

IB CHEMISTRY – DEFINITIONS (v.1)

Topic 1 - Stoichiometry

Avogadro's constant: The number of particles in 12g of ^{12}C .

Concentration: the amount of solute per unit of volume of solution

Formula, empirical: The formula obtained by experiment, showing the simplest whole number ratio of atoms of each element in a particle of a substance.

Formula, molecular: The formula showing the actual number of atoms of each element in a particle of a substance.

Formula, structural: Shows the arrangement of atoms and bonds within a molecule.

Limiting reagent: The reactant which will determine the theoretical maximum amount of product formed.

Molar mass: The mass of a mole of a substance.

Mole: The amount of substance that contains a number of specified species equal to Avogadro's constant.

Solute: A substance that is dissolved into another (the solvent)

Solvent: a substance that dissolves another (the solute)

Yield, percentage: The experimental yield as a percentage of the maximum theoretical yield ($\text{experimental/theoretical} \times 100$)

Topic 2 – Atomic theory

Atomic emission spectra: The characteristic line spectrum that occurs as a result of energy being released by individual elements. Coloured lines on a black background.

Atomic absorption spectra: The characteristic line spectrum that occurs as a result of energy being absorbed by individual elements. Black lines on a continuum (coloured) background.

Atomic number: Number of protons in the nucleus.

Mass number: Number of nucleons (protons and neutrons) in the nucleus

Aufbau principle: The principle that states that lowest energy levels are filled first.

Hund's rule: Orbitals within the same sub-shell are filled singly first.

Ionization energy, first: Energy required to remove one mole of electrons from an atom in its gaseous state.

Isotopes: Atoms that contain the same number of protons but a different number of neutrons.

Orbital: A region of space around the nucleus of an atom that is occupied by a maximum of two electrons at any given time.

Pauli's exclusion principle: electrons in single orbital must have opposite spin.

Relative abundances: The percentage of natural occurrence of an isotope of an element.

Relative atomic mass: The weighted mean of all the naturally occurring isotopes of the element relative to ^{12}C . No units.

Valence electrons: The electrons in the highest main energy level.

Topic 3 – Periodicity

Alkali metals: Group 1 elements.

Catalyst: A substance that increases the rate of reaction while being recoverable unchanged at the final stage of the reaction. Examples of catalytic transition metals:

Fe is used in Haber process;

V_2O_5 in Contact process;

Ni in hydrogenation reactions;

MnO_2 in the decomposition of hydrogen peroxide

Catalyst, heterogeneous: In different state than reactants

Catalyst, homogeneous: In the same state as reactants

Colored complex: A complex is a compound in which molecules or ions form dative bonds to a metal atom or ion. Colors are due to e^- transitions between different d orbitals.

Co-ordination number: Number of lone pairs bonded to the metal ion.

Cl^- often gives 4 coordinate bonds, CN^- gives 6, H_2O gives 6 and NH_3 gives 4 or 6.

Electronegativity: Relative measure of the ability an atom has to attract a shared pair of electrons.

Group: Elements with the same number of valence e^- .

Halide ions: Ions of the halogens.

Their presence can be detected by the addition of silver nitrate. $AgCl$ is white, $AgBr$ is cream-colored, and AgI is yellow. Silver halides react with light to form silver metal.

Ligand: A molecule or ion that can donate an electron pair.

Metalloid: An element that possesses some of the properties of a metal and some of a non-metal. While metal oxides tend to be basic and non-metal oxides tend to be acidic, metalloid oxides such as aluminium oxide can be amphoteric.

Transition element: An element that possesses an incomplete d sub-level in one or more of its oxidation states.

Often very efficient catalysts as they can exist in a variety of oxidation states (all except Ti have oxidation state of +2). Form coloured complexes.

Topic 4 – Bonding

Structure, giant covalent: Very hard but brittle. Very high m.p. and b.p. Do not conduct in any state. Insoluble.

Structure, giant ionic: Hard but brittle. High m.p. and b.p. Conduct when molten or aqueous, but not as solids.

Structure, giant metallic: Malleable, not brittle. M.p. and b.p. dependent on no. of valence e^- . Good conductivity.

Structure, molecular covalent: Usually soft and malleable unless hydrogen bonded.

Low m.p. and b.p. Do not conduct in any state. Often soluble in non-aqueous solvents, unless they can hydrogen bond to water.

Allotropes: Occur when an element can exist in different crystalline forms, such as in carbon, which can exist as graphite, fullerene and diamond.

Diamond is exceptionally hard because there is no plane of weakness in the molecule made up of sp^3 hybridized carbon atoms. In graphite, the carbon atoms are sp^2 hybridized. Remaining electrons after the three σ bonds, are delocalized, resulting in the fact that graphite is a good conductor of electricity.

Bond polarity: A polarity caused by a difference in electronegativity between the elements. The greater the difference, the greater the polarity.

Bond, π : Pi bond. A bond formed by the sideways overlap of p orbitals with electron densities concentrated above and below a line drawn through the two nuclei. Double bonds have one π bond, while triple bonds have two which are perpendicular to each other.

Bond, σ : Sigma bond. A bond formed by the head on overlap of atomic orbitals from two different atoms along the line drawn through the two nuclei, with electron densities concentrated along the line. Single, double and triple bonds have one σ bond.

Covalent bond: Bonding by the sharing of electrons. The electrons are shared and attracted by both nuclei resulting in a directional bond between the two atoms.

Dative bond: A bond in which both electrons come from one of the atoms. Also known as coordinate bond.

Ionic bond: A bond by which electrons are transferred from one atom to another to form ions with complete outer shells.

In an ionic compound the + and – ions are attracted to each other by the electrostatic force between them, and build up into a strong lattice. Have relatively high m.p. Ionic bonds occur between elements with a great difference (>1.8) in electronegativity.

Conductivity: The extent to which a substance can conduct electricity. Must possess electrons or ions that are free to move.

Delocalization: The sharing of one electron pair by more than two atoms.

Forces, dipole-dipole: Permanent electrostatic forces of attraction between polar molecules. Stronger than van der Waals'.

Forces, Hydrogen bonding: Occurs when hydrogen attached to a highly electronegative element (N, F, or O) is bonded to another highly electronegative element (N, F, or O). Stronger than dipole:dipole forces.

Forces, van der Waal's: Temporary dipole forces due to momentary unevenness in spread of electrons. Weakest of intermolecular forces. Increase with increasing molar mass.

Hybridization: The mixing of atomic orbitals to create new orbitals of the same energy.

Metallic bonding: The valence electrons in metals become detached from the individual atoms so that the metals consist of a closely packed lattice of + ions in a 'sea' of delocalized electrons. Forces of attraction are between ions and electrons and not between the ions themselves, which means that metals are malleable and ductile.

Molecular polarity: Depends on both the bond polarity and the symmetry.

Resonance hybrid: Structures that arise from the possibility to draw a multiple bond in different positions equivalently. Can be better explained by delocalization.

Solubility: The extent to which one substance dissolves in another.

VSEPR theory: Valence Shell Electron Pair Repulsion theory. States that pairs of electrons arrange themselves around the central atom so that they are as far apart from each other as possible. Greater repulsion between lone pair of electrons than bonded pairs.

Topic 5 – Energetics

Average bond enthalpy: The average enthalpy change of breaking one mole of a bond in a gaseous atom into its constituent gaseous atoms.

Born-Haber cycle: Energy cycles for the formation of ionic compounds. If there is little agreement between the theoretical and experimental values, this could indicate a degree of covalent character.

Electron affinity: Enthalpy change when an electron is added to an isolated atom in the gaseous state.

Endothermic: A reaction in which energy is absorbed. ΔH is +. Reactants more stable than products.

Enthalpy: The internal energy stored in the reactants. Only changes in enthalpy can be measured.

Entropy: A measure of the disorder of a system. Things causing entropy to increase: 1) increase of number of moles of gaseous molecules; 2) change of state from solid to liquid or liquid to gas; 3) increase of temperature

Exothermic: A reaction in which energy is evolved. ΔH is –. Products more stable than reactants.

Gibb's free energy: Must be – for reaction to be spontaneous. $\Delta G = \Delta H - T\Delta S$

Hess' law: Enthalpy change for a reaction depends only on difference between enthalpy of products and enthalpy of reactants. It is independent of pathway.

Lattice enthalpy: The endothermic process of converting a crystalline solid into its gaseous ions, or the reverse exothermic process. The lattice enthalpy increases with decreasing size of the ions and increasing charge.

Spontaneous: A reaction that has a natural tendency to occur.

Standard conditions: 298 K and 1 atm.

Temperature: A measure of the average kinetic energy.

Standard enthalpy of vaporisation: The energy required to vaporise one mole of a liquid.

Enthalpy of atomisation: The energy required to produce one mole of gaseous atoms from an element in its standard state.

Bond dissociation enthalpy: The energy change when one mole of a specific bond is broken or created under standard conditions.

Enthalpy of Combustion: The energy released when one mole of a compound is burned in excess oxygen.

Standard enthalpy of formation: The energy change when one mole of a compound is formed under standard conditions from its constituent elements in their standard states.

Standard enthalpy of solution: The energy change when one mole of a substance is dissolved in an infinite amount of water under standard conditions.

Topic 6 – Kinetics

Activated complex: Created during a bimolecular process. Not a chemical substance which can be isolated, but consists of reacting particles in which bonds are in the process of being broken and formed. Can break down to form either the products or back to the original reactants.

Activation energy: The minimum amount of energy required for a reaction to occur between two particles. The other requirement is that the particles have to have an appropriate geometry of collision.

Arrhenius equation: An equation showing the relationship between the temperature and the rate constant. $K=Ae^{(-E_a/RT)}$

Bimolecular process: A reaction step when *two* species collide and interact.

Catalyst: Provide an alternative pathway for a reaction such that the activation energy required to reach the activation complex is lowered.

Can be divided into two types: homogenous catalysts are in the same phase as the reactants, while heterogeneous ones are in a different phase. Heterogeneous catalysts tend to work by bringing the reactant particles into close alignment by adsorbing them onto the catalytic surface.

Half-life: The time taken for the concentration of the reactant to fall to half of its initial value.

Molecularity: Number of species taking part in any specified step in the reaction.

Order of reaction: The rate is always proportional to the concentration of a reactant raised to a power, where the power is the order of the reaction with respect to that reactant.

Rate constant: The constant of proportionality in the rate expression.

Rate expression: An equation that shows the relationship between the concentrations of the reactants and the rate of the reaction.

Every species in the rate expression must occur in the rate determining step or in an equilibrium occurring before it.

Rate of reaction: The rate of increase of concentration of one of the products or the rate of decrease of concentration of one of the reactants.

Rate-determining step: The slowest step of a reaction (or the step with the lowest activation energy). This determines the rate of the entire reaction.

Unimolecular process: A process in which a single species breaks down into two or more products.

Topic 7 – Equilibrium

Closed system: A system in which neither matter nor energy can be lost or gained. An equilibrium can never occur in a system that is not closed.

Contact process: The synthesis of sulphur trioxide, (V_2O_5 is used as a catalyst).

Equilibrium constant: For a reaction $aA + bB \rightarrow cC + dD$, where the small letters are coefficients and capital letters are the reactants, the equilibrium constant is $[C]^c[D]^d/[A]^a[B]^b$. Variable units.

Equilibrium, dynamic: An equilibrium in which the rates of the forward and reverse reactions are the same.

Haber process: The synthesis of ammonia, where Fe is used as a catalyst.

Homogeneous reaction: A reaction in which all the species involved are in the same phase.

Le Chatelier's principle: If an equilibrium is subjected to a stress, the equilibrium will shift to minimize the effect of the stress.

Phase equilibrium: When the rate of vaporization is equal to the rate of condensation.

Vapour pressure: The partial pressure of a vapour. Boiling occurs when a liquid's vapour pressure equals the external pressure. The stronger the intermolecular forces the lower the vapour pressure at a particular temperature.

Topic 8 – Acids and Bases

Amphoteric: Can have the properties of both a base and an acid, depending on whether it is reacting with a base or an acid.

Brønsted-Lowry: An acid is defined as a proton donor, while a base is a proton acceptor.

Buffer: A solution that resists changes in pH when small amounts of acid or alkali are added to it.

When a small amount of acid is added, the excess of H^+ ions causes the equilibrium to shift to the left \rightarrow balances the difference. When a small amount of alkali is added, the OH^- ions react with the H^+ ions to form water. The decrease in $[H^+]$ is compensated for by an equilibrium shift to the right.

Vice versa for alkali buffers. Buffer solutions are made by several means:

**strong base + excess weak acid; **strong acid + excess weak base; **weak acid + same acid's salt; **weak base + same base's salt.

Concentrated: High number of moles of solute per volume of solution.

Conductivity: The more a solution is dissociated into its ions, the greater its conductivity.

Conjugate: The species remaining after an acid has lost a proton (conjugate base) or a base has gained one (conjugate acid). $pK_a + pK_b = pK_w$

Diprotic: Where one mole of an acid produces two moles of hydrogen ions, e.g. H_2SO_4 .

End point: The point at which the indicator changes colour most rapidly.

Equimolar: Containing moles at a ratio equal to the stoichiometric ratio.

Equivalence point: Where the acid and base are in equimolar quantities. Exactly enough to react with each other.

Indicator: A weak acid or base in which the dissociated form is a different colour to the undissociated form. The end point occurs when the pH is approximately equal to

the pK_{in} value. Ideally, the end point corresponds to the equivalence point in a titration.

Lewis theory: An acid is defined as an electron pair acceptor (e.g. BF_3) and a base is an electron donator (e.g. NH_3).

Monoprotic: Where one mole of the acid produces one mole of hydrogen ions, e.g. HCl .

pH: Power of hydrogen. $-\log [H^+]$

Salt hydrolysis: The process by which a salt is broken down by water.

Strong: An acid or a base that dissociates completely into its ions. $K_a \gg 1$.

Some strong acids: hydrochloric, sulphuric, nitric (weaker than other two). Strong bases: hydroxides of alkali metals.

Water, ionic product of: The equilibrium constant for the dissociation of water into its ions, where $[H_2O]$ is taken to be constant. Value of K_w increases as temperature is increased, as the dissociation is an endothermic process.

Weak: An acid or base that only slightly dissociates into its ions. $K_a \ll 1$. Some weak acids: ethanoic, carbonic. *Weak bases: ammonia, aminoethane.

Topic 9 – Oxidation and Reduction

Anode: Where oxidation takes place. In electrolysis, it is the + electrode and anions are attracted here.

Cathode: Where reduction takes place. In electrolysis, it is the – electrode and cations are attracted here.

Electrolysis: Passage of electric current through an electrolyte. Amount of discharge is affected by: 1) current; 2) charge on ion, 3) duration of electrolysis.

Electrolyte: A substance which does not conduct electricity when solid, but does when molten or in aqueous solution and is chemically decomposed in the process.

Electrolytic cell: Used to make non-spontaneous redox reactions occur by providing energy in the form of electricity from an external source.

Electroplating: A process of coating one metal with a thin layer of another metal, by electrolysis.

Half cell: A metal in contact with an aqueous solution of its own ions.

Oxidation: The loss of electrons

Oxidizing agent: A substance that readily oxidizes other substances. Oxidizing agents are thus reduced.

Reactivity: A measure of the readiness of a substance to gain or lose electrons. The stronger the reducing agent or oxidizing agent, the more reactive it is.

Redox reaction: A reaction in which there is a transfer of electrons, i.e. reduction and oxidation occurring simultaneously.

Reducing agent: A substance that readily reduces other substances. Reducing agents are thus oxidized.

Reduction: The gain of electrons

Salt bridge: Allows the free movement of ions in a voltaic cell. Paper dipped in a saturated solution of KNO_3 is an example of a salt bridge.

Shorthand notation: For a voltaic cell. Example: $Cu_{(s)}/Cu^{2+}_{(aq)} || H^+_{(aq)} / H_{2(g)}$

Standard conditions: 298 K, 1 atm, 1.0 M.

Standard electrode potential: The electrode potential of one half-cell compared against another half-cell, by convention, the hydrogen half-cell, which is arbitrarily given a value of 0 V.

Standard cell potential: Difference between the two standard electrode potentials of the two half cells.

Standard hydrogen electrode: Arbitrarily assigned a potential of zero. Electrode consists of an inert metal such as platinum dipped into a 1 M solution of HCl, where hydrogen gas at 1 atm flows in.

Voltaic cell: Two different half-cells connected together to enable to electron transferred during the redox reaction to produce energy in the form of electricity. The electrons are produced at the half-cell that is most easily oxidized.

Topic 10 – Organic Chemistry

Benzene: Hexagonal shape with delocalized π bonds. Undergo substitution rather than addition reactions.

Boiling and melting point: Depend on intermolecular forces. The greater the intermol. forces, the higher the m.p. and b.p.

Bromination: Yellow/orange bromine is decolorized when added to an alkene due to addition reaction. Used to test for alkenes.

Carbocation: A cation in which the carbon carries most of the + charge. Can be formed during S_N1 substitution.

Chiral center: An asymmetric carbon atom, i.e. has four different groups of atoms attached to it.

Cis-isomer: The geometric isomer in which the similar groups are on the same side of the double bond. Commonly polar.

Condensation reaction: Reaction in which two molecules join together with the loss of a small molecule, typically water.

Dehydration: Loss of water. Alcohols can be dehydrated when they are refluxed with condensed sulphuric acid.

Esterification: Process by which an alcohol and a carboxylic acid are converted into an ester and water, with sulphuric acid catalysis.

Fission, heterolytic: Bond breaking in which the more electronegative of the two atoms joined by the bond takes both of the electrons.

Fission, homolytic: Bond breaking in which each atom takes one of the e- in the bond, creating free radicals.

Free radical: A species containing at least one unpaired electron, as a result of homolytic fission. Very reactive.

Halogenoalkane, primary: Halogenoalkanes that have one alkyl group attached to the carbon atom bonded to the halogen. Undergo S_N2 mechanism in nucleophilic substitution.

Halogenoalkane, tertiary: Halogenoalkanes that have three alkyl groups attached to the carbon atom bonded to the halogen. Undergo S_N1 mechanism in nucleophilic substitution.

Homologous series: A group of compounds where neighbouring members differ by $-CH_2$. Have similar chemical properties, but gradually changing physical properties.

Hydration: Addition of water. Ethanol can be formed from addition of water to ethene.

Hydrocarbon: Compounds containing only carbon and hydrogen.

Hydrogenation: Addition of hydrogen. Can be used to reduce number of double bonds in polyunsaturated vegetable oils present in margarine, causing it to become a solid at room temperature.

Hydrolysis: Process by which a molecule is broken down by water.

Isomers: Different compounds that have the same molecular formula but different structure.

Isomers, functional group: Where the isomers contain different functional groups.

Isomers, hydrocarbon chain: Where there is a difference in the structure of the hydrocarbon chain.

Isomers, optical: Where a molecule shows optical activity in its mirror images.

Enantiomers rotate the plane of polarization of light in different directions. Occurs when there is one or more chiral centers.

Isomers, positional: Where the position of the functional group is different.

Isomers, stereo-: Where the molecules have a different spatial arrangement of atoms and hence different 3D shapes. Subdivided into geometric and optical isomers (enantiomers).

Isomers, structural: Where the atoms have a different structural formula altogether.

Subdivided into positional, hydrocarbon chain and functional group isomers.

Mechanism, S_N1 : A unimolecular process by which a halogenoalkane undergoes nucleophilic substitution. A two-step mechanism: a rate-determining step in which the bond between the carbocation and the halogen are broken, followed by a step in which the nucleophile is attracted to the carbocation. Faster than S_N2 , as the formation of the intermediate carbocation is faster than the S_N2 route which involves a transition state with relatively high activation energy.

Mechanism, S_N2 : A bimolecular process by which a halogenoalkane undergoes nucleophilic substitution. Mechanism involves formation of a transition state which involves both of the reactants.

Monomer: Components of a polymer.

Nucleophile: The species that donates the electron pair in an organic chemical reaction. A nucleophile is also a Lewis base. Typical nucleophiles are CN^- , OH^- and NH_3 .

Nucleophilic substitution: Substitution that occurs with a halogenoalkane reacting with a nucleophile.

Peptide bond: $-C=ONH-$. Bond formed as the result of condensation reaction between a carboxyl group and an amino group.

Peptide, di-: Two amino-acids joined together.

Peptide, poly-: More than 20 amino-acids joined together.

Peptide: Molecule formed by aminoacids joined together by peptide bonds (by condensation reaction in which water is lost).

Polymer: Very long molecule made up of repeating units.

Polymerization, addition: Forming a polymer by addition of monomers.

Polymerization, condensation: Forming a polymer by substitution reaction between monomers, each having two functional groups.

Reaction, addition: A reaction in which the reactant is added across a $C=C$ bond, converting it to a $C-C$ bond. Addition reactions with water requires an H_2SO_4 catalyst. Addition reactions with hydrogen use Ni as catalyst.

Reaction, substitution: A reaction in which one group is substituted for another.

Substitution reactions with halogenoalkanes are nucleophilic substitutions. Benzene does not undergo substitution reactions readily as its π bonds are delocalized.

Reflux: A condenser which causes any vapour produced to condense and returns to the flask and continues to react. If the carboxylic acid is desired from the oxidation of a primary alcohol, this must be done under reflux. On the other hand, if the aldehyde is desired, this can be distilled from the reaction mixture as soon as it is formed.

Saturated: Containing only single bonds. Alkanes are saturated.

Spectrometry, mass: Separating ions according to mass.

Spectroscopy, IR: Analyzing the bonds present within a molecule by sending infrared light through it, causing the bonds to absorb radiation of characteristic frequencies.

Spectroscopy, NMR: Analysis of hydrogen environments to deduce the structure of a molecule.

Trans-isomer: The geometric isomer in which the similar groups are on different sides of the double bond. Commonly non-polar.

Unsaturated: Containing double bonds between carbon atoms. Alkenes are unsaturated. Can be tested for by bromination.