Lecture 5 Outline

5.1 Stoichiometry, the mole etc.

5.2 Chemical Equations

5.3 Molarity

5.4 Limiting reagents and yields

5.5 Reaction enthalpies and Gibbs free energy

5.6 Catalyst

Lecture 5

Stoichiometry

Derived from the Greek *stoicheion* (*"element"*) and *metron* (*"measure"*)

Stoichiometry is based on atomic masses and on the **Law of Conservation of mass**: *The total mass of all substances present after a chemical reaction is the same as the total mass before the reaction.*

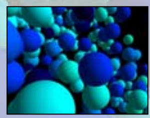
Stoichiometry

Reminder !!!

mole - the amount of a substance that contains the same number of entities as there are atoms in exactly 12g of carbon-12.

Dozen = 12

Pair = 2



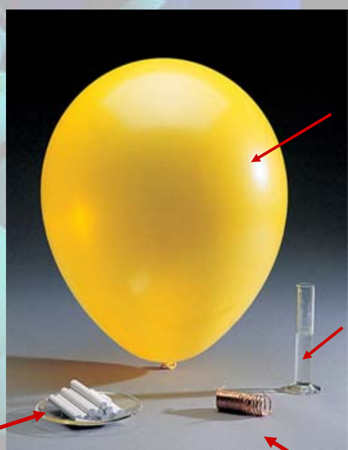
$6.022x10^{23}$ = mole

This amount is $6.022x10^{23}$. The number is called Avogadro's number and is abbreviated as ***N.***

One mole (1 mol) contains $6.022x10^{23}$ entities (to four significant figures)

Counting Objects of Fixed Relative Mass

55.85g Fe = 6.022×10^{23} atoms Fe
32.07g S = 6.022×10^{23} atoms S



Oxygen 32.00 g

Water 18.02 g

$CaCO_3$ 100.09 g

Copper 63.55 g

Summary of Mass Terminology

Term	Definition	Unit
Isotopic mass	Mass of an isotope of an element	amu
Atomic mass (also called atomic weight)	Average of the masses of the naturally occurring isotopes of an element weighted according to their abundance	amu
Molecular (or formula) mass (also called molecular weight)	Sum of the atomic masses of the atoms (or ions) in a molecule (or formula unit)	amu
Molar mass (Mm) (also called gram-molecular weight)	Mass of 1 mole of chemical entities (atoms, ions, molecules, formula units)	g/mol

$$\text{Number of moles (n)} = \frac{\text{Mass (g)}}{\text{Molar Mass (g mol-1)}}$$

$M = m/n$

$$n = \frac{m}{M}$$

$m = n \cdot M$

$$\text{No. of entities} = \text{no. of moles} \times \frac{6.022\times10^{23}\ \text{entities}}{1\ \text{mol}}$$

Sample Problem — **Calculating the Mass and the Number of Atoms in a Given Number of Moles of an Element**

PROBLEM: **(a)** Silver (Ag) is used in jewelry and tableware but no longer in U.S. coins. How many grams of Ag are in 0.0342mol of Ag?

(b) Iron (Fe), the main component of steel, is the most important metal in industrial society. How many Fe atoms are in 95.8g of Fe?

(a) SOLUTION: $m = n \cdot M$

$$0.0342\,\text{mol} \times \frac{107.9\text{ g}}{\text{mol}} = 3.69\text{g}$$

3.69 g Ag

(b) SOLUTION: $n = m/M$

$$95.8\text{ g} \times \frac{\text{mol}}{55.85\text{ g}} = 1.72\text{ mol}$$

$$1.72\text{mol} \times \frac{6.022\text{x}10^{23}\text{atoms}}{\text{mol}} = 1.04\text{x}10^{24}\text{ atoms}$$

$1.04\text{x}10^{24}$ Fe atoms

Mass %

Mass % of element X =

$$\frac{\text{moles of X in formula x molar mass of X (amu)}}{\text{molecular (or formula) mass of compound (amu)}} \times 100$$

Sample Problem — **Determining the Empirical Formula from Masses of Elements**

PROBLEM: Elemental analysis of a sample of an ionic compound gave the following results: 2.82g of Na, 4.35g of Cl, and 7.83g of O. What are the empirical formula and name of the compound?

PLAN: Once we find the relative number of moles of each element, we can divide by the lowest mol amount to find the relative mol ratios (empirical formula).

SOLUTION: $n = m/M$

$$2.82\text{g Na}\ \frac{\text{mol Na}}{22.99\text{g Na}} = 0.123\ \text{mol Na}$$

$$4.35\text{g Cl}\ \frac{\text{mol Cl}}{35.45\text{g Cl}} = 0.123\ \text{mol Cl}$$

$$7.83\text{g O}\ \frac{\text{mol O}}{16.00\ \text{O}} = 0.489\ \text{mol O}$$

$Na_1\ Cl_1\ O_{3.98}$ ⟶ $NaClO_4$

$NaClO_4$ is sodium perchlorate.

Sample Problem 3.5 — **Determining a Molecular Formula from Elemental Analysis and Molar Mass**

PROBLEM: During physical activity lactic acid (M=90.08g/mol) forms in muscle tissue and is responsible for muscle soreness. Elemental analysis shows that it contains 40.0 mass% C, 6.71 mass% H, and 53.3 mass% O.

(a) Determine the empirical formula of lactic acid.

(b) Determine the molecular formula.

Trick:

Assume an amount: e.g. 100g

⇨ amount (mol) of each element

⇨ preliminary formula

⇨ convert to integer subscripts

⇩

empirical formula

divide mol mass by mass of empirical formula to get a multiplier

⇧

molecular formula

Sample Problem **Determining a Molecular Formula from Elemental Analysis and Molar Mass**

continued

SOLUTION: Assuming there are 100.0g of lactic acid, the constituents are

$n = m/M$

$40.0\text{g} \times \frac{\text{mol}}{12.01\text{g}}$ = 3.33 mol C	$6.71\text{g} \times \frac{\text{mol}}{1.008\text{g}}$ = 6.66 mol H	$53.3\text{g} \times \frac{\text{mol}}{16.00\text{g}}$ = 3.33 mol O

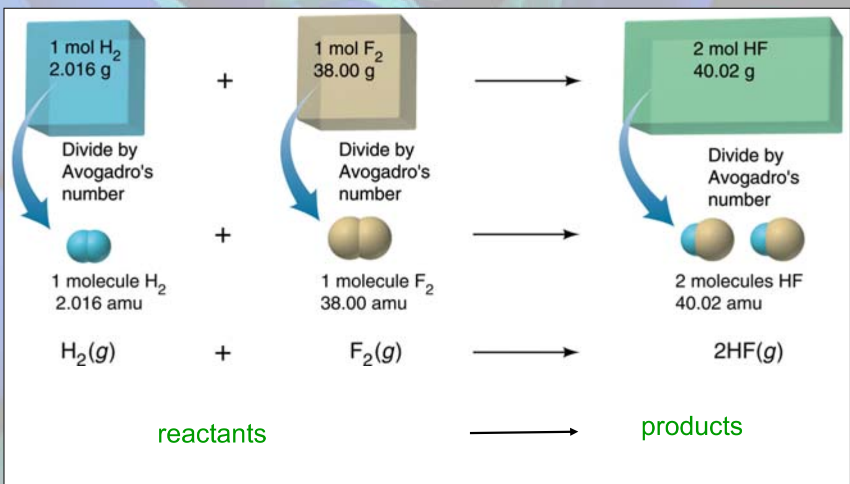
$$\frac{C_{3.33}}{3.33} \frac{H_{6.66}}{3.33} \frac{O_{3.33}}{3.33} \longrightarrow CH_2O \quad \text{empirical formula}$$

$M(CH_2O) = 30.03$ g/mol

M(lactic acid) = 90.08 g/mol $\longrightarrow$ 3 $\longrightarrow$ $C_3H_6O_3$ is the molecular formula

Chemical Equations

The formation of HF gas on the macroscopic and molecular levels



The Chemical Reaction — Important aspects

1) The stoechiometric factor specifies how many entities of a chemical species are involved in a chemical reaction

$H + H \Rightarrow H_2$ oder $2\,H \Rightarrow H_2$

2) Distinguishing between reactants (left from the arrow) and products (on the right)

$H_2 + Cl_2 \Rightarrow 2\,HCl$

3) Conservation of mass

$SiO_2 + 4\,HF \Rightarrow SiF_4 + 2\,H_2O$

4) Neutral Charge

$Mg^{2+} + 2\,F^- \Rightarrow MgF_2$

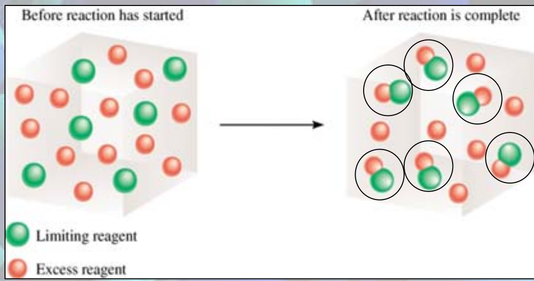
Sample Problem — Balancing Chemical Equations

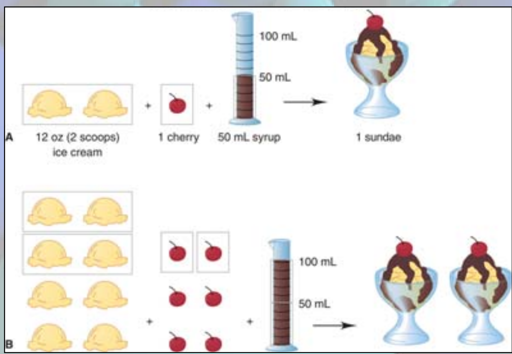
PROBLEM: Within the cylinders of a car's engine, the hydrocarbon octane (C_8H_{18}), one of many components of gasoline, mixes with oxygen from the air and burns to form carbon dioxide and water vapor. Write a balanced equation for this reaction.

PLAN:	SOLUTION:
translate the statement	$C_8H_{18} + O_2 \rightarrow CO_2 + H_2O$
balance the atoms	$C_8H_{18} + 25/2\,O_2 \rightarrow 8\,CO_2 + 9\,H_2O$
adjust the coefficients	$2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$
check the atom balance	$2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O$
specify states of matter	$2C_8H_{18}(l) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(g)$

Limiting Reagents

The limiting reagent determines the yield of the product





An Ice Cream Sundae Analogy for Limiting Reactions

What does this mean in chemistry?

Limiting Reagents?

In one process, 124 g of Al are reacted with 601 g of Fe_2O_3

$2Al + Fe_2O_3 \longrightarrow Al_2O_3 + 2Fe$

Which is the limiting reagent?

n = m/M !!!

g Al → mol Al → mol Fe_2O_3 needed → g Fe_2O_3 needed

$\frac{124 \text{ g Al}}{27.0 \text{ g/mol Al}} = 4.59 \text{ mol Al}$

2 mol Al react with 1 mol Fe_2O_3

4.59/2 = 2.30 mol Fe_2O_3 → Mass (g) Fe_2O_3 = 2.30 mol x 159.7 g mol^{-1}

= 367 g Fe_2O_3

Start with 124 g Al ⟶ need 367 g Fe_2O_3

Have more Fe_2O_3 (601 g) so Al is limiting reagent

Yield of a Reaction

Theoretical is the amount of product that would result if all the limiting reagent reacted.

Actual Yield is the amount of product actually obtained from a reaction.

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

Fundamentals of Solution Stoichiometry

- Solute: The substance that dissolves in the solvent
- Solvent: The substance in which the solute(s) dissolve

Molarity is the number of moles of solute per liter of solution.

$$c = \frac{\text{Number of moles}}{\text{Volume}} \qquad \left[\frac{\text{mol}}{\text{L}} = \text{M} \right]$$

also called: concentration: Symbol: ***c or [ ] (sometimes M)***

$c(H_2O)$ = 5 mol/L
$[H_2O]$ = 5 mol/L

$$c = \frac{n}{V}$$

Sample Problem **Calculating Mass of Solute in a Given Volume of Solution**

PROBLEM: How many grams of solute are in 1.75L of 0.460M sodium monohydrogen phosphate?

c = n/V → n ⇢ n = m/M ⇢ m

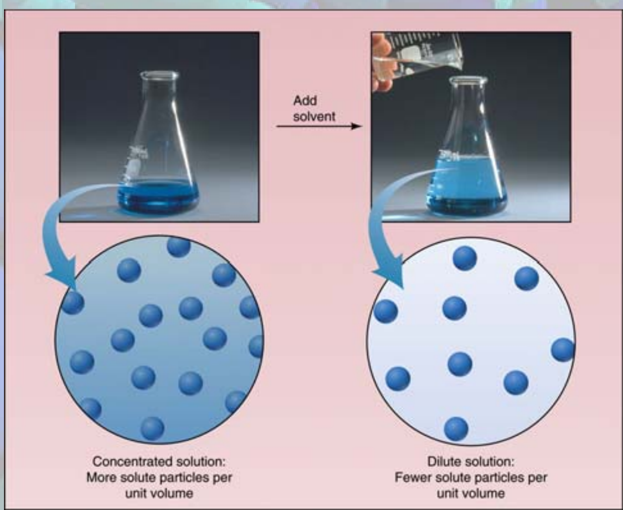
SOLUTION:

$$1.75\text{L} \times \frac{0.460\text{moles}}{1\text{ L}} = 0.805\text{mol } Na_2HPO_4$$

$$0.805\text{mol } Na_2HPO_4 \times \frac{141.96\text{g } Na_2HPO_4}{\text{mol } Na_2HPO_4}$$

$= 114\text{g } Na_2HPO_4$

Converting a Concentrated Solution to a Dilute Solution

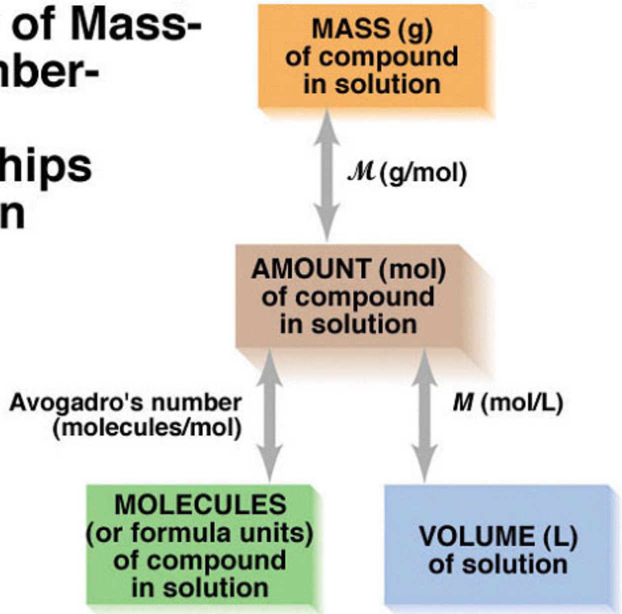


molarity

or

concentration

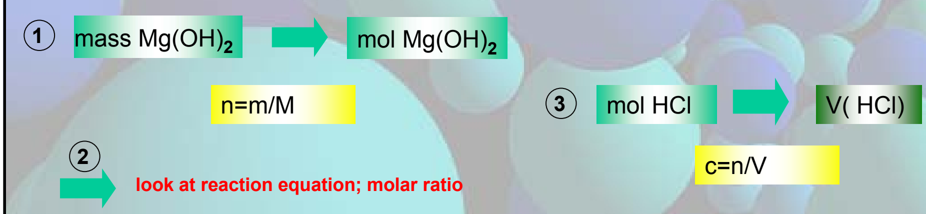
Summary of Mass-Mole-Number-Volume Relationships in Solution



Sample Problem **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.



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

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

n=m/M

$$n(Mg(OH)_2) = \frac{0.10g}{58.33g/mol} = 1.7x10^{-3} \text{ mol } Mg(OH)_2$$

The reaction ratio is: 1 mole of $Mg(OH)_2$ reacts with 2 moles HCl

$1.7x10^{-3}$ mol x 2 = $3.4x10^{-3}$ mol

c = n/V

$$\frac{3.4x10^{-3} \text{ mol}}{0.10mol/L} = 3.4x10^{-2} \text{ L HCl}$$

Chemical Reactions

….. Energetic Effects

….. more from the physical chemistry section !!!!

Reaction heat of a chemical reaction that takes place at constant pressure is called *reaction enthalpie* (ΔH).

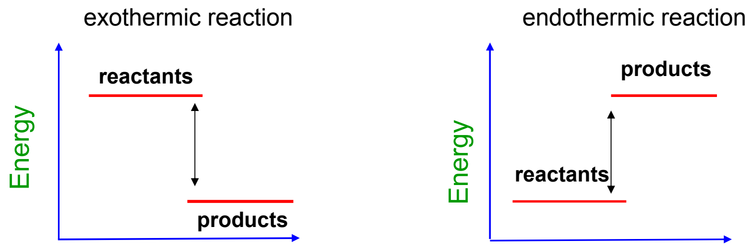
ΔH positive: endotherm
↓
heat is released

ΔH positive: exotherm
↓
heat is used/needed

Reaction enthalpies ΔH

Stoechimetric factors have to be considered

$$\Delta H = \Sigma H_{reactants} - \Sigma H_{products}$$



$H_2 + Cl_2 \Longrightarrow 2\,HCl$ $\quad$ ΔH = -184,8 kJ/mol

$N_2 + O_2 \Longrightarrow 2\,NO$ $\quad$ ΔH = +180,6 kJ/mol

If just 1 mol: ½ ΔH

ΔH: does not tell us if a reaction "occurs freely on its own"

….. description of the state of a chemical system

$$\Delta G = \Delta H - T \cdot \Delta S$$

Gibbs-Helmholtz Equation

free reaction enthalpie (ΔG)

entropy (ΔS)

all systems strive for a maximum disorder;
Increase of particles during a reaction

$\Delta G < 0$: spontaneous reaction — exergonic reaction
$\Delta G = 0$: equilibrium
$\Delta G < 0$: not a spontaneous reaction — endergonic reaction

Entropy changes are especially high if during the reaction if the number of moles of gases increases.

$$\Delta G = \Delta H - T \cdot \Delta S$$

A positive ΔG value can get compensated if ΔS is positive

→ **Thermal Energy**

$N_2 + O_2 + E_{therm.} \Rightarrow 2\,NO \quad \Delta G = +174$ kJ/mol

→ **Light Energy**

$AgBr + h\nu \Rightarrow Ag + \frac{1}{2} Br_2 \quad \Delta G = +97$ kJ/mol

→ **Electrical Energy**

$H_2O + E_{elekt.} \Rightarrow H_2 + \frac{1}{2} O_2 \quad \Delta G = +237$ kJ/mol

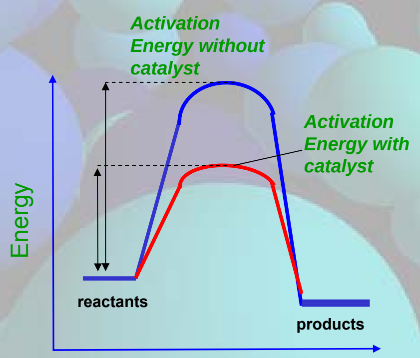
Velocity of Reactions ……. Kinetic

a) Reactions can occur with different velocity

b) Higher temperature → higher reaction velocity

c) Some reactions are irreversible, some are reversible

→ Increase of the reaction velocity → catalysis



The catalyst is not used during the reaction !!

Example: V_2O_5 catalysis of the H_2SO_4 Synthesis

sulphuric acid

$S + O_2 \longrightarrow SO_2$

$SO_2 + ½ O_2 \longrightarrow SO_3 \xrightarrow{H_2O} H_2SO_4$

Decomposes at high temperatures but reaction has a high activation energy

Catalytic Process:

a) $V_2O_5 + SO_2 \Longrightarrow SO_3 + 2\ VO_2$

b) $2\ VO_2 + ½ O_2 \Longrightarrow V_2O_5$