CHAPTER 3 CALCULATIONS WITH CHEMICAL FORMULAS AND EQUATIONS

Dr. Yuan Dan

3.1 Molecular Mass and Formula Mass

- **Molecular mass**: the sum of the atomic masses of all the atoms in a molecule of the substance

H_2O: 18 amu

- **Formula mass**: the sum of the atomic masses of all atoms in a formula unit of the compound, whether molecular or not

NaCl: 58.44 amu

P88 Example 3.1

Calculate the formula mass of each of the following to three significant figures, using a table of atomic masses (AM): a. chloroform, $CHCl_3$; b. iron(III) sulfate, $Fe_2(SO_4)_3$.

$$\begin{aligned}
1 \times \text{AM of C} &= & 12.0 \text{ amu} \\
1 \times \text{AM of H} &= & 1.0 \text{ amu} \\
3 \times \text{AM of Cl} &= 3 \times 35.45 \text{ amu} = & \underline{106.4 \text{ amu}} \\
\text{FM of } CHCl_3 &= & 119.4 \text{ amu}
\end{aligned}$$

$$\begin{aligned}
2 \times \text{AM of Fe} &= 2 \times 55.8 \text{ amu} = & 111.6 \text{ amu} \\
3 \times \text{AM of S} &= 3 \times 32.1 \text{ amu} = & 96.3 \text{ amu} \\
3 \times 4 \times \text{AM of O} &= 12 \times 16.00 \text{ amu} = & \underline{192.0 \text{ amu}} \\
\text{FM of } Fe_2(SO_4)_3 &= & 399.9 \text{ amu}
\end{aligned}$$

3.2 The Mole Concept

- A mole: the quantity of a given substance that contains as many molecules or formula units as the number of atoms in exactly 12 g of C-12.
- Avogadro's number (N_A): 6.02×10^{23}

How many Na^+, O?

- Molar mass: the mass of one mole of the substance (unit: g/mol)

How many moles
What's the weight
?

$$1 \text{ mol } C_2H_5OH = 46.1 \text{ g } C_2H_5OH$$

$$10.0 \cancel{\text{ g } C_2H_5OH} \times \frac{1 \text{ mol } C_2H_5OH}{46.1 \cancel{\text{ g } C_2H_5OH}} = 0.217 \text{ mol } C_2H_5OH$$

P90 Example 3.3

$Cl: 35.5 g/mol$

$$\text{Mass of a Cl atom} = \frac{35.5\ \text{g}}{6.02 \times 10^{23}} = \mathbf{5.90 \times 10^{-23}\ g}$$

a. What is the mass in grams of a chlorine atom, Cl?

克

b. What is the mass in grams of a hydrogen chloride molecule, HCl?

$$\text{Mass of an HCl molecule} = \frac{36.5\ \text{g}}{6.02 \times 10^{23}} = \mathbf{6.06 \times 10^{-23}\ g}$$

P90 Example 3.4

Zinc iodide, ZnI_2, can be prepared by the direct combination of elements. A chemist determines from the amounts of elements that 0.0654 mol ZnI_2 can form. How many grams of zinc iodide is this?

$$0.0654\ \cancel{\text{mol ZnI}_2} \times \frac{319\ \text{g ZnI}_2}{1\ \cancel{\text{mol ZnI}_2}} = \mathbf{20.9\ g\ ZnI_2}$$

3.3 Mass Percentages from the Formula

- Percentage Composition

$$\text{Mass\% } A = \frac{\text{mass of } A \text{ in the whole}}{\text{mass of the whole}} \times 100\%$$

P94 Example 3.7

Formaldehyde, CH_2O, is a toxic gas with a pungent odor. Large quantities are consumed in the manufacture of plastics, and a water solution of the compound is used to preserve biological specimens. Calculate the mass percentages of the elements in formaldehyde (give answers to three significant figures).

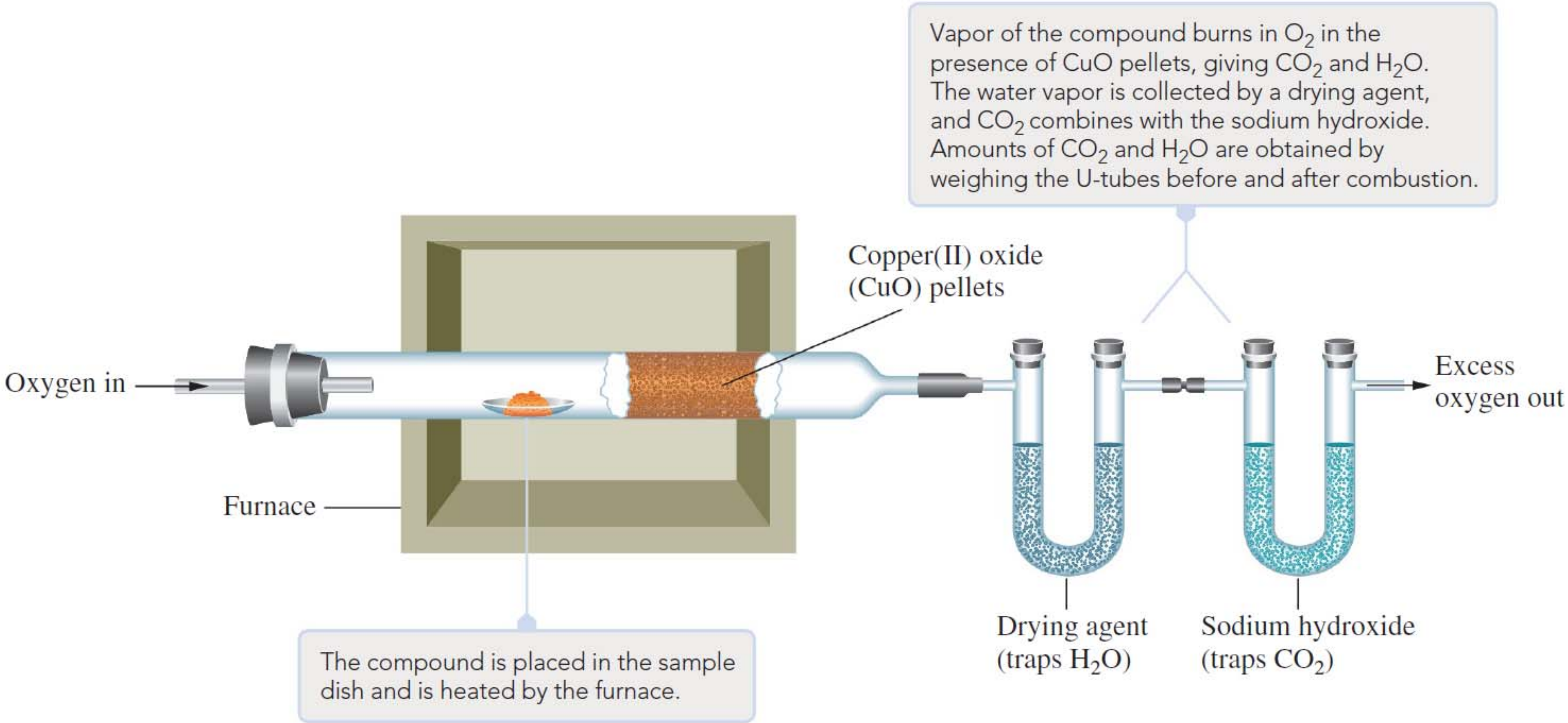
$$\% \text{ C} = \frac{12.0 \text{ g}}{30.0 \text{ g}} \times 100\% = \mathbf{40.0\%}$$

$$\% \text{ H} = \frac{2 \times 1.01 \text{ g}}{30.0 \text{ g}} \times 100\% = \mathbf{6.73\%}$$

$$\% \text{ O} = 100\% - (40.0\% + 6.73\%) = \mathbf{53.3\%}$$

3.4 Elemental Analysis

- **Combustion method**

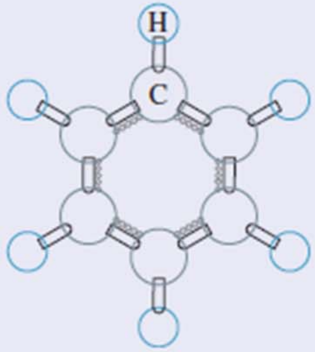


3.5 Determining Formulas

- Empirical formula: a formula written with the smallest integer subscripts

TABLE 3.1 Molecular Models of Two Compounds That Have the Empirical Formula CH

Although benzene and acetylene have the same empirical formula, they do not have the same molecular formula or structure.

Compound	Empirical Formula	Molecular Formula	Molecular Model
Acetylene	CH	C_2H_2	
Benzene	CH	C_6H_6	

3.5 Determining Formulas

- **Molecular Formula from Empirical Formula**

$$n = \frac{\text{molecular weight}}{\text{empirical formula weight}}$$

P101 Example 3.12

In Example 3.9, we found the percentage composition of acetic acid to be 39.9% C, 6.7% H, and 53.4% O. Determine the empirical formula. The molecular mass of acetic acid was determined by experiment to be 60.0 amu. What is its molecular formula? $C_2H_4O_2$

3.6 Molar Interpretation of a Chemical Equation

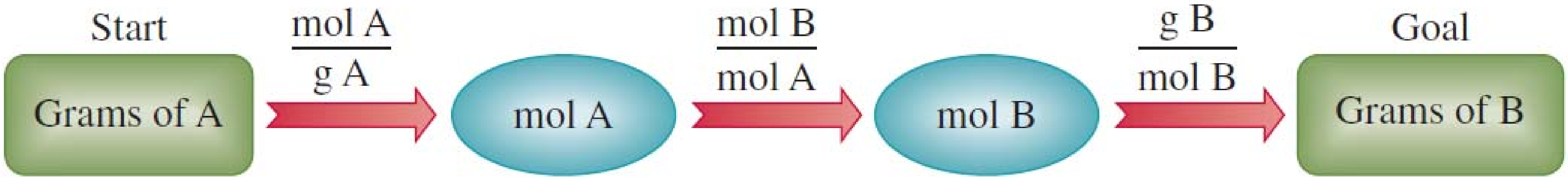
- Stoichiometry

  The calculation of the quantities of reactants and products involved in a chemical reaction.

$$
\begin{array}{ccccc}
N_2 & + & 3H_2 & \longrightarrow & 2NH_3 \\
1 \text{ molecule } N_2 & + & 3 \text{ molecules } H_2 & \longrightarrow & 2 \text{ molecules } NH_3 \\
1 \text{ mol } N_2 & + & 3 \text{ mol } H_2 & \longrightarrow & 2 \text{ mol } NH_3 \\
28.0 \text{ g } N_2 & + & 3 \times 2.02 \text{ g } H_2 & \longrightarrow & 2 \times 17.0 \text{ g } NH_3
\end{array}
$$

3.7 Amounts of Substances in a Chemical Reaction

- **Steps in a stoichiometric calculation**



$$\begin{array}{ccccc}
N_2 & + & 3H_2 & \longrightarrow & 2NH_3 \\
1\ \text{molecule}\ N_2 & + & 3\ \text{molecules}\ H_2 & \longrightarrow & 2\ \text{molecules}\ NH_3 \\
1\ \text{mol}\ N_2 & + & 3\ \text{mol}\ H_2 & \longrightarrow & 2\ \text{mol}\ NH_3 \\
28.0\ \text{g}\ N_2 & + & 3 \times 2.02\ \text{g}\ H_2 & \longrightarrow & 2 \times 17.0\ \text{g}\ NH_3
\end{array}$$

? kg **907 kg**

P105 Example 3.13

Hematite, Fe_2O_3, is an important ore of iron. (An ore is a natural substance from which the metal can be profitably obtained.) The free metal is obtained by reacting hematite with carbon monoxide, CO, in a blast furnace. Carbon monoxide is formed in the furnace by partial combustion of carbon. The reaction is

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

How many grams of iron can be produced from 1.00 kg Fe_2O_3?

P105 Example 3.13

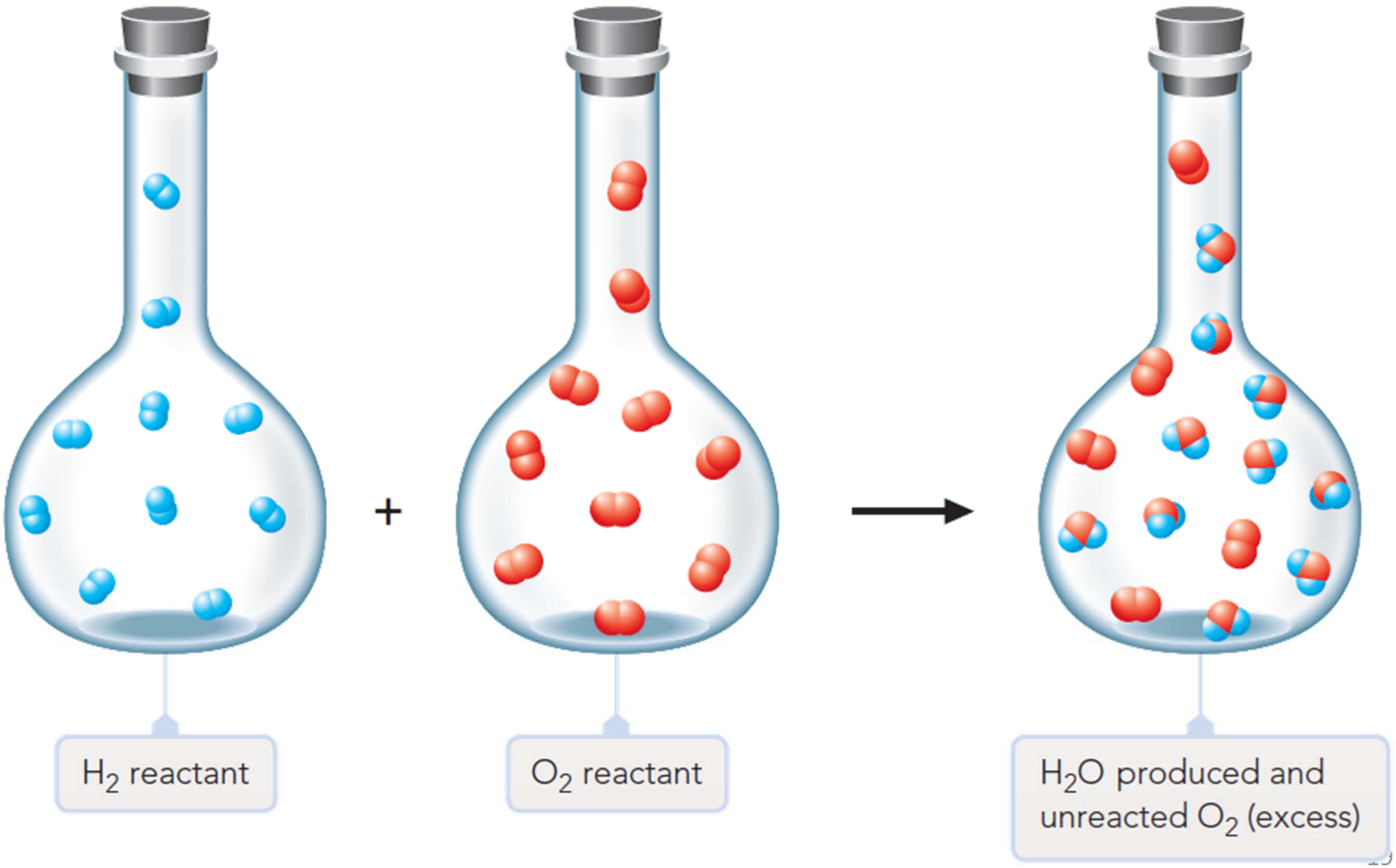
$$1.00 \times 10^3\ \cancel{\text{g Fe}_2\text{O}_3} \times \frac{1\ \cancel{\text{mol Fe}_2\text{O}_3}}{160\ \cancel{\text{g Fe}_2\text{O}_3}} \times \frac{2\ \cancel{\text{mol Fe}}}{1\ \cancel{\text{mol Fe}_2\text{O}_3}} \times \frac{55.8\ \text{g Fe}}{1\ \cancel{\text{mol Fe}}} = \mathbf{698\ g\ Fe}$$

3.8 Limiting Reactant; Theoretical and Percentage Yields

- **Limiting reactant:** the reactant that is entirely consumed when a reaction goes to completion
- The moles of product are always determined by the starting moles of limiting reactant.

3.8 Limiting Reactant; Theoretical and Percentage Yields

Limiting Reactant



3.8 Limiting Reactant; Theoretical and Percentage Yields

- **Theoretical yield:** the maximum amount of product that can be obtained by a reaction from given amounts of reactants
- **Percentage yield:** the actual yield (experimentally determined) expressed as a percentage of the theoretical yield (calculated)

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