Stoichiometry

A. The Meaning of Coefficients in a Reaction Equation

1. Consider the following reaction:

$$2H_2 + O_2 \rightarrow 2H_2O$$

The **coefficients** in the equation tell us that two hydrogen molecules react with one oxygen molecule to produce two molecules of water.

As long as the 2:1:2 ratio is maintained, the reaction is balanced, so this reaction is also balanced when written as

$$200\ H_2 + 100\ O_2 \rightarrow 200\ H_2O$$

or

$$2 \times (6.02 \times 10^{23})\ H_2 + 1 \times (6.02 \times 10^{23})\ O_2 \rightarrow 2 \times (6.02 \times 10^{23})\ H_2O$$

Which is the same as

$$2\ \text{mol}\ H_2 + 1\ \text{mol}\ O_2 \rightarrow 2\ \text{mol}\ H_2O$$

Thus the coefficients in a balanced equation simply gives us the **ratio of reactants and products** in terms of **atoms and molecule** or in terms of **moles of atoms and molecules.**

In other words, the balanced equation provides us with a **MOLE RATIO** that relates reactants and products.

STOICHIOMETRY

The relationship between the amounts of reactants used in a chemical reaction and the amounts of products produced by the reaction.

EXAMPLE 7.1	**RATIOS IN TERMS OF MOLECULES**
Problem	Consider the reaction equation: $$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$ How many molecules of N_2 are required to react with 15 molecules of H_2?
Solution	According to the balanced equation, 1 molecule of N_2 reacts with 3 molecules of H_2. $$\#\ N_2 = 15 \text{ molecules } H_2 \times \frac{1 \text{ molecule } N_2}{3 \text{ molecules } H_2}$$ $$= 5 \text{ molecules } N_2$$

EXAMPLE 7.2	**RATIOS IN TERMS OF MOLES**
Problem	Consider the reaction equation: $$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$ How many moles of NH_3 are produced when 18 mol of H_2 are reacted?
Solution	According to the balanced equation, 2 moles of NH_3 are produced when 3 moles of H_2 react. $$\#\ NH_3 = 18 \text{ moles } H_2 \times \frac{2 \text{ moles } NH_3}{3 \text{ moles } H_2} = 12 \text{ moles } NH_3$$

SAMPLE PROBLEM 7.1	**RATIOS IN TERMS OF MOLES**
Problem	Consider the reaction equation: $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$ (a) How many molecules of NH_3 are formed from the reaction of 54 H_2? (b) How many moles of N_2 are required to react with 27 moles of H_2?
Solution	(a) (b)

B. Stoichiometry Calculations Involving Moles, Mass, Gas Volume, and Molecules

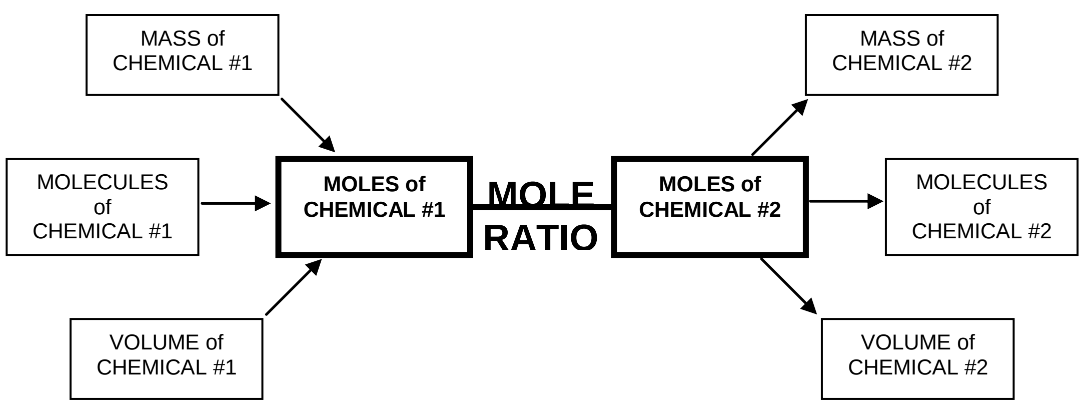
1. Stoichiometry calculations allow us to find out how much of chemical #1 is involved in a chemical reaction based on the amount of chemical #2 involved. A typical problem might be

"How many grams of chemical #1 must be reacted to produce 25.0 g of chemical #2?"

or

"What volume of chemical #1 at STP will be produced when 15.0 g of chemical #2 is reacted?"

In most cases, the quantities of the chemicals will be given in terms of molecules, mass, or volume of a gas at STP. It is important to remember that the **balanced** equation provides with a **MOLE RATIO** that relates reactants and products. As such, before we can use the ratio, the **quantities that are given must be converted to moles** first.



EXAMPLE 7.3	CALCULATIONS INVOLVING MASS
Problem	Consider the balanced equation: $$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$ What mass of C_3H_8 is required to produce 100.0 g of H_2O?
Solution	mass $H_2O \rightarrow$ mol $H_2O \rightarrow$ mol $C_3H_8 \rightarrow$ mass C_3H_8 $$\text{mass} = 100.0\text{ g } H_2O \times \frac{1\text{ mol}}{18.0\text{ g}} \times \frac{1\ C_3H_8}{4\ H_2O} \times \frac{44.0\text{ g}}{1\text{ mol}}$$ $$= 61.1\text{ g } C_3H_8$$

EXAMPLE 7.4	CALCULATIONS INVOLVING VOLUME OF A GAS
Problem	Consider the balanced equation: $$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$ If a sample of propane is burned what mass of $H_2O(l)$ is produced if the reaction also produces 50.0 L of $CO_2(g)$ at STP?
Solution	volume $CO_2 \rightarrow$ mol $CO_2 \rightarrow$ mol $H_2O \rightarrow$ mass H_2O $$\text{mass } H_2O = 50.0\text{ L } CO_2 \times \frac{1\text{ mol}}{22.4\text{ L}} \times \frac{4H_2O}{3CO_2} \times \frac{18.0\text{ g}}{1\text{mol}}$$ $$= 53.6\text{ g } H_2O$$

EXAMPLE 7.5	**CALCULATIONS INVOLVING MOLECULES**
Problem	Consider the balanced equation: $$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$ A sample of porous, gas–bearing rock is crushed and 1.35 × 10^{-6} g of $C_3H_8(g)$ is extracted from the powdered rock. How many molecules of CO_2 are produced if the gas sample is burned in the presence of an excess of $O_2(g)$?
Solution	mass C_3H_8 → mol C_3H_8 → mol CO_2 → molecules CO_2 $$1.35 \times 10^{-6}\text{ g } C_3H_8 \times \frac{1\text{ mol}}{44.0\text{ g}} \times \frac{3CO_2}{1\ C_3H_8} \times \frac{6.02 \text{ x } 10^{23}}{1\text{ mol}}$$ $$= 5.54 \times 10^{16}\text{ molecules } CO_2$$

SAMPLE PROBLEM 7.2	**CALCULATIONS INVOLVING MASS, VOLUME, AND MOLECULES**
Problem	Consider the reaction equation: $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$ (a) What mass of NH_3 is formed from the reaction of 25.0 g of H_2? (b) What volume of N_2 at STP is required to react with 30.0 g of H_2? (c) How many molecules of NH_3 are produced from the reaction of 15.0 g of N_2?
Solution	(a) (b) (c)

C. Stoichiometry Involving Molar Concentrations

1. Recall that molar concentration calculations involve the use of the equation:

$$M = \frac{mol}{V}$$

Since stoichiometry involves finding relationships between moles of one chemical to another, the equation can be re–arranged to give moles

$$mol = M \times V$$

If a volume is mentioned in a question, and the problem involves molarity, **DO NOT** assume that 22.4 L should be used. The relationship 22.4 L = 1 mole only applies to gases at STP.

EXAMPLE 7.6	**CALCULATIONS INVOLVING VOLUME OF A SOLUTION**
Problem	A tablet of Tums has a mass of 0.750 g. What volume of stomach acid having [HCl] = 0.0010 M is neutralized by a 0.750 g portion of $CaCO_3$? $$CaCO_3 + 2HCl \rightarrow CaCl_2 + CO_2 + H_2O$$
Solution	$$\text{moles of } CaCO_3 = 0.750\text{ g } CaCO_3 \times \frac{1\text{ mol}}{100.1\text{ g}}$$ $$= 0.00750\text{ moles}$$ $$\text{moles of HCl} = 0.0075\text{ moles } CaCO_3 \times \frac{2\text{ HCl}}{1\text{ } CaCO_3}$$ $$= 0.0150\text{ moles}$$ $$\text{Volume of HCl} = \frac{\text{mol}}{\text{V}} = \frac{0.0150\text{ mol}}{0.0010\text{ mol/L}} = 15\text{ L}$$ or $$0.750\text{ g } CaCO_3 \times \frac{1\text{ mol}}{100.1\text{ g}} \times \frac{2\text{ HCl}}{1\text{ } CaCO_3} \times \frac{1\text{ L}}{0.0010\text{ mol}}$$ $$= 15\text{ L}$$

EXAMPLE 7.7	CALCULATIONS INVOLVING VOLUME OF A GAS
Problem	What volume of $CO_2(g)$ at STP is produced if 1.25 L of 0.0055 M HCl reacts with an excess of $CaCO_3$? $CaCO_3 + 2HCl \rightarrow CaCl_2 + CO_2 + H_2O$
Solution	$\text{mole of HCl} = 1.25\text{ L} \times \frac{0.0055\text{ mol}}{\text{L}} = 0.006875\text{ mol}$ $\text{moles of } CO_2 = 0.006875\text{ moles HCl} \times \frac{1\ CO_2}{2\ HCl}$ $= 0.003438\text{ mol } CO_2$ $\text{volume of } CO_2 = 0.003438\text{ mol} \times \frac{22.4\text{ L}}{1\text{ mol}} = 0.077\text{ L}$ or $1.25\text{ L} \times \frac{0.0055\text{ mol}}{\text{L}} \times \frac{1\ CO_2}{2\ HCl} \times \frac{22.4\text{ L}}{1\text{ mol}} = 0.077\text{ L}$

2. A special process called **TITRATION** is used to find the unknown concentration of a chemical in solution.

> **TITRATION** is a process in which a measured amount of a solution is reacted with an known volume of another substance (of unknown concentration) until a desired equivalence point is reached.

The **EQUIVALENCE POINT** is the point in a titration where the ratio of the moles of each species involved exactly equals the ratio of the coefficients of the species in the balanced equation.

EXAMPLE 7.8	**TITRATION CALCULATION**
Problem	If 19.8 mL of H_3PO_4 with an unknown molarity reacts with 25.0 mL of 0.500 M KOH according to the following reaction. What is the molarity of the H_3PO_4? $H_3PO_4 + 3KOH \rightarrow K_3PO_4 + 3H_2O$
Solution	$\text{moles of KOH} = 0.0250\text{ L} \times \frac{0.500\text{ mol}}{\text{L}} = 0.0125\text{ mol}$ $\text{moles of } H_3PO_4 = 0.0125\text{ mol KOH} \times \frac{1\ H_3PO_4}{3\text{ KOH}}$ $= 0.00417\text{ mol}$ $[H_3PO_4] = \frac{\text{mol}}{\text{V}} = \frac{0.00417\text{ mol}}{0.0198\text{ L}} = 0.210\text{ M}$ or $0.0250\text{ L} \times \frac{0.500\text{ mol KOH}}{\text{L}} \times \frac{1\ H_3PO_4}{3\text{ KOH}} \times \frac{1}{0.0198\text{ L}}$ $= 0.210\text{ M}$

SAMPLE PROBLEM 7.3	**TITRATION CALCULATION**
Problem	Calculate the [H_3PO_4] if 23.46 mL of 0.750 M KOH is required to titrate 15.00 mL of H_3PO_4 according to the reaction: $H_3PO_4 + 3KOH \rightarrow K_3PO_4 + 3H_2O$
Solution	

D. Stoichiometry of Excess Quantities

1. In all of the previous stoichiometric calculations we assumed that a given reactant was **completely used up during a reaction.** Reactions are frequently carried out in such a way that one or more of the reactants are present in **EXCESS** amounts. Some reasons for having an excess amount include:

   i) to make sure all of a second reactant is completely used (the second reactant may be too expensive to waste or harmful to the environment).

   ii) to unavoidably have a reactant in excess because a limited amount of another reactant is available.

2. In these types of calculations, the reactant that it present in lesser amount is called the **LIMITING REACTANT**. Since the limiting reactant gets completely used up first, it sets the limit on the amount of product that can be formed and the amount of the excess reactant used in the reaction.

LIMITING REACTANT is the reactant that sets a limit on the amount of product that can be formed (completely used up in a chemical reaction).

EXCESS REACTANT is the reactant that is not completely used up in a chemical reaction.

EXAMPLE 7.9	**LIMITING REACTANTS AND EXCESS**
Problem	If 20.0 g of $H_2(g)$ reacts with 100.0 g of $O_2(g)$ according to the reaction: $$2H_2(g) + O_2(g) \rightarrow 2H_2O(g)$$ which reactant is in excess and by how much?
Solution	To determine the reactant in excess, calculate the mass of some arbitrarily–selected product. Find how much H_2O can be formed. Using H_2 $$\text{mass of } H_2O = 20.0 \text{ g } H_2 \times \frac{1 \text{ mol}}{2.0 \text{ g}} \times \frac{2\ H_2O}{2H_2} \times \frac{18.0 \text{ g}}{1 \text{ mol}}$$ $$= 180.0 \text{ g}$$ Using O_2 $$\text{mass of } H_2O = 100.0 \text{ g } O_2 \times \frac{1 \text{ mol}}{32.0 \text{ g}} \times \frac{2\ H_2O}{1\ O_2} \times \frac{18.0 \text{ g}}{1 \text{ mol}}$$ $$= 112.5 \text{ g}$$

	Although there is enough H_2 to make 180.0 g of H_2O, there is only enough O_2 to make 112.5 g of H_2O therefore, O_2 is called the limiting reactant and H_2 is the excess reactant. The limiting reactant is used to calculate how much H_2 is reacted. $\text{mass of } H_2 \text{ (reacted)} = 100.0 \text{ g } O_2 \times \frac{1 \text{ mol}}{32.0 \text{ g}} \times \frac{2\ H_2}{1\ O_2} \times \frac{2.0 \text{ g}}{1 \text{ mol}}$ $= 12.5 \text{ g}$ mass of H_2 in excess = 20.0 g – 12.5 g = 7.5 g

EXAMPLE 7.10	**LIMITING REACTANTS AND EXCESS**
Problem	If 56.8 g of $FeCl_2$, 14.0 g of KNO_3, and 40.0 g of HCl are mixed and allowed to react according to the reaction: $3FeCl_2 + KNO_3 + 4HCl \rightarrow 3FeCl_3 + NO + 2H_2O + KCl$ (a) which reactant is the limiting reactant? (b) how many grams of each "excess reactant" remains?
Solution	(a) Arbitrarily find the mass of NO which can be produced $\text{mass NO} = 56.8\text{ g }FeCl_2 \times \frac{1\text{ mol}}{126.8\text{ g}} \times \frac{1\text{ NO}}{3\ FeCl_2} \times \frac{30.0\text{ g}}{1\text{ mol}}$ $= 4.48\text{ g}$ $\text{mass NO} = 14.0\text{ g }KNO_3 \times \frac{1\text{ mol}}{101.1\text{ g}} \times \frac{1\text{ NO}}{1\ KNO_3} \times \frac{30.0\text{ g}}{1\text{ mol}}$ $= 4.15\text{ g}$ $\text{mass NO} = 40.0\text{ g HCl} \times \frac{1\text{ mol}}{36.5\text{ g}} \times \frac{1\text{ NO}}{4\text{ HCl}} \times \frac{30.0\text{ g}}{1\text{ mol}}$ $= 8.22\text{ g}$ Since KNO_3 produces the least amount of NO, KNO_3 is the limiting reactant. (b) Use the limiting reactant, KNO_3, to calculate the mass of $FeCl_2$ and HCl reacted. $\text{mass }FeCl_2 = 14.0\text{ g }KNO_3 \times \frac{1\text{ mol}}{101.1\text{ g}} \times \frac{3\ FeCl_2}{1\ KNO_3} \times \frac{126.8\text{ g}}{1\text{ mol}}$ $= 52.7\text{ g}$ mass of $FeCl_2$ in excess = 56.8 g – 52.7 g = 4.1 g

	$$\text{mass of HCl} = 14.0\text{ g }KNO_3 \times \frac{1\text{ mol}}{101.1\text{ g}} \times \frac{4\text{ HCl}}{1\text{ }KNO_3} \times \frac{36.5\text{ g}}{1\text{ mol}}$$ $$= 20.2\text{ g}$$ mass of HCl in excess = 40.0 g – 20.2 g = 19.8 g

SAMPLE PROBLEM 7.4	**LIMITING REACTANTS AND EXCESS**
Problem	If 35.0 g of H_2 reacts with 4.68 g of N_2 according to the reaction: $$N_2 + 3H_2 \rightarrow 2NH_3$$ what is the limiting reactant and by how many grams?
Solution	

E. Percentage Yield and Percentage Purity

1. Sometimes 100% of the expected amount of products cannot be obtained from a reaction. The term **“PERCENTAGE YIELD”** is used to describe the **amount of product actually obtained as a percentage of the expected amount.** There are two major reasons for this reduced yield of products.

   i) The reactants may not all react because not all the pure material reacts or the reactants may be less than 100% pure.

   ii) Some of the products are lost during experimental procedures such as filtering.

$$\text{Percentage Yield} = \frac{\text{mass of product obtained}}{\text{mass of product expected}} \times 100\%$$

$$\text{Percentage Purity} = \frac{\text{mass of pure reactant}}{\text{mass of impure reactant}} \times 100\%$$

2. Percentage yield calculations fall into three categories.

   i) Find the percentage yield, given the mass of reactant used and mass of product formed.

   ii) Find the mass of product formed, given the mass of reactant used and the percentage yield.

   iii) Find the mass of reactant used, given the mass of product formed and the percentage yield.

EXAMPLE 7.11	**FINDING PERCENTAGE YIELD**
Problem	When 15.0 g of CH_4 is reacted with an excess of Cl_2 according to the reaction $CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$ a total of 29.7 g of CH_3Cl is formed. What is the percentage yield of the reaction?
Solution	(1) Find expected (theoretical yield) mass of CH_3Cl $\text{mass of } CH_3Cl = 15.0 \text{ g } CH_4 \times \frac{1 \text{ mol}}{16.0 \text{ g}} \times \frac{1\ CH_3Cl}{1\ CH_4} \times \frac{50.5 \text{ g}}{1 \text{ mol}}$ $= 47.34 \text{ g}$ (2) now: $\text{percentage yield} = \frac{29.7 \text{ g}}{47.34 \text{ g}} \times 100\% = 62.7\%$

EXAMPLE 7.12	**FINDING MASS OF PRODUCT**
Problem	What mass of K_2CO_3 is produced when 1.50 g of KO_2 is reacted with an excess of CO_2 according to the reaction $4KO_2 + 2CO_2 \rightarrow 2K_2CO_3 + 3O_2$ if the reaction has a 76.0% yield?
Solution	(1) Find expected (theoretical yield) mass of K_2CO_3 $1.50\text{ g }KO_2 \times \frac{1\text{ mol}}{71.1\text{ g}} \times \frac{2\ K_2CO_3}{4\ KO_2} \times \frac{138.2\text{ g}}{1\text{ mol}} = 1.458\text{ g}$ (2) now since the percentage yield is only 76.0% $\text{percentage yield} = \frac{\text{actual}}{\text{expected}}$ $0.760 = \frac{\text{actual}}{1.458\text{ g}}$ actual mass of K_2CO_3 = 1.458 g × 0.760 = 1.11 g

EXAMPLE 7.13	**FINDING MASS OF REACTANT USED**
Problem	What mass of CuO is required to make 10.0 g of Cu according to the reaction $$2NH_3 + 3CuO \rightarrow N_2 + 3Cu + 3H_2O$$ if the reaction has a 58.0% yield?
Solution	(1) The actual yield is 10.0 g, we need to expect to produce more than 10.0 g of Cu since only 58.0% of what is expected will actually be produced. $$\text{percentage yield} = \frac{\text{actual}}{\text{expected}} \qquad 0.580 = \frac{10.0\text{ g}}{\text{expected}}$$ $$\text{expected} = \frac{10.0\text{ g}}{0.580} = 17.24\text{ g}$$ This means that we must attempt to produce 17.24 g of Cu if we are to actually obtain 10.0 g of Cu. (2) Now calculate how much CuO is required to produce 17.2 g of Cu. $$\text{mass of CuO} = 17.24\text{ g Cu} \times \frac{1\text{ mol}}{63.5\text{ g}} \times \frac{3\text{ CuO}}{3\text{ Cu}} \times \frac{79.5\text{ g}}{1\text{ mol}}$$ $$= 21.6\text{ g}$$

SAMPLE PROBLEM 7.5	**PERCENTAGE YIELD**
Problem	When 25.0 g of H_2 are reacted with excess N_2 according to the reaction: $$N_2 + 3H_2 \rightarrow 2NH_3$$ a total of 135.2 g of NH_3 is formed. What is the percentage yield?
Solution	