (1.00\ \text{g}\ \cancel{C_6H_{12}O_6})\left(\frac{1\ \cancel{\text{mol}\ C_6H_{12}O_6}}{180.0\ \text{g}\ \cancel{C_6H_{12}O_6}}\right)\left(\frac{6\ \cancel{\text{mol}\ H_2O}}{1\ \cancel{\text{mol}\ C_6H_{12}O_6}}\right)\left(\frac{18.0\ \text{g}\ H_2O}{1\ \cancel{\text{mol}\ H_2O}}\right)$$

$$= 0.600\ \text{g}\ H_2O$$

Check We can check how reasonable our result is by doing a ballpark estimate of the mass of H_2O. Because the molar mass of glucose is 180 g/mol, 1 g of glucose equals 1/180 mol. Because 1 mol of glucose yields 6 mol H_2O, we would have 6/180 = 1/30 mol H_2O. The molar mass of water is 18 g/mol, so we have 1/30 × 18 = 6/10 = 0.6 g of H_2O, which agrees with the full calculation. The units, grams H_2O, are correct. The initial data had three significant figures, so three significant figures for the answer is correct.

Sample Exercise 3.16 Calculating Amounts of Reactants and Products

Continued

Practice Exercise 1

Sodium hydroxide reacts with carbon dioxide to form sodium carbonate and water:

$$2\ NaOH(s) + CO_2(g) \rightarrow Na_2CO_3(s) + H_2O(l)$$

How many grams of Na_2CO_3 can be prepared from 2.40 g of NaOH? (**a**) 3.18 g, (**b**) 6.36 g, (**c**) 1.20 g, (**d**) 0.0300 g.

Practice Exercise 2

Decomposition of $KClO_3$ is sometimes used to prepare small amounts of O_2 in the laboratory: $2\ KClO_3(s) \rightarrow 2\ KCl(s) + 3\ O_2(g)$. How many grams of O_2 can be prepared from 4.50 g of $KClO_3$?

Sample Exercise 3.17 Calculating Amounts of Reactants and Products

Solid lithium hydroxide is used in space vehicles to remove the carbon dioxide gas exhaled by astronauts. The hydroxide reacts with the carbon dioxide to form solid lithium carbonate and liquid water. How many grams of carbon dioxide can be absorbed by 1.00 g of lithium hydroxide?

Solution

Analyze We are given a verbal description of a reaction and asked to calculate the number of grams of one reactant that reacts with 1.00 g of another.

Plan The verbal description of the reaction can be used to write a balanced equation:

$$2\ \mathrm{LiOH}(s) + \mathrm{CO_2}(g) \rightarrow \mathrm{Li_2CO_3}(s) + \mathrm{H_2O}(l)$$

We are given the mass in grams of LiOH and asked to calculate the mass in grams of CO_2. We can accomplish this with the three conversion steps in Figure 3.16. The conversion of Step 1 requires the molar mass of LiOH (6.94 + 16.00 + 1.01 = 23.95 g/mol). The conversion of Step 2 is based on a stoichiometric relationship from the balanced chemical equation: 2 mol LiOH $\simeq$ mol CO_2. For the Step 3 conversion, we use the molar mass of CO_2 12.01 + 2(16.00) = 44.01 g/mol.

Solve

$$(1.00\ \mathrm{g}\ \cancel{\mathrm{LiOH}})\left(\frac{1\ \cancel{\mathrm{mol\ LiOH}}}{23.95\ \cancel{\mathrm{g\ LiOH}}}\right)\left(\frac{1\ \cancel{\mathrm{mol\ CO_2}}}{2\ \cancel{\mathrm{mol\ LiOH}}}\right)\left(\frac{44.01\ \mathrm{g\ CO_2}}{1\ \cancel{\mathrm{mol\ CO_2}}}\right) = 0.919\ \mathrm{g\ CO_2}$$

Sample Exercise 3.17 Calculating Amounts of Reactants and Products

Continued

Check Notice that 23.95 g LiOH/mol ≈ 24 g LiOH/mol, 24 g LiOH/mol × 2 mol LiOH = 48 g LiOH, and (44 g CO_2/mol)/(48 g LiOH) is slightly less than 1. Thus, the magnitude of our answer, 0.919 g CO_2, is reasonable based on the amount of starting LiOH. The number of significant figures and units are also appropriate.

Practice Exercise 1

Propane, C_3H_8 (Figure 3.8), is a common fuel used for cooking and home heating. What mass of O_2 is consumed in the combustion of 1.00 g of propane? **(a)** 5.00 g, **(b)** 0.726 g, **(c)** 2.18 g, **(d)** 3.63 g.

Practice Exercise 2

Methanol, CH_3OH, reacts with oxygen from air in a combustion reaction to form water and carbon dioxide. What mass of water is produced in the combustion of 23.6 g of methanol?

Sample Exercise 3.18 Calculating the Amount of Product Formed from a Limiting Reactant

The most important commercial process for converting N_2 from the air into nitrogen-containing compounds is based on the reaction of N_2 and H_2 to form ammonia (NH_3):

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

How many moles of NH_3 can be formed from 3.0 mol of N_2 and 6.0 mol of H_2?

Solution

Analyze We are asked to calculate the number of moles of product, NH_3, given the quantities of each reactant, N_2 and H_2, available in a reaction. This is a limiting reactant problem.

Plan If we assume one reactant is completely consumed, we can calculate how much of the second reactant is needed. By comparing the calculated quantity of the second reactant with the amount available, we can determine which reactant is limiting. We then proceed with the calculation, using the quantity of the limiting reactant.

Solve The number of moles of H_2 needed for complete consumption of 3.0 mol of N_2 is

$$\text{Moles } H_2 = (3.0\ \cancel{\text{mol } N_2})\left(\frac{3\ \text{mol } H_2}{1\ \cancel{\text{mol } N_2}}\right) = 9.0\ \text{mol } H_2$$

Sample Exercise 3.18 Calculating the Amount of Product Formed from a Limiting Reactant

Continued

Because only 6.0 mol H_2 is available, we will run out of H_2 before the N_2 is gone, which tells us that H_2 is the limiting reactant. Therefore, we use the quantity of H_2 to calculate the quantity of NH_3 produced:

$$\text{Moles } NH_3 = (6.0\ \cancel{\text{mol } H_2})\left(\frac{2\text{ mol } NH_3}{3\ \cancel{\text{mol } H_2}}\right) = 4.0\text{ mol } NH_3$$

Comment It is useful to summarize the reaction data in a table:

	$N_2(g)$	+	$3\ H_2(g)$	$\longrightarrow$	$2\ NH_3(g)$
Before reaction:	3.0 mol		6.0 mol		0 mol
Change (reaction):	−2.0 mol		−6.0 mol		+4.0 mol
After reaction:	1.0 mol		0 mol		4.0 mol

Notice that we can calculate not only the number of moles of NH_3 formed but also the number of moles of each reactant remaining after the reaction. Notice also that although the initial (before) number of moles of H_2 is greater than the final (after) number of moles of N_2, H_2 is nevertheless the limiting reactant because of its larger coefficient in the balanced equation.

Sample Exercise 3.18 Calculating the Amount of Product Formed from a Limiting Reactant

Continued

Check Examine the Change row of the summary table to see that the mole ratio of reactants consumed and product formed, 2:6:4, is a multiple of the coefficients in the balanced equation, 1:3:2. We confirm that H_2 is the limiting reactant because it is completely consumed in the reaction, leaving 0 mol at the end. Because 6.0 mol H_2 has two significant figures, our answer has two significant figures.

Practice Exercise 1

When 24 mol of methanol and 15 mol of oxygen combine in the combustion reaction $2\ CH_3OH(l) + 3\ O_2(g) \rightarrow 2\ CO_2(g) + 4\ H_2O(g)$, what is the excess reactant and how many moles of it remains at the end of the reaction? **(a)** 9 mol $CH_3OH(l)$, **(b)** 10 mol $CO_2(g)$, **(c)** 10 mol $CH_3OH(l)$, **(d)** 14 mol $CH_3OH(l)$, **(e)** 1 mol $O_2(g)$.

Practice Exercise 2

(a) When 1.50 mol of Al and 3.00 mol of Cl_2 combine in the reaction $2\ Al(s) + 3\ Cl_2(g) \rightarrow 2\ AlCl_3(s)$, which is the limiting reactant? **(b)** How many moles of $AlCl_3$ are formed? **(c)** How many moles of the excess reactant remain at the end of the reaction?

Sample Exercise 3.19 Calculating the Amount of Product Formed from a Limiting Reactant

The reaction

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

is used to produce electricity in a hydrogen fuel cell. Suppose a fuel cell contains 150 g of $H_2(g)$ and 1500 g of $O_2(g)$ (each measured to two significant figures). How many grams of water can form?

Solution

Analyze We are asked to calculate the amount of a product, given the amounts of two reactants, so this is a limiting reactant problem.

Plan To identify the limiting reactant, we can calculate the number of moles of each reactant and compare their ratio with the ratio of coefficients in the balanced equation. We then use the quantity of the limiting reactant to calculate the mass of water that forms.

Solve From the balanced equation, we have the stoichiometric relations

$$2\ \text{mol}\ H_2 \simeq \text{mol}\ O_2 \simeq 2\ \text{mol}\ H_2O$$

Sample Exercise 3.19 Calculating the Amount of Product Formed from a Limiting Reactant

Continued

Using the molar mass of each substance, we calculate the number of moles of each reactant:

$$\text{Moles } H_2 = (150 \cancel{\text{g } H_2})\left(\frac{1 \text{ mol } H_2}{2.02 \cancel{\text{g } H_2}}\right) = 74 \text{ mol } H_2$$

$$\text{Moles } O_2 = (1500 \cancel{\text{g } O_2})\left(\frac{1 \text{ mol } O_2}{32.0 \cancel{\text{g } O_2}}\right) = 47 \text{ mol } O_2$$

The coefficients in the balanced equation indicate that the reaction requires 2 mol of H_2 for every 1 mol of O_2. Therefore, for all the O_2 to completely react, we would need 2 × 47 = 94 mol of H_2. Since there are only 74 mol of H_2, all of the O_2 cannot react, so it is the excess reactant, and H_2 must be the limiting reactant. (Notice that the limiting reactant is not necessarily the one present in the lowest amount.)

We use the given quantity of H_2 (the limiting reactant) to calculate the quantity of water formed. We could begin this calculation with the given H_2 mass, 150 g, but we can save a step by starting with the moles of H_2, 74 mol, we just calculated:

$$\text{Grams } H_2O = (74 \cancel{\text{mol } H_2})\left(\frac{2 \cancel{\text{mol } H_2O}}{2 \cancel{\text{mol } H_2}}\right)\left(\frac{18.0 \text{ g } H_2O}{1 \cancel{\text{mol } H_2O}}\right)$$
$$= 1.3 \times 10^2 \text{ g } H_2O$$

Sample Exercise 3.19 Calculating the Amount of Product Formed from a Limiting Reactant

Continued

Check The magnitude of the answer seems reasonable based on the amounts of the reactants. The units are correct, and the number of significant figures (two) corresponds to those in the values given in the problem statement.

Comment The quantity of the limiting reactant, H_2, can also be used to determine the quantity of O_2 used:

$$\text{Grams } O_2 = (74\ \cancel{\text{mol } H_2})\left(\frac{1\ \cancel{\text{mol } O_2}}{2\ \cancel{\text{mol } H_2}}\right)\left(\frac{32.0\text{ g } O_2}{1\ \cancel{\text{mol } O_2}}\right)$$
$$= 1.2 \times 10^3\text{ g } O_2$$

The mass of O_2 remaining at the end of the reaction equals the starting amount minus the amount consumed:

$$1500\text{ g} - 1200\text{ g} = 300\text{ g}.$$

Practice Exercise 1

Molten gallium reacts with arsenic to form the semiconductor, gallium arsenide, GaAs, used in light–emitting diodes and solar cells:

$$\text{Ga}(l) + \text{As}(s) \rightarrow \text{GaAs}(s)$$

Sample Exercise 3.19 Calculating the Amount of Product Formed from a Limiting Reactant

Continued

If 4.00 g of gallium is reacted with 5.50 g of arsenic, how many grams of the excess reactant are left at the end of the reaction?
(a) 4.94 g As, **(b)** 0.56 g As, **(c)** 8.94 g Ga, or **(d)** 1.50 g As.

Practice Exercise 2

When a 2.00-g strip of zinc metal is placed in an aqueous solution containing 2.50 g of silver nitrate, the reaction is

$$Zn(s) + 2\ AgNO_3(aq) \rightarrow 2\ Ag(s) + Zn(NO_3)_2(aq)$$

(a) Which reactant is limiting? **(b)** How many grams of Ag form? **(c)** How many grams of $Zn(NO_3)_2$ form?
(d) How many grams of the excess reactant are left at the end of the reaction?

Sample Exercise 3.20 Calculating Theoretical Yield and Percent Yield

Adipic acid, $H_2C_6H_8O_4$, used to produce nylon, is made commercially by a reaction between cyclohexane (C_6H_{12}) and O_2:

$$2\ C_6H_{12}\,(l) + 5\ O_2(g) \rightarrow 2\ H_2C_6H_3O_4(l) + 2\ H_2O(g)$$

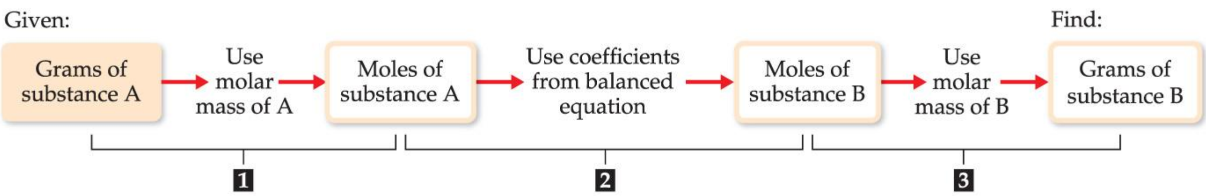
(a) Assume that you carry out this reaction with 25.0 g of cyclohexane and that cyclohexane is the limiting reactant. What is the theoretical yield of adipic acid? **(b)** If you obtain 33.5 g of adipic acid, what is the percent yield for the reaction?

Solution

Analyze We are given a chemical equation and the quantity of the limiting reactant (25.0 g of C_6H_{12}). We are asked to calculate the theoretical yield of a product $H_2C_6H_3O_4$ and the percent yield if only 33.5 g of product is obtained.

Plan

(a) The theoretical yield, which is the calculated quantity of adipic acid formed, can be calculated using the sequence of conversions shown in Figure 3.16.



(b) The percent yield is calculated by using Equation 3.14 to compare the given actual yield (33.5 g) with the theoretical yield.

Sample Exercise 3.20 Calculating Theoretical Yield and Percent Yield

Continued

Solve

(a) The theoretical yield is

$$\text{Grams } H_2C_6H_8O_4 = (25.0\ \cancel{g\ C_6H_{12}})\left(\frac{1\ \cancel{mol\ C_6H_{12}}}{84.0\ \cancel{g\ C_6H_{12}}}\right)\left(\frac{2\ \cancel{mol\ H_2C_6H_8O_4}}{2\ \cancel{mol\ C_6H_{12}}}\right)\left(\frac{146.0\ g\ H_2C_6H_8O_4}{1\ \cancel{mol\ H_2C_6H_8O_4}}\right)$$

$$= 43.5\ g\ H_2C_6H_8O_4$$

(b) $$\text{Percent yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100\% = \frac{33.5\ g}{43.5\ g} \times 100\% = 77.0\%$$

Check We can check our answer in **(a)** by doing a ballpark calculation. From the balanced equation we know that each mole of cyclohexane gives 1 mol adipic acid. We have $25/84 \approx 25/75 = 0.3$ mol hexane, so we expect 0.3 mol adipic acid, which equals about $0.3 \times 150 = 45$ g, about the same magnitude as the 43.5 g obtained in the more detailed calculation given previously. In addition, our answer has the appropriate units and number of significant figures. In **(b)** the answer is less than 100%, as it must be from the definition of percent yield.

Sample Exercise 3.20 Calculating Theoretical Yield and Percent Yield

Continued

Practice Exercise 1

If 3.00 g of titanium metal is reacted with 6.00 g of chlorine gas, Cl_2, to form 7.7 g of titanium (IV) chloride in a combination reaction, what is the percent yield of the product? **(a)** 65%, **(b)** 96%, **(c)** 48%, or **(d)** 86%.

Practice Exercise 2

Imagine you are working on ways to improve the process by which iron ore containing Fe_2O_3 is converted into iron:

$$Fe_2O_3(s) + 3\ CO(g) \rightarrow 2\ Fe(s) + 3\ CO_2(g)$$

(a) If you start with 150 g of Fe_2O_3 as the limiting reactant, what is the theoretical yield of Fe?
(b) If your actual yield is 87.9 g, what is the percent yield?