CHEMICAL REACTIONS AND YIELD

stoichiometry = the numerical relationships between chemical amounts in a reaction.

$2C_8H_{18}(l) + 25O_2 \longrightarrow 16CO_2(g) + 18H_2O(g)$

From the equation, 16 moles of CO_2 (a greenhouse gas resulting in global warming) are produced for every 2 moles of octane burned (by combustion).

Estimate the mass of CO_2 produced in 2004 by the combustion of 3.4×10^{15} g gasoline.

Solution: **number of moles = mass/molar mass**; *molar mass = molecular mass*
molecular masses: C_8H_{18} = 114.22; CO_2 = 44.01 $gmol^{-1}$

$4.4 \times 10^{15}/114.22 = 3.882 \times 10^{13}$ moles C8H18.

stoichiometric ratio CO_2: C_8H_{18} = 16:2 $\Rightarrow$ $3.882 \times 10^{13} \times (16/2) = 3.056 \times 10^{14}$ moles CO_2
$= 1.3 \times 10^{16}$ g CO_2.

limiting reactant (or reagent) = the reactant that limits the amount of product
excess reactants = reactants not completely consumed
theoretical yield = the amount of product that can be made from the limiting reactant
actual yield = the amount of product that is made in a reaction actual yield
generally less than the theoretical yield, never more!
percent yield = the efficiency of product recovery

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

When 28.6 kg of C reacts with 88.2 kg of TiO_2, 42.8 kg of Ti are obtained. Find the Limiting Reactant, Theoretical Yield, and Percent Yield.
$TiO_2(s) + 2\,C(s) \rightarrow Ti(s) + 2CO(g)$

Solution: 1 mole TiO_2 gives 1 mole Ti; 2 moles C gives 1 mole Ti.
molar masses C = 12.01; TiO_2 = 79.87; Ti = 47.87 $gmol^{-1}$.

Number of moles of C = 2.38×10^3 moles $\Rightarrow$ 1.191×10^3 moles Ti
Number of moles of TiO_2 = 2.38×10^3 moles $\Rightarrow$ 1.104×10^3 moles Ti

TiO_2 = limiting reactant $\Rightarrow$ $1.104 \times 10^3 \times 47.87$ = 52.9 kg Ti = theoretical yield

Percent yield = 100% x 42.8 / 52.9 = 80.9 %.

PRACTICE EXAMPLE ONE

Mining companies use the following reaction to obtain iron from iron ore:

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

The reaction of 167g of Fe_2O_3 with 85.8g of CO produces 72.3g Fe. Find the limiting reagent, theoretical yield and percent yield.

Making aqueous solutions

When an ionic compound **dissolves** in water, the water molecules surround the cations and anions; e.g. KCl(s) $\rightarrow$ K^+(aq) + Cl^-(aq). Heating the solution increases solubility. Substances such as potassium chloride or hydrogen chloride (strong acid) that completely dissociate into ions are **strong electrolytes** (solution conducts electrical current). **Weak electrolytes** dissolve mostly as molecules but partly dissociate into ions:

$$CH_3COOH(aq) \rightleftharpoons CH_3COO^-(aq) + H^+(aq)$$

dilute (淡的) **solutions** = small amount of solute (溶质) compared to solvent (溶剂)

concentrated (浓) **solutions** = large amount of solute compared to solvent

$$\textbf{Molarity} = \frac{\text{amount of solute (in moles)}}{\text{amount of solution (in L or dm}^3\text{)}}$$

Find the **molarity, M** (or **concentration, C**) of a solution that has 25.5 g KBr dissolved in 1.75 L of solution

Solution: molar mass KBr = 119.00 gmol-1
number of moles = 25.5 / 119 = 0.214 mol KBr
molarity = 0.214 / 1.75 = **0.122 M** (or mol dm^{-3}).

Dilution = make a solution less concentrated

moles solute in solution 1 = moles solute in solution 2

$M_1V_1 = M_2V_2$

To what volume should you dilute 0.200 L of 15.0 M NaOH to make 3.00 M NaOH?

Solution: $M_2 = M_1V_1 / V_2$ = 15 x 0.2 / 3 = **1.0 M**

PRACTICE EXAMPLE TWO

What volume of a 6.00 M $NaNO_3$ solution should you use to make 0.525 L of a 1.20 M $NaNO_3$ solution?

What volume of 0.150 M KCl is required to completely react with 0.150 L of 0.175 M $Pb(NO_3)_2$ in the reaction $2KCl(aq) + Pb(NO_3)_2(aq) \rightarrow PbCl_2(s) + 2\ KNO_3(aq)$?

1 L $Pb(NO_3)_2$ = 0.175 mol, 1 L KCl = 0.150 mol,
stoichiometry: 1 mol $Pb(NO_3)_2$ reacts with 2 mol KCl

Number of moles of $Pb(NO_3)_2$ used = molarity x volume = 0.0263 moles
Number of moles of KCl used = 0.02625 moles x 2 = 0.0525 moles
volume KCl = moles / molarity = 0.0525 /0.150 = **0.35 L**

PRACTICE EXAMPLE THREE

Consider the following reaction:

$Li_2S(aq) + Co(NO_3)_2(aq) \rightarrow 2LiNO_3(aq) + CoS(aq)$

What volume of 0.150 M Li_2S solution is required to completely react with 125 mL of 0.250 M $Co(NO_3)_2$?

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____[208 mL]

soluble (可溶性) **=** compounds that dissolve in a solvent (e.g. NaCl dissolves in water)
insoluble (不溶性) **=** compounds that do not dissolve (e.g. AgCl does not)

Most Group I compounds are soluble in water (e.g. NaOH, Na_2SO_4). Some Group II compounds are soluble (e.g. $CaCl_2$), slightly soluble e.g. $Ca(OH)_2$, others are not (e.g. $CaSO_4$). Many ammonium NH_4^+ compounds are soluble (e.g. NH_4Cl) and ALL NITRATES (e.g. $Ca(NO_3)_2$) are soluble. **See book table 4.1, p.149.**

Precipitation (沉淀) **reactions** = reactions between aqueous solutions of ionic compounds that produce an ionic compound that is insoluble (**precipitate**) in water:

$2KI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + 2\ KNO_3(aq)$; **$PbI_2(s)$ is the precipitate**

Writing and simplifying equations

molecular equations = equations which describe the chemicals put into the water and the product molecules molecular equations, e.g.

$2KI(aq) + Pb(NO_3)_2(aq) \rightarrow PbI_2(s) + 2\ KNO_3(aq)$

complete ionic equations = equations which describe the actual dissolved species:

$2K^+(aq) + 2I^-(aq) + Pb^{2+}(aq) + 2NO_3^{2-}(aq) \rightarrow 2K^+(aq) + 2NO_3^{2-}(aq) + PbI_2(s)$

- ions that are both reactants and products are called **spectator ions (they do not react and remain in the solution)**

net ionic equation = an ionic equation in which the spectator ions are removed:

$Pb^{2+}(aq) + 2I^{-}(aq) \rightarrow PbI_2(s)$

neutralization reactions = the acid and base neutralize each other's properties

$2HNO_3(aq) + Ca(OH)_2(aq) \rightarrow Ca(NO_3)_2(aq) + 2\ H_2O(l)$

the net ionic equation for an acid-base reaction is:

$H^+(aq) + OH^-(aq) \rightarrow H_2O(l)$

PRACTICE EXAMPLE FOUR

Write complete ionic and net ionic equations for each reaction:

$K_2SO_4(aq) + CaI_2(aq) \rightarrow CaSO_4(s) + KI(aq)$
$NH_4Cl(aq) + NaOH(aq) \rightarrow NH_3(g) + NaCl(aq) + H_2O(l)$

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acids ionize in water to form H^+ ions

more precisely, the H from the acid molecule is donated to a water molecule to form **hydronium ion, H_3O^+**. A proton (H^+) cannot exist on its own in water!

bases dissociate in water to form OH^- ions

bases, such as NH_3, that do not contain OH^- ions, produce OH^- by pulling H off water molecules

acid + base $\rightarrow$ salt + water

titration - a solution's concentration is determined by reacting it with another material and using stoichiometry (involving a chemical equation and calculation). An indicator permanently changes colour at the **end-point** (just finished).

For example, if we know the concentration and precise volume of the alkali but only the volume of acid of unknown concentration, we can determine its concentration. Titration can be used for many ionic reactions.

$$n_1A + n_2B \rightarrow \text{products (e.g. salt + water)}$$

$$\boxed{\frac{C_1 \times V_1}{C_2 \times V_2} = \frac{n_1}{n_2}} \quad \text{or} \quad C_2 = \frac{C_1 \times V_1 \times n_2}{n_1 \times V_2}$$

12.54 mL of 0.100 M NaOH(aq) reacts 10.00 mL of HCl(aq) solution. What is the concentration of the acid? The formula can be used with mL (for both solutions) or converted to L for both solutions.

$NaOH(aq) + HCl(aq) \rightarrow NaCl(aq) + H_2O(l)$

C_1 concentration = 0.100 M NaOH(aq); C_2 = ?
V_1 volume = 12.54 mL NaOH(aq); V_2 = 10.00 mL
n_1 stoichiometric value = 1 for NaOH; n_2 = 1 for HCl

C_2 = 0.100 x 12.54 x 1 / 1 x 10.00 = **0.125 M HCl(aq)**

Some neutralization reactions evolve gases; the intermediate carbonic acid (H_2CO_3) thus decomposes, e.g.

$Na_2CO_3(aq) + 2HNO_3(aq) \rightarrow 2NaNO_3(aq) + \mathbf{CO_2(g)} + H_2O(l)$

PRACTICE EXAMPLE FIVE

A 30.00 mL sample of an unknown H_3PO_4 solution is titrated with a 0.100 M NaOH solution. The end-point (equivalence point) is reached when 26.38 mL of NaOH solution is added. What is the concentration of the unknown H_3PO_4 solution?

$3NaOH(aq) + H_3PO_4(aq) \rightarrow Na_3PO_4(aq) + 3H_2O(l)$

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REDOX REACTIONS

REDOX (oxidation-reduction) reactions = transferring electrons from one atom to another
Many involve the use of O_2, Cl_2 etc.

$4 Fe(s) + 3O_2(g) \rightarrow 2 Fe_2O_3(s)$; the iron has transferred its electrons to the oxygen atoms

Combustion (molecular - involve the use of O_2) is also REDOX, e.g.

$H_2(g) + O_2(g) \rightarrow 2H_2O(l)$

oxidation occurs when an atom's oxidation state **increases** during a reaction (Fe(0) to Fe +3). **LOSS OF ELECTRONS**

reduction occurs when an atom's oxidation state **decreases** during a reaction (O (0) to O (-2). **GAIN OF ELECTRONS**

In a REDOX reaction, the oxidizing agent is always reduced and the reducing agent always oxidized.

$C + 2S \rightarrow CS_2$ carbon is the **reducing agent** (0 to +4) and sulphur the **oxidizing agent** (0 to -2).

Oxidation state and ionic charges are not to be confused; for single atoms with a charge (e.g. Fe^{3+}, O^{2-}) the oxidation state is often the charge!

- oxygen is nearly always -2 (exception KO_2).
- Group I = +1; Group 2 = +2
- Transition metals have variable oxidation states (e.g. chromium from +2 to +6) $K_2Cr_2O_7$: Cr = +6 = potassium chromate(VI)
- elements (e.g. O_2 oxidation state = zero (0).
- Metals have positive oxidation states.
- In a neutral atom or formula the sum (Σ) of the oxidation states = 0.
- An ion is equal to the charge of the ion.

SO_4^{2-}, and H_2SO_4 sulphur has oxidation state of +6.

PRACTICE EXAMPLE SIX

What is the oxidation state of Cl in each ion?

1. a) ClO^- b)ClO_2^- c)ClO_3^- d)ClO_4^-

2. Determine the *oxidizing* and *reducing* agent:

a) Al(s) + 3Ag+(aq) $\rightarrow$ Al^{3+}(aq) + 2Ag(s)
b) NaI_2(aq) + Cl_2(g) $\rightarrow$ 2NaCl(aq) + I_2(aq)

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COMBUSTION REACTIONS

We have encountered several combustion reactions so far. Common ones include burning elemental carbon, hydrogen, sulphur, phosphorous, hydrocarbons (e.g. methane) or alcohol in air or oxygen. They give off heat (exothermic, $\Delta H < 0$ typically about 2000 $KJmol^{-1}$) and light. **Equations must be balanced in an exam (number of atoms on the left = number of atoms on the right).**