OCR (A) Chemistry A-Level

Module 6 - Organic Chemistry & Analysis

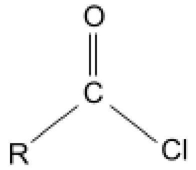
Definitions and Concepts

Definitions and Concepts for OCR (A) Chemistry A-level

Module 6 - Organic Chemistry & Analysis

6.1.1 - Aromatic Compounds

Acyl Chloride: a molecule containing the functional group below.



Aromatic Compound: a compound containing at least one benzene ring.

Delocalised Model of Benzene: the p-orbitals of the 6 carbon atoms overlap to form a delocalised π system. This model is supported by experimental evidence: all the C-C bond lengths in benzene are the same, the enthalpy change of hydrogenation is less exothermic than would be expected for cyclohex-1,3,5-triene and the benzene does not undergo addition reactions.

Electron Density: a representation of the probability of finding an electron at a specific point around an atom/ molecule. Benzene has a lower electron density than an alkene. In benzene, the electron density is delocalised into the π system across 6 carbon atoms while in an alkene, the pair of electrons is localised between 2 carbon atoms in a π bond.

Electron Donating Groups: groups which donate electrons into the aromatic ring when they are attached to a carbon in the ring. OH, an electron donating group, is 2- and 4-directing, meaning that substituents will be substituted at positions 2 and 4 during an electrophilic substitution reaction.

Electron Withdrawing Groups: groups which pull electron density away from the delocalised π system of benzene. NO_2, an electron withdrawing group, is 3-directing meaning that substituents will be substituted at carbon 3 during an electrophilic substitution reaction.

Electrophilic Substitution: a reaction in which an electrophile (an electron pair acceptor) reacts with another compound to replace an atom / group of atoms.

Haloalkane: an organic compound containing a halogen atom (F/Cl/Br/I) bound to an alkyl chain.

Halogen Carrier: a Lewis acid that can bind to a halogen molecule, weakening the halogen bond and allowing the halogen to function as an electrophile and attack electrons in an aromatic ring. Examples of halogen carriers include iron, iron halides and aluminium halides.

Kekulé's Structure of Benzene: a model of benzene which contains alternating C=C double and C-C single bonds in a hexagonal ring, with each carbon atom bound to one hydrogen atom.

Phenol: a weak acid that reacts with NaOH but not carbonates. Phenol has an aromatic ring with an OH group attached. Phenol can undergo electrophilic substitution reactions more easily than benzene as the lone pair in the p-orbital of oxygen is donated into the π system of phenol, increasing its electron density. As a result of this electron donation, phenol is more susceptible to electrophilic attack than benzene.

6.1.2 - Carbonyl Compounds

2,4-dinitrophenylhydrazine: also known as Brady's reagent, this compound forms an orange precipitate in the presence of aldehydes and ketones. The melting point of the 2,4-DNP derivative of a carbonyl can be used to identify the carbonyl compound.

Aldehyde: a compound containing the -CHO functional group at the end of an alkyl chain. Aldehydes can be oxidised to carboxylic acids using $Cr_2O_7^{2-}$/ H^+.

Carbonyl: the C=O group. Aldehydes and ketones are carbonyl compounds.

Nucleophile: an electron pair donor.

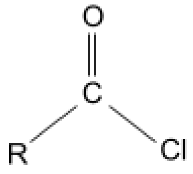
Nucleophilic Addition: a reaction in which an electrophilic π bond reacts with a nucleophile, breaking the π bond and forming 2 new σ bonds. Examples include carbonyl compounds reacting with $NaBH_4$ to form alcohols or with HCN to form hydroxynitriles.

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

Tollens' Reagent: also known as ammoniacal silver nitrate, this reagent forms a silver mirror in the presence of an aldehyde and can be used to distinguish between aldehydes and ketones. An aldehyde is oxidised to a carboxylic acid while silver ions in Tollens' are reduced to silver.

6.1.3 - Carboxylic Acids and Esters

Acyl Chloride: a compound containing the functional group shown below. Acyl chlorides can be made from carboxylic acids and $SOCl_2$ and they are used to form esters, carboxylic acids and primary and secondary amides.



Bronsted-Lowry Acid: a proton donor.

Bronsted-Lowry Base: a proton acceptor.

Carboxylic Acid: an organic compound containing the -COOH functional group. Carboxylic acids react with metals as well as bases such as carbonates, metal oxides and alkalis.

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 a reaction between carboxylic acids and alcohols in the presence of an acid catalyst or by a reaction between acid anhydrides and alcohols.

Hydrolysis: a reaction in which water is used to break down a compound. Esters can either be hydrolysed with hot aqueous acid (forming carboxylic acids and alcohols) or with hot aqueous alkali (forming carboxylate salts and alcohols).

Water Soluble: a compound that can dissolve in water. Carboxylic acids are water soluble as they can form hydrogen bonds with the H_2O molecules.

6.2.1 - Amines

Aliphatic Amine: an amine which only contains straight or branched alkyl chains. Aliphatic amines can be formed via a substitution reaction of haloalkanes with either ammonia or amines in ethanol solvent.

Amines: compounds that contain the NR_3 functional group (where R could be hydrogen atoms or alkyl chains). Amines are basic as the nitrogen lone pair allows the acceptance of a proton. In a reaction between amines and dilute acids, salts are formed.

Aromatic Amine: an amine which contains a benzene ring directly attached to the nitrogen atom. Aromatic amines can be formed by reducing nitroarenes with tin and concentrated HCl.

6.2.2 - Amino Acids, Amides and Chirality

α-Amino Acid: a compound with the general formula $RCH(NH_2)COOH$, where an amino group and a carboxylic acid group are bonded to the same carbon atom. The carboxylic acid group of an amino acid reacts with alkalis or can be used to form esters. The amine group of an amino acid reacts with acids.

Amine Group: the $-NH_2$ group in an organic compound.

Carboxylic Acid Group: the -COOH group in an organic compound.

Chiral Centre: a carbon atom which is bonded to 4 different groups.

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

Optical Isomerism: a type of stereoisomerism in which compounds are non-superimposable mirror images of one another (caused by the presence of a chiral centre).

Primary Amide: an organic compound which contains the functional group RNH_2 (where R is an alkyl chain).

Secondary Amide: an organic compound which contains the functional group R_2NH (where R is an alkyl chain).

Stereoisomers: compounds with the same structural formula but a different arrangement of atoms in space.

6.2.3 - Polyesters and Polyamides

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

Amide Hydrolysis: amides can either be hydrolysed under acidic conditions (forming carboxylic acids and ammonium salts) or under alkaline conditions (forming carboxylate salts and either ammonia or an amine). Polyamides can be hydrolysed in a similar way.

Condensation Polymerisation: a long chain molecule formed when monomers react together with the release of small molecules such as water. Types of condensation polymers are polyamides (formed from carboxylic acids / acyl chlorides and amines) and polyesters (formed from carboxylic acids/ acyl chlorides and alcohols).

Ester Hydrolysis: esters can either be hydrolysed with hot aqueous acid (forming carboxylic acids and alcohols) or with hot aqueous alkali (forming carboxylate salts and alcohols). Polyesters can be hydrolysed in a similar way.

Monomer: a small molecule that is used to form polymers.

Polymer: a large molecule made from many small units that have been bonded together.

Polymerisation: the process of making a polymer from its monomers. There are two types: addition polymerisation and condensation polymerisation.

Repeat Unit: a structure within a polymer that appears over and over again. Joining many repeat units together would form the polymer.

6.2.4 - Carbon-Carbon Bond Formation

Acylation: a reaction that is used to form substituted aromatic compounds, using an acyl chloride to form a C-C bond in the presence of a halogen carrier.

Acid Hydrolysis: the breakdown of a compound using aqueous acid. Nitriles can be hydrolysed to form carboxylic acids.

Alkylation: a reaction which is used to form substituted aromatic compounds, using a haloalkane to form a C-C bond in the presence of a halogen carrier.

Carbonyl: a compound which contains the C=O functional group.

Friedel-Crafts Reactions: reactions which were developed to attach substituents to an aromatic ring. Acylation and alkylation are the 2 main types of Friedel-Craft reactions.

Halogen Carrier: a Lewis acid that can bind to a halogen molecule, weakening the halogen bond and allowing the halogen to function as an electrophile and attack electrons in an aromatic ring. Examples of halogen carriers include iron, iron halides and aluminium halides.

Nitrile: an organic compound which contains a -C≡N group bound to an alkyl chain.

Nucleophile: an electron pair donor.

Nucleophilic Addition: a reaction in which an electrophilic π bond reacts with a nucleophile, breaking the π bond and forming 2 new σ bonds. One example is the reaction of carbonyl compounds with HCN to form hydroxynitriles.

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. One example is the reaction of haloalkanes with CN^- and ethanol to form nitriles.

Reduction: gain of electrons/ decrease in oxidation number. Nitriles can be reduced to amines with H_2/Ni.

6.2.5 - Organic Synthesis

Distillation: a technique in which a liquid is heated then the vapour is cooled and collected in a separate flask to the reaction mixture. During distillation, the condenser must be positioned horizontally.

Filtration Under Reduced Pressure: a technique used to separate and dry an organic solid. A Büchner funnel is inserted into the top of a side-arm flask and a vacuum is applied. The solution is poured onto filter paper in the Büchner funnel so that the solid product can be separated.

Functional Group: a group of atoms responsible for the characteristic reactions of a compound.

Melting Point Apparatus: a piece of apparatus used to determine the melting point of a sample. The recorded melting point range is compared with known values to determine whether the sample is pure.

Quickfit Apparatus: glassware that easily fits together in a variety of arrangements.

Recrystallisation: a technique used to purify an organic solid. The sample is dissolved in the minimum volume of hot solvent and filtered. The filtrate is then cooled before being filtered under reduced pressure. The purified solid will collect on the filter paper in the Büchner funnel.

Reflux: the continual boiling and condensing of a reaction mixture. This is to ensure that the reaction goes to completion. During reflux, the condenser must be positioned vertically.

Synthetic Route: a series of steps that are followed to make a specific compound.

6.3.1 - Chromatography and Qualitative Analysis

Aldehyde: an organic compound containing the C=O functional group at the end of an alkyl chain. Aldehydes form a silver mirror when reacted with Tollens' reagent. Aldehydes can be oxidised to carboxylic acids with acidified potassium dichromate, causing a colour change from orange to green.

Alkene: an organic compound containing the C=C functional group. Alkenes decolourise bromine water.

Carbonyl: an organic compound containing the C=O functional group. Carbonyl compounds react with 2,4-DNP to form an orange precipitate.

Carboxylic Acid: an organic compound containing the -COOH functional group. Carboxylic acids react with CO_3^{2-}, causing effervescence.

Chromatography: a technique used to separate and identify components in a mixture. There are several different types of chromatography, including: thin layer chromatography, and gas chromatography. Separation during chromatography depends on the balance between solubility in the mobile phase and retention by the stationary phase.

Gas Chromatography: a type of chromatography in which a column is packed with a solid (or a solid coated in a liquid) and a gas is passed through the column under pressure at high temperature. Mass spectrometry may be used to analyse components separated by GC.

Haloalkane: an organic compound containing a halogen atom attached to an alkyl chain. The test for haloalkanes is a reaction with aqueous silver nitrate in ethanol. Chloroalkanes form a white precipitate, bromoalkanes form a cream precipitate and iodoalkanes form a yellow precipitate.

Mobile Phase: a substance that moves through the chromatography system to separate the mixture. This may be a gas (GC) or a liquid (TLC).

Phenol: an organic compound containing an aromatic ring with an -OH group attached. Phenols are weak acids but do not react with CO_3^{2-}.

Primary Alcohol: an organic compound with the general formula RCH_2OH. Primary alcohols can be oxidised with acidified dichromate, causing a colour change from orange to green.

Qualitative Analysis: techniques that are used to identify whether or not an element, functional group or ion is present in a sample.

Retention Time: the time taken for a sample to travel from the inlet to the detector in GC. The recorded retention time can be compared with standards to identify the substances in the mixture.

R_f value: in TLC, the R_f values can be calculated as shown below then compared with standards to identify what substances present in a mixture.

$$R_f = \text{distance moved by substance} \div \text{distance moved by solvent}$$

Secondary Alcohol: an organic compound with the general formula R_2CHOH. Secondary alcohols can be oxidised with acidified dichromate, causing a colour change from orange to green.

Stationary Phase: a substance through which the mobile phase moves in chromatography. This is typically a solid although a solid coated in a liquid may be used in GC.

Thin Layer Chromatography (TLC): a type of chromatography in which a plate is coated with a solid and a solvent moves up the plate.

6.3.2 - Spectroscopy

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 show what environments are present.

Chemical Shift: the shift of a carbon or proton environment relative to standard (TMS). The chemical shift value (δ) depends on the molecular environment of the proton/ carbon atom.

Coupling: interaction between adjacent non-equivalent protons during NMR spectroscopy.

D_2O Exchange: as O-H and N-H peaks can appear across a wide range of chemical shift values on a proton NMR spectrum, D_2O exchange can be used to identify which peaks are caused by O-H and N-H protons. Firstly, a proton NMR is run on a sample. The sample is then shaken with D_2O and a second proton NMR is run. Any peaks that are due to O-H or N-H protons will disappear on the second spectrum as these protons will be exchanged for deuterium.

Deuterated Solvent: a solvent, such as $CDCl_3$, in which all of the hydrogen atoms have been replaced by deuterium (^2H). Deuterated solvents are used in order to prevent the appearance of a solvent peak on the ^1H NMR spectrum.

Doublet: a signal on a ^1H NMR spectra made up of 2 peaks, indicating that there is 1 adjacent non-equivalent proton.

Elemental Analysis: a sample is analysed to determine the proportion of elements that make up the compound present. This is done by converting a known amount of an unknown sample into simple known compounds.

Environment: in NMR spectroscopy, a proton or carbon environment considers the atoms/ groups that are adjacent to that hydrogen/ carbon atom. If 2 protons / carbons are surrounded by different groups of atoms, they are in different environments.

Equivalent protons: protons that are in the same environment.

IR Spectroscopy: a technique used to identify particular bonds and functional groups within a molecule. Infrared radiation is absorbed by covalent bonds in molecules, causing them to vibrate at a specific frequency.

Mass Spectroscopy: a technique used to identify compounds and determine relative molecular mass by measuring their mass to charge ratio.

n+1 Rule: used to determine spin-spin splitting patterns of adjacent non-equivalent protons. A proton with n adjacent non-equivalent protons will have a signal made up of n+1 peaks on a ^{1}H NMR spectrum.

Nuclear Magnetic Resonance (NMR): a technique that uses the absorption of electromagnetic radiation by a 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 show the type of environments. The integration trace (equivalent to 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.

Quartet: a signal on a ^{1}H NMR spectra made up of 4 peaks, indicating that there are 3 adjacent non-equivalent protons.

Spin-Spin Splitting: an interaction between adjacent non-equivalent protons. When protons couple (interact with one another), the signal on the ^{1}H NMR spectrum is split into a multiplet according to the n+1 rule.

Tetramethylsilane (TMS): the standard for chemical shift measurement in NMR spectroscopy.

Triplet: a signal on a ^{1}H NMR spectra made up of 3 peaks, indicating that there are 2 adjacent non-equivalent protons.