WJEC (Wales) Chemistry A-level

Unit 2: Energy, Rate and Chemistry of Carbon Compounds

Definitions and Concepts

Definitions and Concepts for WJEC (Wales) Chemistry A-level

Unit 2: Energy, Rate and Chemistry of Carbon Compounds

2.1 Thermochemistry

Bond enthalpy: The amount of energy required to break one mole of the stated bond in the gas phase.

Enthalpy change (ΔH): The heat energy change measured under a constant pressure.

Enthalpy change of reaction: The enthalpy change when quantities of substances in standard states react completely.

Enthalpy of combustion: The enthalpy change when one mole of a substance is burned in excess oxygen.

Hess's law: The enthalpy change of a reaction is independent of the route taken.

Mean bond enthalpy: The enthalpy change when one mole of a specified covalent bond is broken averaged out across the range of compounds.

Standard enthalpy of formation ($\Delta_f H^\ominus$): The enthalpy change when one mole of a substance in its standard state under standard conditions is formed from its elements under standard conditions.

2.2 Rates of Reaction

Activation energy: The minimum amount of energy for particles to collide with for a successful reaction to take place.

Catalyst: A substance that increases the rate of a reaction without being changed in chemical composition or amount. They work by providing an alternative reaction pathway with a lower activation energy.

Collision theory: Reactions can only occur when collisions take place between particles that have sufficient energy.

Colorimetry: This method is used to calculate the concentration of a specific coloured compound in a solution by measuring the extent to which it absorbs certain wavelengths of light. This is measured with a colorimeter.

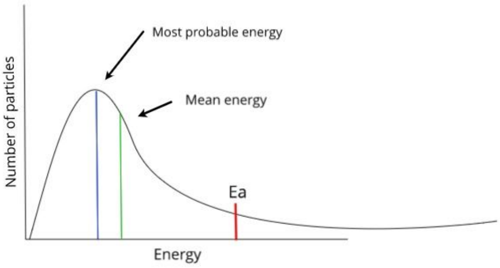
Effect of concentration on reaction rate: As the concentration of reactants increases, the reacting particles get closer together meaning they will collide more often. As a result, there will be a higher rate of successful collisions and a faster rate of reaction.

Effect of pressure on reaction rate: As the pressure of gaseous reactants increases, the reacting particles get closer together meaning they will collide more often. As a result, there will be a higher rate of successful collisions and a faster rate of reaction.

Effect of temperature on reaction rate: Increasing the temperature means the particles will have more kinetic energy and so will move faster. If the molecules are moving faster they will collide more often and, since they've gained kinetic energy, a larger proportion of the particles will have at least the activation energy. For both these reasons the rate of reaction increases.

Energy profile: A graph used to show the relative energy of reaction species (including reactants and products) as a reaction proceeds.

Maxwell-Boltzmann distribution: Shows the distribution of the molecular energies in a gas at a constant temperature. The area under the curve indicates the total number of particles present. Example distribution:



Rate of reaction: The measure of the amount of product formed or reactant used over time. The units of rate of reaction may be given as g/s, cm^3/s or mol/s.

2.3 The Wider Impact of Chemistry

Biofuels: Fuels made from once-living organic matter. These fuels are renewable and sustainable and are an alternative to fossil fuels.

Synthesis: The process of combining different elements and compounds to build new molecules.

Sustainability: The process of using resources at a rate that allows their supply to be maintained.

Green chemistry: Chemistry that aims to be sustainable in terms of energy and resources and restricts pollution.

2.4 Organic Compounds

Alcohol: An organic compound containing the functional group -OH.

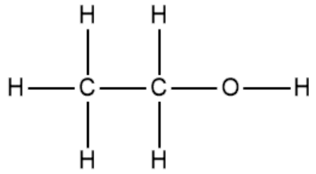
Alkane: A homologous series of saturated hydrocarbons with the general formula C_nH_{2n+2}.

Alkene: An hydrocarbon containing at least one C=C double bond with the general formula C_nH_{2n}.

Boiling temperature: The temperature at which a substance changes from a liquid state to a gaseous state.

Carboxylic acid: An organic compound containing the -COOH functional group.

Displayed formula: The relative positions of atoms and the bonds between them. e.g. Ethanol:



Electrophile: A species that can accept electrons in a reaction, to form a chemical bond. Electrophiles are attracted to areas with a lot of electrons/high negative charge.

Functional group: An atom/group of atoms responsible for the characteristic reactions of a compound.

Halogenoalkane: A saturated molecule where one or more of the hydrogen atoms in an alkane have been substituted for a halogen.

Heterolytic (bond breaking): The type of bond breaking in which both the electrons from the bond move together to one of the bonding atoms.

Homolytic (bond breaking): The type of bond breaking in which the electrons from the bond move separately, one goes to each of the atoms of the bonding pair.

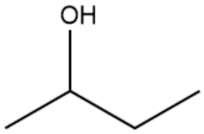
Melting temperature: The melting point of a substance is the temperature at which it changes from solid state to liquid state.

Nucleophile: An atom or molecule that donates an electron pair to form a covalent bond. Attracted to electron-deficient areas.

Organic compound: A carbon-containing compound.

Radical: A species with an unpaired electron. Represented in mechanisms by a single dot.

Skeletal formula: The simplified organic formula, shown by removing hydrogen atoms from alkyl chains, leaving the carbon skeleton and the functional groups. E.g. butan-2-ol:



Solubility: The ability of a given substance to dissolve in a solvent.

Structural formula: Shows the arrangement of atoms in a molecule. E.g. butane: $CH_3(CH_2)_2CH_3$.

Structural isomer: Structural isomers are compounds that have the same molecular formula but a different structural formula. Structural isomers include chain isomers, functional group isomers and position isomers.

2.5 Hydrocarbons

Addition polymerisation: The formation of a long chain molecule when many monomers join together (the polymer is the only product).

Alkane: A homologous series of saturated hydrocarbons with the general formula C_nH_{2n+2}.

Alkane fuel: Alkanes are good fuels as they are considered to burn cleanly, they undergo combustion in excess oxygen to produce only carbon dioxide and water.

Alkene: An hydrocarbon containing at least one C=C double bond with the general formula C_nH_{2n}.

Combustion of alkanes: Combustion of alkanes releases energy. During combustion, the carbon and hydrogen in the fuels are oxidised. Alkanes can undergo complete or incomplete combustion. Water and carbon dioxide are the only products of complete combustion, whereas carbon monoxide and carbon particulates can be produced in incomplete combustion.

E/Z isomerism: A type of stereoisomerism that occurs due to the restricted rotation around the carbon double bond. This results in two different groups on either end of the double bond. If the highest priority groups for each carbon are found on the same side of the molecule, then it is the Z-isomer. If the highest priority groups for each carbon are found on opposite sides of the molecule, then it is the E-isomer.

Electrophilic addition: A reaction where a π bond is broken and 2 new σ bonds form due to the addition of an electrophile.

Free radical substitution: A photochemical reaction between halogens and alkanes to form halogenoalkanes. The reaction requires UV light and involves three stages: initiation, propagation and termination. Initiation creates a radical species. Propagation involves a series of chain reactions where free radicals bond to molecules to form new free radicals. Termination involves the reaction of free radicals with other free radicals to form new molecules.

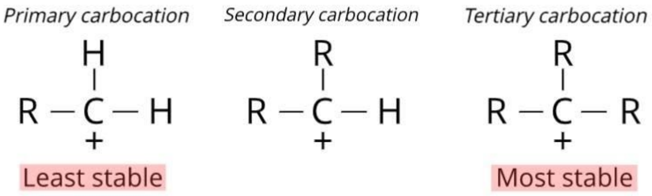
Free radicals: A species with an unpaired electron. These are represented in mechanisms by a single dot.

Hydrocarbon: A compound consisting of hydrogen and carbon atoms only.

Hydrogenation: A reaction between H_2 and an alkene to form an alkane. These reactions usually require a catalyst like nickel.

Initiation step: The first step in a radical substitution mechanism, involving the formation of the radicals.

Major/minor products: Major and minor products are formed from electrophilic addition due to the relative stabilities of the primary/secondary/tertiary carbocation intermediates. The major product is formed from the most stable intermediate and the minor product is formed from the least stable intermediate.



π-bond: A type of covalent bond formed when adjacent p orbitals overlap above and below the σ single carbon bond. Pi (π) bonds can't be rotated. As π-bonds have low bond enthalpy, alkenes are more reactive than alkanes.

Propagation step: Propagation involves a series of chain reactions where free radicals react with molecules to form new free radicals.

σ-bond: A covalent bond formed of overlapping s orbitals.

Termination: The final steps in a radical substitution mechanism in which two radicals react together to form a species that only contains paired electrons.

Unsaturated bond: A type of bond made up of both a σ-bond and a π-bond.

2.6 Halogenoalkanes

Bond enthalpy: The amount of energy required to break one mole of the stated bond in the gas phase.

Chlorofluorocarbons (CFCs): Compounds containing carbon, hydrogen, chlorine and fluorine atoms. In the atmosphere, they form radicals which result in the depletion of the ozone layer.

Elimination: A reaction in which a molecule loses atoms or groups of atoms to form a C=C bond.

Halogenoalkane: A saturated molecule where one or more of the hydrogen atoms in an alkane have been substituted for a halogen.

Hydrolysis: A reaction in which water is used to break down a compound.

Nucleophile: An atom or molecule that donates an electron pair to form a covalent bond. Attracted to electron-deficient areas.

Nucleophilic substitution: A reaction in which an electron pair donor attacks an electrophilic atom (an atom with a partial or full positive charge) to replace an atom/group of atoms.

Ozone: Ozone is formed naturally in the upper atmosphere. It is beneficial because it absorbs ultraviolet radiation and this prevents harmful radiation reaching the earth.

Polar bond: A covalent bond in which there is an unequal distribution of the electrons between the two atoms due to the differing electronegativities of the bonding atoms. One atom will have a partial positive charge while the other will have a partial negative charge.

Reflux: The continual boiling and condensing of a reaction mixture. This technique is often used to make sure a volatile liquid reaches a high enough temperature to ensure that the reaction goes to completion.

Solvent: A liquid that can dissolve other substances.

Toxicity: A measure of how poisonous a chemical substance is.

2.7 Alcohols and carboxylic acids

Alcohol: An organic compound containing the functional group -OH.

Aldehyde: A compound containing the -CHO functional group at the end of an alkyl chain. Aldehydes can be oxidised to carboxylic acids by heating them under reflux with $Cr_2O_7^{2-}$/ H^+.

Biofuels: Fuels made from once-living organic matter. These fuels are renewable and sustainable and are an alternative to fossil fuels.

Carbon neutrality (fuels): A fuel is described as carbon-neutral if the production and use of the fuel has no net increase on the amount of carbon dioxide in the atmosphere.

Carboxylic acid: An organic compound containing the -COOH functional group.

Dehydration: A reaction in a water molecule is lost from a molecule/compound.

Distillation: A technique used to purify a liquid by heating and cooling. When the liquid evaporates it moves into a condenser where it is cooled, recondenses and collected.

Ester: A compound containing the R-COO-R’ functional group (where R and R’ are alkyl groups).

Esterification: The process of making esters. Esters can be made by the reaction between carboxylic acids and alcohols in the presence of an acid catalyst, or by the reaction between acid anhydrides and alcohols.

Fermentation: The process by ethanol is produced from organic sugars, such as glucose. This process requires yeast and anaerobic conditions.

Ketone: A compound containing the C=O functional group within an alkyl chain. Ketones cannot be oxidised further.

Oxidation: The loss of electrons/increase in oxidation number.

Oxidising agent: A substance that can oxidise another species by being reduced.

Primary alcohol: An alcohol in which the -OH is attached to a primary carbon atom (i.e. RCH_2OH). Primary alcohols can be oxidised with $Cr_2O_7^{2-}/H^+$ to form either an aldehyde or a carboxylic acid, depending on the conditions.

Secondary alcohol: An alcohol in which the -OH is attached to a secondary carbon atom (i.e. R_2CHOH). Secondary alcohols can be oxidised under reflux with $Cr_2O_7^{2-}/H^+$ to form a ketone.

Tertiary alcohol: An alcohol in which the -OH is attached to a tertiary carbon atom (i.e. R_3COH). Tertiary alcohols cannot be oxidised.

2.8 Instrumental analysis

Carbon-13 NMR spectroscopy: A type of NMR spectroscopy which analyses ^{13}C nuclei. The number of peaks in the spectrum shows the number of different environments and the chemical shifts represent the environments present.

Fingerprint Region: The region on an IR spectrum below 1500 cm^{-1} which is unique to each molecule.

Infrared Spectroscopy: An analytical technique used to identify particular bonds and functional groups within a molecule.

Mass spectrometry: A technique used to identify compounds and determine their relative molecular mass.

Molecular ion peak: The peak on a mass spectrum with the highest m/z value, this is used to determine the molecular mass of a compound.

Nuclear Magnetic Resonance (NMR): A technique that uses the absorption of electromagnetic radiation by an atomic nucleus in an external magnetic field to analyse the structure of a compound. Typically, either ^{13}C or ^{1}H nuclei are analysed. ^{13}C NMR spectra are generally simpler than ^{1}H NMR spectra.

Proton NMR spectroscopy: A type of NMR spectroscopy which analyses ^{1}H nuclei. The number of peaks on the spectrum shows the number of proton environments and the chemical shifts represent the environments. The area under each peak shows the relative number of protons in each environment. The splitting pattern can be used to work out the number of adjacent protons.

Relative peak height: In mass spectra the peak heights show the relative abundances of the substance that made the peak.

Wavenumber: Represents the energy and frequency of infrared radiation absorbed by a bond in a molecule. This is the x-axis on IR spectra.