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Chemical Calculations

Definitions

- Molar mass is the mass in grams of one mole of that substance.
- A solution is a homogenous mixture of solute and solvent.
- A solute is the substance that is dissolved in the solution.
- A solvent is the substance in which another substance is dissolved, forming a solution.
- Concentration is the amount of solute per unit volume of solution.
- Yield is a measure of the extent of a reaction, generally measured by comparing the amount of product against the amount of product that is possible.

Concepts

- The mole is the SI unit for amount of substance.
- One mole contains Avogadro's number of particles ($6,02 \times 10^{23}$)

m - Mass in grams

n - Number of moles

M - Molar Mass (From periodic table)

V - Volume in decimetres cubed (To convert cm³/ml to dm³ divide by 1000)

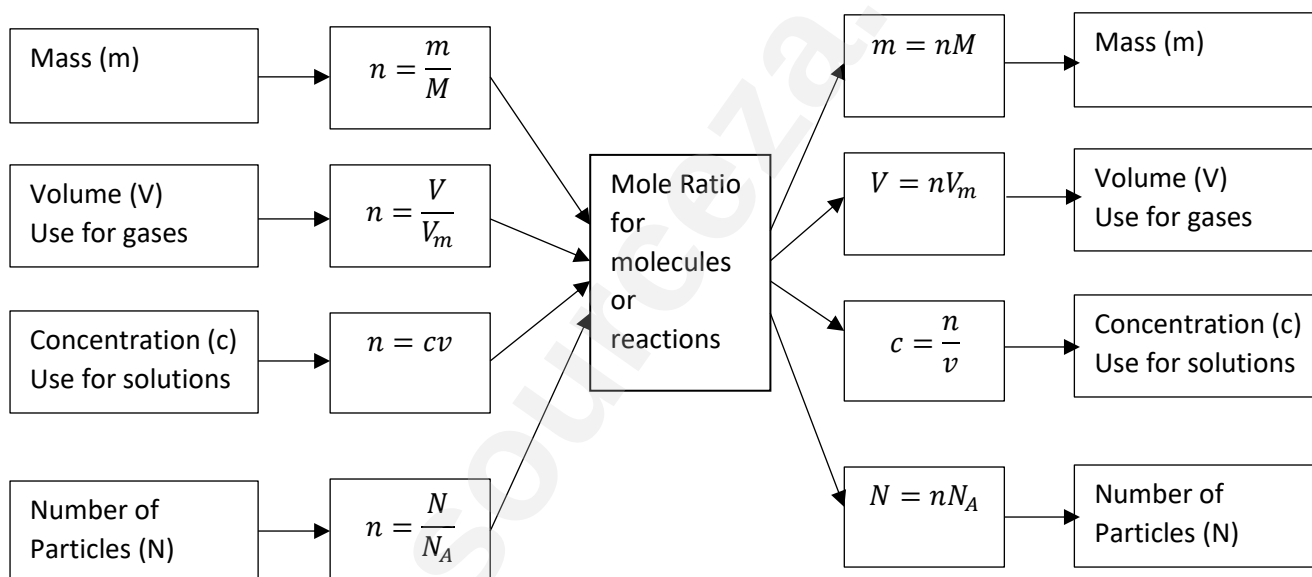
c - Concentration in mols.dm⁻³

N – Number of particles/atoms/molecules/ions.

N_A – Avogadro's Number (6.02 x 10²³)

V_m – Molar Volume = 22.4 dm³ at STP (0° or 273 K/ 101.3 kPa)

Basic Stoichiometry



Percentage Yield

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

1. Convert whatever quantity of the reactant that is given to number of moles using the relevant formula.
2. Using mole ratio find the theoretical yield of the product for which you are given the actual yield.
3. Use the above formula and calculate the percentage yield.

Percentage Purity

$$\%Purity = \frac{Pure\ Mass}{Impure\ Mass} \times 100$$

1. Convert quantity of the reactant or product to number of moles using the relevant formula. NB. DO NOT USE THE IMPURE MASS.
2. Use mole ratio to calculate the pure moles of the impure substance.
3. Convert the moles of the pure substance to mass.
4. Use the above formula to calculate the percentage purity.

Limiting Reagent

The limiting reagent (or limiting reactant, LR) in a chemical reaction is the substance that is totally consumed when the chemical reaction is complete. The amount of product formed is limited by this reagent, since the reaction cannot continue without it.

1. Convert the quantities of both reactants to number of moles using the relevant formulae.
2. Determine which reactant is the limiting reagent, then the other reactant will be in excess.
3. With the number of moles of the limiting reagent as the basis, use mole ratio to determine what the question requires.

Empirical Formulae

When the final mole ratio has:

- 0,5 multiply by 2
- 0,33 or 0,67 multiply by 3
- 0,25 or 0,75 multiply by 4

STUDY GUIDE

ORGANIC CHEMISTRY



DEFINITIONS

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- *Hydrocarbon is a compound containing only carbon and hydrogen atoms*
- *A saturated compound is a compound in which all of the bonds between carbon atoms are single bonds*
- *An unsaturated compound is a compound in which there is at least one double and/or triple bond between carbon atoms*
- *A functional group is an atom or a group of atoms that form the centre of chemical activity in the molecule*
- *A homologous series is a series of similar compounds which have the same functional group and have the same general formula, in which each member differs from the previous one by a single CH_2 unit*
- *Structural isomers are compounds having the same molecular formula but different structural formulae*

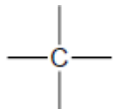
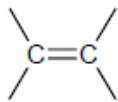
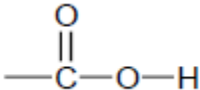
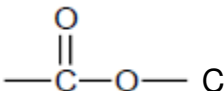
KNOWLEDGE & SKILLS

- Describe organic molecules as molecules containing carbon atoms with the exception of carbon dioxide, carbon monoxide, diamond, graphite, carbonates (or bicarbonates), carbides and cyanides
- Identify compounds that are hydrocarbons
- Identify compounds that are saturated and unsaturated
- Identify the functional group of compounds belonging to the following homologous series:
- Write the IUPAC name when given the formula of compounds in the following homologous series: alkanes, alkenes, haloalkanes, alcohols, carboxylic acids and esters (up to 8 carbon atoms)
- Write down, identify and apply the general formula for alkanes ($\text{C}_n\text{H}_{2n+2}$) and alkenes (C_nH_{2n})
- Draw structural, condensed structural and molecular formulae for compounds belonging to the following homologous series: alkanes, alkenes, haloalkanes, alcohols, carboxylic acids and esters (up to 8 carbon atoms)
- Identify compounds that are structural isomers (up to 8 carbon atoms)
- Recognise and explain the relationship between melting point/ boiling point and the strength of the intermolecular forces
- Know that many organic compounds are flammable and suggest a suitable method of heating organic liquids
- Classify and identify the following GENERAL reaction TYPES: combustion (oxidation), substitution, addition, elimination and condensation (esterification)
- State that combustion reactions are exothermic and hence explain the importance of fossil fuels in terms of their ability to transfer chemical potential energy into heat energy
- Write balanced chemical equations to represent the complete combustion of alkanes, alkenes and alcohols with excess oxygen to produce water and carbon dioxide
- When given the appropriate reaction conditions, write balanced equations to show the formation of substitution products
- When given the appropriate reaction conditions write balanced equations to show the formation of addition products
- When given the appropriate reaction conditions write balanced equations to show the formation of elimination products
- State or identify the appropriate reaction conditions and write balanced equations to show the formation of esters
- State that an acid catalysed condensation reaction between an alcohol and a carboxylic acid produces an ester and water
- Identify the alcohol and carboxylic acid used to prepare any given ester
- Given any alcohol and carboxylic acid, identify the ester produced
- Write an equation to represent the preparation of an ester

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HOMOLOGOUS SERIES & FUNCTIONAL GROUP

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Homologous Series	Functional Groups		Suffix	Formula
	Structure	Name/Description		
Alkanes		<u>Saturated hydrocarbons:</u> Single bonds between carbon atoms.	-ane	C_nH_{2n+2}
Alkenes		<u>Unsaturated hydrocarbons:</u> At least one double bond between carbon atoms.	-ene	C_nH_{2n}
Haloalkanes (Alkyl halides)	---X Where X = F, Cl, Br, or I	At least one <u>halogen</u> bonded to a carbon atom. F – Fluoro Cl – Chloro Br – Bromo I – Iodo	-ane	$C_nH_{2n+1}X$
Alcohols	---O---H	<u>Hydroxyl:</u> At least one OH only bonded to a carbon atom	-ol	$C_nH_{2n+1}OH$
Carboxylic Acid		<u>Carboxyl:</u> At least one OH and O bonded to the same carbon atom.	-oic acid	---COOH
Esters		<u>Ester Group:</u> An oxygen in between 2 carbon atoms with another oxygen bonded to one of the 2 carbon atoms.	-oate	$R\text{---COOC---}R$

Prefixes for Number of Carbon Atoms

Number of Carbon Atoms	Prefix
1	Meth -
2	Eth -
3	Prop -
4	But -
5	Pent -
6	Hex -
7	Hept -
8	Oct -

Alkyl Groups

Name of Alkyl Group	Structure
Methyl	---CH_3
Ethyl	$\text{---C}_2\text{H}_5$

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IUPAC Rule for Naming Organic Compounds

1. Identify the longest carbon chain. Remember a chain is not necessarily in a straight line.
2. Identify the functional group, halogens and alkyl groups in the structure.

Numbering the main chain

3. Number the carbon atoms in the main chain such that the function group, or branch (halogens/alkyl groups) gets the lowest possible number.
4. When naming haloalkanes, the halogen atoms do not get preference over alkyl groups – numbering should start from the end nearest to the first substituent, either the alkyl group or the halogen. In haloalkanes, where e.g. a Br and a Cl have the same number when numbered from different ends of chain, Br gets alphabetical preference.

Writing the name of substituents

5. When writing IUPAC names of substituents (methyl, ethyl, fluoro, chloro, bromo, iodo), write the number of the carbon atom the substituent is attached to followed by the prefix. The number and prefix should be separated by a hyphen.

Examples

2-fluoro means that a fluorine is on carbon number 2 of the main chain.

4-methyl means that a methyl group is found on carbon number 4 of the main chain.

6. If there are more than one substituents, the substituents should be written in alphabetical order.

Examples

3-ethyl-2-fluoro means that there is an ethyl group on carbon 3 and a fluorine on carbon 2, but ethyl takes alphabetical preference.

7. If there are more than one of the same substituent we use the following prefixes:

di- for two of the same.

tri- for three of the same.

tetra- for 4 of the same.

When using alphabetical preference, these prefixes are ignored.

Examples

4,5-dichloro-3-methyl means that there are 1 chlorine on carbon 4 and 1 chlorine on carbon 5, 1 methyl on carbon 3. However, chloro takes alphabetical preference.

8. When writing IUPAC names, the following conventions must be followed:

- Numbers are separated from letters using a dash (-)
- Numbers are separated from numbers using a comma (,)
- Letters are not separated at all (i.e. no space is used), with the exceptions being esters (e.g. methyl ethanoate) and carboxylic acids (e.g. propanoic acid)

Writing the name of the main chain

9. When writing the name of the main chain the first part of the name takes the prefix according to the number of carbon atoms. The second part of the name takes the suffix according to the homologous series.

Examples

Pentane Is an alkane with 5 carbon atoms.

10. For alkenes and alcohols, the number of the carbon atom containing the functional group need to appear between the prefix and suffix. If there are more than one functional group we use the prefix di and tri.

Examples

Penta-1,3-diene Means there is a double bond between the carbon 1 and 2, and a double bond between carbon 3 and 4.

Butane-2,3-diol Means there is a hydroxyl group on carbon 2 and 3

Euphonic rule for diols

11. For euphonic purposes, the vowel "e" is generally removed from the name before the suffix, e.g. butan-1-ol instead of butane-1-ol. However, this is not done for diols, e.g. butane-1,2-diol is correct, and not butan-1,2-diol.

Euphonic rule for dienes

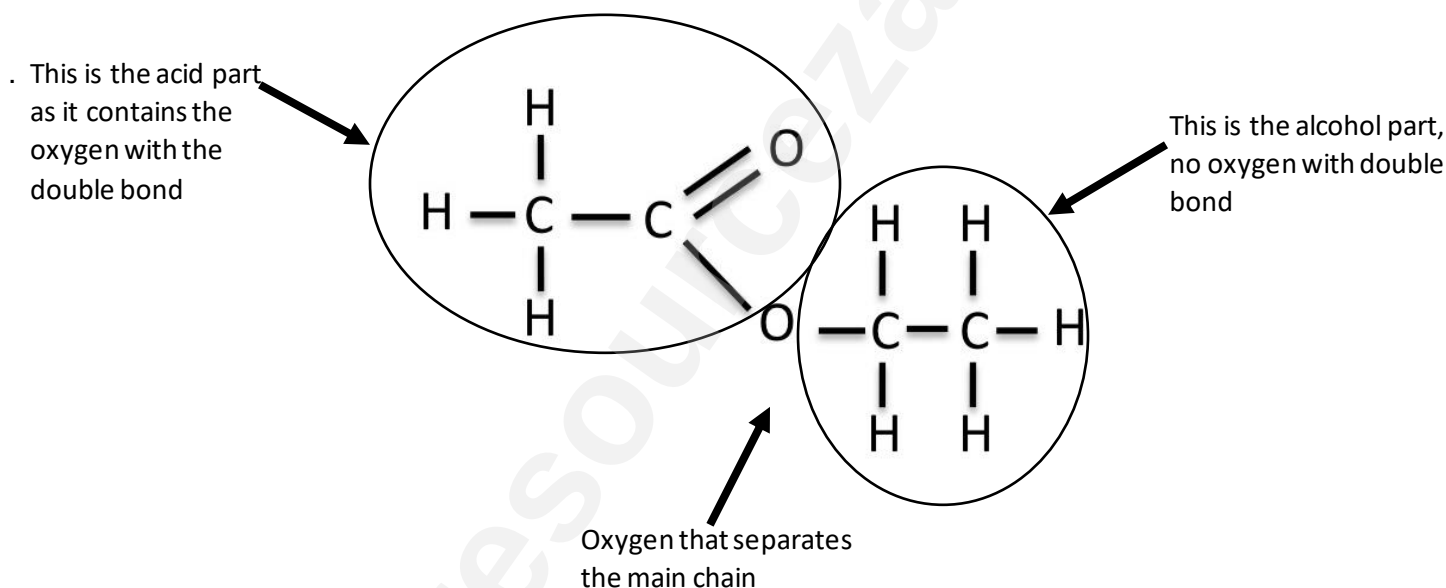
12. For euphonic purposes, the vowel "a" must be added to the name before the suffix for dienes, e.g. buta-1,3-diene is correct, and not but-1,3-diene.

Redundancy rule

13. Although in some, especially smaller, molecules numbering becomes redundant, redundancy will not be penalised. For example, methylbut-2-ene may be written as 2-methylbut-2-ene without penalty. The only exception to this is if numbering is always redundant, e.g. for a carboxylic acid: butan-1-oic acid will be penalised, as it must be written as butanoic acid.

Naming of an Ester

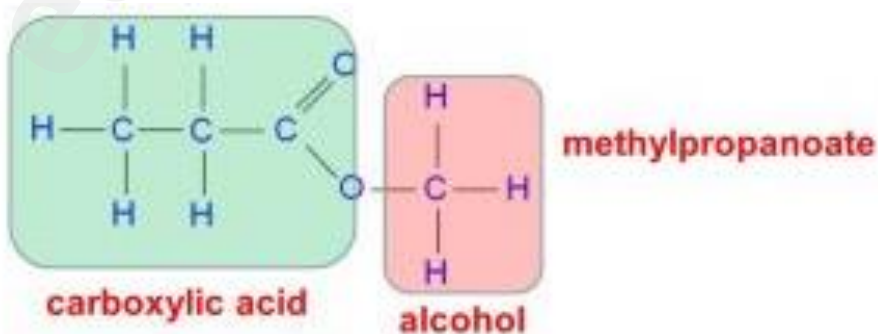
14. An ester is a product from the reaction of an alcohol and a carboxylic acid, hence the name of an ester is derived from the alcohol and carboxylic acid from which they are produced. The two parts are separated by the oxygen atom in the main chain.



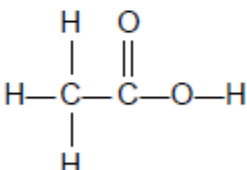
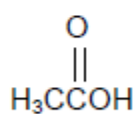
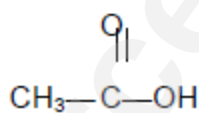
15. The first part of the name comes from the alcohol part and the second part comes from the acid part. The name ends with the suffix of the homologous series.

Example

Ethyl ethanoate from example above



Examples of different types of formulae for ethanoic acid

Structural	Condensed structural	Molecular
Atoms are represented by their chemical symbols and lines are used to represent ALL of the bonds between atoms.	The way in which atoms are bonded but NOT ALL bond lines are shown.	This is a chemical formula that indicates the type of atoms and the correct number of each in a molecule.
	CH₃COOH or  or 	C ₂ H ₄ O ₂

1. Start by drawing the main carbon chain.
2. Number the carbon atoms.
3. Add functional groups substituents to the relevant carbon atoms.
4. Ensure each carbon atom forms 4 bonds by adding hydrogens.

Structural Isomers

Types of structural isomers	Description	Examples
1) Chain isomers	Different type of chain structure, i.e. branching	Butane and methylpropane
2) Positional isomers	Different positions of the same functional group on the parent chain	• 1-chloropropane and 2-chloropropane • But-1-ene and but-2-ene • Ethyl methanoate and methyl ethanoate
3) Functional isomers	Different functional groups. Carboxylic acid and ester are functional isomers	Propanoic acid and ethylmethanoate

ORGANIC COMPOUNDS – PHYSICAL PROPERTIES

Homologous Series	Type of Bonds	Strength of Bond	Type of Molecule	Relationship Between Physical Properties & Structure
Alkanes	Van Der Waals (London/Dispersion)	Weak	Non Polar	Low melting and boiling points due to the weak intermolecular forces.
Alkenes	Van Der Waals (London/Dispersion)	Weak	Non Polar	Low melting and boiling points due to the weak intermolecular forces.
Halo Alkanes	Van Der Waals Dipole Dipole	Stronger than London/Dispersion	Polar	Melting and boiling points are higher than hydrocarbons but lower than alcohols and carboxylic acids due to the stronger intermolecular forces.
Alcohols	Hydrogen Bonds	Strong	Polar	High melting and boiling point due to the hydrogen bonds existing between hydroxyl group and adjacent molecules
Carboxylic Acid	Hydrogen Bonds	Strong	Polar	Has a higher melting and boiling points than Alcohols because each molecule can form 2 hydrogen bonds due to 2 oxygens
Esters	Van Der Waals Dipole Dipole	Stronger than London/Dispersion	Polar	Melting and boiling points are higher than hydrocarbons but lower than alcohols and carboxylic acids due to the stronger intermolecular forces.

Length of Main Chains

Eg. London forces in hydrocarbons

- All hydrocarbons have induced dipole forces or London forces between their molecules.
- The larger molecules have a greater interactive surface and have a greater electron density.
- Bigger temporary dipoles are set up **or** easier dispersion of electrons therefore longer lasting dipoles. These factors result in STRONGER London forces.
- More energy is needed to overcome the stronger intermolecular forces (NOT bonds) therefore larger molecules have higher boiling points.

Branches

Molecules with branches have fewer points of contact for intermolecular forces therefore the forces will be weaker.

Eg. Explain why butane has a higher boiling point than methylpropane

- Both butane and methylpropane have London forces between their molecules.
- Unbranched butane molecules have a larger interacting surface than branched molecules of methylpropane.
- Butane has a longer unbranched chain, therefore can develop larger temporary dipoles than methylpropane which has a branched chain.
- Butane has stronger London forces which require more energy to overcome, therefore butane has the higher boiling point.

Multiple hydrogen bonds

- Carboxylic acids are able to form TWO hydrogen bonds with another carboxylic acid molecule.
- Alcohols can only form ONE hydrogen bond with another alcohol molecule.
- TWO hydrogen bonds per molecule are collectively stronger than ONE.
- More energy is needed to overcome two H-bonds compared with one H-bond, therefore, carboxylic acids have a higher boiling point.

ORGANIC REACTIONS

Type of Reaction	Name of Reaction	Reactant/s	Product	Reaction Dynamics/Conditions		Catalyst
Combustion 2 Reactants→ 2 Products		Alkane Alkene + O ₂ Alcohol Esters	H ₂ O + CO ₂ + Heat	Hydrocarbons are used extensively as fuels because they combine with oxygen to release large quantities of heat and produce the non-toxic products, carbon dioxide and water.		
Substitution 2 Reactants→ 2 Products	Halogenation	Alkane + Halogen	Haloalkane + Hydrogen Halide	Reaction is slow and only takes place in sunlight or UV light or heat		
	Hydrolysis	Haloalkane + NaOH (dil) + Heat	Alcohol + Sodium Halide	Heat under reflux in a dilute alkali solution.		
Addition 2 Reactant→ 1 Products	Hydrogenation	Alkene + H ₂	Alkane	Alkene dissolved in a non-polar solvent with the catalyst in a H ₂ atmosphere		Ni, Pt or Pd
	Halogenation	Alkene + Halogen	Haloalkane	Discolouration of the Bromine occurs Use as test for alkenes.		
	Hydrohalogenation	Alkene + Hydrogen Halide	Haloalkane	No water present	H atom bonds to the carbon atom which already has the larger number of H atoms bonded to it	
	Hydration	Alkene + H ₂ O(g)	Alcohol	Water must be steam		Phosphoric Acid
Elimination 1 Reactants→ 2 Products	Dehydrohalogenation	Haloalkane	Alkene + Hydrogen Halide/ Alkene+Alkali Metal + water	Hot concentrated solution of NaOH or KOH in an ethanol solvent ie, absence of water		
	Dehydration	Alcohol	Alkene + H ₂ O	Heating of alcohol in a water bath. H ₂ SO ₄ acts as a dehydrating agent		H ₂ SO ₄ (conc)
	Cracking	Alkane Alkenes	Smaller Hydrocarbon molecules	Cracking is the breaking up of large hydrocarbon molecules into smaller and more useful molecules	Thermal cracking -high pressures and temperatures without a catalyst; Catalytic cracking -lower temperatures and pressures in the presence of a catalyst	
Esterfication 2 Reactants→ 2 Products	Condensation	Carboxylic Acid + Alcohol	Ester + H ₂ O	Reaction needs to be heated in a water bath as alcohol is flammable.		H ₂ SO ₄ (conc)

REDOX REACTIONS

Definitions

- Redox reaction is a reaction involving the transfer of electrons.
- Oxidation is the loss of electrons.
- Reduction is the gain of electrons.
- Oxidising agent is a substance that accepts electrons.
- Reducing agent is a substance that donates electrons.
- Anode is the electrode where oxidation takes place.
- Cathode is the electrode where reduction takes place.
- An electrolyte is a substance that can conduct electricity by forming free ions when molten or dissolved in solution.

Skills

Use the table of standard electrode potentials (SEP table) to:

Redox Reactions

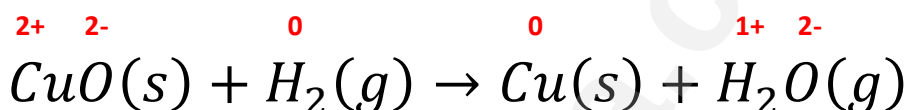
- Predict the chemical species which is oxidised in a redox reaction and write an equation for the oxidation half-reaction.
- Predict the chemical species which is reduced in a redox reaction and write an equation for the reduction half-reaction.
- Write the overall balanced ionic reaction equation by combining the two half-reactions
- Identify the oxidising agent and the reducing agent for a redox reaction.
- Determine the spontaneity of a redox reaction under standard conditions.
- Identify the spectator ion in a redox process and know that the spectator ion does not take part in the electron transfer.

Galvanic

- Describe the galvanic cell as a self-sustaining electrode reaction, where a chemical reaction produces an electric current.
- Describe that chemical energy is converted to electrical energy.
- Predict the half-cell in which oxidation will take place and identify the anode.
- Predict the half-cell in which reduction will take place and identify the cathode.
- Use the SEP table (or other given half-reactions and relevant information) to write equations for half-reactions taking place at the anode and cathode.
- Write the overall ionic cell reaction by combining two half-reactions.
- Describe the movement of ions through the solutions, the electron flow in the external circuit of the cell and the observations in the half-cells
- State the functions of the salt bridge.
- Describe how the salt bridge maintains electrical neutrality in the half-cells by referring to the movement of ions in and out of the salt bridge
- Use cell notation to represent a galvanic cell.

- $$E_{cell}^0 = E_{oxidizing\ agent}^0 - E_{reducing\ agent}^0$$

- ### Example 1


$$RHR: \quad Cu^{2+}(aq) + 2e^{-} \rightarrow Cu(s)$$
$$OHR: H_2(g) \rightarrow 2H^+(aq) + 2e^-$$

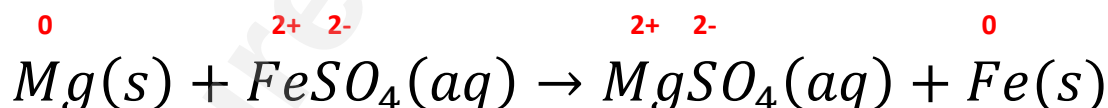
Overall Net Ionic Reaction: $Cu^{2+} + H_2 \rightleftharpoons Cu(s) + 2H^+(aq)$

Reducing Agent: H_2 Oxidizing Agent: Cu^{2+}

$$E_{cell}^0 = E_{oxidizing\ agent}^0 - E_{reducing\ agent}^0 = 0,34 - 0 = 0,34\ V$$

$E_{cell}^0 > 0$ Therefore reaction is spontaneous

Example 2



Fe^{2+} is being reduced, Mg is being oxidized, SO_4^{2-} is a spectator ion

RHR: $Fe^{2+}(aq) + 2e^- \rightarrow Fe(s)$

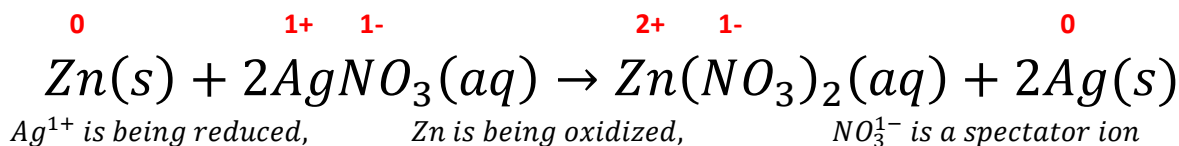
$$\text{OHR: } \text{Mg(s)} \rightarrow \text{Mg}^{2+}(\text{aq}) + 2\text{e}^{-}$$

Overall Net Ionic Reaction: $Fe^{2+}(aq) + Mg(s) \rightleftharpoons Fe(s) + Mg^{2+}(aq)$

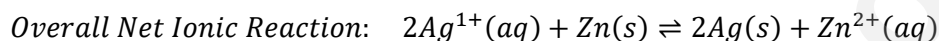
Reducing Agent: Mg Oxidizing Agent: Fe^{2+}

$$E_{cell}^0 = E_{oxidizing\ agent}^0 - E_{reducing\ agent}^0 = -0,44 - (-2,37) = 1,93\ V$$

$E_{cell}^0 > 0$ Therefore reaction is spontaneous

Example 3

Multiple RHR by 2

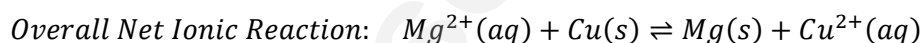
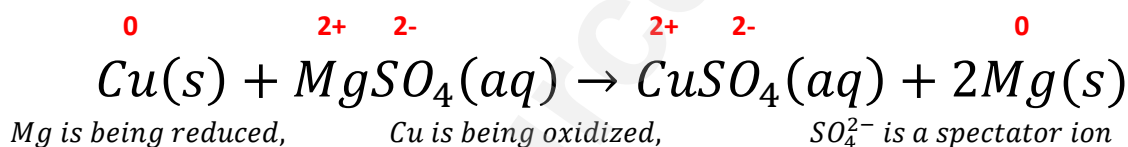


Reducing Agent: Zn

Oxidizing Agent: Ag^{1+}

$$E_{\text{cell}}^0 = E_{\text{oxidizing agent}}^0 - E_{\text{reducing agent}}^0 = 0,80 - (-0,76) = 1,56$$

$E_{\text{cell}}^0 > 0$ Therefore reaction is spontaneous

Example 4

Reducing Agent: Cu

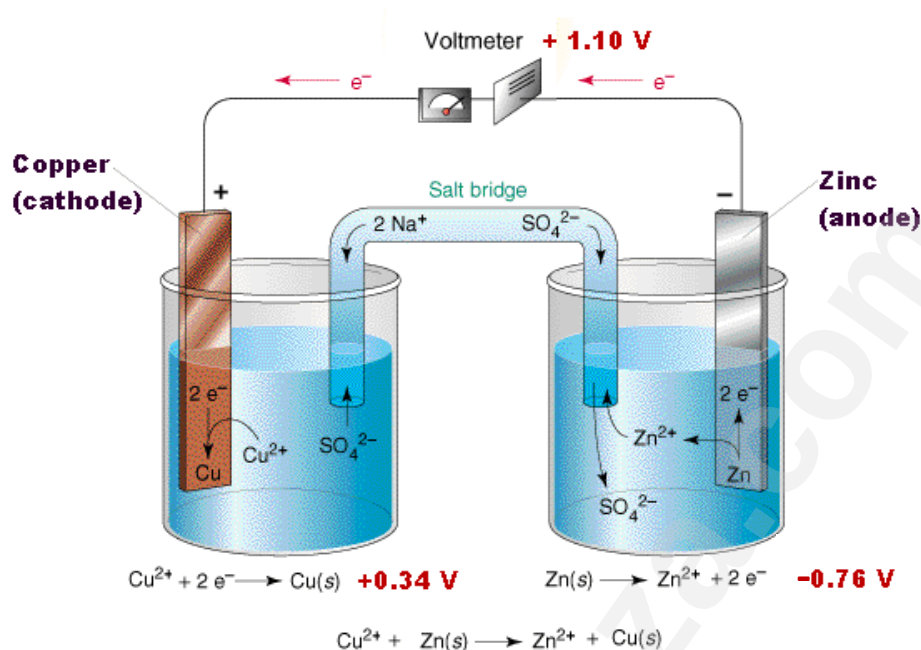
Oxidizing Agent: Mg^{2+}

$$E_{\text{cell}}^0 = E_{\text{oxidizing agent}}^0 - E_{\text{reducing agent}}^0 = -2,37 - 0,34 = -2,71$$

$E_{\text{cell}}^0 < 0$ Therefore reaction is non spontaneous

GALVANIC CELLS

ZINC-COPPER GALVANIC CELL



<https://users.stlcc.edu/gkrishnan/electrochem.html>

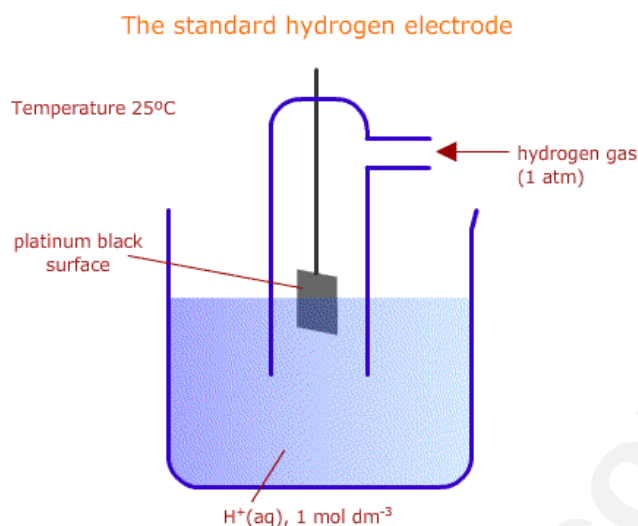
- Cell notation is written in the following way.
reducing agent | oxidised species || oxidising agent | reduced species

CELL NOTATION: $\text{Zn(s)} / \text{Zn}^{2+}(\text{aq}) (1\text{mol.dm}^{-3}) // \text{Cu}^{2+}(\text{aq}) (1\text{mol.dm}^{-3}, 25^{\circ}\text{C}) / \text{Cu(s)}$ at 25°C

The Standard Electrode Potentials

- Conditions under standard electrode is: $T = 25^{\circ} / 298 \text{ K}$, $\text{Conc.} = 1 \text{ mol.dm}^{-3}$.
- The standard electrode is the hydrogen electrode and the standard electrode potentials for all other substances can be determined using this as the reference electrode.
- For the purpose of measuring the standard electrode, the hydrogen standard half cell is regarded as the anode.
- A positive potential indicates that the substance is an oxidising agent.
- A negative potential indicates that the substance is a reducing agent.
- To calculate the potential of any cell, we use the following formula:

$$E^{\circ}_{\text{cell}} = E^{\circ}_{\text{cathode}} - E^{\circ}_{\text{anode}}$$
- If a cell/reaction has a positive potential, this indicates that the reaction is spontaneous under standard conditions.



Why is Platinum used?

- Platinum conducts electricity.
- Platinum is an inert metal.

Setting up a galvanic (Voltiac Cell)

1. Identify both reactions in the Standard Electrode Potentials tables.
2. The reaction with the higher potential proceeds in the forward direction and the reaction with the lower potential proceeds in the reverse direction.
3. Identify the oxidation half reaction and the reduction half reaction.
4. Balance the half reactions by multiplying each half reaction by suitable numbers (if required).
5. Add both reactions to get the overall balance reaction.
6. Anode(-) is where oxidation takes place and cathode(+) is where reduction takes place.
7. Anode decreases in mass and cathode increases in mass.
8. Write the Cell Notation.

Movement of ions and electrons

- Ions flow from via the salt bridge.
- Positive ions (Cations) flow from the anode to the cathode in the internal circuit.
- Negative ions (Anions) flow from the cathode to the anode in the internal circuit.
- Electrons flow through the voltmeter in the external circuit.
- Electrons flow from the anode to the cathode in the external circuit.

Functions of salt bridge

- Complete the circuit.
- Maintain electrical neutrality in the electrolytes.

The electrons move through the wire from the anode to the cathode, leaving the unbalanced positive charge in this vessel. In order to maintain neutrality, the negatively charged ions in the salt bridge will migrate into the anode half-cell. A similar (but reversed) situation is found in the cathode half-cell, where cations ions are being consumed, and therefore electrical neutrality is maintained by the migration of cations ions from the salt bridge into this half-cell.

Cell Notation

- Electrodes, including inert electrodes, are written on the outside of the cell notation
- A single vertical line (|) represents a phase boundary and is drawn between two chemical species that are in different phases but in contact with each other.
- The salt bridge is represented by two vertical lines (||). The identity of the salt bridge need not be shown in the cell notation.
- Cell notation is written using the following order convention:
reducing agent | oxidised species || oxidising agent | reduced species
- Examples:
 $\text{Zn} | \text{Zn}^{2+} || \text{Cu}^{2+} | \text{Cu}$
 $\text{Pt} | \text{Cl}^- | \text{Cl}_2 || \text{F}_2 | \text{F}^- | \text{Pt}$
- When both chemical species in a half-cell are in the same phase then they are separated by a comma
- State symbols need only be shown when requested
Example:
 $\text{Pt(s)} | \text{Sn}^{2+}(\text{aq}), \text{Sn}^{4+}(\text{aq}) || \text{Fe}^{3+}(\text{aq}), \text{Fe}^{2+}(\text{aq}) | \text{Pt(s)}$
- If requested, standard conditions are given in brackets after:
 - o Aqueous solutions of ions (aq, 1 mol.dm⁻³)
 - o Gases (g, 1 atm)
 - o Temperature (at 25 °C) is shown at the end of the cell notationExample:
 $\text{Zn(s)} | \text{Zn}^{2+}(\text{aq}, 1 \text{ mol.dm}^{-3}) || \text{Cu}^{2+}(\text{aq}, 1 \text{ mol.dm}^{-3}) | \text{Cu(s)} \text{ at } 25^\circ\text{C}$

Relation of Current and Potential to Rate and Equilibrium

1. When a galvanic cell reaches completion (IE. When the anode is totally oxidised) or when the reaction reaches equilibrium, no current flows and the voltmeter reads zero volts.
2. The reactions in galvanic cells are reversible.
3. All factors that favour the forward reaction will cause an increase in the voltage.
4. All factors that favour the reverse reaction will cause a decrease in the voltage.

Relation of Current and Potential to Electrodes

Increasing the surface area of the terminals increase the current, but the emf remains the same.

Relation of Current and Potential to Salt Bridge

The wider, shorter and more conductive salt bridge, lowers internal resistance thereby increasing the capacity of the cell to deliver current but does not affect the emf of the cell.

ELECTROLYTIC CELL

- An electrolytic cell is where electrode reactions that are sustained by a supply of electrical energy.
- Electrical energy is converted into chemical energy.

Skills

- Draw an annotated diagram of an electrolytic cell.
- Write equations for half-reactions taking place at the anode and cathode.
- Deduce the overall ionic cell reaction by combining two half reactions.
- Predict the half reaction and identify the electrode at which oxidation takes place (anode).
- Predict the half reaction and identify the electrode at which reduction takes place (cathode).
- Identify the oxidising agent and the reducing agent for an electrolytic reaction.

Application

- Electrolysis of Copper Chloride
- Electroplating of silver and copper
- Refining of Copper
- Chloro Alkali Industry – Production of chlorine, hydrogen and sodium hydroxide.
- Recovery of Aluminium

Participating species: Cu^{2+} , Cl^- , H_2O

For a concentrated solution of CuCl_2

Oxidation Half Reactions: $2\text{Cl}^-(\text{aq}) \rightarrow \text{Cl}_2(\text{g}) + 2\text{e}^-$

Reduction Half Reactions: $\text{Cu}^{2+}(\text{aq}) + 2\text{e}^- \rightarrow \text{Cu}(\text{s})$

NETT OVERALL REACTION: $2\text{Cl}^-(\text{aq}) + \text{Cu}^{2+}(\text{aq}) \rightarrow \text{Cl}_2(\text{g}) + \text{Cu}(\text{s})$

For a dilute solution of CuCl_2

Possibility of H_2O or Cl^- being oxidized as they will be attracted to the positive terminal (anode).

H_2O is a stronger reducing agent than Cl^- , therefore the H_2O will be oxidized to O_2 gas

Possibility of H_2O or Cu^{2+} being reduced as they will be attracted to the negative terminal (cathode)

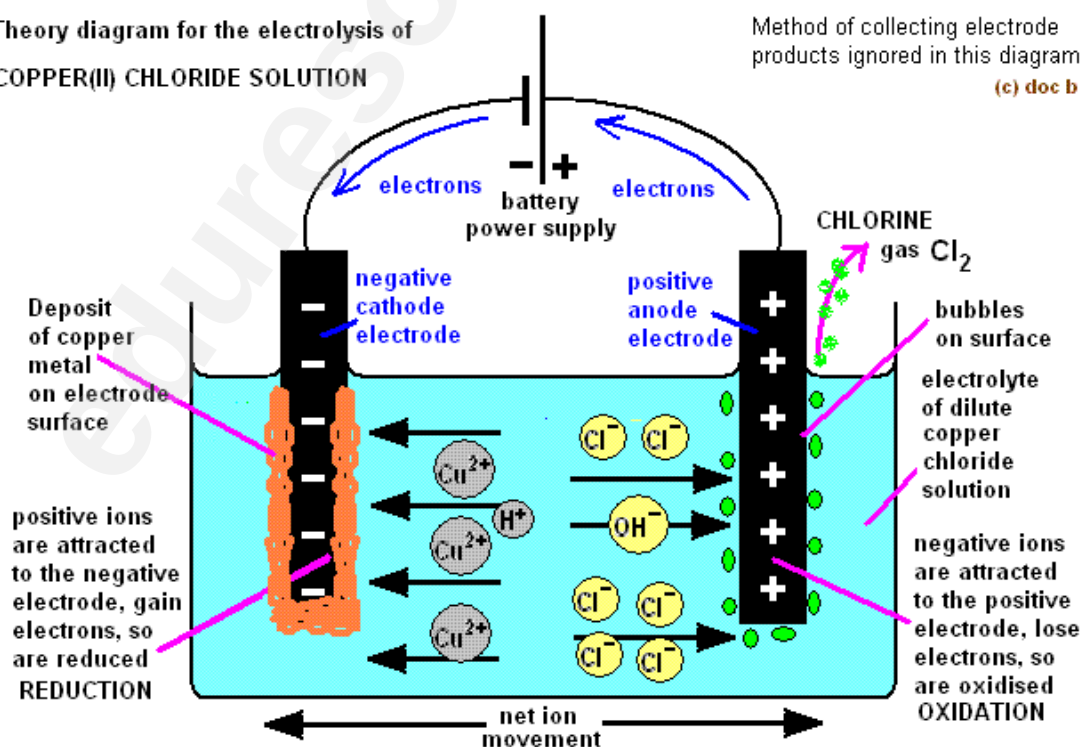
Cu^{2+} is a stronger oxidising agent than H_2O , therefore the Cu^{2+} will be reduced.

Oxidation Half Reactions: $4\text{OH}^-(\text{aq}) \rightarrow 2\text{H}_2\text{O}(\text{g}) + \text{O}_2 + 2\text{e}^-$

Reduction Half Reactions: $\text{Cu}^{2+}(\text{aq}) + 2\text{e}^- \rightarrow \text{Cu}(\text{s})$

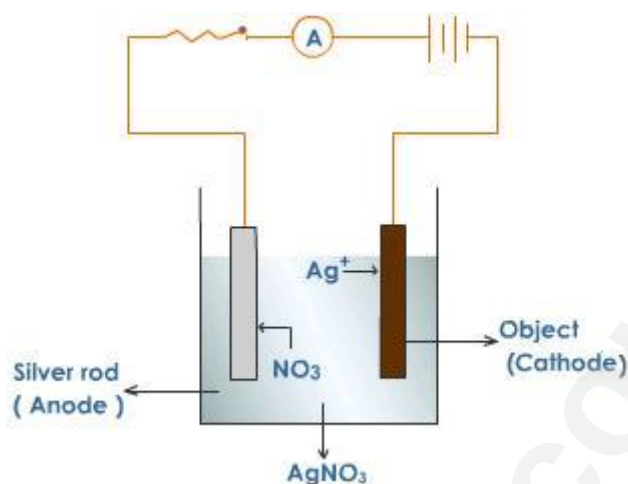
NETT OVERALL REACTION: $4\text{OH}^-(\text{aq}) + \text{Cu}^{2+}(\text{aq}) \rightarrow 2\text{H}_2\text{O}(\text{g}) + \text{O}_2 + \text{Cu}(\text{s})$

Theory diagram for the electrolysis of
COPPER(II) CHLORIDE SOLUTION



ELECTROPLATING OF SILVER AND COPPER

Participating species: Ag^+ , Ag , NO_3^- , H_2O

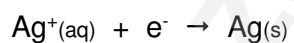


<http://images.tutorvista.com/content/electricity/electroplating-of-silver.jpeg>

Oxidation Half Reactions:



Reduction Half Reactions:



NETT OVERALL REACTION:



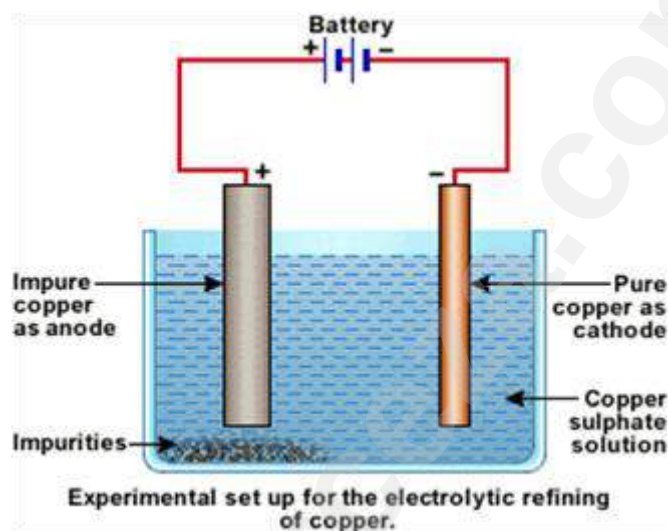
REFINING OF COPPER

Participating species: Cu^{2+} , Cu

Impurities: lead, zinc, nickel, arsenic, selenium, tellurium, and several precious metals including gold and silver.

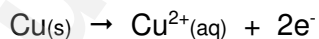
Impurities below copper are not oxidized and sink to the bottom.

Impurities above copper will be oxidized and discarded as sludge.

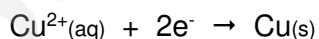


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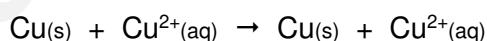
Oxidation Half Reactions:



Reduction Half Reactions:



NETT OVERALL REACTION:



CHLORO ALKALI INDUSTRY

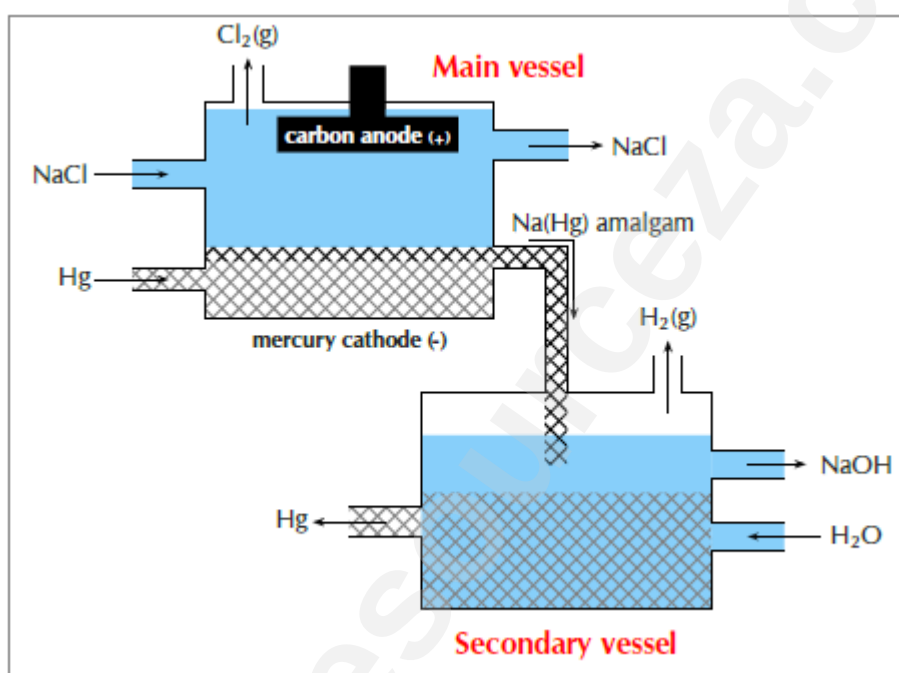
The Chloro-Alkali industry revolves around the electrolysis of brine, a concentrated solution of sodium chloride (NaCl) to produce chlorine. This is an electrolytic cell in which electrical energy is converted to chemical energy.

Participating Species: Na^+ , Cl^- , H_2O

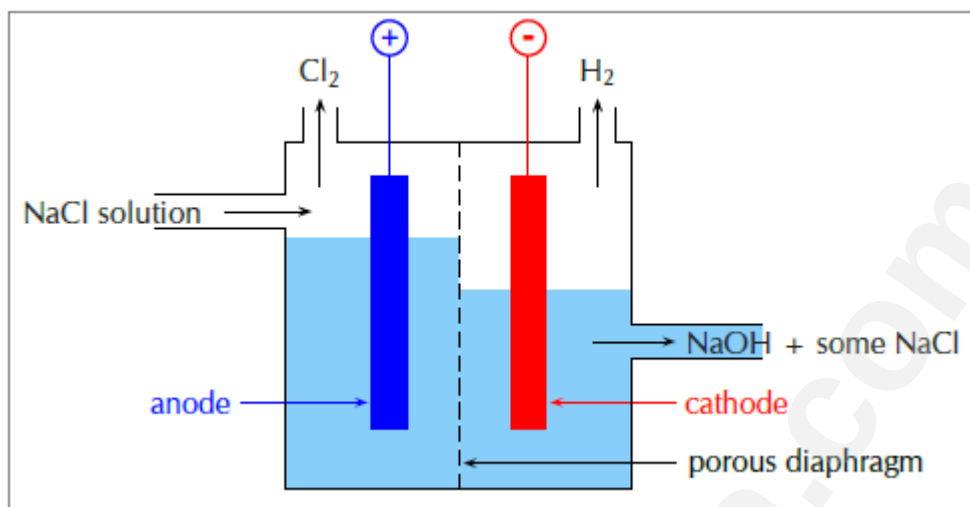
Possibility of Na^+ and H_2O being reduced as they will be attracted to the negative terminal (cathode). Na^+ is a stronger reducing agent than water therefore the water is reduced to H_2 gas.

Possibility of Cl^- and H_2O being oxidized as they will be attracted to the positive terminal (anode). H_2O is a stronger reducing agent therefore water will preferably be oxidized. However, since the solution is concentrated with Cl^- ions, the chloride ions will be oxidized.

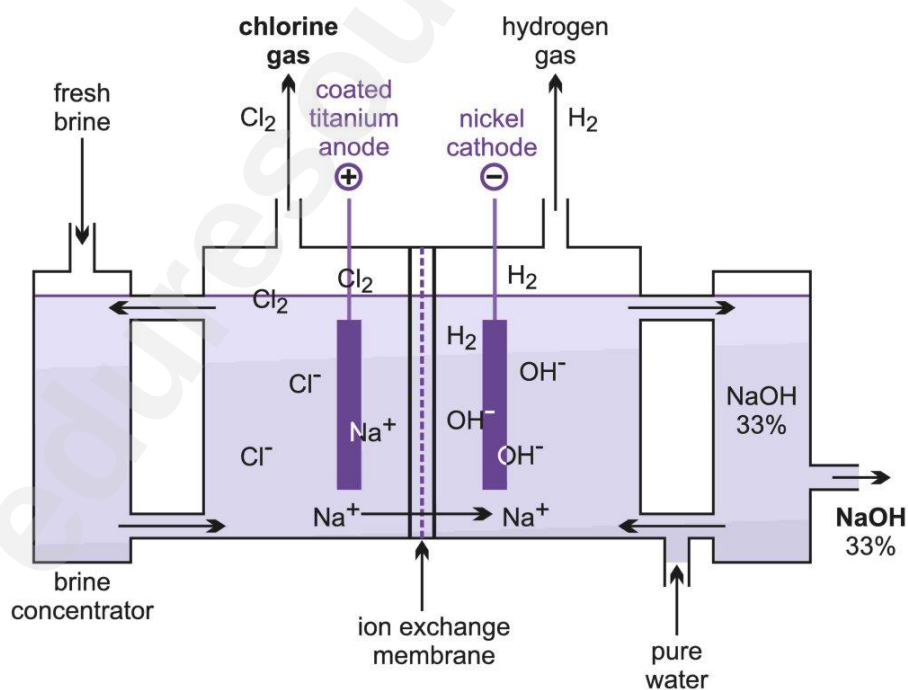
The Mercury Cell



The Diaphragm Cell

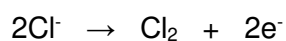


The Membrane Cell

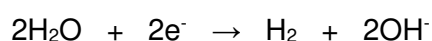


[http://www.essentialchemicalindustry.org/images/stories/250_chlorine/25-Chlorine_05_\(3\).jpg](http://www.essentialchemicalindustry.org/images/stories/250_chlorine/25-Chlorine_05_(3).jpg)

Oxidation Half Reaction:

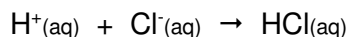


Reduction Half Reaction:



NETT OVERALL REACTION:



Possible Competitive Reactions that may occur**Product Uses**

Hydrogen (H ₂)	Chlorine (Cl ₂)	Sodium Hydroxide (NaOH)
Making ammonia for use in fertilizers	Used in insecticides and disinfectants	Used in the manufacture of aluminium
Hardening of vegetable oils for margarine	Kills bacteria in the purification of water	Making of soaps and detergents
Making hydrogen peroxide		

The three types of cells used

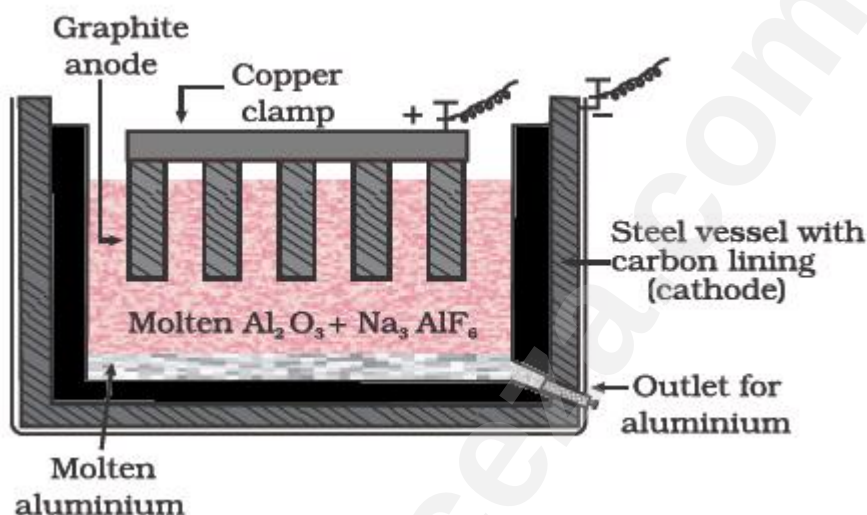
	Membrane Cell	Mercury Cell	Diaphragm Cell
Anode	Titanium	Graphite	Titanium
Cathode	Nickel	Mercury	Steel
Advantages	There are no environmental risks. Lowest energy consumption Cheapest		
Disadvantages		Highly volatile. Mercury contamination occurs. Mercury is highly poisonous The cost of building & running is high. Mercury losses are expensive	Process is discontinued because asbestos is used in the cell. Asbestos has a negative impact on the environment and for humans.
Special features	The membrane cell contains a cation-permeable membrane that allows sodium ions to pass through but not the chloride ions		

RECOVERY OF ALUMINIUM FROM BAUXITE

Hall-Heroult Process

- Bauxite is about 60% aluminium(III)oxide (Al_2O_3) with the remainder being iron oxide and silicon oxide.
- Aluminium is extracted from bauxite using an electrolytic cell

Participating Species: Al^{3+} , O^{2-} , C



http://www.askiitians.com/onlinetest/ForumsImages/246-1369_Capture.PNG

Oxidation Half Reaction: $2\text{O}^{2-} \rightarrow \text{O}_2 + 2\text{e}^-$

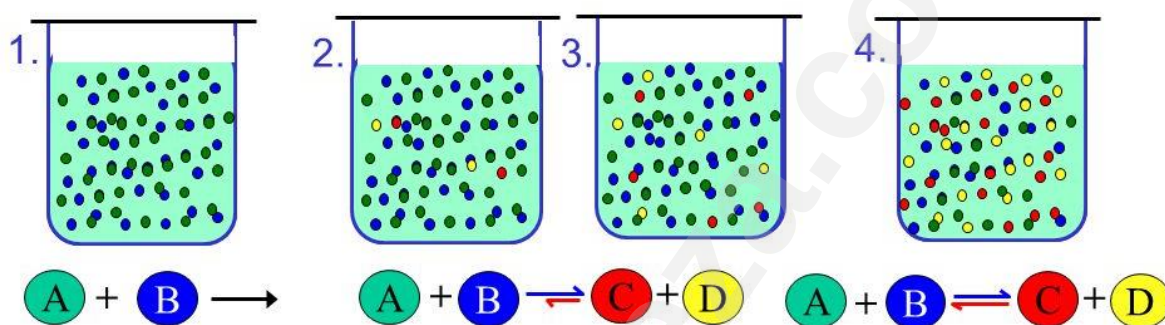
Reduction Half Reaction: $\text{Al}^{3+} + 3\text{e}^- \rightarrow \text{Al}$

NETT OVERALL REACTION: $6\text{O}^{2-} + 2\text{Al}^{3+} \rightarrow 2\text{Al} + 3\text{O}_2$

- Aluminium is melted along with cryolite (Na_3AlF_6) which acts as the electrolyte.
- Cryolite helps to lower the melting point and dissolve the ore.
- Cryolite gives off green house gases which is harmful to the environment.
- The carbon rod anode provides a site for the oxidation of O^{2-} and F^- ions.
- $\text{C} + \text{O}_2 \rightarrow \text{CO}_2$
- Oxygen and fluorine gas are given off at the anode and also result in anode consumption.
- The anode eventually corrodes due to the oxygen reacting with carbon to produce carbon dioxide.

STUDY GUIDE

CHEMICAL EQUILIBRIUM



- Yield is a measure of the extent of a reaction, generally measured by comparing the amount of product against the amount of product that is possible.
- A closed system (in chemistry) is one in which mass is conserved inside the system but energy can enter or leave the system freely.
- An open system (in chemistry) is one in which both energy and matter can be exchanged between the system and its surroundings.

LAWS & PRINCIPLES

- Le Chatelier's principle: 'When an external stress (change in pressure, temperature or concentration) is applied to a system in chemical equilibrium, the equilibrium point will change in such a way as to counteract the stress'

CONCEPTS

- Reversible reaction: A chemical system is reversible if the products of the reaction can change back into the reactants.
- Dynamic equilibrium – Rate of the forward reaction equals to the rate of the reverse reaction. The equilibrium is dynamic because the forward and the reverse reaction is taking place at the same time.

KNOWLEDGE & SKILLS

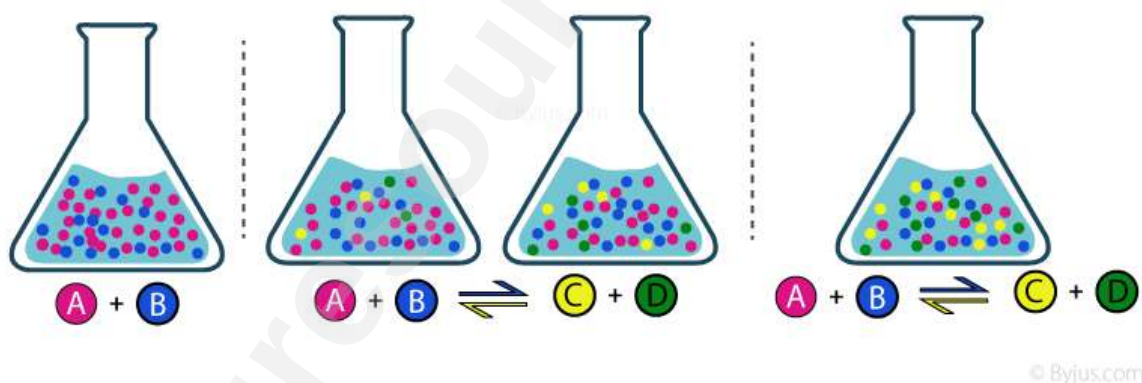
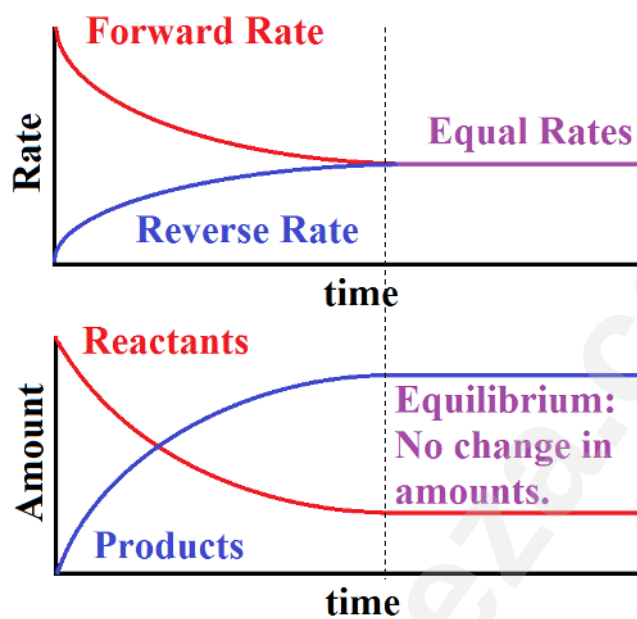
- Explain what is meant by: Open and closed systems, A reversible reaction and Dynamic equilibrium.
- List the external factors which shift the position of a particular reaction viz: temperature, pressure and concentration.
- State Le Chatelier's principle.
- Use Le Chatelier's principle to predict the effects of changes of pressure, temperature, and concentration (common ion effect) on the concentrations and amounts of each substance in an equilibrium mixture.
- Use collision theory to explain the changes predicted by Le Chatelier's principle
- State that the addition of a catalyst to a system in equilibrium will speed up both the forward and reverse reactions equally and hence have no effect on the position of equilibrium.
- Interpret rate graphs
- Interpret amount vs time graphs for chemical reactions in a closed system
- Define yield.
- When given chemical equations, diagrams or flow charts, apply rate and equilibrium principles to describe how yields are affected in the following industrial processes:
 - NH_3 – Haber process
 - HNO_3 – Ostwald process
 - H_2SO_4 – including the Contact process
- Write down an expression for the equilibrium constant having been given the equation for the reaction
- State that temperature is the only factor which influences the value of the equilibrium constant.
- Predict and explain how temperature influences the K_c value for a particular equilibrium reaction
- Calculate K_c given equilibrium concentrations or moles and volumes of all relevant species, initial concentrations (or moles) of all species and the equilibrium concentration (or moles) of one species.
- Calculate the equilibrium concentration of one of the reactants or one of the products given the value of K_c and other relevant information
- Explain the significance of high and low values of the equilibrium constant

CHEMICAL EQUILIBRIUM

Given a reversible reaction: $aA + bB \rightleftharpoons cC + dD$

Forward Reaction: $aA + bB \rightarrow cC + dD$

Reverse Reaction: $cC + dD \rightarrow aA + bB$



Changing Concentration

- Changing concentration can be done by adding or removing reactants or products.

Reaction Details	Change	Explanation
Reactants	Increase	Stress: Increase in the concentration of reactants. Response: The rate of the forward reaction increases. Reason: Forward reaction decreases the concentration of the reactants which relieves the stress. Effect: Depends on question. (Could be yield or colour change).
	Decrease	Stress: Decrease in the concentration of reactants. Response: The rate of the reverse reaction increases Reason: The reverse reaction increases the concentration of the reactants which relieves the stress. Effect: Depends on question. (Could be yield or colour change)
Products	Increase	Stress: Increase in the concentration of products. Response: The rate of the reverse reaction increases. Reason: Reverse reaction decreases the concentration of the products which relieves the stress. Effect: Depends on question. (Could be yield or colour change).
	Decrease	Stress: Decrease in the concentration of products. Response: The rate of the forward reaction increases. Reason: Forward reaction increases the concentration of the products which relieves the stress. Effect: Depends on question. (Could be yield or colour change).

Changing Temperature

- The forward reaction is exothermic when $\Delta H < 0$, ΔH is negative. Then the reverse reaction is endothermic
- The forward reaction is endothermic when $\Delta H > 0$, ΔH is positive. Then the reverse reaction is exothermic

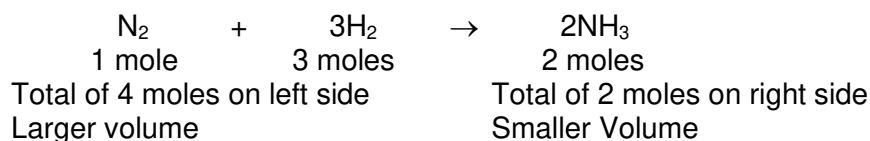
Reaction Details	Change	Explanation
Forward reaction is exothermic, reverse reaction is endothermic	Increase	Stress: Increase in temperature. Response: The rate of the reverse reaction increases. Reason: Reverse reaction absorbs the heat which relieves the stress. Effect: Depends on question. (Could be yield or colour change).
	Decrease	Stress: Decrease in temperature. Response: The rate of the forward reaction increases Reason: The forward reaction produces heat which relieves the stress. Effect: Depends on question. (Could be yield or colour change)
Forward reaction is endothermic, reverse reaction is exothermic	Increase	Stress: Increase in temperature. Response: The rate of the forward reaction increases. Reason: Forward reaction absorbs heat which relieves the stress. Effect: Depends on question. (Could be yield or colour change).
	Decrease	Stress: Decrease in temperature. Response: The rate of the reverse reaction increases. Reason: Reverse reaction produces heat which relieves the stress. Effect: Depends on question. (Could be yield or colour change).

Changing Pressure

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- Increase pressure causes a decrease in volume according to Boyle's Law, and VICE VERSA.
- Volume is related to the number of moles on each side of the reaction.

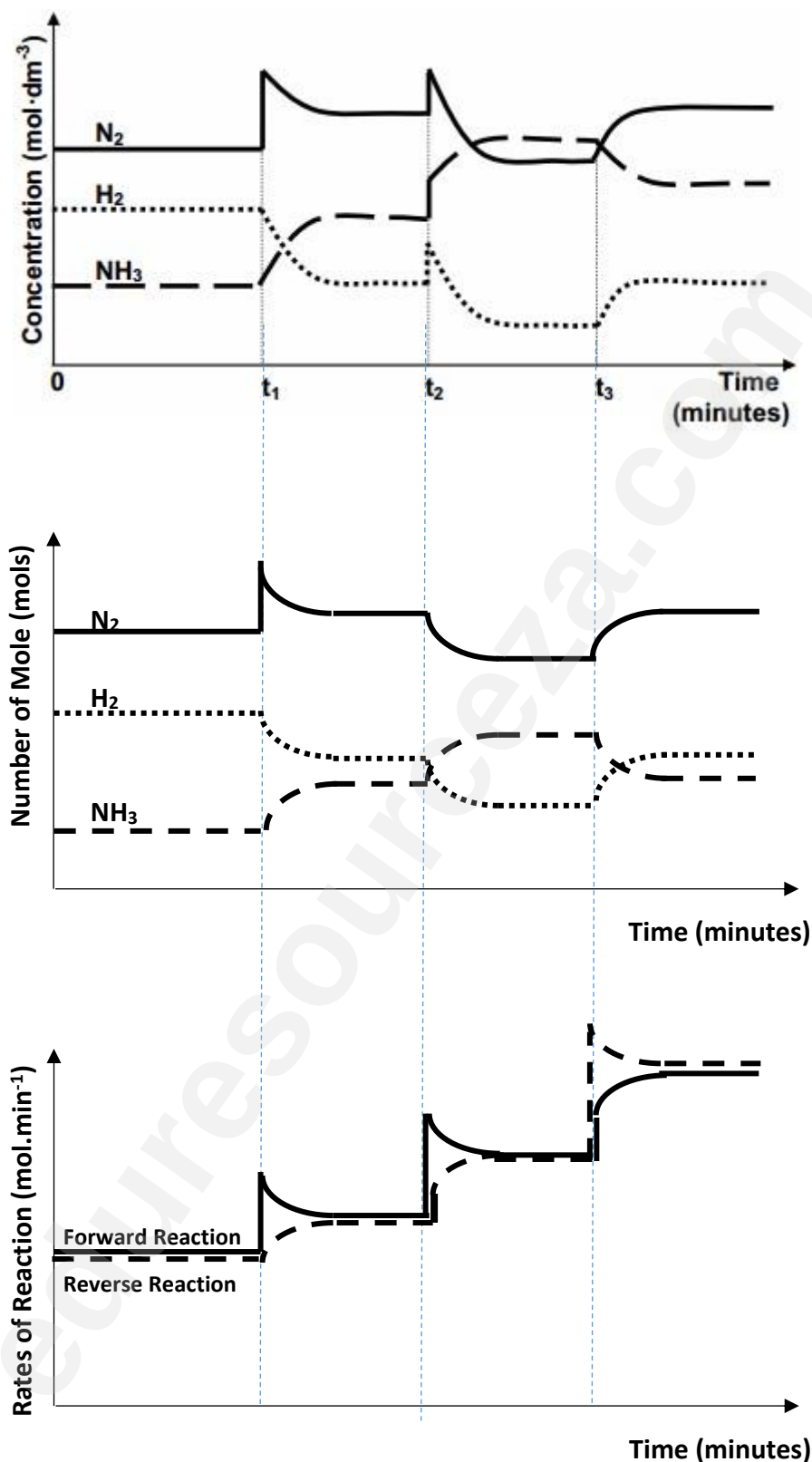
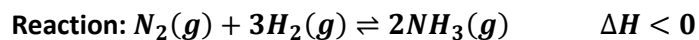
Example



Reaction Details	Change	Explanation
Left side has greater number of moles	Increase	Stress: Increase in pressure. Response: The rate of the forward reaction increases. Reason: Forward reaction produces less number of moles which relieves the stress. Effect: Depends on question. (Could be yield or colour change).
	Decrease	Stress: Decrease in pressure. Response: The rate of the reverse reaction increases Reason: The reverse reaction produces more number of moles which relieves the stress. Effect: Depends on question. (Could be yield or colour change)
Right side has greater number of moles	Increase	Stress: Increase in pressure. Response: The rate of the reverse reaction increases. Reason: Reverse reaction produces less number of moles which relieves the stress. Effect: Depends on question. (Could be yield or colour change).
	Decrease	Stress: Decrease in pressure. Response: The rate of the forward reaction increases. Reason: Forward reaction produces more number of moles which relieves the stress. Effect: Depends on question. (Could be yield or colour change).
Left & Right side has same number of moles	Increase and Decrease	No Effect on equilibrium

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GRAPHICAL REPRESENTATION OF STRESSES



<http://www.smartlearner.mobi/science/VideoPastPapers/Equilibrium/Equilibrium.htm>

0 – t₁

- System is in equilibrium.
- Concentration of reactants and products are constant.

At t₁ Reactant has been added

- N₂ has been added (Seen by the spike)
- Rate of forward reaction would increase,
- Forward reaction decreases the concentration of N₂.
- H₂ decreases in concentration while NH₃ increases in concentration.

0 – t₂

- New equilibrium has been established.

At t₂ Change in pressure

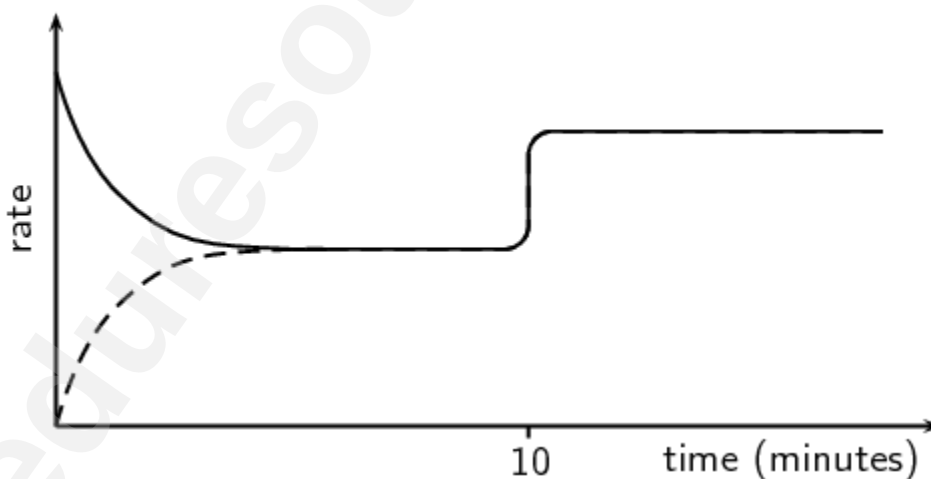
- Pressure is increased.
- Concentration of both reactants and products has increased due to a decrease in volume.
- However, the concentration of NH₃ continue to increase while N₂ and H₂ decreases.
- This indicates that the rate of the forward reaction has increased.
- Right side having a smaller number of moles.

t₂ – t₃

- New equilibrium has been established.

At t₃ Change in temperature

- Temperature is increased.
- The rate of both the forward and reverse reactions increase, however the reverse reaction increases more indicating that the reverse reaction was favoured.
- The reverse reaction consumes the excess heat thereby relieving the stress.
- Concentration of the reactants increases while the concentration of the products decreases

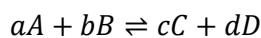
EFFECT OF CATALYST

Calculating K_c values

- The equilibrium constant (K_c) is the ratio between the concentration of products and reactants in a chemical reaction.

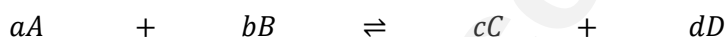
$$K_c = \frac{[\text{Products}]}{[\text{Reactants}]}$$

- Determine the K_c value as follows:



$$K_c = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$

- Only gases and aqueous phases appear in the K_c value. Solids and liquids do not appear in the K_c value.
- When solving problems relating to K_c, use the following table:



Ratio	a	b	c	d
Initially				
Change				
Equilibrium				
Concentration				

- The mole ratio is applied to row 3.

The meaning of K_c values

- The formula for K_c has the concentration of the products in the numerator and the concentration of reactants in the denominator.
- The formula for K_c has a K_c value greater than 1 means that the equilibrium lies to the right there are more products than reactants.
- The formula for K_c has a K_c value between 0 and 1 means that the equilibrium lies to the left more reactants than products.
- When the concentration of the reactants is much larger than the concentration of the products K_c will be small (normally less than one).
- When the concentration of the reactants is much less than that of the products K_c will be large (normally greater than one).

A high K _c value	A low K _c value
the concentration of products is high	the concentration of reactants is high
the equilibrium lies far to the right	the equilibrium lies far to the left
the reaction has a high yield	the reaction has a low yield

Factors that influence the value of K_c (ESCNT)

Concentration, pressure, and temperature all affect the equilibrium position of a reaction, and a catalyst affects reaction rates. However, only temperature affects the value of K_c .

Changing concentration:

- Changing the concentration of a reactant or product results in one of the reactions (forward or reverse) being favoured.
- This change in reaction rate minimises the effect of the change and restores the concentration ratio between reactants and products. There will just be more reactants and products.
- K_c will remain the same.

Changing pressure:

- Changing the pressure of the system will change the ratio between the reactant and product concentrations.
- The equilibrium then shifts to minimise the effect of the change and restores the ratio between reactant and product concentrations.
- K_c will remain the same.

Adding a catalyst to the system:

- Both the forward and reverse reactions rates are increased.
- Therefore the ratio between reactant and product concentrations will remain the same.
- K_c will remain the same.

Changing temperature:

- Changing the temperature will favour either the endothermic or exothermic reaction.
- The ratio between the concentration of the reactants and products will change.
- K_c will change.

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Energy Changes & Rates of Reactions

Definitions

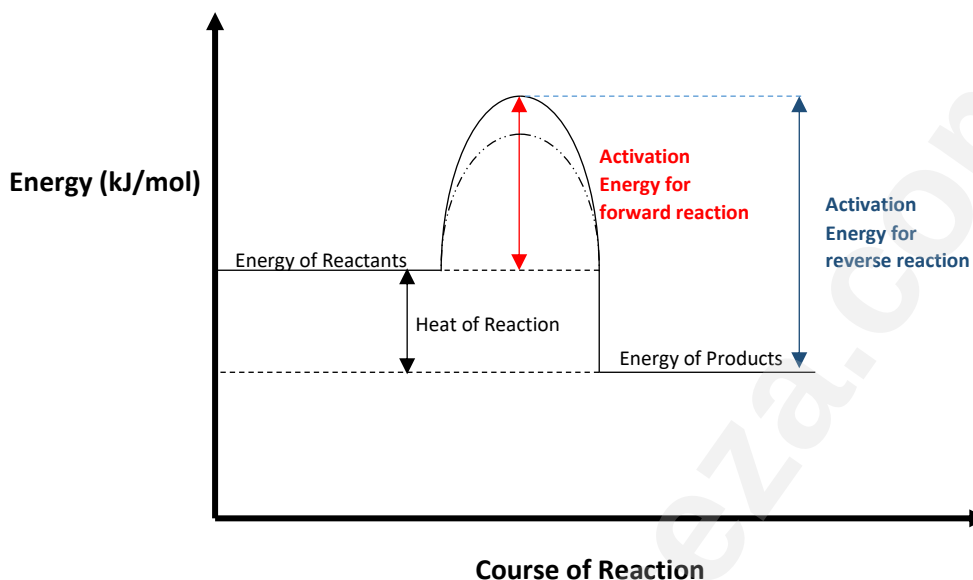
- Heat of reaction (ΔH) is the net change of chemical potential energy of the system.
- Exothermic reactions are reactions which transform chemical potential energy into thermal energy.
- Endothermic reactions are reactions which transform thermal energy into chemical potential energy.
- Activation energy is the minimum energy required to start a chemical reaction OR the energy required to form the activated complex.
- The activated complex is a high energy, unstable, temporary transition state between the reactants and the products.
- Reaction rate is the change in concentration per unit time of either a reactant or product.
- Catalyst is a substance that increases the rate of the reaction but remains unchanged at the end of the reaction

Skills

- Identify that bond breaking is endothermic and that bond formation is exothermic. (No calculations will be required).
- Identify that a stronger bond requires more energy to break and releases more energy when formed.
- Predict that $\Delta H > 0$ for endothermic reactions.
- Predict that $\Delta H < 0$ for exothermic reactions.
- Know that exothermic reactions release heat and thus increase the temperature of the reaction mixture.
- Know that endothermic reactions absorb heat and thus decrease the temperature of the reaction mixture.
- Draw and interpret potential energy profile graphs of catalysed and uncatalysed endothermic reactions and exothermic reactions (with reactants, products, activation energy, activated complex and ΔH labelled).
- Calculate average reaction rate, with appropriate units, in terms of change in mass, volume, or number of moles per unit time
- Distinguish between average and instantaneous reaction rates
- List the factors that affect the rate of chemical reactions.
- Explain that the collision theory is a model that explains that a reaction will only proceed when reactant particles collide effectively.
- Explain in terms of the collision theory that reaction rate is directly proportional to the number of effective collisions per unit time.
- Explain in terms of the collision theory how the various factors affect the rate of chemical reactions.
- Suggest and explain suitable experimental techniques for measuring the rate of a given reaction.
- Answer questions and interpret data (tables or graphs) on different experimental techniques for measuring the rate of a given reaction.
- Apply collision theory to explain the changes in the distribution of molecular energies (number of particles against their kinetic energy, i.e. Maxwell-Boltzmann distribution) due to changes in temperature, concentration of reactants and the presence of a catalyst.
- Use any other suitable graph (including e.g. energy profile graph, rate vs time or amount vs time) to show how changing concentration, pressure, surface area, or adding a catalyst affects the rate of reaction

- An effective (or successful) collision is one in which the colliding reactant particles have:
 - the correct orientation
 - sufficient energy, i.e. kinetic energy equal to or greater than the activation energy.

Energy Profile Curve for Exothermic Reaction

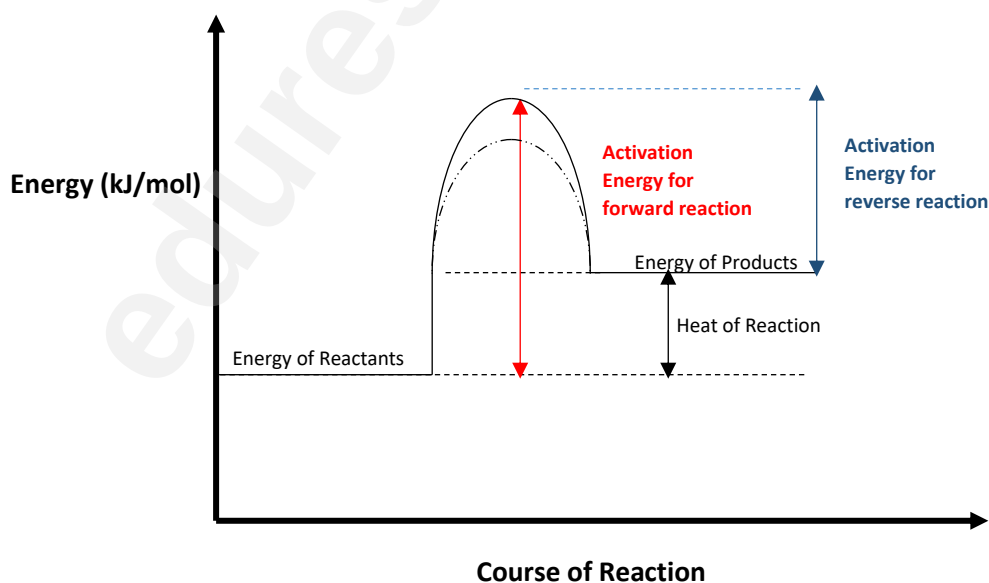


$$\Delta H = E_{\text{products}} - E_{\text{reactants}} < 0 \text{ for forward reaction}$$

$$\Delta H > 0 \text{ for reverse reaction, endothermic reaction}$$

----- Alternate path with catalyst

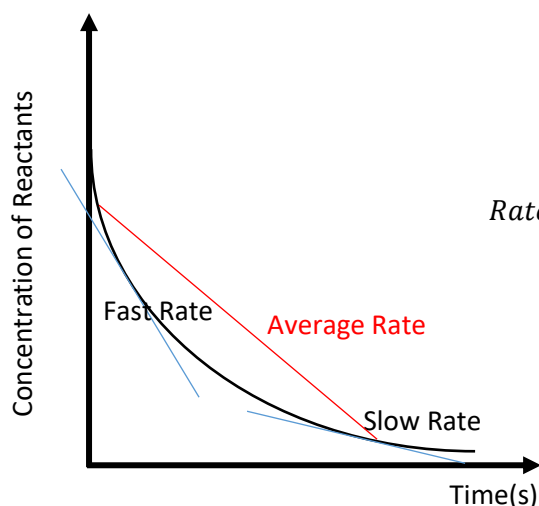
Energy Profile Curve for Endothermic Reaction



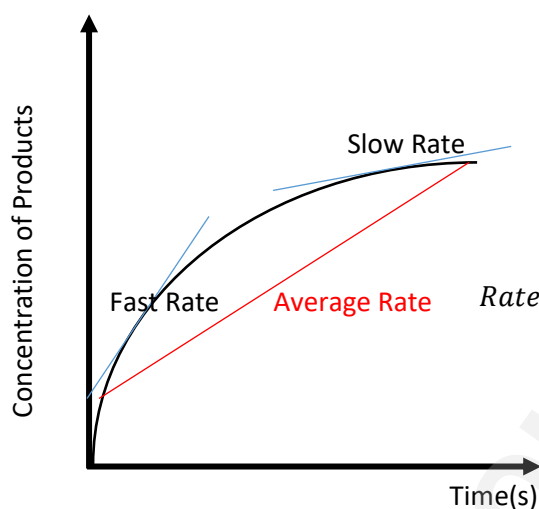
$$\Delta H = E_{\text{products}} - E_{\text{reactants}} > 0 \text{ for forward reaction}$$

$$\Delta H < 0 \text{ for reverse reaction, exothermic reaction}$$

----- Alternate path with catalyst



$$\text{Rate of Reaction} = \frac{\Delta \text{Concentration of Reactants}}{\Delta t}$$



$$\text{Rate of Reaction} = \frac{\Delta \text{Concentration of Products}}{\Delta t}$$

- The concentration of reactants/products can either be mass, volume or number of moles.
- The relevant units for rate of reaction will vary depending on how the quantity of the reactant/product is measured.
- When we measure the change in concentration of reactants/products over a long time interval this will give us the average reaction rate. (Red Line)
- When we measure the change in concentration of reactants/products over a short time interval this will give us the instantaneous reaction rate. (Blue Line)

Collision Theory

Reactant particles must collide effectively for the reactants to change into products.

To collide effectively the colliding reactant particles must:

1. Have the correct orientation: To break the existing bonds (in the reactants) and form new bonds (in the products).
2. Have sufficient energy: Kinetic energy equal to or greater than the activation energy.

More effective collisions will result in a higher rate of reaction.

Factor that affect the rate of a reaction

1. Nature of Reactants

- Bonds between reactants are broken.
- More particles have the correct orientation.
- Increase in the number of effective collisions per unit time.
- Higher reaction rate.

2. Surface area of solid

- A higher surface area means that there is a greater number of surface particles exposed to collisions.
- Increase in the number of collisions (between reactant particles) per unit time.
- Increase in the number of effective collisions per unit time.
- Higher reaction rate.

3. Concentration of solutions (aqueous)

- Increase in concentration, greater number of particles per unit volume.
- Increase in the number of collisions (between reactant particles) per unit time.
- Increase in the number of effective collisions per unit time.
- Higher reaction rate.

4. Pressure of a gas

- Increase in pressure, decreases volume, greater number of particles per unit volume.
- Increase in the number of collisions (between reactant particles) per unit time.
- Increase in the number of effective collisions per unit time.
- Higher reaction rate.

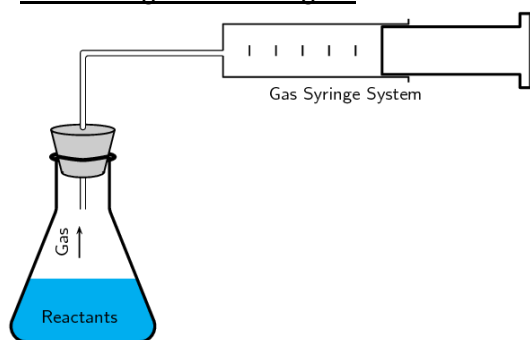
5. Temperature

- A higher temperature means that the particles have a greater average kinetic energy.
- Minor effect: there is an increase in the number of collisions per unit time.
Major effect: there is a greater proportion of particles with sufficient kinetic energy to overcome the activation energy.
- Increase in the number of effective collisions per unit time.
- Higher reaction rate.

6. Catalyst

- A catalyst offers a reaction pathway of lower activation energy.
- There is thus a greater proportion of particles with sufficient kinetic energy to overcome the activation energy.
- Increase in the number of effective collisions per unit time.
- Higher reaction rate.

1. Measuring volume of gas.

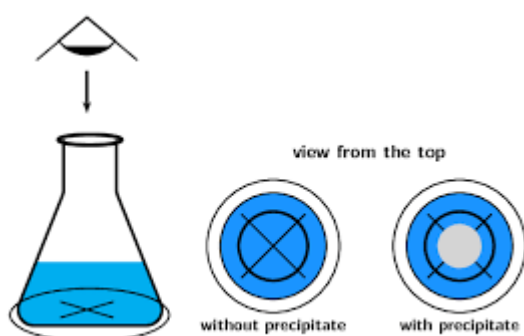


When a reaction produces a gas like CO_2 , the gas can be collected in a syringe using a delivery tube.

The volume of the gas is measured

The rate of the reaction can be calculated by taking the volume of gas formed divided by the time.

2. Measuring turbidity (Precipitation formation)

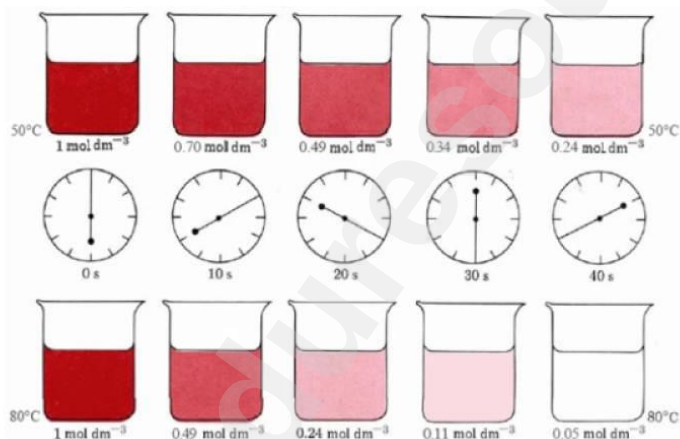


When a precipitate like sulphur is formed in the solution the turbidity can be used as a measure of products formed.

The time taken for the cross to disappear is recorded.

Since the amount of products formed in each case is constant, $1/\text{time}$ can be used as a measure of the rate of reaction.

3. Change of colour

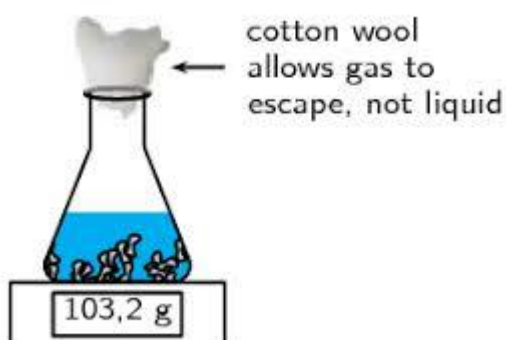


Using a spectrophotometer which measures the amount of light of a specific wavelength that is absorbed by the mixture.

Product formed can be quantified using the degree of colour.

The rate of reaction can be calculated by taking the degree of colour over time.

4. Change of mass

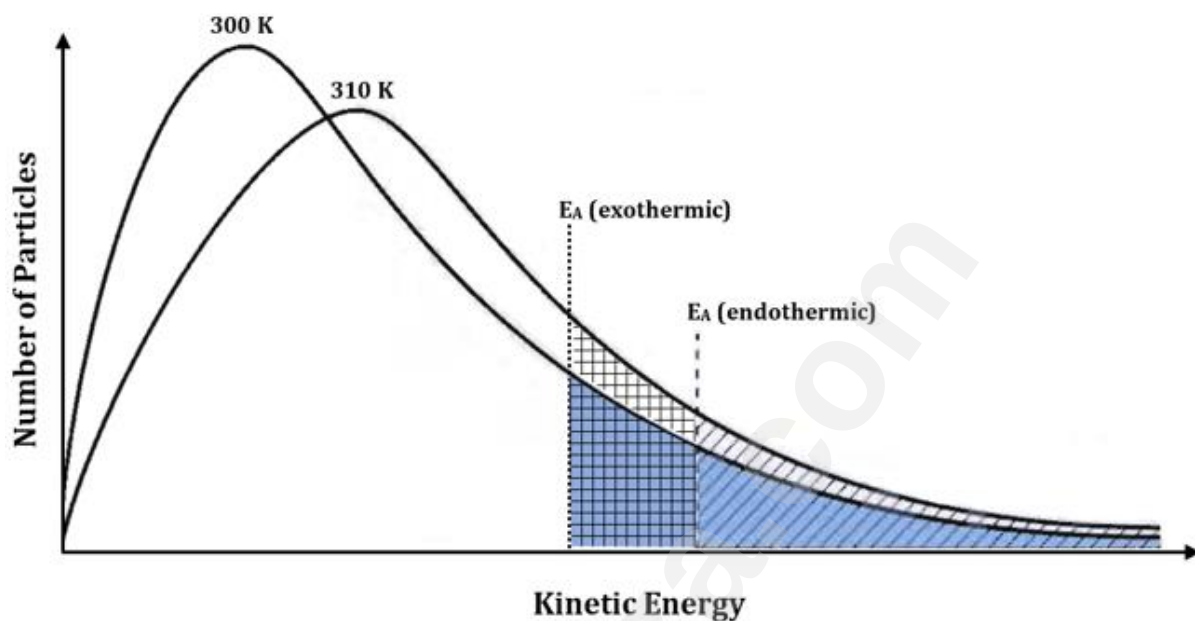


When one of the products is a gas like CO_2 , the mass of the contents decreases.

The decrease in mass is the amount of products formed.

The rate of reaction can be calculated by taking the loss in mass over time.

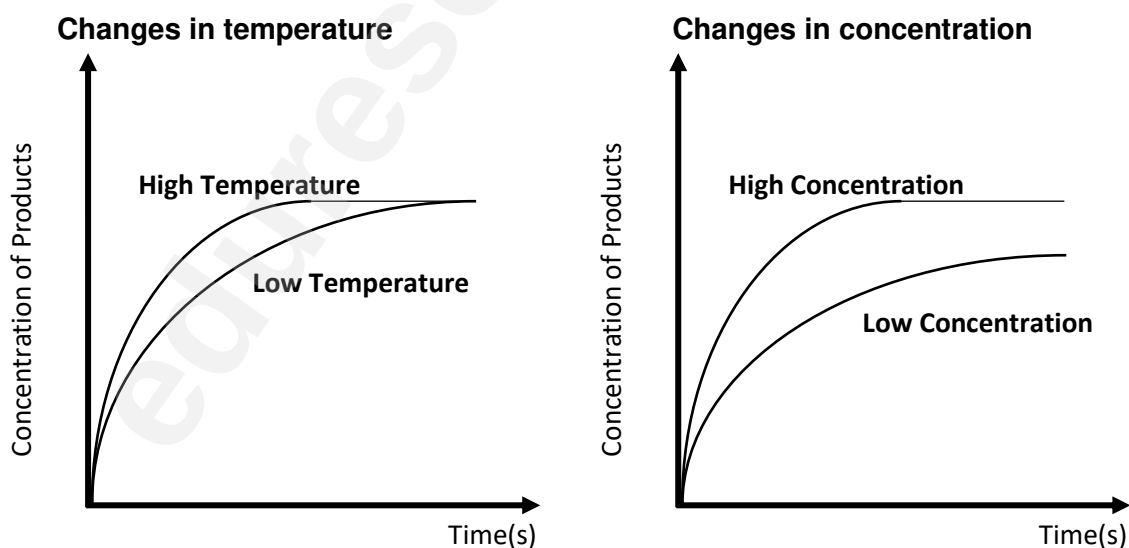
1. Maxwell-Boltzmann Distribution Curve



The higher the activation energy, the greater the percentage increase in the proportion of particles with $E_K > E_A$ (shaded area):

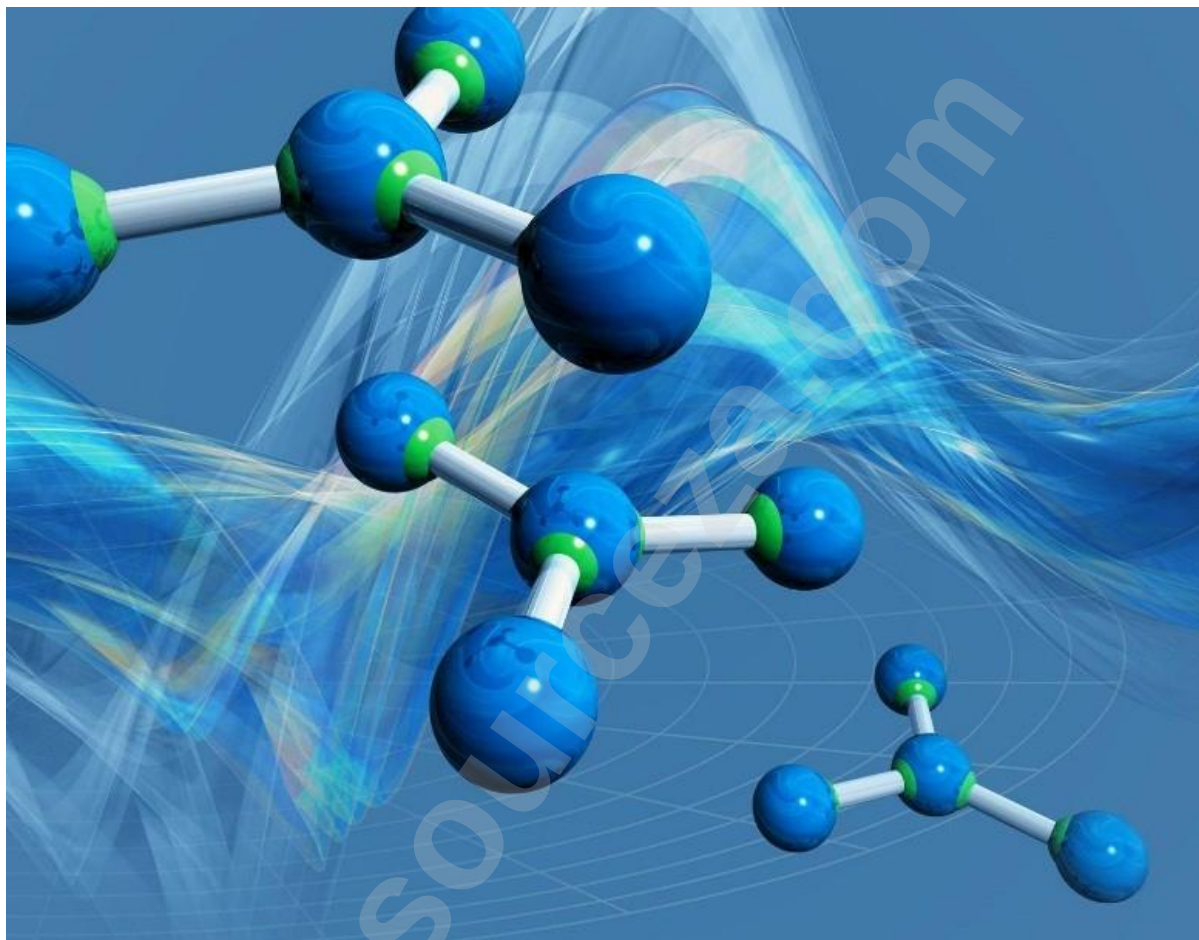
- Increase in temperature, peak moves right.
- Decrease in temperature, peak moves left.
- Increase in concentration, peak moves up.
- Decrease in concentration, peak moves down.
-

2. Graphical effect of factors affecting reaction rate.



NOTES

CHEMICAL BONDING



- An intramolecular bond occurs between atoms within molecules.
- Electronegativity is a measure of the tendency of an atom to attract a bonding pair of electrons
- A covalent bond is a sharing of at least one pair of electrons by two atoms that are non-metals
 - Non - polar covalent (pure covalent) is an equal sharing of electrons
 - Polar covalent is unequal sharing of electrons leading to a dipole forming (as a result of electronegativity difference)
- An ionic bond is a transfer of electrons and subsequent electrostatic attraction. It is between a metals and non-metals.
- Metallic bonding is between a positive kernel and a sea of delocalised electrons.
- Intermolecular force is a weak force of attraction between molecules or between atoms of noble gases.

KNOWLEDGE & SKILLS

- Use electronegativity numbers to determine the specific type of covalent bond and know that
 - a zero difference in electronegativity indicates a non-polar(pure) covalent bond
 - a non-zero difference in electronegativity indicates a polar covalent bond
 - the greater the difference in electronegativity the more polar the bond
- Identify that in a liquid or a solid there must be forces between the molecules causing them to be attracted to one another, otherwise, the molecules would move apart and become a gas.
- Distinguish between intermolecular forces and intramolecular bonds
- State that van der Waals forces are intermolecular forces
- Name and explain the origin of the following different types of van der Waals forces:
 - Dipole-dipole forces/interactions
 - London forces (induced dipole or dispersion forces)
 - Hydrogen bonding as a special case of dipole-dipole forces
- Know that hydrogen bonds exist between polar molecules in which hydrogen is bonded to:
 - a small atom
 - of high electronegativity
 - with at least one lone pair of electrons
- Know that all interactions between particles involve some sort of London forces.
- Explain how the strength of London forces is influenced by the size of the temporary dipoles, which is influenced by:
 - The number of electrons
 - The interacting surface of the molecule (e.g. long unbranched chain vs branched chain – see organic chemistry section)
- Identify the predominant (strongest) intermolecular force in a substance
- Explain that in giant structures such as diamond, graphite and silicon dioxide melting and boiling points are high due to the large amount of energy needed to break the many strong covalent bonds
- Explain that in giant ionic solids (e.g. sodium chloride), the melting points and boiling points are determined by electrostatic forces of attraction (ionic bonds) between the cations and the anions in the lattice structure

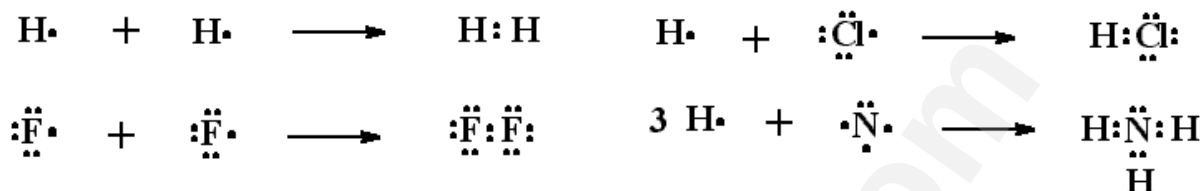
- Downloaded from eduresourceza.com
- Identify that for simple molecular substances the melting and boiling points are affected by the strength and the relative number (for hydrogen bonds) of the intermolecular forces
 - Explain that when comparing the melting and boiling points of substances in the same group on the Periodic Table (e.g. halogens, hydrides of elements in groups 15, 16 and 17) or the same homologous series (see organic chemistry section), the difference in melting points and boiling points is mainly due to the London forces, the exception being those that experience hydrogen bonds (e.g. H_2S vs H_2O)
 - Explain that when comparing the melting and boiling points of substances of similar mass in different groups on the Periodic Table or different homologous series (see organic chemistry section) the difference in melting and/or boiling point is due to the presence of other intermolecular forces (dipole-dipole and/or hydrogen bonds) besides the London forces which are present between all particles
 - Explain that when comparing the melting and boiling points of substances that involve hydrogen bonding, the difference in melting and/or boiling point is due to the relative number of hydrogen bonds that occur between the particles (e.g. HF vs H_2O or propanol vs propanoic acid – see organic chemistry section)
 - Explain that metals and graphite conduct electricity due to the presence of free (mobile) valence electrons.
 - Explain that ionic compounds only conduct electricity when molten or in aqueous solution due to the presence of free (mobile) ions, which are not present in the solid state.

POLYATOMIC IONS

No	Name	Formula	Oxidation Number
1	Ammonium	NH_4^+	+1
2	Chlorate	ClO_3^{-1}	-1
3	Ethanoate	$\text{C}_2\text{H}_3\text{O}_2^-$	-1
4	Hydroxide	OH^-	-1
5	Nitrate	NO_3^-	-1
6	Nitrite	NO_2^-	-1
7	Permanganate	MnO_4^-	-1
8	Carbonate	CO_3^{2-}	-2
9	Hydrogen Carbonate	HCO_3^-	-1
10	Sulphate	SO_4^{2-}	-2
11	Hydrogen Sulphate	HSO_4^-	-1
12	Thiosulphate	$\text{S}_2\text{O}_3^{2-}$	-2
13	Sulphite	SO_3^{2-}	-2
14	Phosphate	PO_4^{3-}	-3
15	Dichromate	$\text{Cr}_2\text{O}_7^{2-}$	-2

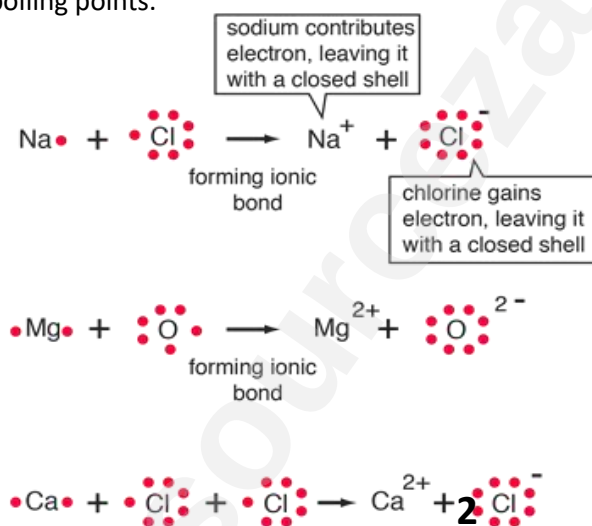
Covalent Bond

Covalent bonds involve the sharing of one or more pairs of electrons. There are two types of covalent bonds. Non polar / pure covalent bond which is the equal sharing of electrons, when the electronegativities of both the atoms are the same. Polar covalent bonds which is the unequal sharing of electrons, when the electronegativities of both the atoms are different. The greater the difference in electronegativities, the stronger the polar covalent bond.



Ionic Bonds

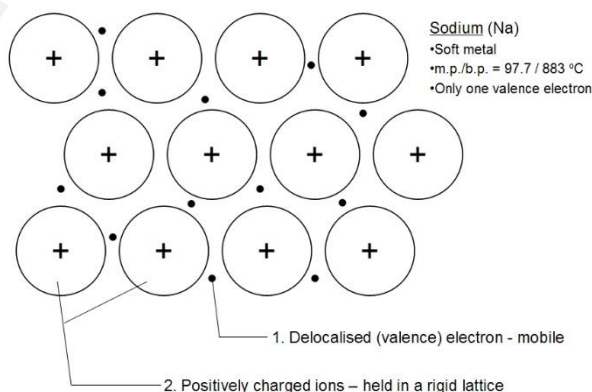
Ionic bonds involves the transfer of one or more electrons. Metals loose electrons to form positive ion (Cation) and non metals accept electrons to form negative ions (anions). Ionic compounds have high melting and boiling points.

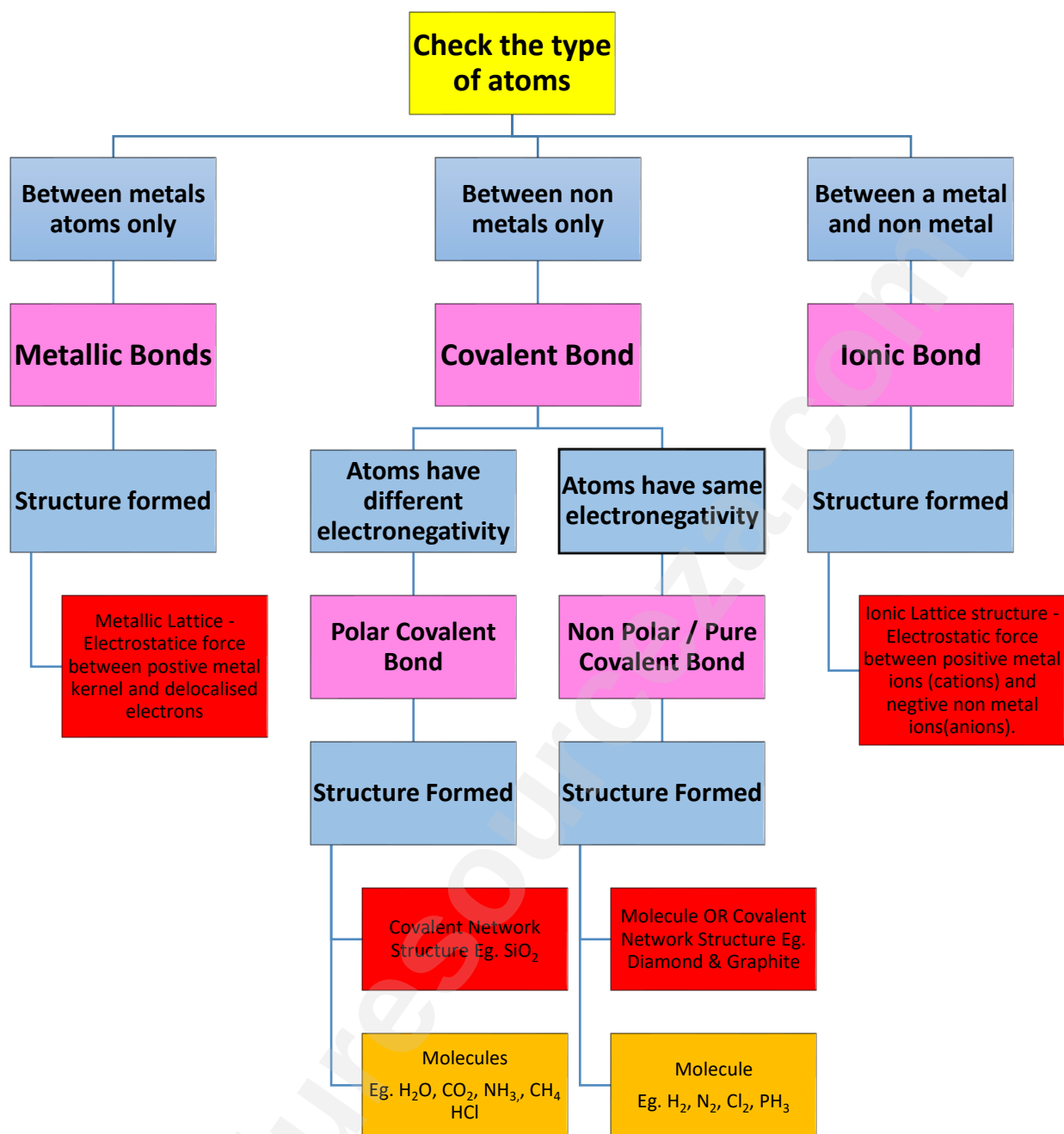


Metallic Bonds

Metallic are electrostatic forces of attraction between positive metal kernels and delocalized electrons. Metals have high melting and boiling points

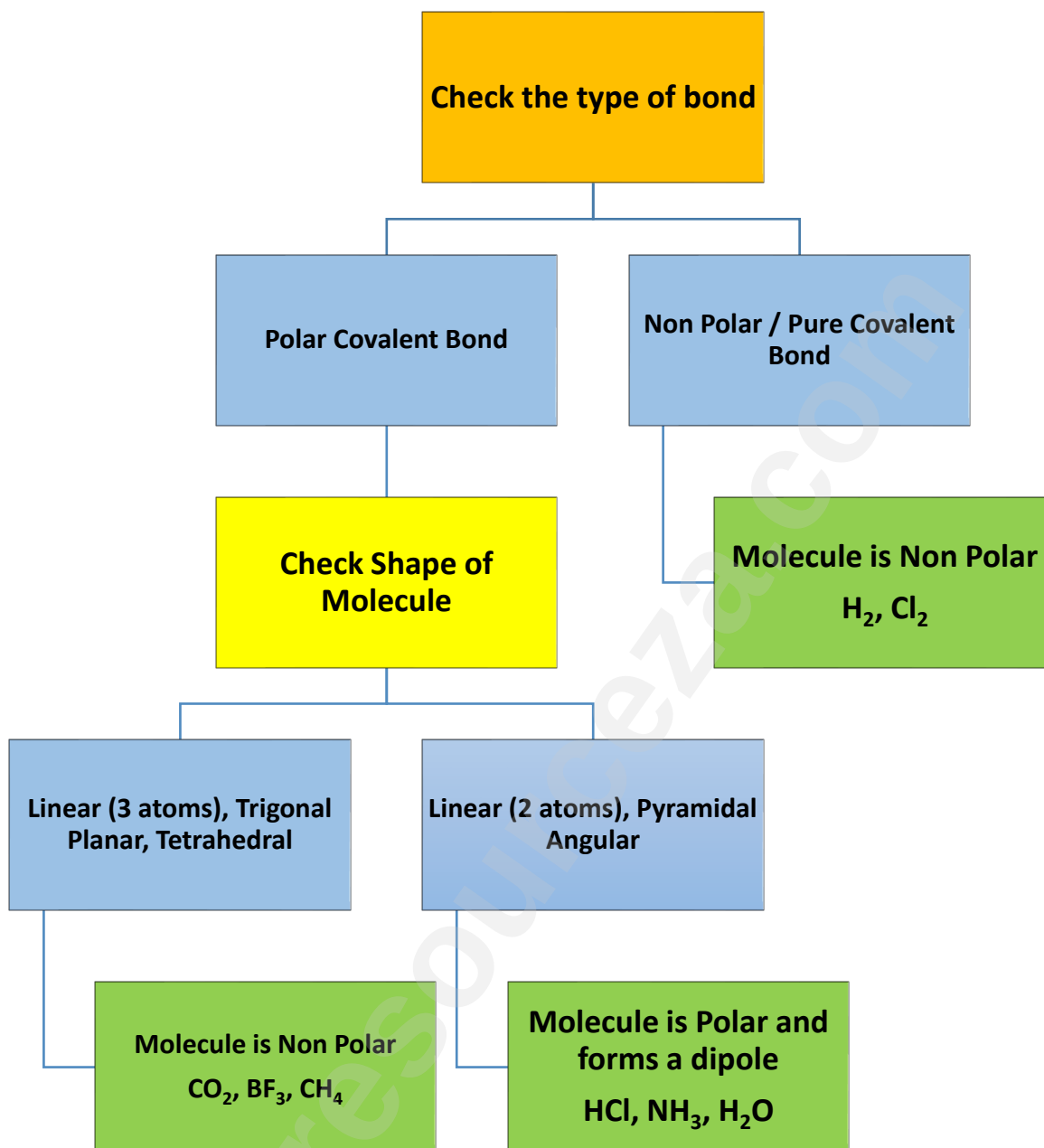
Metallic Bonding





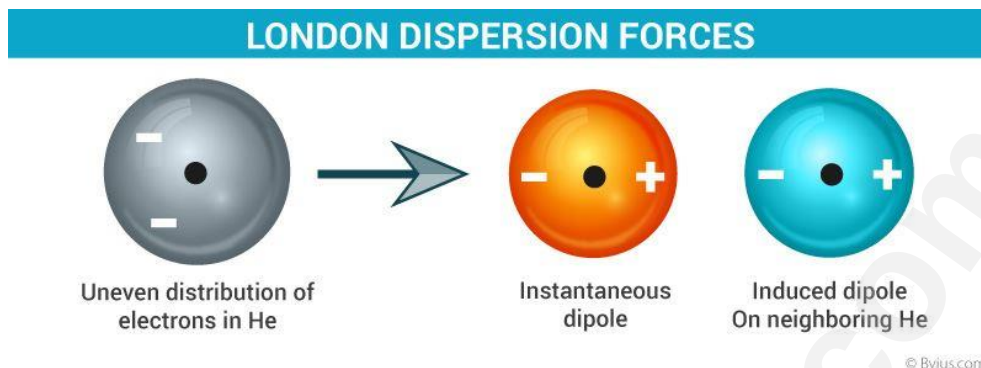
PREDICTING SHAPES OF MOLECULES

No of Atoms	Lone Pairs around central atom	Bonding Pairs	Shape	Symmetrical / Asymmetrical	Examples
2	3	1	Linear	Asymmetrical	HCl, HI
3	0	2	Linear	Symmetrical	BeCl_2
3	0	2 x 2 (2 double bonds)	Linear	Symmetrical	CO_2 ,
3	2	2	Angular/Bent	Asymmetrical	H_2O , H_2S
4	0	3	Trigonal Planar	Symmetrical	BF_3
4	1	3	Pyramidal	Asymmetrical	NH_3 , PCl_3
5	0	4	Tetrahedral	Symmetrical	CH_4 , CCl_4 ,



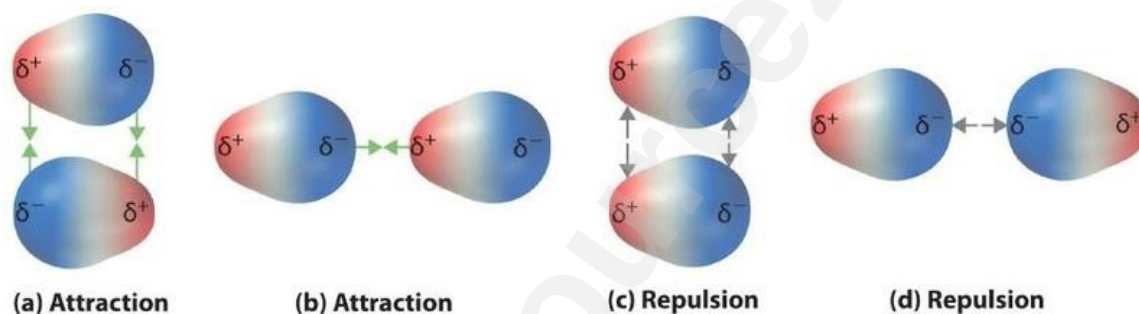
London Forces / Dispersion Forces / Induced Dipole – Induced Dipole Forces (Van Der Waals Forces)

London forces, also known as dispersion forces, originate between any two molecules that are weakly attracted to each other by means of small instantaneous dipoles that occur as a result of the varying positions of the electrons during their movement about their nuclei.



Dipole Dipole Forces (Van Der Waals Forces)

Dipole-dipole interactions are electrostatic interactions between molecules that have polar covalent bonds and have permanent dipoles.

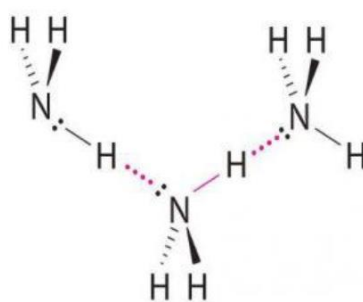
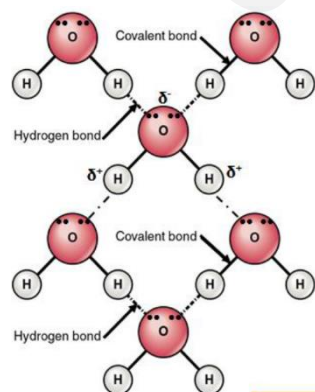


Hydrogen Bonds

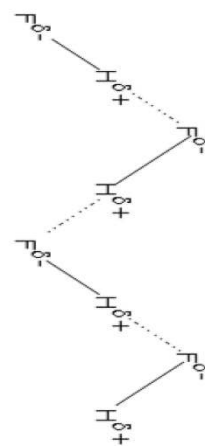
These are a special case of dipole-dipole forces. They are **STRONGER** than any other van der Waals forces and exist between polar molecules in which hydrogen is bonded to ...

- a small atom
- of high electronegativity
- with at least one lone pair of electrons

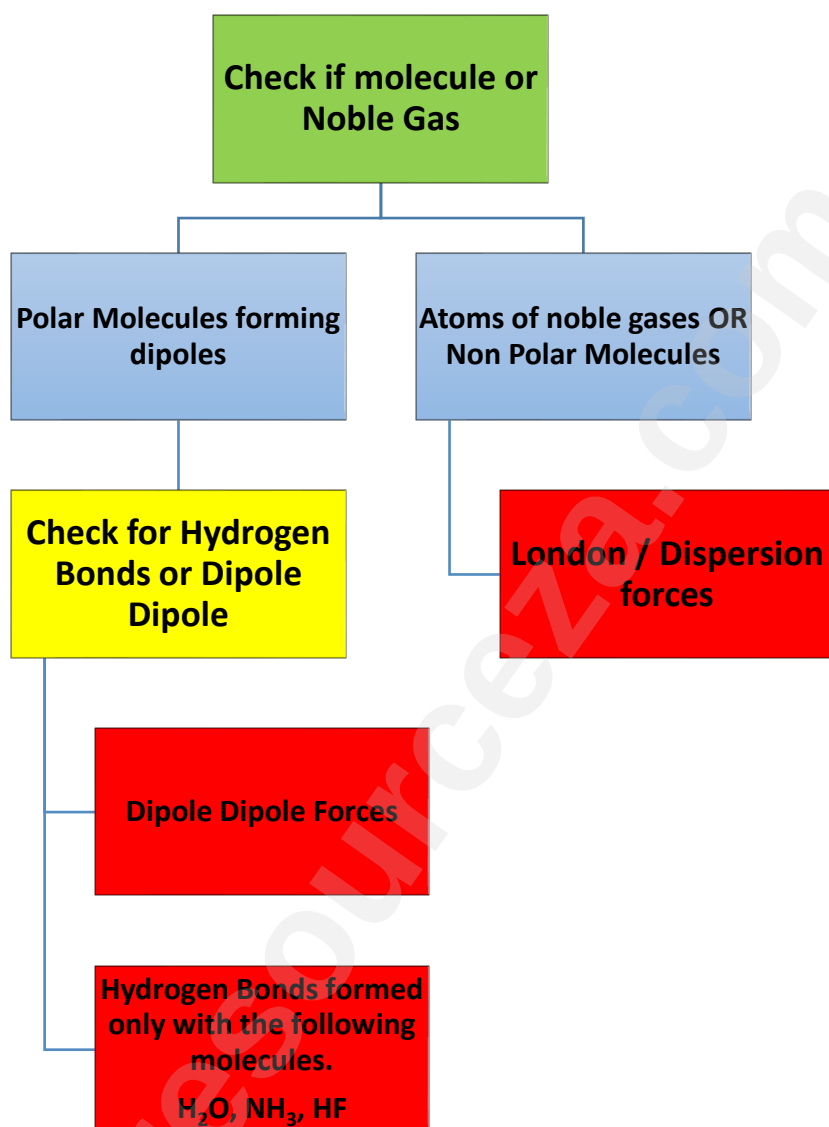
A hydrogen bond forms when the strong partially positive (δ^+) hydrogen atom of one molecule attracts a lone pair of electrons on the highly electronegative atom of a neighbouring molecule.



Hydrogen bonding in ammonia



PREDICTING INTERMOLECULAR FORCES



EXPLAINING TRENDS – BOILING & MELTING POINTS

Same intermolecular forces different sizes (London forces)

Eg. The strength of London forces is influenced by: The number of electrons

- Larger molecules have more electrons
- Can develop larger temporary dipoles and stronger London forces.
- When descending a group in the periodic table the size of the molecules increases and the strength of the London forces increases.
- More energy is required to overcome the London forces in larger molecules.
- High melting and boiling points.

Same group, different type of IMF

Eg. Explain why HF has a higher boiling point than HCl

- HF has hydrogen bonds between its molecules.
- HCl has dipole-dipole forces between its molecules.
- HF has stronger intermolecular forces.
- More energy is needed to overcome the stronger intermolecular forces, therefore HF has the higher boiling point.

Same group, same type of IMF

Eg. Explain why HI has a higher boiling point than HCl

- HCl and HI have dipole-dipole forces between their molecules.
- HI has bigger molecules which have more electrons than molecules of HCl
- Therefore HI has larger temporary dipoles than HCl
- HI has stronger dipole-dipole which require more energy to overcome, therefore HI has the higher boiling point.

Number of hydrogen bonds

Eg. Explain why H₂O has a higher boiling point than HF

- Water forms FOUR hydrogen bonds per molecule.
- Hydrogen fluoride forms TWO hydrogen bonds per molecule.
- Four hydrogen bonds is stronger than two
- More energy is needed to overcome the greater number of hydrogen bonds, therefore water has the higher boiling point.

Hydrogen bonds		
NUMBER of hydrogen bonds in H ₂ O	NUMBER of hydrogen bonds in NH ₃	NUMBER of hydrogen bonds in HF
On average each H ₂ O molecule forms FOUR H-bonds to other H ₂ O molecules. Each molecule has two δ^+ hydrogen atoms and two lone pairs of electrons so that every one of them can be involved in hydrogen bonding.	On average each NH ₃ molecule forms TWO H-bonds to other NH ₃ molecules. Each ammonia molecule can form one hydrogen bond using its lone pair and one involving one of its δ^+ hydrogens. (The other 2 hydrogen atoms are "wasted".)	On average each HF molecule forms TWO H-bonds to other HF molecules. Each molecule can only form one hydrogen bond using its δ^+ hydrogen and one involving one of its lone pairs. (The other 2 lone pairs are essentially "wasted".)

Number of weak intermolecular forces versus strong intermolecular forces

Eg. Explain why I_2 has a higher boiling point than H_2O

- I_2 has London forces between its molecules
- H_2O has hydrogen bonds between its molecules
- Since there are a large number of London forces in I_2 , the London forces is stronger than the hydrogen bonds in H_2O .
- More energy is needed to overcome the London forces in I_2 .
- I_2 has higher melting and boiling points

EXPLAINING TRENDS – ELECTRICAL CONDUCTIVITY

Covalent Compounds

Covalent compounds do not conduct electricity in the pure form as they do not have free electrons or ions to conduct electricity. An exception is graphite

- Graphite has delocalised electrons, just like metals.
- These electrons are free to move between the layers in graphite, so graphite can conduct electricity.
- The forces between the layers in graphite are weak.
- This means that the layers can slide over each other.

Ionic Compounds

Ionic compounds do not conduct electricity in the solid state, but conducts electricity in the molten and aqueous state.

Molten State

- When ionic compounds are melted at very high temperatures, the ionic bonds break.
- Ions are now free to move.
- With an application of an EMF, the ions begin to move.
- Ionic compounds conduct electricity in the molten state.

Aqueous State

- When ionic compounds are dissolved in water, the ionic bonds break.
- Ions are now free to move.
- With an application of an EMF, the ions begin to move.
- Ionic compounds conduct electricity in the molten state.

Metals

- Metals have delocalized electrons, which are free to move.
- With an application of an EMF, the electrons begin to move.
- Metals are able to conduct electricity.

Acids & Bases

Definitions

- An acid is defined as a proton donor.
- A base is defined as a proton acceptor.
- A strong acid is an acid that ionises almost completely in an aqueous solution.
- A weak acid is an acid that only ionises partially in an aqueous solution.
- Ionisation is the reaction of a molecular substance with water to produce ions.
- Dissociation is the splitting of an ionic compound into its ions.
- A strong base is a base that dissociates almost completely in an aqueous solution.
- A weak base is a base that only dissociates/ionises partially in an aqueous solution.
- An amphoteric (or amphiprotic) substance is a substance that can act as either an acid or a base. EG. H_2O , HSO_4^- , HCO_3^- .
- A standard solution is a solution of known concentration.
- A salt is a substance in which the hydrogen of an acid has been replaced by a cation.
- Neutralisation is the point where an acid and base have reacted so neither is in excess. (Also defined as the equivalence point)
- Hydrolysis of a salt is a reaction with water where water itself is decomposed.

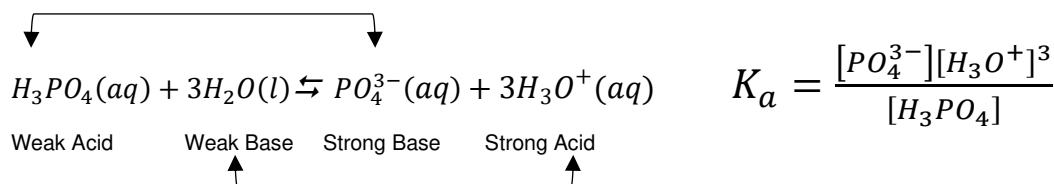
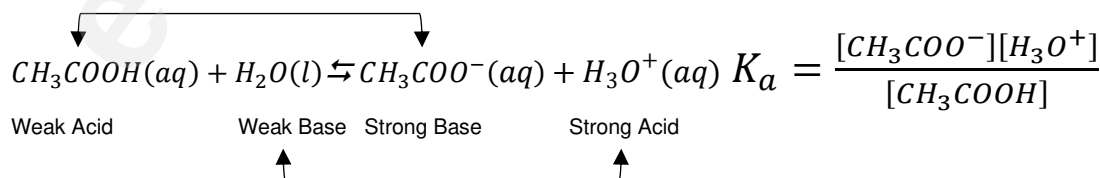
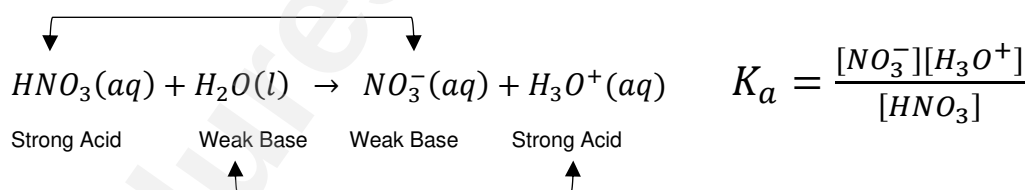
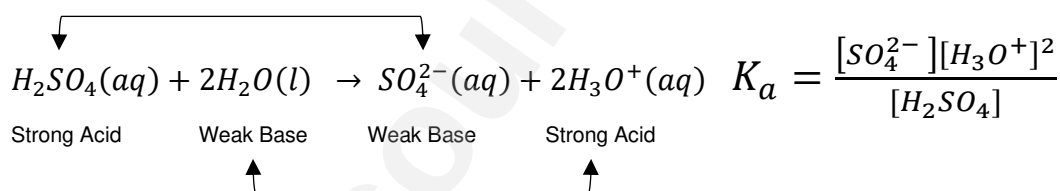
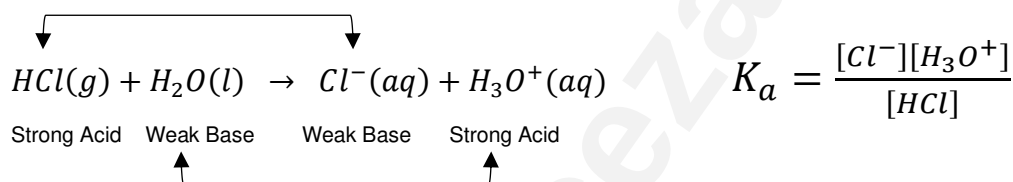
Skills

- Name and write the formula of the following common strong and weak acids.
- Classify acids as strong when given sufficient information, e.g. K_a values.
- Identify polyprotic acids on the basis of being able to donate more than one proton
- Distinguish between monoprotic, diprotic and triprotic acids and give examples of each.
- Write reaction equations for the ionisation of any known or given acids dissolving in water, using single arrows for strong acids and double arrows for weak acids.
- Name and write the formula of some common strong and weak.
- Write the reaction equations (using single arrows) for the dissociation of any known or given metal hydroxides dissolving in water.
- Name and write the formula of ammonia solution $NH_3(aq)$ or $NH_4OH(aq)$ and know that it is a weak base which only ionises partially in aqueous solution.
- Write the reaction equation for the ionisation of ammonia in water.
- Know that metal carbonates and metal hydrogen carbonates are weak base salts.
- State what is meant by a concentrated acid and a concentrated base.
- State what is meant by a dilute acid and a dilute base.
- Identify a substance as amphoteric (or amphiprotic), e.g. H_2O , HCO_3^- , HSO_4^-
- Write equations to show how an amphoteric (or amphiprotic) substance can act as an acid or a base.
- Identify conjugate acid-base pairs for given compounds or reactions.
- Know that a strong acid has a very weak conjugate base and a strong base has a very weak conjugate acid.

Name	Common Name	Symbol	Strength
Hydrogen Chloride	Hydrochloric Acid	HCl	Strong
Hydrogen Sulphate	Sulphuric Acid	H ₂ SO ₄	Strong
Hydrogen Nitrate	Nitric Acid	HNO ₃	Strong
Hydronium/Oxonium Ions		H ₃ O ⁺	Strong
Hydrogen Fluoride	Hydrofluoric Acid	HF	Weak
Hydrogen Phosphate	Phosphoric Acid	H ₃ PO ₄	Weak
Hydrogen Sulphite	Sulphurous Acid	H ₂ SO ₃	Weak
Ethanoic Acid	Acetic Acid	CH ₃ COOH	Weak
Oxalic Acid	Oxalic Acid	(COOH) ₂	Weak

- Polyprotic acids are able to donate more than one proton. Diprotic acid are able to donate two protons.
- A concentrated acid is an acid that has a high concentration of hydronium/oxonium ions.
- A dilute acid is an acid that has a low concentration of hydronium/oxonium ions.

Ionisation of Acids

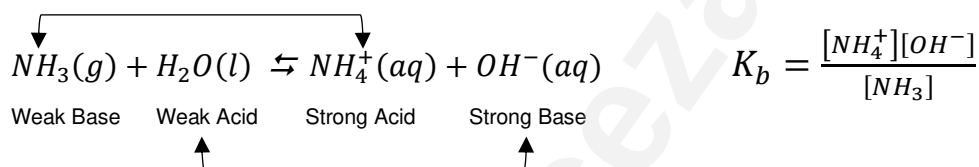


- A strong acid forms a weak conjugate base.
- A weak acid forms a strong conjugate base.
- A strong acid is an acid that ionises almost completely in an aqueous solution.
- A weak acid is an acid that only ionises partially in an aqueous solution.
- K_a is the ionisation constant of an acid
- Acids with high K_a values are strong. K_a values measures the strength of an acid.
- Conductivity can be used as a measure of acid strength, strong acids have a high concentration of ions, which increases the conductivity of the acid.

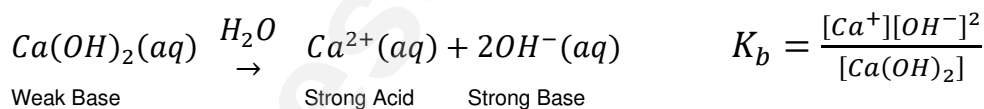
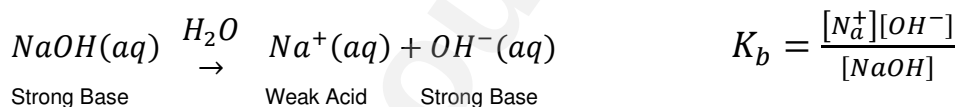
Name	Common Name	Symbol	Strength
<i>Group 1 Metal Hydroxides are strong</i>			
Sodium Hydroxide	Caustic Soda	NaOH	Strong
Potassium Hydroxide	Caustic Potash	KOH	Strong
Lithium Hydroxide		LiOH	Strong
Hydroxide Ion		OH ⁻	Strong
<i>All other Metal Hydroxides are weak</i>			
Calcium Hydroxide		Ca(OH) ₂	Weak
Magnesium Hydroxide		Mg(OH) ₂	Weak
Ammonium Hydroxide		NH ₄ OH	Weak
Ammonia		NH ₃	Weak
Metal Carbonates		MetalCO ₃	Weak

- A concentrated base is a base that has a high concentration of hydroxide ions.
- A dilute base is a base that has a low concentration of hydroxide ions.

Ionisation of Bases



Dissociation of Bases



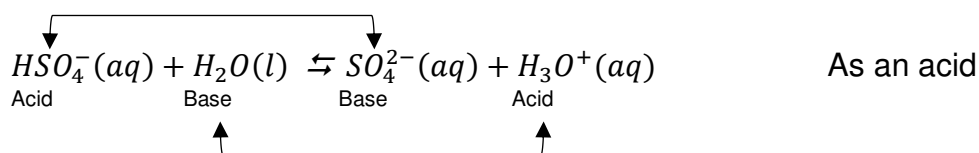
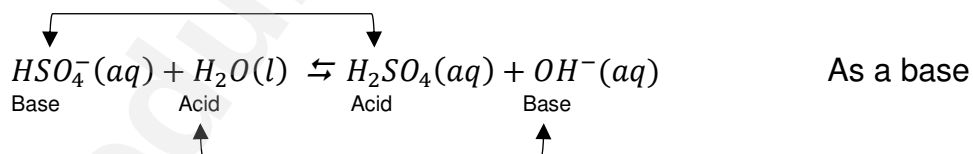
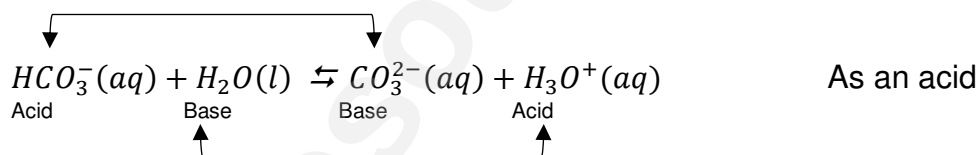
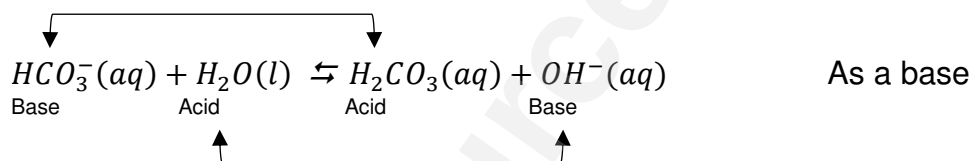
- A strong base produces a weak conjugate acid.
- A weak base produces a strong conjugate acid.
- K_b is the dissociation constant of a base.
- Bases with high K_b values are strong. K_b values measures the strength of a base.
- A strong base is a base that dissociates almost completely in an aqueous solution.
- A weak base is a base that only dissociates partially in an aqueous solution.

	Acid	Base
Strong	high percentage forms ions in solution	high percentage forms ions in solution
Weak	only a small percentage forms ions in solution	only a small percentage forms ions in solution
Concentrated	large number of moles of acid in solution	large number of moles of base in solution
Dilute	small number of moles of acid in solution	small number of moles of base in solution

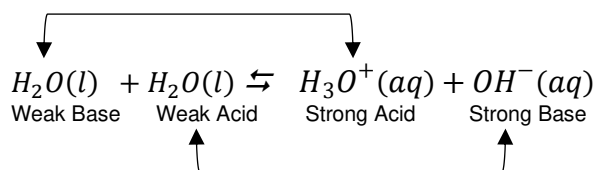
Amphoteric Substances

Name	Common Name	Symbol	Strength
Hydrogen Oxide	Water	H ₂ O	
Hydrogen Carbonate Ion		HCO ₃ ⁻	
Hydrogen Sulfate Ion		HSO ₄ ⁻	

Ionisation of Amphoteric Substances



This type of reaction (the transfer of a proton between identical molecules) is known as auto-protolysis.



$$K_w = [H_3O^+][OH^-] = 1 \times 10^{-14} \text{ at } 25^\circ\text{C}$$

pH Scale

The pH scale is the measure of hydronium ion (H_3O^+) concentration in water at 25°C .

- $\text{pH} < 7$ is acidic $[H_3O^+] > [OH^-]$
- $\text{pH} = 7$ is neutral $[H_3O^+] = [OH^-]$
- $\text{pH} > 7$ is basic $[H_3O^+] < [OH^-]$

Acid and Base Reactions

acid + active metal $\rightarrow$ salt + hydrogen (NB: A redox reaction)

Only metals above hydrogen will react since hydrogen is a stronger oxidising agent.

acid + metal oxide $\rightarrow$ salt + water

acid + metal hydroxide $\rightarrow$ salt + water

acid + metal carbonate $\rightarrow$ salt + carbon dioxide + water

acid + metal hydrogen carbonate $\rightarrow$ salt + carbon dioxide + water

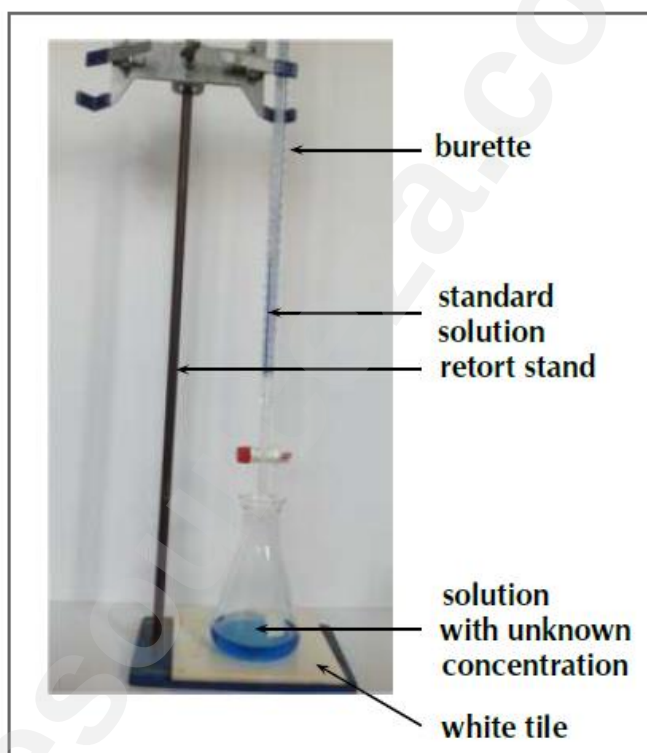
Hydrolysis of Salts

A salt is a substance in which the hydrogen of an acid has been replaced by a cation.

	Neutral Salts	Acidic Salts	Basic Salts
Examples	$NaCl, KNO_3$ A neutral salt is formed from a strong acid and a strong base.	$NH_4Cl, MgSO_4$ An acidic salt is formed from a strong acid and a weak base.	CH_3COONa, K_2CO_3 A basic salt is formed from a weak acid and a strong base.
Determining the acid and base that forms the salt Replace the cation with hydrogen to determine the acid and replace the anion with hydroxide for the base.	$HCl + NaOH \rightarrow NaCl + H_2O$ $HNO_3 + KOH \rightarrow KNO_3 + H_2O$	$HCl + NH_4OH \rightarrow NH_4Cl + H_2O$ $H_2SO_4 + Mg(OH)_2 \rightarrow MgSO_4 + 2H_2O$	$CH_3COOH + NaOH \rightarrow CH_3COONa + H_2O$ $H_2CO_3 + 2KOH \rightarrow K_2CO_3 + 2H_2O$
Hydrolysis reactions of salts Hydrolysis of a salt is a reaction with water where water itself is decomposed	Anions of strong acids (Cl^- , NO_3^-) and the cations of strong bases (Na^+ , K^+) do not undergo hydrolysis. A solution of this type of salt will be neutral. $NaCl \xrightleftharpoons{H_2O} Na^+ + Cl^-$ $KNO_3 \xrightleftharpoons{H_2O} K^+ + NO_3^-$	Cations of weak bases (NH_4^+ , Mg^{2+}) undergo hydrolysis but the anions of strong acids (Cl^- , SO_4^{2-}) do not. $NH_4Cl \xrightleftharpoons{H_2O} NH_4^+ + Cl^-$ $NH_4^+ + H_2O \rightarrow NH_3 + H_3O^+$ $MgSO_4 \xrightleftharpoons{H_2O} Mg^{2+} + SO_4^{2-}$ $Mg^{2+} + 2H_2O \rightarrow Mg(OH)_2 + H_3O^+$	Anions of weak acids (CH_3COO^- , CO_3^{2-}) undergo hydrolysis but the cations of strong bases (Na^+ , K^+) do not. $CH_3COONa \xrightleftharpoons{H_2O} CH_3COO^- + Na^+$ $CH_3COO^- + H_2O \rightarrow CH_3COOH + OH^-$ $K_2CO_3 \xrightleftharpoons{H_2O} K^+ + CO_3^{2-}$ $CO_3^{2-} + H_2O \rightarrow HCO_3^- + OH^-$
Salts of Weak Acid and Weak Bases	Both cations and anions undergo hydrolysis. The pH of this type of solution depends on the relative strengths of the acids and bases.		

Titration

- The method used to determine the concentration of a known substance using another, standard, solution.
- In a titration: a known volume of a standard solution (A) is added to a known volume of a solution with unknown concentration (B). The concentration of B can then be determined.
- The point of neutralisation is called the end-point of the reaction.
- A colour change caused by a suitable indicator determines the end point.
- Neutralisation/Equivalent point is the point where an acid and base have reacted so neither is in excess.



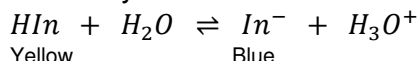
Indicators

Examples of Indicators

- Indicators are weak acids that changes colour according to certain conditions.
- Le Chatelier's principle can be used predict colour changes in indicators.

Example

1. Bromothymol Blue:



Titration type	Preferred indicator	Colour of acid	Colour of end-point	Colour of base	pH range
strong acid + strong base	bromothymol blue	yellow	green	blue	6,0 - 7,6
weak acid + strong base	phenolphthalein	colourless	faint pink	pink	8,3 - 10,0
strong acid + weak base	bromocresol green	yellow	green	blue	3,8 - 5,4

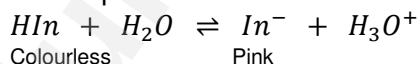
Adding acids

- Stress: If an acid is added concentration of H_3O^+ ions increase.
- Response: This causes the reverse reaction to be favoured, increasing the rate of the reverse reaction.
- Reason: To decrease the concentration of H_3O^+ ions.
- Effect: Solution turns yellow.

Adding bases

- Stress: If a base is added concentration of H_3O^+ ions decreases due to the OH^- ions reacting with the H_3O^+ ions to form water.
- Response: This causes the forward reaction to be favoured, increasing the rate of the forward reaction.
- Reason: To increase the concentration of H_3O^+ ions.
- Effect: Solution turns blue.

2. Phenolphthalein:

**Adding acids**

- Stress: If an acid is added concentration of H_3O^+ ions increase.
- Response: This causes the reverse reaction to be favoured, increasing the rate of the reverse reaction.
- Reason: To decrease the concentration of H_3O^+ ions.
- Effect: Solution turns colourless.

Adding bases

- Stress: If a base is added concentration of H_3O^+ ions decreases due to the OH^- ions reacting with the H_3O^+ ions to form water.
- Response: This causes the forward reaction to be favoured, increasing the rate of the forward reaction.
- Reason: To increase the concentration of H_3O^+ ions.
- Effect: Solution turns pink.