Mole - Mass Relationships in Chemical Systems

Mole Concept

1 mole = 6.022×10^{23} = Avogadro's number

- **convenient in measuring the amounts of reactants & products in chemical reactions**

- **1 mole of a substance =**

  Atomic Mass in grams of an element or

  Molecular Mass in grams of a compound

Examples:

	Mg	+	S	------>	MgS
atoms:				------>	**formula units**
moles:				------>	
atoms:				------>	**formula units**
mass:				------>	

2 Mg + O_2 ------> 2 MgO

atoms: ------> formula units

moles: ------>

------> formula units

mass: ------>

Stoichiometric Equivalencies

- **Ratio in which the elements occur in a compound**

  e.g. Al_2O_3

  2 Al^{3+} : 3 O^{2-}

  2 mol Al^{3+} : 3 mol O^{2-}

  2 mol Al : 3 mol O

  54.0 g Al : 48.0 g O

Sample Problems:

1. **How many moles of Al are needed to react with 2.7 mol oxygen *atoms* to make Al_2O_3?**

   Ans. = 1.8 mol Al

2. **How many moles of Al are needed to make 3.0 mol Al_2O_3?**

   Ans. = 4.5 mol Al

3. **How many moles of oxygen *atoms* are needed to make 3.0 mol Al_2O_3?**

Ans. = 9.0 mol O atoms

4. **How many moles of oxygen *molecules* are needed to make 3.0 mol Al_2O_3?**

Ans. = 4.5 mol O_2 molecules

Measuring Moles of Elements and Compounds

- **Atomic Mass or Molecular Mass in grams (Molar Mass):**
  - **Contains 1 mole (Avogadro's number) of atoms or molecules**

Some Examples:

SUBSTANCE	MOLAR MASS (g/mol)
Au	196.9665
O	15.9994
O_2	32.000
H_2O	18.00
$Ca(OH)_2$	74.094
$CaCl_2 \cdot 2H_2O$	147.015

Mass <------> Mole conversions

- **Use molar mass as conversion factor**

Examples:

1. How many moles of gold are in 19.70 g Au?

2. How many moles of water are in 72.0 g water?

3. How many moles of oxygen molecules are in 16.0 g oxygen?

4. How many grams of water are in 3.5 mol water?

5. How many grams of gold are in 1.97×10^{12} atoms of gold?

6. How can you determine the mass of *one* water molecule?

Answers:
1. 0.1000 mole Au; 2. 4.00 mol H2O; 3. 0.500 mol O2;
4. 63.0 g H2O; 5. 6.44×10^{-10} g Au

Applications of Stoichiometry

1. How many grams of chlorine *atoms* are needed to combine with 24.4 g silicon to produce silicon tetrachloride?

Answer: 123 g Cl

a. How many chlorine atoms are needed?

Ans. 2.09×10^{24} Cl atoms

b. How many chlorine molecules are needed?

Ans. 1.04×10^{24} Cl_2 molecules

Percentage Composition

- **Mass % of each element in the compound:**

  % by mass of element = [mass of element / mass of sample] * 100

  - **Intensive property**
  - **Used in determining the formulas of new compounds**

Examples

1. **5.58 g Fe react with oxygen gas to yield 7.98 g iron oxide. Calculate the % composition of the product and then determine if the product is iron (II) oxide or iron (III) oxide.**

2. **Which oxide of nitrogen has a % composition of 25.94% N and 74.06% O, N_2O, NO, N_2O_3, N_2O_4, or N_2O_5?**

Empirical and Molecular formulas

Empirical Formula

- **Smallest <u>whole</u> number ratio of atoms in the compound that agrees with the elemental analysis of the compound**

Molecular Formula

- **True formula of a compound as it exists in nature**
- **A multiple of the empirical formula**

Remember...

The formula of compound represents the *mole* ratio of the elements present in the compound

Table 3.3

Some Compounds with Empirical Formula CH_2O (Composition by Mass 40.0% C, 6.71% H, 53.3%O)

Molecular Formula	*M* (g/mol)	Name	Use or Function
CH_2O	30.03	Formaldehyde	Disinfectant; Biological preservative
$C_2H_4O_2$	60.05	Acetic acid	Acetate polymers; vinegar (5% solution)
$C_3H_6O_3$	90.08	Lactic acid	Causes milk to sour; forms in muscle during exercise
$C_4H_8O_4$	120.10	Erythrose	Forms during sugar metabolism
$C_5H_{10}O_5$	150.13	Ribose	Component of many nucleic acids and vitamin B_2
$C_6H_{12}O_6$	180.16	Glucose	Major nutrient for energy in cells

Examples...

1. **Calculate the empirical formula of magnesium oxide if 2.431 g Mg react with oxygen to yield 4.031 g of product.**

2. **Determine the empirical formula of a compound that is 25.94% Nitrogen and 74.06% Oxygen.**

Empirical Formulas from % Composition: Assume you have 100 g of the compound!!!! Why???

Steps to Determine Empirical Formulas

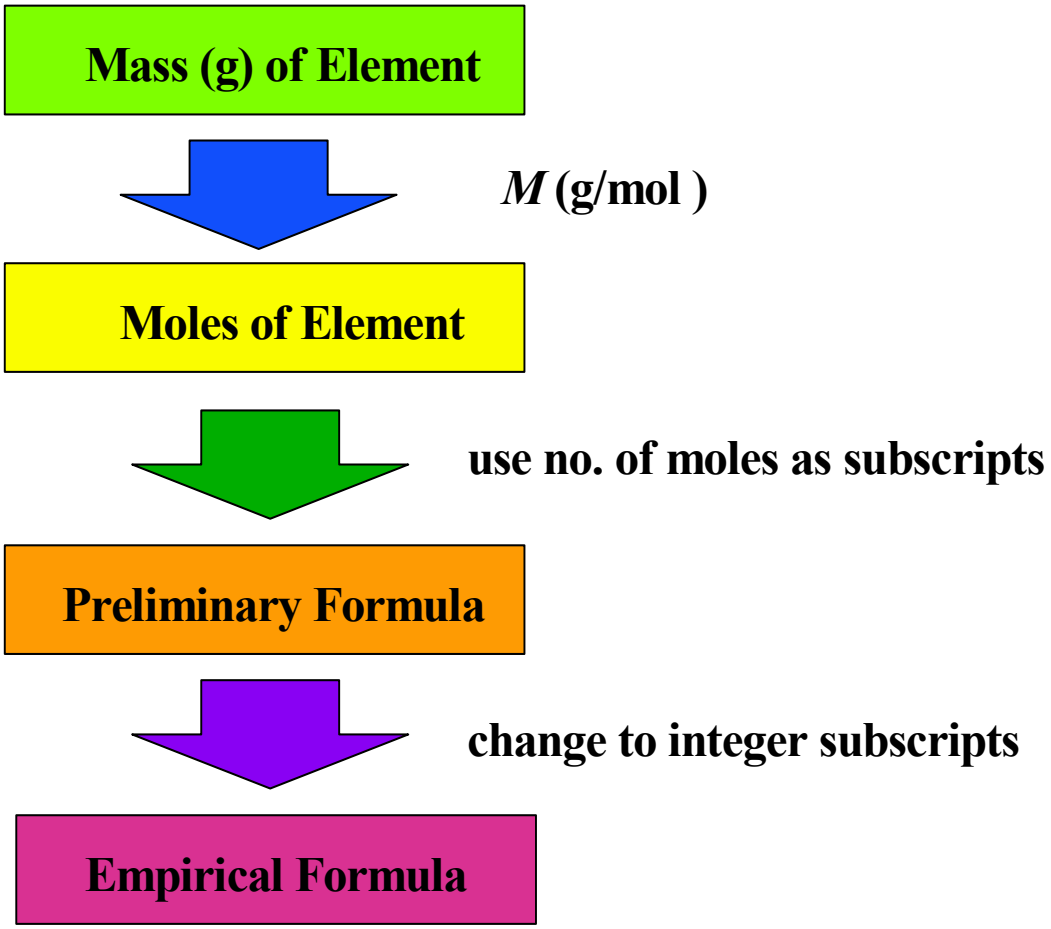
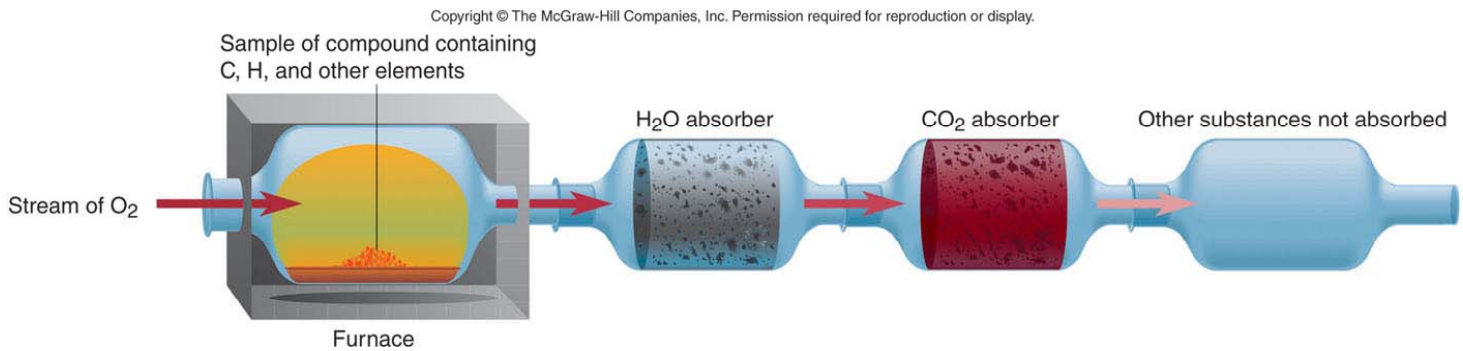


Figure 3.4

Combustion Train for the Determination of the Chemical Composition of Organic Compounds.



$$C_nH_m + (n+\frac{m}{2})\,O_2 \rightarrow n\,CO_2(g) + \frac{m}{2}\,H_2O$$

Where does each of the following come from?

1. **Carbon in the Carbon in the CO_2?**
2. **Hydrogen in the H_2O?**
3. **Oxygen in the CO_2?**
4. **Oxygen in the H_2O?**

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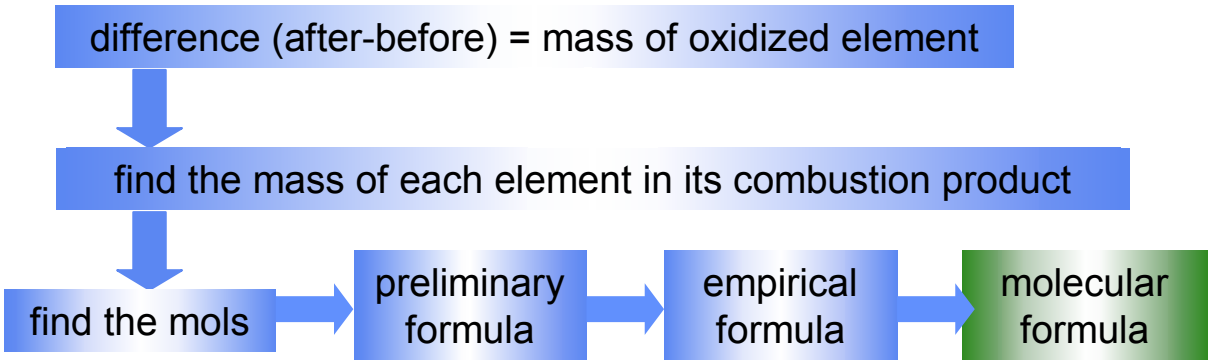
Sample Problem 3.6 Determining a Molecular Formula from Combustion Analysis

PROBLEM: Vitamin C (M=176.12g/mol) is a compound of C,H, and O found in many natural sources especially citrus fruits. When a 1.000-g sample of vitamin C is placed in a combustion chamber and burned, the following data are obtained:

mass of CO_2 absorber after combustion	=85.35g
mass of CO_2 absorber before combustion	=83.85g
mass of H_2O absorber after combustion	=37.96g
mass of H_2O absorber before combustion	=37.55g

What is the molecular formula of vitamin C?

PLAN:



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Sample Problem 3.6 Determining a Molecular Formula from Combustion Analysis

continued

SOLUTION:

CO_2 85.35g-83.85g = 1.50g H_2O 37.96g-37.55g = 0.41g

There are 12.01g C per mol CO_2. $1.50g\ CO_2 \dfrac{12.01g\ CO_2}{44.01g\ CO_2} = 0.409g\ C$

There are 2.016g H per mol H_2O. $0.41g\ H_2O \dfrac{2.016g\ H_2O}{18.02g\ H_2O} = 0.046g\ H$

O must be the difference: 1.000g - (0.409 + 0.049) = 0.545

$\dfrac{0.409g\ C}{12.01g\ C} = 0.0341mol\ C$ $\dfrac{0.046g\ H}{1.008g\ H} = 0.0461mol\ H$ $\dfrac{0.545g\ O}{16.00g\ O} = 0.0341mol\ O$

$C_1H_{1.3}O_1 \longrightarrow C_3H_4O_3 \longrightarrow \dfrac{176.12g/mol}{88.06g} = 2.000$ $C_6H_8O_6$

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Determining the Molecular Formula of a Compound

- **Stuff Needed:**
  - **Empirical formula of the compound**
  - **Molecular mass of the compound**

- **Remember....**
  - **The molecular formula is a multiple of the empirical formula. Therefore.....**
  - **The molecular formula mass is a multiple of the empirical formula mass.**

Examples...

1. **The empirical formula of a sugar is CH_2O. Determine the molecular formula if the molecular mass is 180.0 g/mol.**

2. **Explain how you could determine the empirical and molecular formulas of a compound that contains the elements Hg, C, H, and O from the following data.**

   A compound of mercury with a formula mass of 519 g/mol has the following % composition by mass:

   77.26% Hg, 9.25% C, 1.17% H,
   and the balance consisting of Oxygen.

Writing and Balancing Chemical Equations

- **What do Chemical Equations Show?**
  - **Mole ratios of reactants and products**
  - **States of reactants and products: (s), (l), (g), (aq)**
  - **Energetics**

- **Balancing Chemical Equations: trial and error method**
  1. Write correct formulas for reactants and products
  2. Adjust *coefficients* to get equal numbers of each type of atom on each side of the equation

$$Fe_2O_3\ (s) + C\ (s) \rightarrow Fe\ (s) + CO_2\ (g)$$

$$C_4H_{10}\ (g) + O_2\ (g) \rightarrow$$

$$AgNO_3\ (aq) + CaCl_2\ (aq) \rightarrow AgCl\ (s) + NaNO_3\ (aq)$$

$$NaHCO_3\ (aq) + H_2SO_4\ (aq) \rightarrow Na_2SO_4\ (aq) + H_2O\ (l) + CO_2\ (g)$$

Some reactions are nearly impossible to balance by trial and error. E.g. "Redox" reactions will be covered next chapter!

Using Chemical Equations in Calculations

Recall:

Coefficients in *Balanced* Chemical Reactions give the *Mole* Ratios between all Reactants and Products!!!

e.g. Rusting of Iron:

$$Fe\ (s) + O_2\ (g) \rightarrow Fe_2O_3\ (s)$$

1. If 2 moles of iron react, how many moles of ....

a. oxygen will react?

b. rust will form?

2. If 27.9 grams of iron rust completely, how many.....

a. Moles of oxygen will react?

b. Molecules of oxygen reat?

c. Grams of oxygen?

d. Moles of rust will form?

e. Grams of rust?

Fe = 55.85 g/mol; O = 16.00 g/mol; Fe_2O_3 = 159.6 g/mol

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3. How many kg of gasoline must react to produce 100. lbs of carbon dioxide? Assume that gasoline contains only octane, C_8H_{18} and that carbon dioxide and water are the only two products.

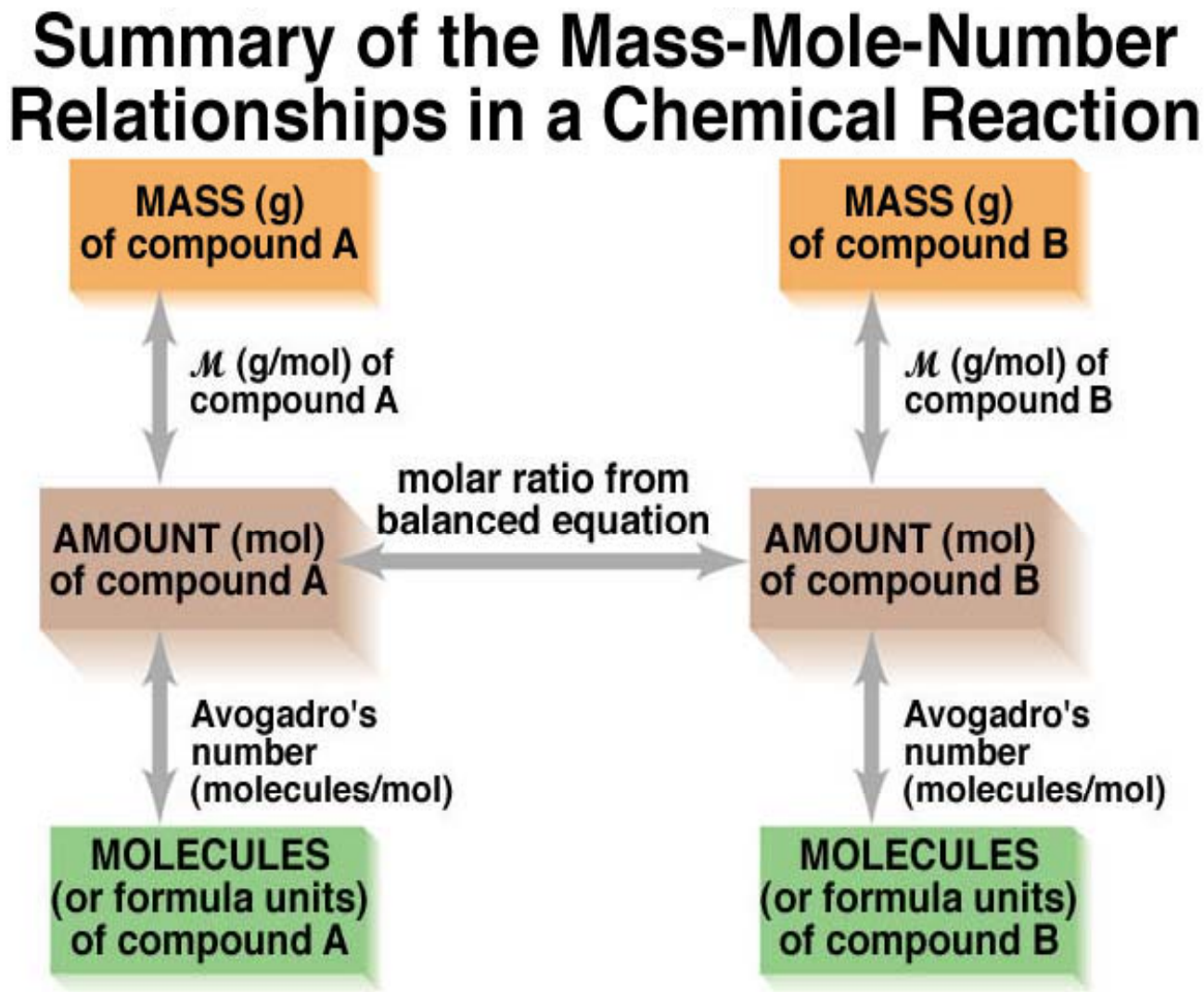
Summary of the Mass-Mole-Number Relationships in a Chemical Reaction
MASS (g) of compound A
MASS (g) of compound B
$\mathcal{M}$ (g/mol) of compound A
$\mathcal{M}$ (g/mol) of compound B
molar ratio from balanced equation
AMOUNT (mol) of compound A
AMOUNT (mol) of compound B
Avogadro's number (molecules/mol)
Avogadro's number (molecules/mol)
MOLECULES (or formula units) of compound A
MOLECULES (or formula units) of compound B

Fig. 3.8

Limiting Reactant:

- Reactant that is consumed completely
- Limits or determines the amount of product produced
- The reactant that produces the least amount of product is the limiting reactant

An Ice Cream Sundae Analogy for Limiting Reactions

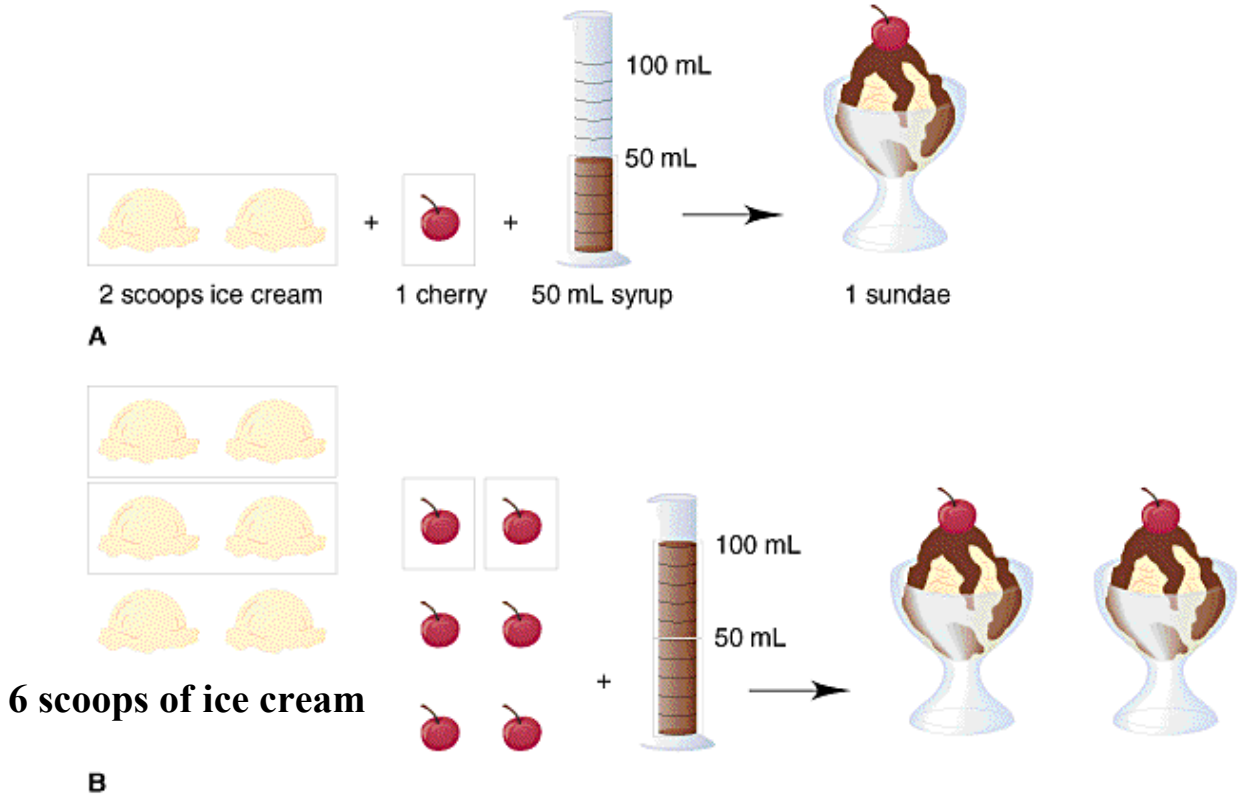

Fig. 3.10

How do you know if a problem is a limiting Reactant Problem???

e.g. 32.0 g Zinc and 32.0 g sulfur reacted to form zinc sulfide:

32.0 g		32.0 g		?? g
Zn	+	**S**	→	**ZnS**

a. Which chemical is the limiting reactant?
b. How many grams of ZnS can be formed?
c. How many grams of excess reactant will be left after the reaction?

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e.g. O.360 mol phosphorus pentachloride was slowly added to 2.88 mole of water.

0.360 mol		2.88 mol				
PCl_5	+	$4\ H_2O$	→	H_3PO_4	+	$5\ HCl$

a. Which reactant, if either, is the limiting reactant?

b. Calculate the theoretical yields in moles of each product.

Theoretical Yield and % Yield Problems

- **Theoretical Yield:**
  Yield (amount of product) obtained if *all* of the limiting reactant is converted to product and none product is lost
- **Yields are almost never 100%. Why?**
  - **Incomplete reaction (e.g. Chemical Equilibrium)**
  - **Product may be slightly soluble**
  - **Product may be volatile**
  - **Competing reactions occur**
  - **Product sticks to container**

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

Question 3.81 (Page 126 Silberberg 3ed)

What is the % yield of a reaction in which 41.5 g tungsten (VI) oxide, $W0_3$, reacts with excess hydrogen gas to produce metallic tungsten and 9.50 mL water. d_{water} = 1.000 g/mL,
H_2O = 18.0 g/mol, W = 183.5 g/mol, $W0_3$ = 231.5 g/mol

$$W0_{3\,(s)} + 2\ H_{2\,(g)} \rightarrow W_{(s)} + 2\ H_2O_{(l)}$$

Ans. 98.1%

Question 3.83 (Page 126 Silberberg 3ed)

When 153 g methane and 43.0 g chlorine gas undergo a reaction that has an 80.0% yield, what mass of chloromethane, CH_3Cl, forms? Hydrogen chloride gas is also produced.

$$CH_{4\,(g)} + Cl_{2\,(g)} \rightarrow CH_3Cl_{(g)} + HCl_{(g)}$$

16.0 g/mol	**70.90 g/mol**	**50.45 g/mol**	**36.45 g/mol**

Ans: 24.5 g CH_3Cl

Concentration of solutions

$$\text{Molarity} = \frac{\text{moles solute}}{\text{Liters of Solution}} = \frac{\text{moles}}{\text{L}}$$

- **Solute substance dissolved in the solvent—usually water**
- **Solution: solute and solvent**

Preparing a Solution

- Prepare a solution of Sodium Phosphate by dissolving 3.95g of Sodium Phosphate into water and diluting it to 300.0 ml or 0.300 l !

- What is the Molarity of the salt and each of the ions?

- $Na_3PO_{4\,(s)} + H_2O_{(solvent)} = 3\,Na^+_{(aq)} + PO_4^{-3}{}_{(aq)}$

Preparing a Solution - II

- Mol wt of Na_3PO_4 = 163.94 g / mol
- 3.95 g / 163.94 g/mol = 0.0241 mol Na_3PO_4
- dissolve and dilute to 300.0 ml
- M = 0.0241 mol Na_3PO_4 / 0.300 l = 0.0803 M Na_3PO_4
- for PO_4^{-3} ions = **0.0803 M**
- for Na^+ ions = 3 x 0.0803 M = **0.241 M**

Make a Solution of Potassium Permanganate

Problem: What is the molarity of a solution that is prepared a solution by dissolving 1.58 grams of $KMnO_4$ into sufficient water to make 250.00 ml of solution? What is the concentration of each ion is the solution?

$KMnO_4$ = 158.04 g / mole

$$1.58 \text{ g } KMnO_4 \times \frac{1 \text{ mole } KMnO_4}{158.04 \text{ g } KMnO_4} = \mathbf{0.0100 \text{ moles } KMnO_4}$$

$$\text{Molarity} = \frac{0.0100 \text{ moles } KMnO_4}{0.250 \text{ liters}} = \mathbf{0.0400 \text{ M}}$$

Molarity of K^+ ion = $[K^+]$ ion = $[MnO_4^-]$ ion = 0.0400 M

Dilution of Solutions

- Take 25.00 ml of the 0.0400 M $KMnO_4$
- Dilute the 25.00 ml to 1.000 Liter. What is the resulting Molarity of the diluted solution?
- # moles = Vol x M
- 0.0250 L x 0.0400 M = 0.00100 Moles
- 0.00100 Mol / 1.000 L = **0.00100 M**

Another example…

Preparation of a less concentrated from a more concentrated solution

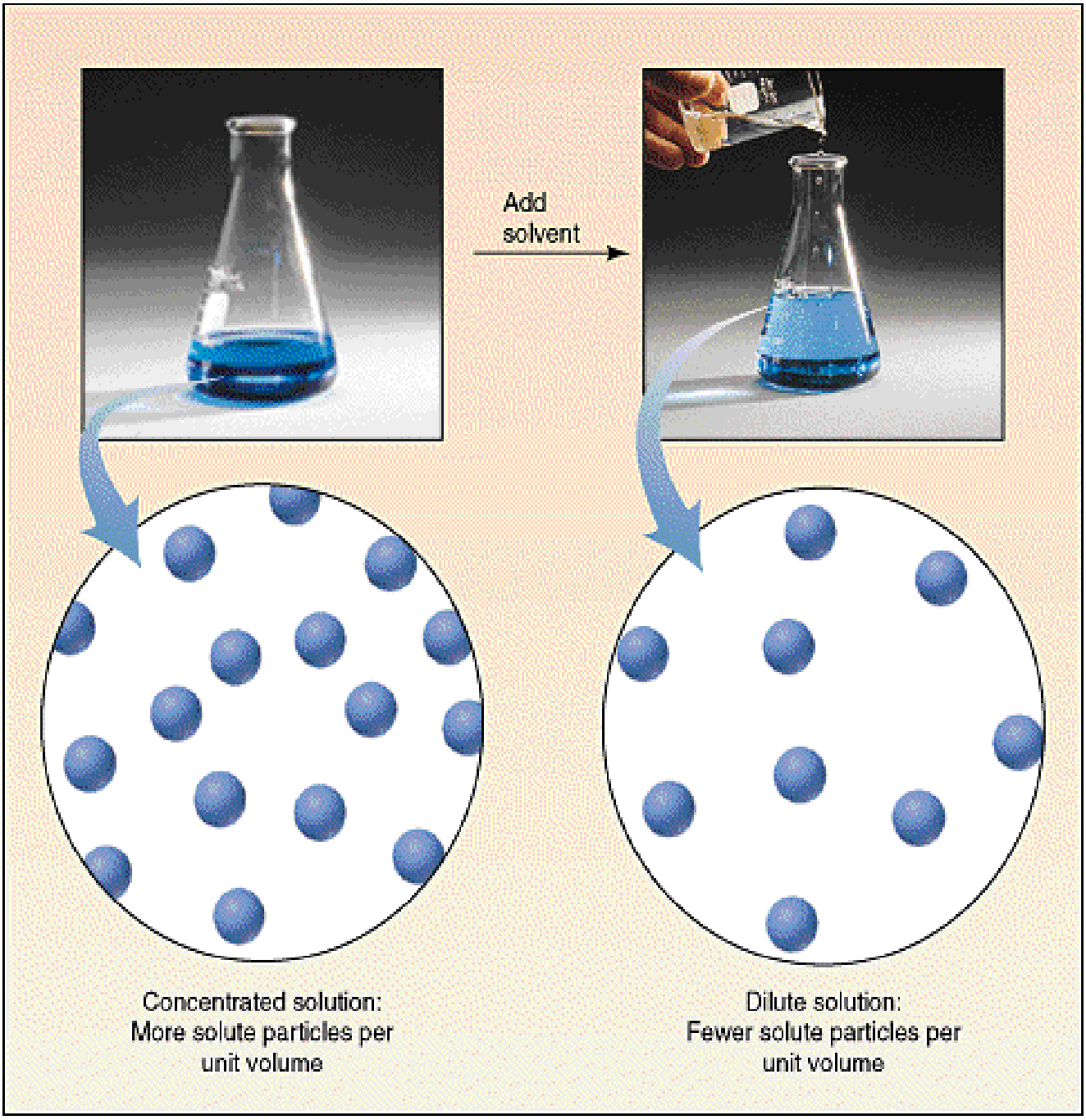
e.g. How would you prepare 500. mL of 0.10 M HCl from a stock solution of concentrated reagent, 12 M HCl?

$$\mathbf{V_{dil} \cdot M_{dil} = V_{conc} \cdot M_{conc}}$$

Would you add the acid to the water or the water to the the acid?

Answer: 4.2 mL 12M HCl is needed

Fig. 3.13


Add
solvent
Concentrated solution:
More solute particles per
unit volume
Dilute solution:
Fewer solute particles per
unit volume

Calculating Mass of Solute from a Given Volume of Solution

Volume (L) of Solution

Molarity = M = (mol solute / Liters of solution) = mol/L

Moles of Solute

Molar Mass (*M*) = (mass / mole) = g/mol

Mass (g) of Solute

Calculating Amounts of Reactants and Products for a Reaction in Solution

$$Al(OH)_{3\,(s)} + 3\ HCl_{(aq)} \rightarrow 3\ H_2O_{(l)} + AlCl_{3\,(aq)}$$

Mass (g) of $Al(OH)_3$

↓ ***M*** **(g/mol)**

Moles of $Al(OH)_3$

↓ **molar ratio**

Moles of HCl

↓ **M (mol/L)**

Volume (L) of HCl

Given 10.0 g $Al(OH)_3$, what volume of 1.50 M HCl is required to neutralize the base?

$$\frac{10.0\ g\ Al(OH)_3}{78.00\ g/mol} = \mathbf{0.128\ mol\ Al(OH)_3}$$

$$0.128\ mol\ Al(OH)_3 \times \frac{3\ moles\ HCl}{moles\ Al(OH)_3} =$$

0.385 Moles HCl

$$\textbf{Vol HCl} = \frac{1.00\ L\ HCl}{1.50\ Moles\ HCl} \times 0.385\ Moles\ HCl$$

Vol HCl = 0.256 L = **256 ml HCl**

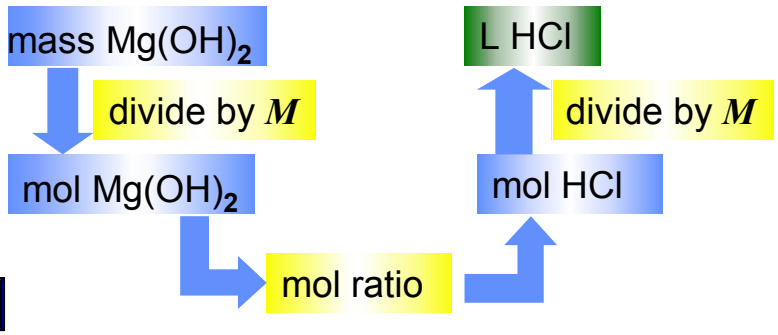
1. What volume in mL of O.200 M HCl is needed to neutralize 25.00 mL of 0.400 M NaOH?

Answer: 50.0 mL 0.200 M HCl

Sample Problem 3.15 Calculating Amounts of Reactants and Products for a Reaction in Solution

PROBLEM: Specialized cells in the stomach release HCl to aid digestion. If they release too much, the excess can be neutralized with antacids. A common antacid contains magnesium hydroxide, which reacts with the acid to form water and magnesium chloride solution. As a government chemist testing commercial antacids, you use 0.10M HCl to simulate the acid concentration in the stomach. How many liters of "stomach acid" react with a tablet containing 0.10g of magnesium hydroxide?

PLAN: Write a balanced equation for the reaction; find the grams of $Mg(OH)_2$; determine the mol ratio of reactants and products; use mols to convert to molarity.



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Sample Problem 3.15 Calculating Amounts of Reactants and Products for a Reaction in Solution

continued

SOLUTION: $Mg(OH)_2(s) + 2HCl(aq) \longrightarrow MgCl_2(aq) + 2H_2O(l)$

$$0.10\text{g } Mg(OH)_2 \frac{\text{mol } Mg(OH)_2}{58.33\text{g } Mg(OH)_2} = 1.7\text{x}10^{-3} \text{ mol } Mg(OH)_2$$

$$1.7\text{x}10^{-3} \text{ mol } Mg(OH)_2 \frac{2 \text{ mol HCl}}{1 \text{ mol } Mg(OH)_2} = 3.4\text{x}10^{-3} \text{ mol HCl}$$

$$3.4\text{x}10^{-3} \text{ mol HCl} \frac{1\text{L}}{0.10\text{mol HCl}} = 3.4\text{x}10^{-2} \text{ L HCl}$$

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