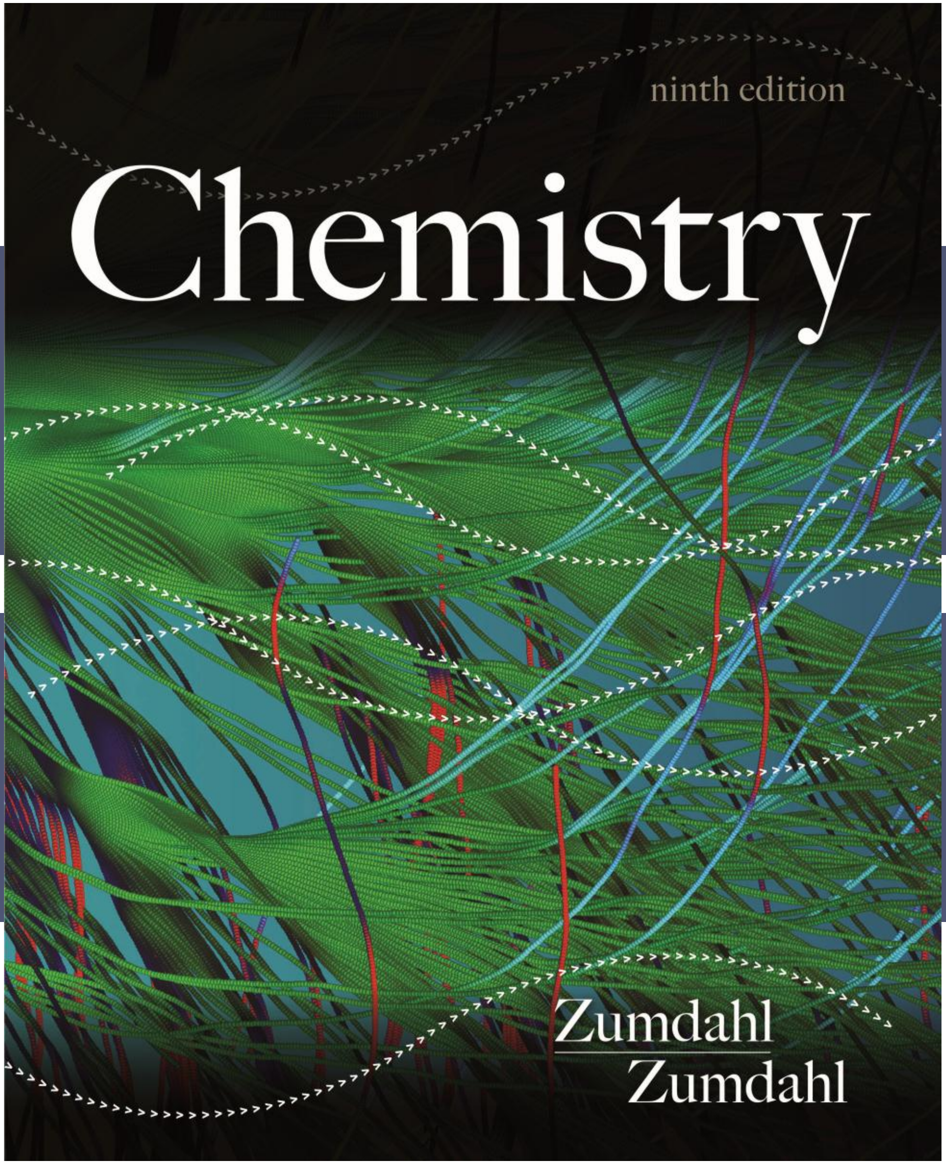

Chapter 3

Stoichiometry

Chapter 3
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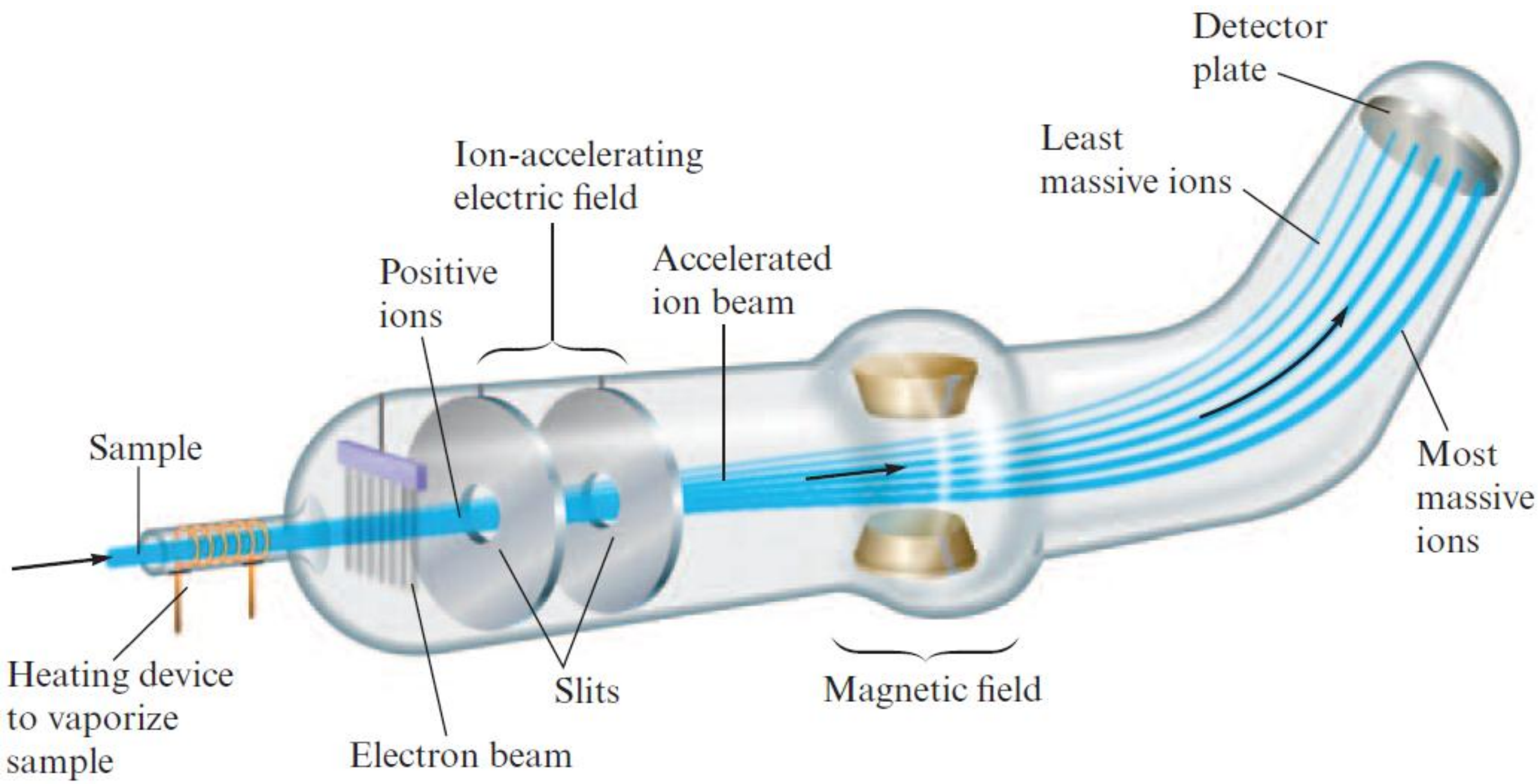
Chemical Stoichiometry

- The study of quantities of materials consumed and produced in chemical reactions
- Requires the understanding of the concept of relative atomic masses

An Overview of Stoichiometry

- The average mass of objects is required to count the objects by weighing
  - Objects behave as though they are all identical
- Chemists deal with samples of matter that contain huge numbers of atoms
  - Number of atoms in a sample can be determined by finding its mass

Figure 3.1 - Schematic Diagram of a Mass Spectrometer



Mass Spectrometer and the Mass of an Ion

- In a mass spectrometer, the amount of path deflection of an ion depends on its mass
  - Massive ions are deflected in the smallest amount
    - Causes separation of ions
- Position where the ions hit the detector plate provides accurate values of their relative masses

Average Atomic Mass of Elements

- Atomic mass or average mass of an element
- All elements occur in nature as mixtures of isotopes
  - Atomic masses of all elements are average values based on the isotopic composition of naturally occurring elements

Average Atomic Mass of Carbon

- Natural carbon is a mixture of three isotopes - ^{12}C, ^{13}C, and ^{14}C
  - Atomic mass of carbon is an average value of the three isotopes
- Natural carbon is composed of:
  - 98.89% ^{12}C atoms (mass = 12 u)
  - 1.11% ^{13}C atoms (mass = 13.003355 u)

Average Atomic Mass of Carbon (Continued)

- The average atomic mass of natural carbon can be calculated as follows:

98.89% of 12 u + 1.11% of 13.0034 u =

$$(0.9889)(12\text{ u}) + (0.0111)(13.0034\text{ u}) = 12.01\text{ u}$$

  - For stoichiometric purposes, assume that carbon is composed of only one type of atom with a mass of 12.01

Uses of Mass Spectrometer

- Helps determine accurate mass values for individual atoms
- Ascertains the isotopic composition of naturally occurring elements

Geoff Tompkinson/Photo Researchers, Inc.

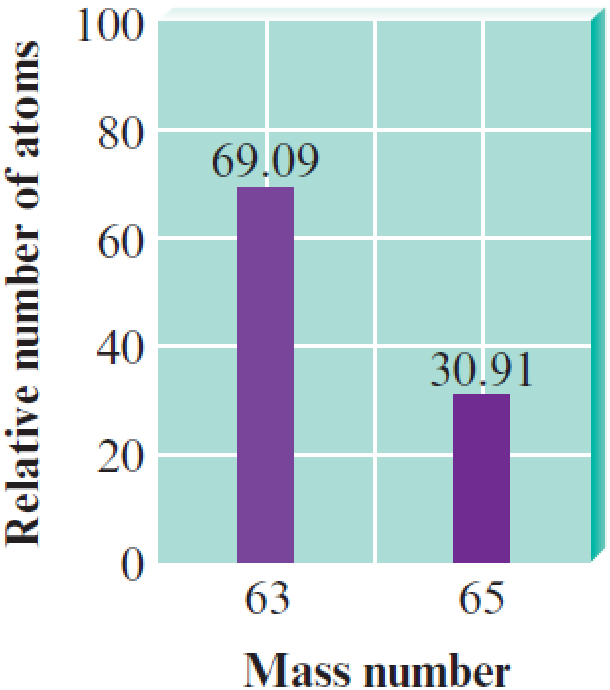
Exercise

- An element consists of:
  - 1.40% of an isotope with mass 203.973 u
  - 24.10% of an isotope with mass 205.9745 u
  - 22.10% of an isotope with mass 206.9759 u
  - 52.40% of an isotope with mass 207.9766 u
    - Calculate the average atomic mass, and identify the element

Mass = 207.2 u
The element is lead (Pb)

Example 3.1 - The Average Mass of an Element

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



Example 3.1 - Solution

- Where are we going?
  - To calculate the average mass of natural copper
- What do we know?
  - ^{63}Cu mass = 62.93 u
  - ^{65}Cu mass = 64.93 u
- How do we get there?
  - As shown by the graph, of every 100 atoms of natural copper, 69.09 are ^{63}Cu and 30.91 are ^{65}Cu

Example 3.1 - Solution (Continued 1)

- Thus, the mass of 100 atoms of natural copper is

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

- The average mass of a copper atom is

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

  - This mass value is used in doing calculations involving the reactions of copper

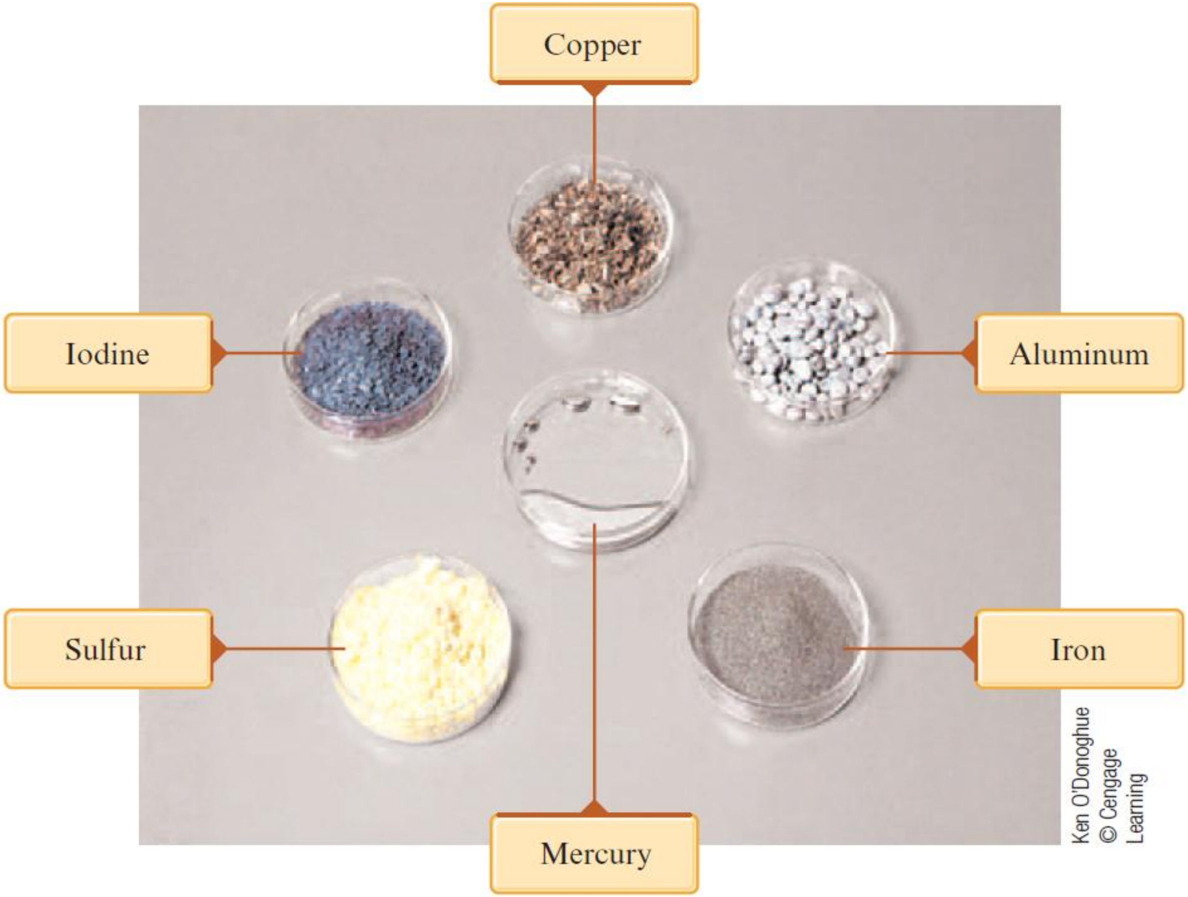
Example 3.1 - Solution (Continued 2)

- Reality check
  - The answer of 63.55 u is between the masses of the atoms that make up natural copper
  - This makes sense
  - The answer could not be smaller than 62.93 u or larger than 64.93 u

Mole (mol)

- Number of carbon atoms in exactly 12 grams of pure ^{12}C
  - Determined to be 6.02214×10^{23} using the technique of mass spectrometry
  - **Avogadro's number**: 1 mole of something consists of 6.022×10^{23} units of that substance

Figure 3.4 - One Mole Samples of Several Elements



Critical Thinking

- What if you were offered \$1 million to count from 1 to 6×10^{23} at a rate of one number each second?
  - Determine your hourly wage
  - Would you do it? Could you do it?

Using the Mole in Chemical Calculations

- Avogadro's number is defined as the number of atoms in exactly 12 g of ^{12}C
  - 1 mol C = 6.022×10^{23} atoms
- 12.01-g sample of natural carbon contains 6.022×10^{23} atoms

Using the Mole in Chemical Calculations (Continued)

- Ratio of masses of both samples - 12 g/12.01 g
- Ratio of masses of individual components - 12 u/12.01 u
  - Therefore, both samples contain the same number of atoms

Table 3.1 - Comparison of 1 Mole Samples of Various Elements

Element	Number of Atoms Present	Mass of Sample (g)
Aluminum	6.022×10^{23}	26.98
Copper	6.022×10^{23}	63.55
Iron	6.022×10^{23}	55.85
Sulfur	6.022×10^{23}	32.07
Iodine	6.022×10^{23}	126.9
Mercury	6.022×10^{23}	200.6

Defining the Mole

- Sample of a natural element whose mass equals the element's atomic mass expressed in grams contains 1 mole of atoms
- Relationship between the atomic mass unit and the gram:

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

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

Critical Thinking

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

Interactive Example 3.5 - Calculating the Number of Moles and Mass

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

Interactive Example 3.5 - Solution

- Where are we going?
  - To calculate the number of moles and the mass of a sample of Co
- What do we know?
  - Sample contains 5.00×10^{20} atoms of Co

Interactive Example 3.5 - Solution (Continued 1)

- How do we get there?
  - Note that the sample of 5.00 × 10^{20} atoms of cobalt is less than 1 mole (6.022 × 10^{23} atoms) of cobalt
    - What fraction of a mole it represents can be determined as follows:

$$5.00 \times 10^{20}\ \cancel{\text{atoms}}\ \text{Co} \times \frac{1\ \text{mol Co}}{6.022 \times 10^{23}\ \cancel{\text{atoms}}\ \text{Co}}$$

$$= 8.30 \times 10^{-4}\ \text{mol Co}$$

Interactive Example 3.5 - Solution (Continued 2)

- Since the mass of 1 mole of cobalt atoms is 58.93 g, the mass of 5.00×10^{23} atoms can be determined as follows:

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

Interactive Example 3.5 - Solution (Continued 3)

- Reality check
  - The sample contains 5×10^{20} atoms, which is approximately 1/1000 of a mole
    - The sample should have a mass of about (1/1000)(58.93) ≅ 0.06
    - The answer of ~ 0.05 makes sense

Exercise

- Diamond is a natural form of pure carbon
  - What number of atoms of carbon are in a 1.00-carat diamond (1.00 carat = 0.200 g)?

1.00×10^{22} atoms C

Molar Mass - An Introduction

- Mass in grams of one mole of a substance
  - Obtained by finding the sum of masses of a compound's constituent atoms
- Example - Mass of 1 mole of methane (CH_4) can be computed by summing the masses of C and H
  - Mass of 1 mol of C = 12.01 g
  - Mass of 4 mol of H = 4 × 1.008 g = 4.03 g
    - Therefore, mass of 1 mol CH_4 = 16.04 g

Interactive Example 3.7 - Calculating Molar Mass II

- Calcium carbonate ($CaCO_3$), also called calcite, is the principal mineral found in limestone, marble, chalk, pearls, and the shells of marine animals such as clams
  a. Calculate the molar mass of calcium carbonate
  b. A certain sample of calcium carbonate contains 4.86 moles
     - What is the mass in grams of this sample? What is the mass of the CO_3^{2-} ions present?

Interactive Example 3.7 - Solution (a)

- Calcium carbonate is an ionic compound composed of Ca^{2+} and CO_3^{2-} ions
  - In 1 mole of calcium carbonate, there are 1 mole of Ca^{2+} ions and 1 mole of CO_3^{2-} ions
  - Molar mass is calculated by summing the masses of the components

Interactive Example 3.7 - Solution (a) (Continued)

1 Ca^{2+}:	1×40.08 g	=	40.08 g
1 CO_3^{2-}:			
1 C:	1×12.01 g	=	12.01 g
3 O:	3×16.00 g	=	48.00 g
Mass of 1 mol $CaCO_3$		=	100.09 g

- Thus, the mass of 1 mole of $CaCO_3$ (1 mole of Ca^{2+} plus 1 mole of CO_3^{2-}) is 100.09 g
  - This is the molar mass

Interactive Example 3.7 - Solution (b)

- The mass of 1 mole of $CaCO_3$ is 100.09 g
  - The sample contains nearly 5 moles, or close to 500 g
  - The exact amount is determined as follows:

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

Interactive Example 3.7 - Solution (b) (Continued 1)

- To find the mass of carbonate ions (CO_3^{2-}) present in this sample, realize that 4.86 moles of $CaCO_3$ contains 4.86 moles of Ca^{2+} ions and 4.86 moles of CO_3^{2-} ions
- The mass of 1 mole of CO_3^{2-} ions is calculated as follows:

1 C:	1×12.01	=	12.01 g
3 O:	3×16.00	=	48.00 g
Mass of 1 mol CO_3^{2-}		=	60.01 g

Interactive Example 3.7 - Solution (b) (Continued 2)

- Thus, the mass of 4.86 moles of CO_3^{2-} ions is

$$4.86\ \cancel{\text{mol}\ CO_3^{2-}} \times \frac{60.01\ \text{g}\ CO_3^{2-}}{1\ \cancel{\text{mol}\ CO_3^{2-}}} = 292\ \text{g}\ CO_3^{2-}$$

Interactive Example 3.8 - Molar Mass and Numbers of Molecules

- Isopentyl acetate ($C_7H_{14}O_2$) is the compound responsible for the scent of bananas
  - Interestingly, bees release about 1 μg (1×10^{-6} g) of this compound when they sting
    - The resulting scent attracts other bees to join the attack
    - How many molecules of isopentyl acetate are released in a typical bee sting?
    - How many atoms of carbon are present?

Interactive Example 3.8 - Solution

- Where are we going?
  - To calculate the number of molecules of isopentyl acetate and the number of carbon atoms in a bee sting
- What do we know?
  - Mass of isopentyl acetate in a typical bee sting is 1 microgram = 1×10^{-6} g

Interactive Example 3.8 - Solution (Continued 1)

- How do we get there?
  - Since we are given a mass of isopentyl acetate and want to find the number of molecules, we must first compute the molar mass of $C_7H_{14}O_2$

$$7\ \cancel{\text{mol}}\ \text{C} \times 12.01\ \frac{\text{g}}{\cancel{\text{mol}}} = 84.07\ \text{g C}$$

$$14\ \cancel{\text{mol}}\ \text{H} \times 1.008\ \frac{\text{g}}{\cancel{\text{mol}}} = 14.11\ \text{g H}$$

Interactive Example 3.8 - Solution (Continued 2)

$$2\ \cancel{\text{mol}}\ \text{O} \times 16.00\ \frac{\text{g}}{\cancel{\text{mol}}} = 32.00\ \text{g O}$$

$$\text{Molar mass of } C_7H_{14}O_2 = 84.07\ \text{g C} + 14.11\ \text{g H} + 32.00\ \text{g O}$$
$$= 130.18\ \text{g}$$

- This means that 1 mole of isopentyl acetate (6.022×10^{23} molecules) has a mass of 130.18 g

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

Interactive Example 3.8 - Solution (Continued 3)

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

- Since 1 mole is 6.022×10^{23} units, we can determine the number of molecules

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

Interactive Example 3.8 - Solution (Continued 4)

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

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

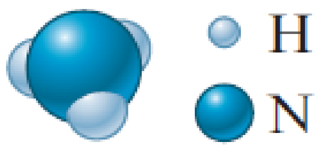
Interactive Example 3.8 - Solution (Continued 5)

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

Exercise

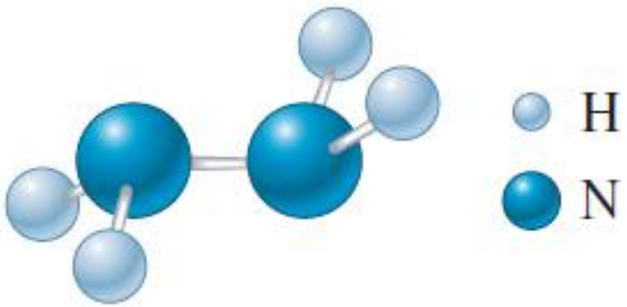
- Calculate the molar mass of the following substances:

a.



17.03 g/mol

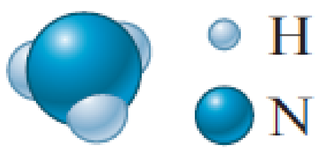
b.



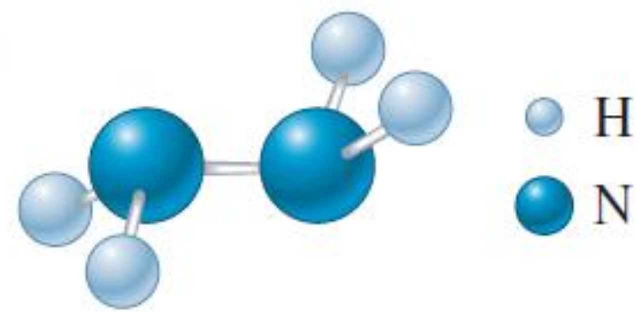
32.05 g/mol

Exercise (Continued)

- What number of atoms of nitrogen are present in 1.00 g of each of the following compounds?

a. 

3.54×10^{22} atoms

b. 

3.76×10^{22} atoms

Conceptual Problem Solving

- Method that will help solve problems in a flexible and creative manner
  - Based on the understanding of fundamental concepts of chemistry
- Goal of the text
  - To help one solve new problems on their own

Methods of Approaching a Problem

- Pigeonhole method
  - Emphasizes memorization
  - Involves labeling the problem
    - Slotting the problem into the apt pigeonhole
  - Provides steps that one can memorize and store in an appropriate slot for each different problem
  - Challenge
    - Requirement of a new pigeonhole for every new problem

Methods of Approaching a Problem (Continued)

- Conceptual problem solving
  - Helps understand the reality of the situation
  - Involves looking for a solution within the problem
    - Each problem is assumed as a new one
    - The problem should guide you as you solve it
  - Involves asking a series of questions while proceeding with the problem
    - One uses his/her knowledge of fundamental chemistry principles to answer the questions

Conceptual Problem Solving - The Approach

- Where are we going?
  - Read the problem and decide on the final goal
  - Sort through the given facts and focus on the key words
  - Draw a diagram of the problem
  - This stage involves a simple, visual analysis of the problem

Conceptual Problem Solving - The Approach (Continued)

- How do we get there?
  - Work backward from the final goal to decide where to start
- Reality check
  - Check if the answer makes sense
  - Check whether the answer is reasonable

Methods of Describing a Compound's Composition

- In terms of the numbers of the compound's atoms
- In terms of **mass percent** (weight percent)

$$\text{mass \%} = \frac{\text{mass of an element in 1 mol of the compound}}{\text{mass of 1 mol of the compound}} \times 100\%$$

Interactive Example 3.9 - Calculating Mass Percent

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

Interactive Example 3.9 - Solution

- Where are we going?
  - To find the mass percent of each element in carvone
- What do we know?
  - Molecular formula is $C_{10}H_{14}O$
- What information do we need to find the mass percent?
  - Mass of each element (we'll use 1 mole of carvone)
  - Molar mass of carvone

Interactive Example 3.9 - Solution (Continued 1)

- How do we get there?
  - Determine the mass of each element in 1 mole of $C_{10}H_{14}O$

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

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

$$\text{Mass of O in 1 mol} = 1\ \cancel{\text{mol}} \times 16.00\frac{\text{g}}{\cancel{\text{mol}}} = 16.00\text{ g}$$

Interactive Example 3.9 - Solution (Continued 2)

- What is the molar mass of $C_{10}H_{14}O$?

$$\begin{array}{ccccccc} 120.1\text{ g} & + & 14.11\text{ g} & + & 16.00\text{ g} & = & 150.2\text{ g} \\ C_{10} & + & H_{14} & + & O & = & C_{10}H_{14}O \end{array}$$

- What is the mass percent of each element?
  - Find the fraction of the total mass contributed by each element and convert it to a percentage

Interactive Example 3.9 - Solution (Continued 3)

$$\text{Mass percent of C} = \frac{120.1\text{ g C}}{150.2\text{ g }C_{10}H_{14}O} \times 100\% = 79.96\%$$

$$\text{Mass percent of H} = \frac{14.11\text{ g H}}{150.2\text{ g }C_{10}H_{14}O} \times 100\% = 9.394\%$$

$$\text{Mass percent of O} = \frac{16.00\text{ g C}}{150.2\text{ g }C_{10}H_{14}O} \times 100\% = 10.65\%$$

- Reality check
  - The percentages add up to 100%

Exercise

- Calculate the percent composition by mass of the following compounds that are important starting materials for synthetic polymers:
  a. $C_3H_4O_2$ (acrylic acid, from which acrylic plastics are made)

     50.00% C, 5.595% H, and 44.41% O

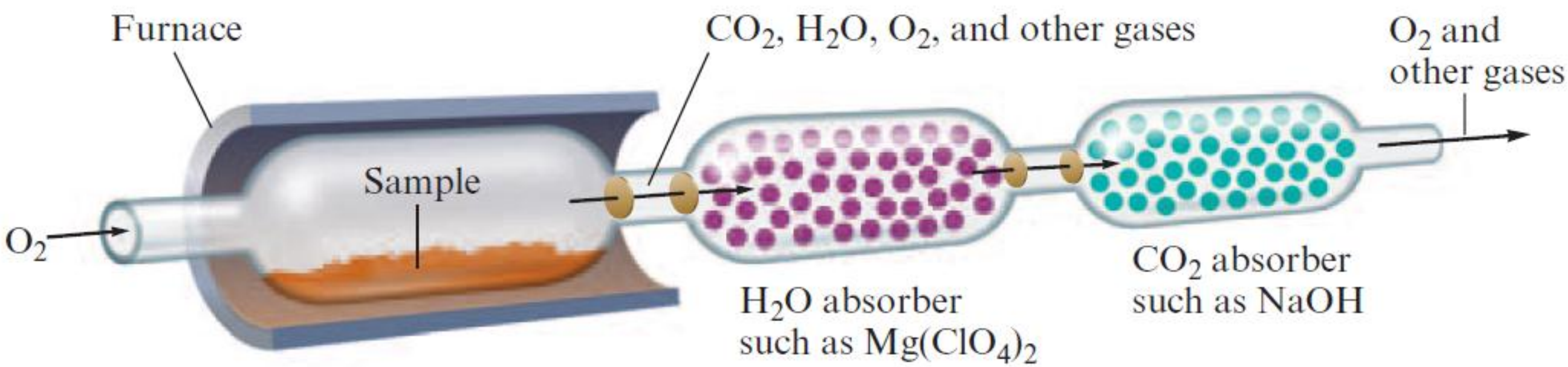
  b. $C_4H_6O_2$ (methyl acrylate, from which Plexiglas is made)

     55.80% C, 7.025% H, and 37.18% O

Determining the Formula of a Compound

- Weigh the sample of the compound
- Decompose the sample into its constituent elements or react it with oxygen
- Combustion device
  - Used to analyze substances for hydrogen and carbon
  - Helps determine the mass percent of each element in a compound

Figure 3.5 - A Schematic Diagram of a Combustion Device



Empirical Formula

- Any molecule that can be represented as $(CH_5N)_n$ has the empirical formula CH_5N
  - *n* - Integer
  - **Molecular formula**: Exact formula of the molecules present in a substance
    - Requires the knowledge of the molar mass

Problem-Solving Strategy - Empirical Formula Determination

- Mass percentage gives the number of grams of a particular element per 100 g of compound
  - Therefore, base the calculation on 100 g of compound
  - Each percent will then represent the mass in grams of that element
- Determine the number of moles of each element present in 100 g of compound
  - Use the atomic masses of the elements present

Problem-Solving Strategy - Empirical Formula Determination (Continued)

- Divide each value of the number of moles by the smallest of the values
  - If each resulting number is a whole number (after appropriate rounding), these numbers represent the subscripts of the elements in the empirical formula
  - If the numbers obtained are not whole numbers, multiply each number by an integer so that the results are all whole numbers

Critical Thinking

- One part of the problem-solving strategy for empirical formula determination is to base the calculation on 100 g of compound
  - What if you chose a mass other than 100 g?
    - Would this work?
  - What if you chose to base the calculation on 100 moles of compound?
    - Would this work?

Problem-Solving Strategy - Determining Molecular Formula from Empirical Formula

- Obtain the empirical formula
- Compute the mass corresponding to the empirical formula
- Calculate the ratio

$$\frac{\text{Molar mass}}{\text{Empirical formula mass}}$$

Problem-Solving Strategy - Determining Molecular Formula from Empirical Formula (Continued)

- Number of empirical formula units in one molecule is represented by the integer from the previous step
  - Molecular formula results when the empirical formula subscripts are multiplied by this integer
  - This procedure is summarized as follows:

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

Interactive Example 3.11 - Determining Empirical and Molecular Formulas II

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

Interactive Example 3.11 - Solution

- Where are we going?
  - To find the empirical and molecular formulas for the given compound
- What do we know?
  - Percent of each element
  - Molar mass of the compound is 283.88 g/mol

Interactive Example 3.11 - Solution (Continued 1)

- What information do we need to find the empirical formula?
  - Mass of each element in 100.00 g of compound
  - Moles of each element
- How do we get there?
  - What is the mass of each element in 100.00 g of compound?

Mass of P = 43.64 g   Mass of O = 56.36 g

Interactive Example 3.11 - Solution (Continued 2)

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

$$43.64\ \cancel{\text{g P}} \times \frac{1\ \text{mol P}}{30.97\ \cancel{\text{g P}}} = 1.409\ \text{mol P}$$

$$56.36\ \cancel{\text{g O}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = 3.523\ \text{mol O}$$

Interactive Example 3.11 - Solution (Continued 3)

- What is the empirical formula for the compound?
  - Dividing each mole value by the smaller one gives:

$$\frac{1.409}{1.409} = 1 \text{ P and } \frac{3.523}{1.409} = 2.5 \text{ O}$$

  - This yields the formula $PO_{2.5}$
  - Since compounds must contain whole numbers of atoms, the empirical formula should contain only whole numbers
  - To obtain the simplest set of whole numbers, we multiply both numbers by 2 to give the empirical formula P_2O_5

Interactive Example 3.11 - Solution (Continued 4)

- What is the molecular formula for the compound?
  - Compare the empirical formula mass to the molar mass

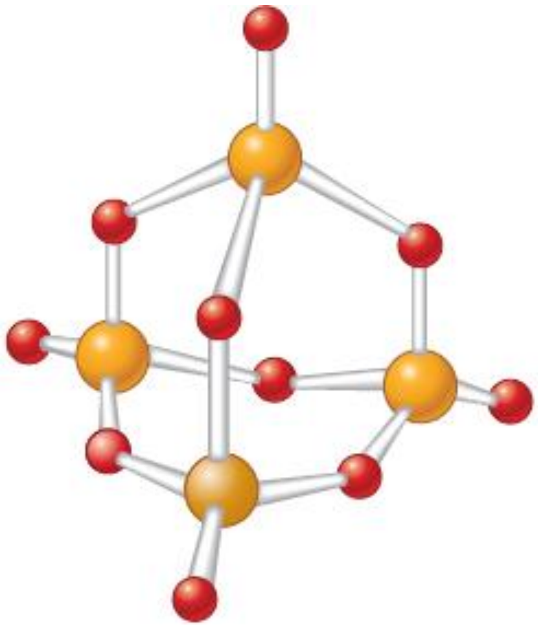
$$\text{Empirical formula mass} = 141.94 \text{ g/mol}$$
$$\text{Given molar mass} = 283.88 \text{ g/mol}$$

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

  - The molecular formula is $(P_2O_5)_2$, or P_4O_{10}

Interactive Example 3.11 - Solution (Continued 5)

- Note - The structural formula for this interesting compound is given below



Exercise

- A compound contains 47.08% carbon, 6.59% hydrogen, and 46.33% chlorine by mass
  - Molar mass of the compound is 153 g/mol
  - What are the empirical and molecular formulas of the compound?

Empirical formula - C_3H_5Cl
Molecular formula - $C_6H_{10}Cl_2$

Problem-Solving Strategy - Determining Molecular Formula from Mass Percent and Molar Mass

- Use the mass percentages and the molar mass to determine the mass of each element present in 1 mole of compound
- Compute the number of moles of each element present in 1 mole of compound
  - Integers in this step represent the subscripts in the molecular formula

Interactive Example 3.12 - Determining a Molecular Formula

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

Interactive Example 3.12 - Solution

- Where are we going?
  - To find the molecular formula for caffeine
- What do we know?
  - Percent of each element
    - 49.48% C
    - 28.87% N
    - 5.15% H
    - 16.49% O
  - Molar mass of caffeine is 194.2 g/mol

Interactive Example 3.12 - Solution (Continued 1)

- What information do we need to find the molecular formula?
  - Mass of each element (in 1 mole of caffeine)
  - Mole of each element (in 1 mole of caffeine)
- How do we get there?
  - What is the mass of each element in 1 mole (194.2 g) of caffeine?

Interactive Example 3.12 - Solution (Continued 2)

$$\frac{49.48 \text{ g C}}{100.0 \cancel{\text{g}} \text{ caffeine}} \times \frac{194.2 \cancel{\text{g}}}{\text{mol}} = \frac{96.09 \text{ g C}}{\text{mol caffeine}}$$

$$\frac{5.15 \text{ g H}}{100.0 \cancel{\text{g}} \text{ caffeine}} \times \frac{194.2 \cancel{\text{g}}}{\text{mol}} = \frac{10.0 \text{ g H}}{\text{mol caffeine}}$$

$$\frac{28.87 \text{ g N}}{100.0 \cancel{\text{g}} \text{ caffeine}} \times \frac{194.2 \cancel{\text{g}}}{\text{mol}} = \frac{56.07 \text{ g N}}{\text{mol caffeine}}$$

$$\frac{16.49 \text{ g O}}{100.0 \cancel{\text{g}} \text{ caffeine}} \times \frac{194.2 \cancel{\text{g}}}{\text{mol}} = \frac{32.02 \text{ g O}}{\text{mol caffeine}}$$

Interactive Example 3.12 - Solution (Continued 3)

- What are the moles of each element in 1 mole of caffeine?

$$\text{Carbon: } \frac{96.09\ \cancel{\text{g C}}}{\text{mol caffeine}} \times \frac{1\ \text{mol C}}{12.01\ \cancel{\text{g C}}} = \frac{8.001\ \text{mol C}}{\text{mol caffeine}}$$

$$\text{Hydrogen: } \frac{10.0\ \cancel{\text{g H}}}{\text{mol caffeine}} \times \frac{1\ \text{mol H}}{1.008\ \cancel{\text{g H}}} = \frac{9.92\ \text{mol H}}{\text{mol caffeine}}$$

Interactive Example 3.12 - Solution (Continued 4)

$$\text{Nitrogen: } \frac{56.07\ \cancel{\text{g N}}}{\text{mol caffeine}} \times \frac{1\ \text{mol N}}{14.01\ \cancel{\text{g N}}} = \frac{4.002\ \text{mol N}}{\text{mol caffeine}}$$

$$\text{Oxygen: } \frac{32.02\ \cancel{\text{g O}}}{\text{mol caffeine}} \times \frac{1\ \text{mol O}}{16.00\ \cancel{\text{g O}}} = \frac{2.001\ \text{mol O}}{\text{mol caffeine}}$$

- Rounding the numbers to integers gives the molecular formula for caffeine: $C_8H_{10}N_4O_2$

Chemical Reactions

- Chemical change involves the reorganization of atoms in one or more substances
  - Atoms are neither created nor destroyed
- Represented by a **chemical equation**
  - **Reactants**: Presented on the left side of an arrow
  - **Products**: Presented on the right side of the arrow

$$CH_4 + O_2 \longrightarrow CO_2 + H_2O$$

Reactants — Products

Balancing a Chemical Equation

- All atoms present in the reactants must be accounted for in the products that are formed

$$\text{Unbalanced equation: } CH_4 + O_2 \longrightarrow CO_2 + H_2O$$

$$\text{Balanced equation: } CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

Reactants	Products
1 C	1 C
4 H	4 H
4 O	4 O

Information Provided by Chemical Equations

- Nature of the reactants and products
- Relative numbers of reactants and products
  - Indicated by coefficients in a balanced equation
- Physical states of reactants and products
- Mass remains constant
  - Atoms are conserved in a chemical reaction

Representing Physical States in a Chemical Equation

State	Symbol
Solid	(*s*)
Liquid	(*l*)
Gas	(*g*)
Dissolved in water (in aqueous solution)	(*aq*)

Things to Remember

- Refrain from considering an unbalanced equation
- Experimental observation determines the identities of the reactants and products of a reaction
- Formulas of compounds must never be changed while balancing a chemical equation
  - Do not change subscripts, and do not add or subtract atoms from a formula

Critical Thinking

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

Problem-Solving Strategy - Writing and Balancing the Equation for a Chemical Reaction

1. Determine what reaction is occurring
   - Determine the reactants, the products, and the physical states involved
2. Write the unbalanced equation that summarizes the reaction

Problem-Solving Strategy - Writing and Balancing the Equation for a Chemical Reaction (Continued)

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

Critical Thinking

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

Interactive Example 3.14 - Balancing a Chemical Equation II

- At 1000° C, ammonia gas, $NH_3(g)$, reacts with oxygen gas to form gaseous nitric oxide, $NO(g)$, and water vapor
  - This reaction is the first step in the commercial production of nitric acid by the Ostwald process
  - Balance the equation for this reaction

Interactive Example 3.14 - Solution

- Steps 1 and 2
  - The unbalanced equation for the reaction is

$$NH_3(g) + O_2(g) \rightarrow NO(g) + H_2O(g)$$

- Step 3
  - Since all the molecules in this equation are of about equal complexity, where we start in balancing it is rather arbitrary

Interactive Example 3.14 - Solution (Continued 1)

- Let's begin by balancing the hydrogen
  - A coefficient of 2 for NH_3 and a coefficient of 3 for H_2O give six atoms of hydrogen on both sides

$$2NH_3(g) + O_2(g) \rightarrow NO(g) + 3H_2O(g)$$

- The nitrogen can be balanced with a coefficient of 2 for NO

$$2NH_3(g) + O_2(g) \rightarrow 2NO(g) + 3H_2O(g)$$

Interactive Example 3.14 - Solution (Continued 2)

- Finally, note that there are two atoms of oxygen on the left and five on the right
  - The oxygen can be balanced with a coefficient of $\frac{5}{2}$ for O_2

$$2NH_3(g) + \frac{5}{2}O_2(g) \rightarrow 2NO(g) + 3H_2O(g)$$

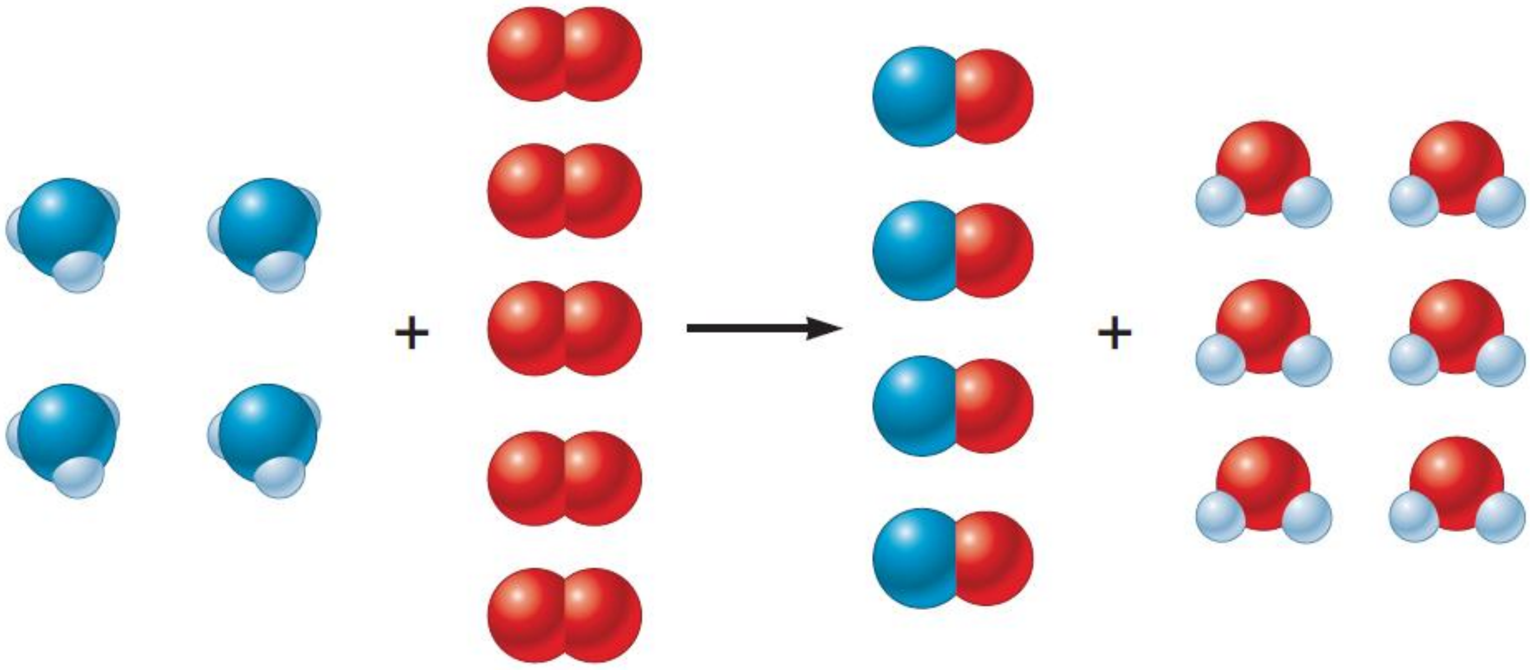
- Usual custom is to have whole-number coefficients
  - We simply multiply the entire equation by 2

$$4NH_3(g) + 5O_2(g) \rightarrow 4NO(g) + 6H_2O(g)$$

- Reality check - There are 4 N, 12 H, and 10 O on both sides, so the equation is balanced

Interactive Example 3.14 - Solution (Continued 3)

- Visual representation of the balanced reaction



Exercise

- Balance the following equations:

a. $Ca(OH)_2(aq) + H_3PO_4(aq) \rightarrow H_2O(l) + Ca_3(PO_4)_2(s)$

$3Ca(OH)_2(aq) + 2H_3PO_4(aq) \rightarrow 6H_2O(l) + Ca_3(PO_4)_2(s)$

b. $AgNO_3(aq) + H_2SO_4(aq) \rightarrow Ag_2SO_4(s) + HNO_3(aq)$

$2AgNO_3(aq) + H_2SO_4(aq) \rightarrow Ag_2SO_4(s) + 2HNO_3(aq)$

Problem-Solving Strategy - Calculating Masses of Reactants and Products in Reactions

1. Balance the equation for the reaction
2. Convert the known mass of the reactant or product to moles of that substance
3. Use the balanced equation to set up the appropriate mole ratios

Problem-Solving Strategy - Calculating Masses of Reactants and Products in Reactions (Continued)

4. Use the appropriate mole ratios to calculate the number of moles of the desired reactant or product
5. Convert from moles back to grams if required by the problem

Critical Thinking

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

Interactive Example 3.15 - Chemical Stoichiometry I

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

Interactive Example 3.15 - Solution

- Where are we going?
  - To find the mass of CO_2 absorbed by 1.00 kg LiOH
- What do we know?
  - Chemical reaction - $\text{LiOH}(s) + \text{CO}_2(g) \rightarrow \text{Li}_2\text{CO}_3(s) + \text{H}_2\text{O}(l)$
  - 1.00 kg LiOH
- What information do we need to find the mass of CO_2?
  - Balanced equation for the reaction

Interactive Example 3.15 - Solution (Continued 1)

- How do we get there?
  1. What is the balanced equation?

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

  2. What are the moles of LiOH?
     - To find the moles of LiOH, we need to know the molar mass

$$\text{Molar mass of LiOH} = 6.941 + 16.00 + 1.008 = 23.95\ \text{g/mol}$$

Interactive Example 3.15 - Solution (Continued 2)

- Now we use the molar mass to find the moles of LiOH

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

3. What is the mole ratio between CO_2 and LiOH in the balanced equation?

$$\frac{1\ \text{mol } CO_2}{2\ \text{mol LiOH}}$$

Interactive Example 3.15 - Solution (Continued 3)

4. What are the moles of CO_2?

$$41.8\ \cancel{\text{mol LiOH}} \times \frac{1\ \text{mol}\ CO_2}{2\ \cancel{\text{mol LiOH}}} = 20.9\ \text{mol}\ CO_2$$

5. What is the mass of CO_2 formed from 1.00 kg LiOH?

$$20.9\ \cancel{\text{mol}\ CO_2} \times \frac{44.0\ \text{g}\ CO_2}{1\ \cancel{\text{mol}\ CO_2}} = 9.20\times10^2\ \text{g}\ CO_2$$

Thus, 920 g of $CO_2(g)$ will be absorbed by 1.00 kg of LiOH(*s*)

Exercise

- Over the years, the thermite reaction has been used for welding railroad rails, in incendiary bombs, and to ignite solid-fuel rocket motors
  - The reaction is as follows:

$$Fe_2O_3(s) + 2Al(s) \rightarrow 2Fe(l) + Al_2O_3(s)$$

  - What masses of iron(III) oxide and aluminum must be used to produce 15.0 g iron? What is the maximum mass of aluminum oxide that could be produced?

Exercise (Continued)

- What masses of iron(III) oxide and aluminum must be used to produce 15.0 g iron?

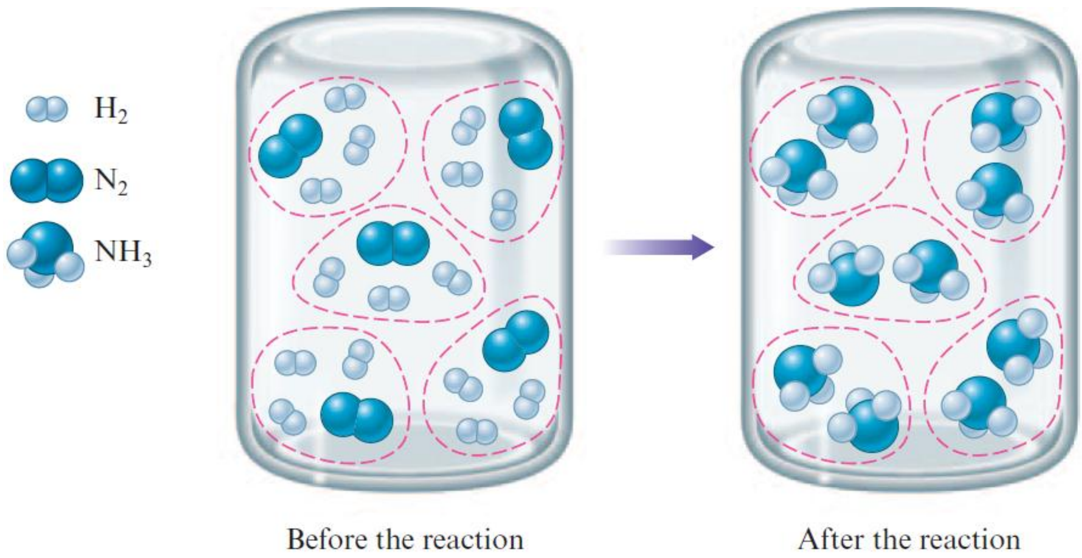
Mass of iron (III) oxide = 21.5 g
Mass of Aluminum = 7.26 g

- What is the maximum mass of aluminum oxide that could be produced?

13.7 g Al_2O_3

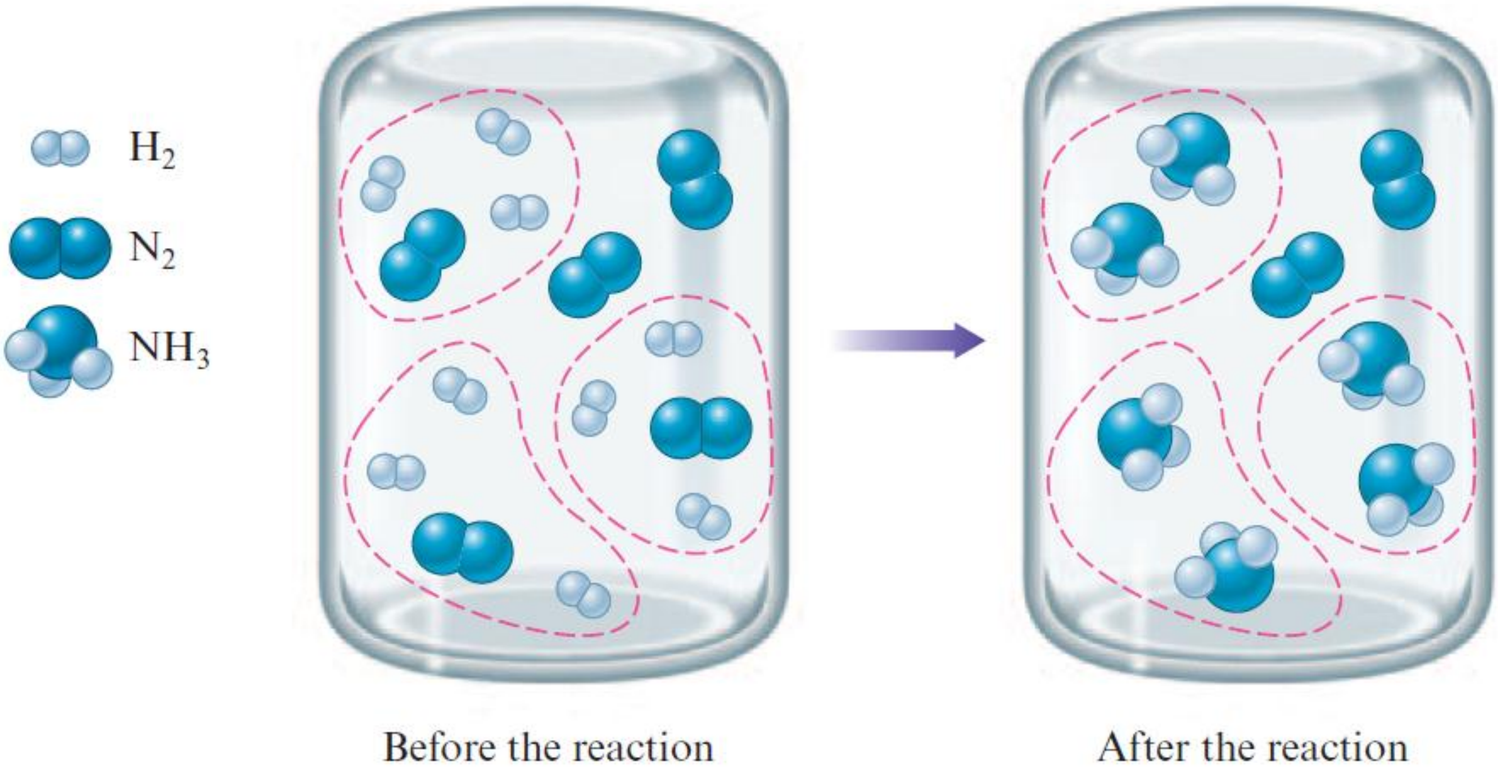
Stoichiometric Mixture

- Contains relative amounts of reactants that match the numbers in the balanced equation



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

When Hydrogen is the Limiting Reactant



Limiting Reactants

- To determine the amount of product that will be formed, ascertain the reactant that is limiting
  - **Limiting reactant**: Runs out first
    - Limits the amounts of products that can be formed
- Some mixtures can be stoichiometric
  - All reactants run out at the same time
  - Requires determining which reactant is limiting

Determination of the Limiting Reactant Using Reactant Quantities

- Compare the moles of reactants to ascertain which runs out first
  - Use moles of molecules instead of individual molecules
- Method
  - Use the balanced equation to determine the limiting reactant

Determination of the Limiting Reactant Using Reactant Quantities (Continued)

- Determine the amount of limiting reactant formed
  - Use the amount of limiting reactant formed to compute the quantity of the product
- Alternative method
  - Compare the mole ratio of substances that are required by the balanced equation with the mole ratio of actual reactants present

Determination of Limiting Reactant Using Quantities of Products Formed

- Use the amounts of products that can be formed by completely consuming each reactant
  - Reactant that produces the smallest amount of product must run out first
    - This is the limiting reactant

Interactive Example 3.17 - Stoichiometry: Limiting Reactant

- Nitrogen gas can be prepared by passing gaseous ammonia over solid copper(II) oxide at high temperatures
  - The other products of the reaction are solid copper and water vapor
  - If a sample containing 18.1 g of NH_3 is reacted with 90.4 g of CuO, which is the limiting reactant?
    - How many grams of N_2 will be formed?

Interactive Example 3.17 - Solution

- Where are we going?
  - To find the limiting reactant
  - To find the mass of N_2 produced
- What do we know?
  - The chemical reaction

$$NH_3(g) + CuO(s) \rightarrow N_2(g) + Cu(s) + H_2O(g)$$

  - 18.1 g NH_3 and 90.4 g CuO

Interactive Example 3.17 - Solution (Continued 1)

- What information do we need?
  - Balanced equation for the reaction
  - Moles of NH_3
  - Moles of CuO
- How do we get there?
  - To find the limiting reactant, determine the balanced equation

$$2NH_3(g) + 3CuO(s) \rightarrow N_2(g) + 3Cu(s) + 3H_2O(g)$$

Interactive Example 3.17 - Solution (Continued 2)

- What are the moles of NH_3 and CuO?
  - To find the moles, we need to know the molar masses

NH_3	17.03 g/mol
CuO	79.55 g/mol

$$18.1\ \cancel{\text{g NH}_3} \times \frac{1\ \text{mol NH}_3}{17.03\ \cancel{\text{g NH}_3}} = 1.06\ \text{mol NH}_3$$

$$90.4\ \cancel{\text{g CuO}} \times \frac{1\ \text{mol CuO}}{79.55\ \cancel{\text{g CuO}}} = 1.14\ \text{mol CuO}$$

Interactive Example 3.17 - Solution (Continued 3)

A. First we will determine the limiting reactant by comparing the moles of reactants to see which one is consumed first
   - What is the mole ratio between NH_3 and CuO in the balanced equation?

$$\frac{3 \text{ mol CuO}}{2 \text{ mol NH}_3}$$

Interactive Example 3.17 - Solution (Continued 4)

- How many moles of CuO are required to react with 1.06 moles of NH_3?

$$1.06 \text{ mol NH}_3 \times \frac{3 \text{ mol CuO}}{2 \text{ mol NH}_3} = 1.59 \text{ mol CuO}$$

  - Thus 1.59 moles of CuO are required to react with 1.06 moles of NH_3
  - Since only 1.14 moles of CuO are actually present, the amount of CuO is limiting; CuO will run out before NH_3 does

Interactive Example 3.17 - Solution (Continued 5)

- We can verify this conclusion by comparing the mole ratio of CuO and NH_3 required by the balanced equation

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

- With the mole ratio actually present

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

- Since the actual ratio is too small (less than 1.5), CuO is the limiting reactant

Interactive Example 3.17 - Solution (Continued 6)

B. Alternatively we can determine the limiting reactant by computing the moles of N_2 that would be formed by complete consumption of NH_3 and CuO

$$1.06\ \cancel{\text{mol NH}_3} \times \frac{1\ \text{mol N}_2}{2\ \cancel{\text{mol NH}_3}} = 0.530\ \text{mol N}_2$$

$$1.14\ \cancel{\text{mol CuO}} \times \frac{1\ \text{mol N}_2}{3\ \cancel{\text{mol CuO}}} = 0.380\ \text{mol N}_2$$

Interactive Example 3.17 - Solution (Continued 7)

- As before, we see that the CuO is limiting since it produces the smaller amount of N_2
- To find the mass of N_2 produced, determine the moles of N_2 formed
  - Because CuO is the limiting reactant, we must use the amount of CuO to calculate the amount of N_2 formed

Interactive Example 3.17 - Solution (Continued 8)

- What is the mole ratio between N_2 and CuO in the balanced equation?

$$\frac{1 \text{ mol } N_2}{3 \text{ mol CuO}}$$

- What are the moles of N_2?

$$1.14 \cancel{\text{ mol CuO}} \times \frac{1 \text{ mol } N_2}{3 \cancel{\text{ mol CuO}}} = 0.380 \text{ mol } N_2$$

Interactive Example 3.17 - Solution (Continued 9)

- What mass of N_2 is produced?
  - Using the molar mass of N_2 (28.02 g/mol), we can calculate the mass of N_2 produced

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

The Concept of Yield

- **Theoretical yield**: Amount of product formed after the limiting reactant is entirely consumed
  - Amount of product predicted is rarely obtained due to side reactions and other complications
- **Percent yield**: Actual yield of product

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

Interactive Example 3.18 - Calculating Percent Yield

- Methanol (CH_3OH), also called methyl alcohol, is the simplest alcohol
  - It is used as a fuel in race cars and is a potential replacement for gasoline
  - Methanol can be manufactured by combining gaseous carbon monoxide and hydrogen

Interactive Example 3.18 - Calculating Percent Yield
(Continued)

- Suppose 68.5 kg CO(*g*) is reacted with 8.60 kg H_2(*g*)
  - Calculate the theoretical yield of methanol
  - If 3.57×10^4 g CH_3OH is actually produced, what is the percent yield of methanol?

Interactive Example 3.18 - Solution

- Where are we going?
  - To calculate the theoretical yield of methanol
  - To calculate the percent yield of methanol
- What do we know?
  - The chemical reaction

$$H_2(g) + CO(g) \rightarrow CH_3OH(l)$$

  - 68.5 kg CO(*g*) and 8.60 kg H_2 (*g*)
  - 3.57×10^4 g CH_3OH is produced

Interactive Example 3.18 - Solution (Continued 1)

- What information do we need?
  - Balanced equation for the reaction
  - Moles of H_2
  - Moles of CO
  - Which reactant is limiting
  - Amount of CH_3OH produced

Interactive Example 3.18 - Solution (Continued 2)

- How do we get there?
  - To find the limiting reactant, balance the chemical equation

$$2H_2(g) + CO(g) \rightarrow CH_3OH(l)$$

  - What are the moles of H_2 and CO?
    - To find the moles, we need to know the molar masses

H_2	2.016 g/mol
CO	28.02 g/mol

Interactive Example 3.18 - Solution (Continued 3)

$$68.5\ \cancel{\text{kg CO}} \times \frac{1000\ \cancel{\text{g CO}}}{1\ \cancel{\text{kg CO}}} \times \frac{1\ \text{mol CO}}{28.02\ \cancel{\text{g CO}}} = 2.44 \times 10^{3}\ \text{mol CO}$$

$$8.60\ \cancel{\text{kg H}_2} \times \frac{1000\ \cancel{\text{g H}_2}}{1\ \cancel{\text{kg H}_2}} \times \frac{1\ \text{mol H}_2}{2.016\ \cancel{\text{g H}_2}} = 4.27 \times 10^{3}\ \text{mol H}_2$$

Interactive Example 3.18 - Solution (Continued 4)

A. Determination of limiting reactant using reactant quantities

- What is the mole ratio between H_2 and CO in the balanced equation?

$$\frac{2 \text{ mol } H_2}{1 \text{ mol CO}}$$

- How does the actual mole ratio compare to the stoichiometric ratio?

Interactive Example 3.18 - Solution (Continued 5)

- To determine which reactant is limiting, we compare the mole ratio of H_2 and CO required by the balanced equation with the actual mole ratio

$$\frac{\text{mol } H_2}{\text{mol CO}}(\text{required}) = \frac{2}{1} = 2$$

$$\frac{\text{mol } H_2}{\text{mol CO}}(\text{actual}) = \frac{4.27 \times 10^3}{2.44 \times 10^3} = 1.75$$

  - Since the actual mole ratio of H_2 to CO is smaller than the required ratio, H_2 is limiting

Interactive Example 3.18 - Solution (Continued 6)

B. Determination of limiting reactant using quantities of products formed

- We can also determine the limiting reactant by calculating the amounts of CH_3OH formed by complete consumption of CO(*g*) and H_2(*g*)

$$2.44 \times 10^3 \ \cancel{\text{mol CO}} \times \frac{1 \text{ mol } CH_3OH}{1 \ \cancel{\text{mol CO}}} = 2.44 \times 10^3 \text{ mol } CH_3OH$$

Interactive Example 3.18 - Solution (Continued 7)

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

- Since complete consumption of the H_2 produces the smaller amount of CH_3OH, the H_2 is the limiting reactant as we determined above

Interactive Example 3.18 - Solution (Continued 8)

- To calculate the theoretical yield of methanol
  - What are the moles of CH_3OH formed?
    - We must use the amount of H_2 and the mole ratio between H_2 and CH_3OH to determine the maximum amount of methanol that can be produced:

$$4.27 \times 10^3 \text{ mol } H_2 \times \frac{1 \text{ mol } CH_3OH}{2 \text{ mol } H_2} = 2.14 \times 10^3 \text{ mol } CH_3OH$$

Interactive Example 3.18 - Solution (Continued 9)

- What is the theoretical yield of CH_3OH in grams?

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

  - Thus, from the amount of reactants given, the maximum amount of CH_3OH that can be formed is 6.86×10^4 g

Interactive Example 3.18 - Solution (Continued 10)

- What is the percent yield of CH_3OH?

$$\text{Percent yield} = \frac{\text{Actual yield (grams)}}{\text{Theoretical yield (grams)}} \times 100$$

$$= \frac{3.57 \times 10^4 \text{ g } CH_3OH}{6.86 \times 10^4 \text{ g } CH_3OH} \times 100\%$$

$$= 52.0\%$$

Problem-Solving Strategy

- Solving a stoichiometry problem involving masses of reactants and products
  1. Write and balance the equation for the reaction
  2. Convert the known masses of substances to moles
  3. Determine which reactant is limiting and its amount
     - Use this amount and the appropriate mole ratios to compute the number of moles of the desired product
  4. Convert from moles to grams, using the molar mass