

OCR (B) Chemistry A-level

Storyline 5: What's in a Medicine? Detailed Notes

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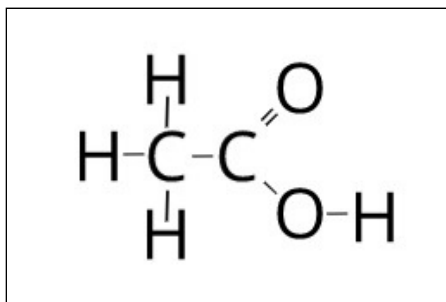


Organic Functional Groups and Reactions

Carboxylic Acids

Carboxylic acids are organic compounds containing the **functional group -COOH**, made of a **carbonyl group (C=O)** and an **-OH acid group**. When naming carboxylic acids, the suffix **-anoic acid** is used. For example, a carboxylic acid containing a chain of four carbon atoms would be called butanoic acid.

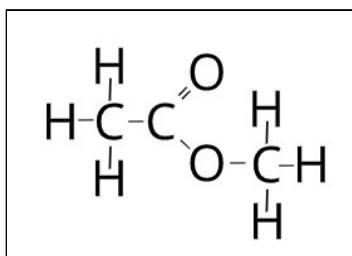
Example: The displayed structure of ethanoic acid.



Esters

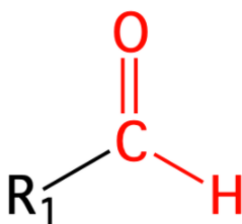
Esters have the functional group **-COO-**. They are named after the **alcohol and carboxylic acid** from which they are formed. For example, the ester formed from methanol and propanoic acid is methyl propanoate and the ester formed from butanol and ethanoic acid is butyl ethanoate.

Example: The displayed structure of methyl ethanoate.



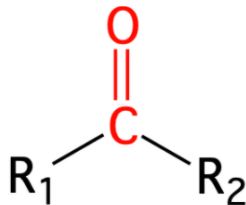
Aldehydes

Aldehydes are produced from the oxidation and distillation of **primary alcohols**. Aldehydes have a carbonyl group at the **end of the carbon chain** (the carbonyl group is only attached to **one other carbon atom**). This gives them the functional group **-CHO**.



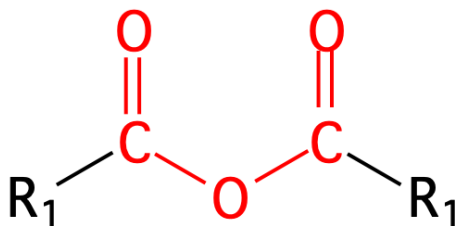
Ketones

Ketones also contain the **functional group -C=O** , a carbonyl group. They are produced from the oxidation of **secondary alcohols** with acidified potassium dichromate(VI). Ketones have a carbonyl group in the middle of a carbon chain (the carbonyl group is attached to **two other carbon atoms**).



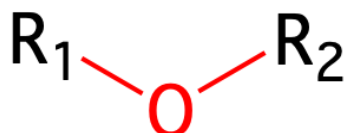
Acid Anhydrides

Acid anhydrides are identified by their functional group **-COOCO-** , which consists of two carbonyl groups joined by an oxygen atom.



Ether

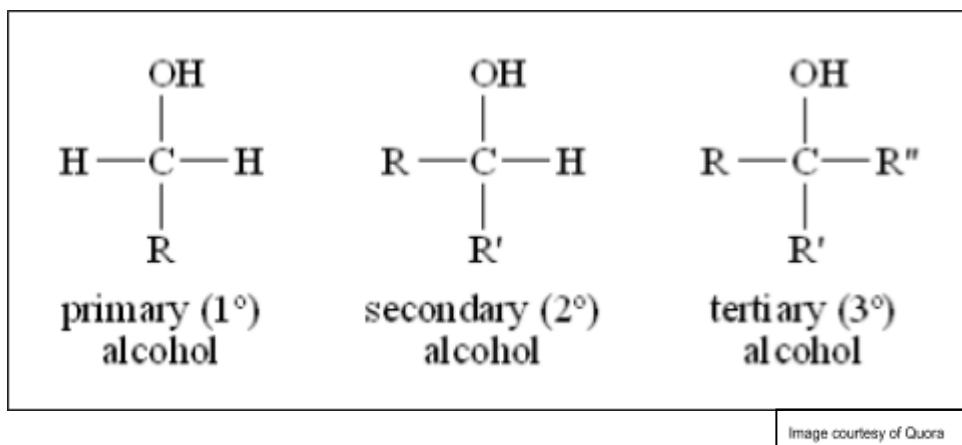
Ethers are identified by their functional group **-O-** , which consists of two alkyl chains connected to a single oxygen atom.



Alcohols

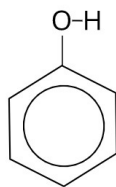
Alcohols contain an **-OH group** and have the general formula **$\text{C}_n\text{H}_{2n+1}\text{OH}$** . They can be produced via methods of fermentation or hydration. Alcohols are named according to **IUPAC** rules and have the suffix **-ol**. Alcohols can be **primary (1°)**, **secondary (2°)** or **tertiary (3°)**, depending on the position of the hydroxyl group.





Phenols

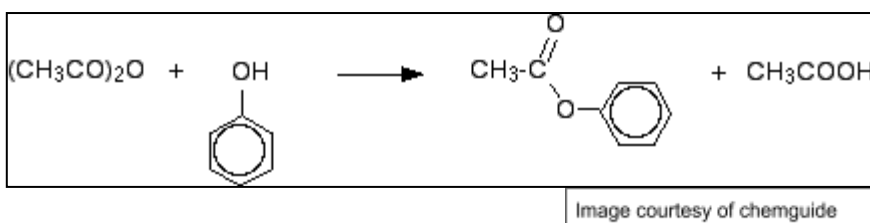
Phenols are organic compounds containing a **benzene ring** with an OH **alcohol group**. This makes them **aromatic alcohols**. Phenols are weak acids. They can be neutralised in a reaction with NaOH but will not react with carbonates.



Phenols can be identified by using neutral iron(III) chloride solution (ferric chloride). When phenol is present, an intense **purple solution** forms.

Production of Esters from Phenol and Acid Anhydride

Phenol reacts like an alcohol to produce an **ester**, this reaction often requires **heating**. The reaction would occur **faster** with acyl chloride than an acid anhydride.



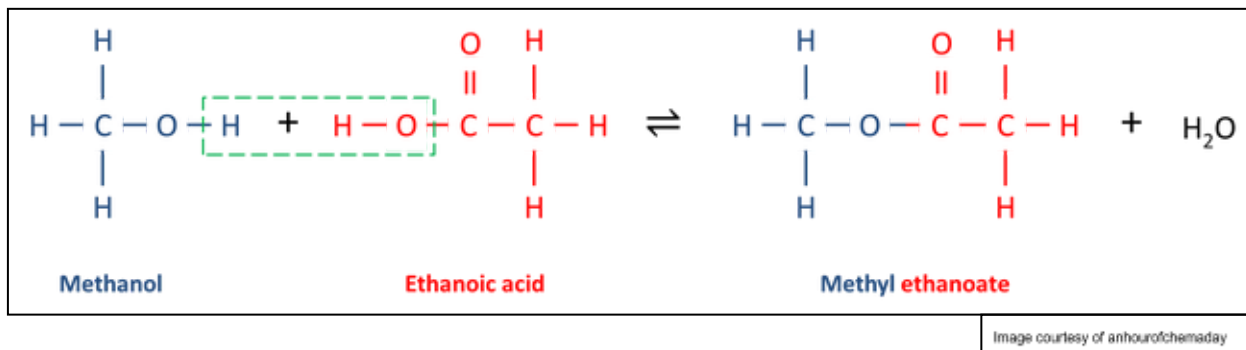
A similar reaction to the one shown above is used in the manufacture of aspirin.

Esterification

Carboxylic acids can **react with alcohols** in the presence of a **strong acid catalyst** (like concentrated sulfuric acid) to form **esters**. **Concentrated sulfuric acid** is often used as the acid catalyst. This reaction is called **esterification** and is carried out under **reflux conditions**.



Example:



A method for remembering the reaction: Remove the -OH from the acid and the hydrogen from the alcohol to make water. Then join the acid and alcohol together.

Esters are **sweet-smelling compounds** used in food flavourings and perfumes. They have **low boiling points** and make **good solvents** for polar molecules.

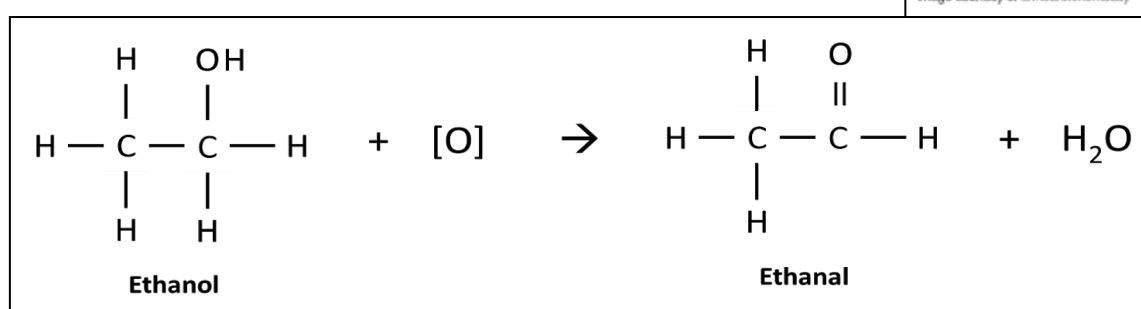
Acid anhydrides can also be used to esterify alcohols. This occurs in an **addition-elimination** mechanism. Acid anhydrides react **less vigorously** than acyl chlorides and do not produce toxic HCl as a side product. As a result, they are often **preferred as a reagent** in esterification.

Oxidation of Alcohols

Primary and **secondary** alcohols can be **oxidised** to produce various products but **tertiary** alcohols are **not easily oxidised**.

When primary alcohols are heated in the presence of **acidified potassium dichromate(VI)**, they are **oxidised** to aldehydes. **Distillation** is required to separate the **aldehyde** product.

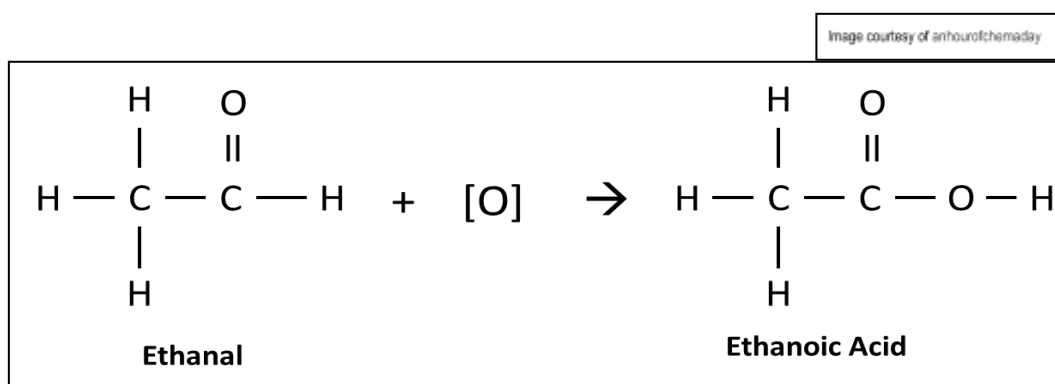
Example: Oxidation of ethanol to ethanal



When an aldehyde is heated further with acidified potassium dichromate(VI) under **reflux** conditions, the aldehyde is **oxidised** to a **carboxylic acid**. Primary alcohols are oxidised to aldehydes and then to carboxylic acids.

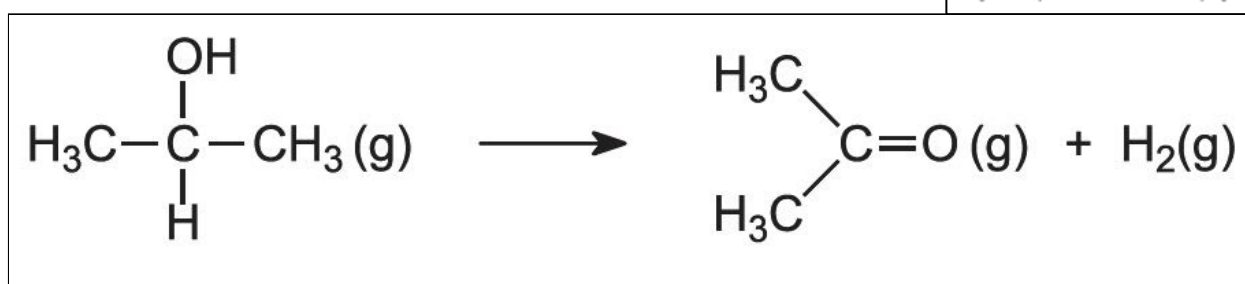


Example: Oxidation of ethanal to ethanoic acid



Secondary alcohols can be oxidised to **ketones** when heated in the presence of **acidified potassium dichromate(VI)**.

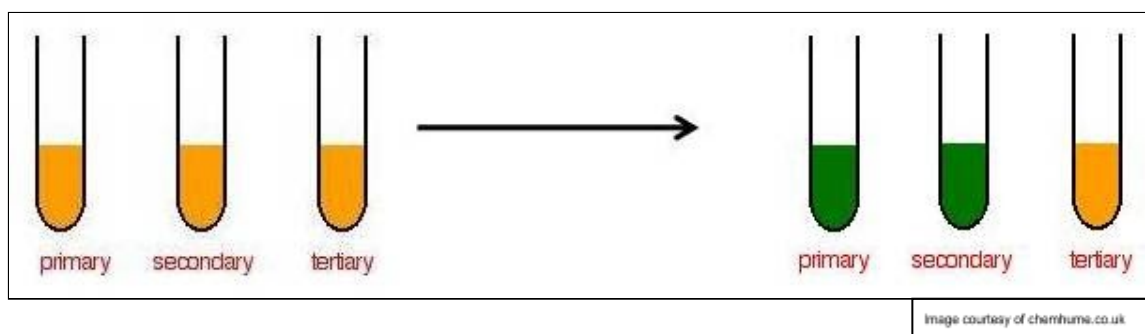
Example: Oxidation of propan-2-ol to propanone



Potassium Dichromate(VI) ($\text{K}_2\text{Cr}_2\text{O}_7$)

Potassium dichromate(VI) is used as an **oxidising agent** in the oxidation of alcohols. As the alcohol is oxidised, potassium dichromate(VI) is **reduced**. This reduction is observed as a colour change from **orange to green**, which indicates the alcohol has undergone oxidation. The colour change occurs due to the change in **oxidation state** of the chromium ion.

Example:



Elimination Reactions

Elimination - a small molecule is **removed** from a larger molecule, often forming a double bond.

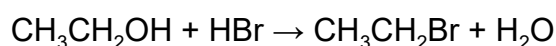


Alkenes can be formed from the **dehydration of alcohols**, where a molecule of **water is removed** from the molecule. In order to do this, the alcohol is heated under reflux with **concentrated sulfuric acid**, or heated using **Al₂O₃**.

Substitution Reactions

Alcohols can react with **halogenating agents** via **nucleophilic substitution**. The **-OH** group is replaced by a **halogen**, producing a **haloalkane**.

A reaction mixture of concentrated **sulfuric acid** and **potassium bromide** can be used to produce **bromoalkanes**. The potassium bromide reacts with the sulfuric acid to form HBr. This then reacts with the alcohol to produce the bromoalkane.

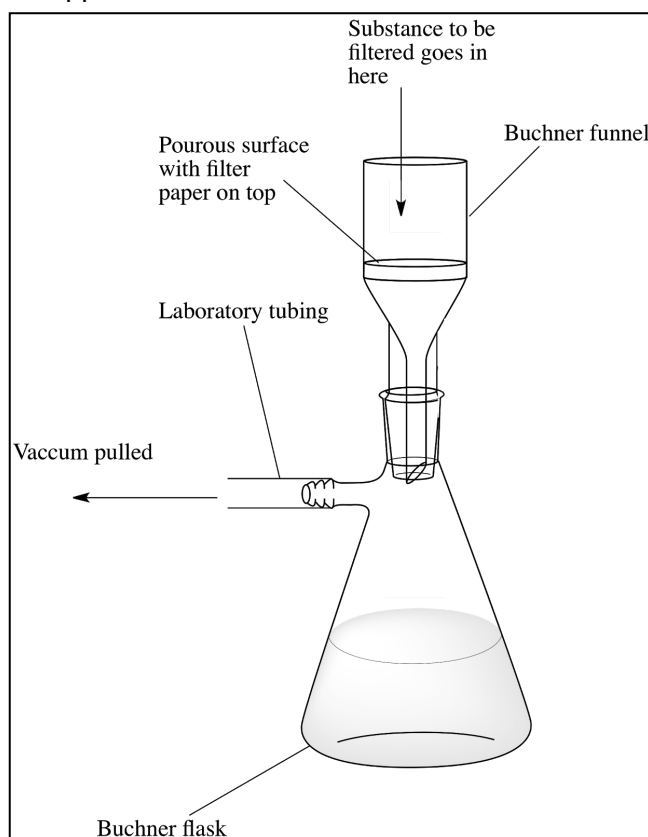


Techniques and Procedures for making a Solid Organic Solvent

Filtration Under Reduced Pressure

This method of filtration is **faster** than gravity filtration due to the solvent and air being pulled through the filter paper.

Diagram: Vacuum filtration apparatus



Recrystallisation

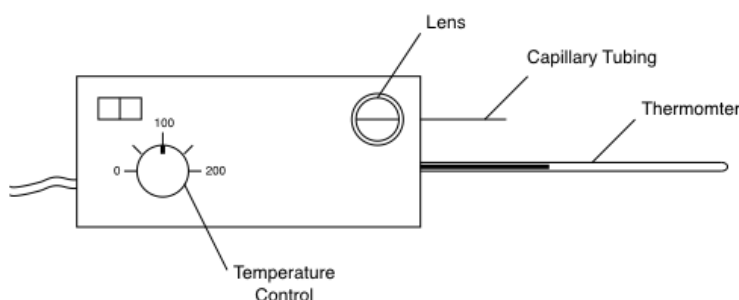
Recrystallization is a method of **purifying an impure compound** using a solvent. This method relies on the fact that the solubility of most organic solids **increases with temperature**. To complete recrystallization an impure solid is dissolved in a **minimum amount** of a **hot solvent**, as the solution is cooled the solubility of the solid decreases and the **crystals** will form.

The solvent used will need to dissolve the solid being purified when hot but not when cold.

Melting Point Determination

The melting point of an organic solid can be found by heating up a sample in a **capillary tube**, where the change of state can be observed.

Diagram: Melting point apparatus



Thin-Layer Chromatography (TLC)

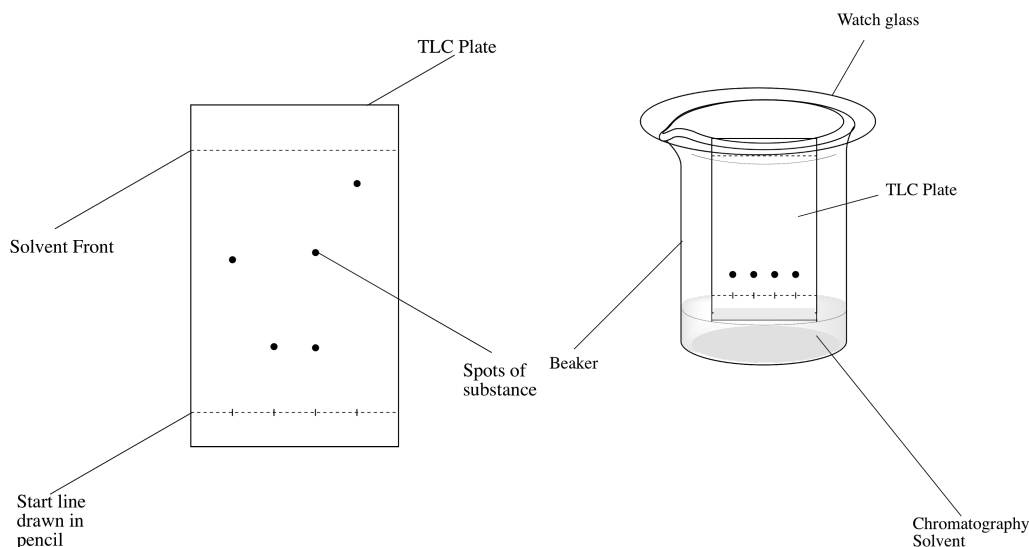
In TLC chromatography, a **metal plate** is coated with a **thin layer of silica** and the sample being analysed is dotted on the plate. These initial samples must be placed above the level of the solvent in the container.

The **solvent** is then allowed to move up the plate, separating the substances within the sample. The plate is taken out of the container and the **solvent front** is marked in pencil when it is roughly 1 cm from the top of the plate. This is the distance that the solvent has traveled - this value is needed for **R_f** value calculations.

The plate is then dried in a **fume cupboard** to reduce toxic fumes. The chemical traces can then be viewed using a **UV lamp** and the distances travelled by the separated substances can be measured. Alternatively, a **developing agent** can be added, such as **iodine**, to allow the **colourless** traces to be seen by the naked eye.



Diagram: TLC plate and TLC plate apparatus



Techniques and Procedures for Preparing and Purifying a Liquid Organic Product

Heating under Reflux

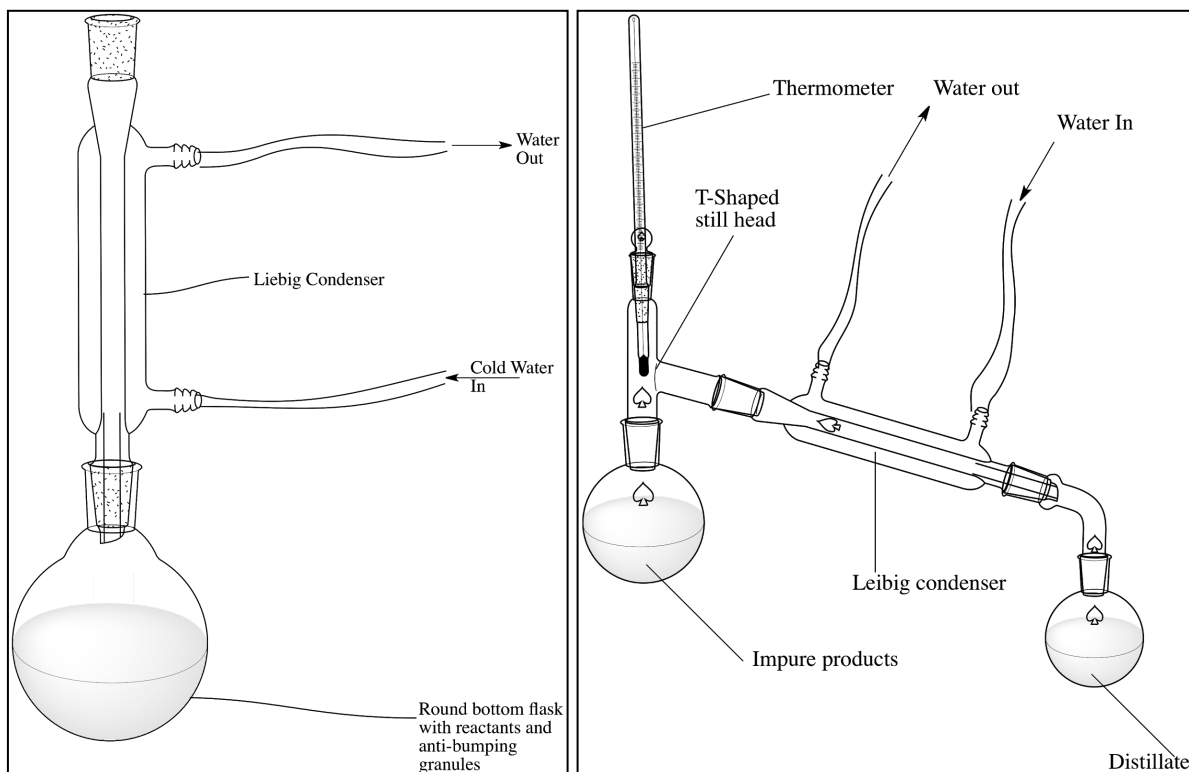
Reflux apparatus is used to **continually heat** the contents of the flask to allow reactions like the **oxidation** of primary alcohols to proceed all the way to the formation of carboxylic acids. The **condenser** helps ensure the vapours condense and **return** to the flask for further heating. This ensures the product vapours do not escape.

Distillation

Distillation apparatus is used to separate liquids with **different boiling points**. The round-bottomed flask is heated and the liquid with the lower boiling point will **evaporate** first. It rises out of the flask and into the attached tubing which is surrounded by a condenser. The condenser causes the vapour to **cool and condense** back into a liquid, which is then collected in a separate flask.



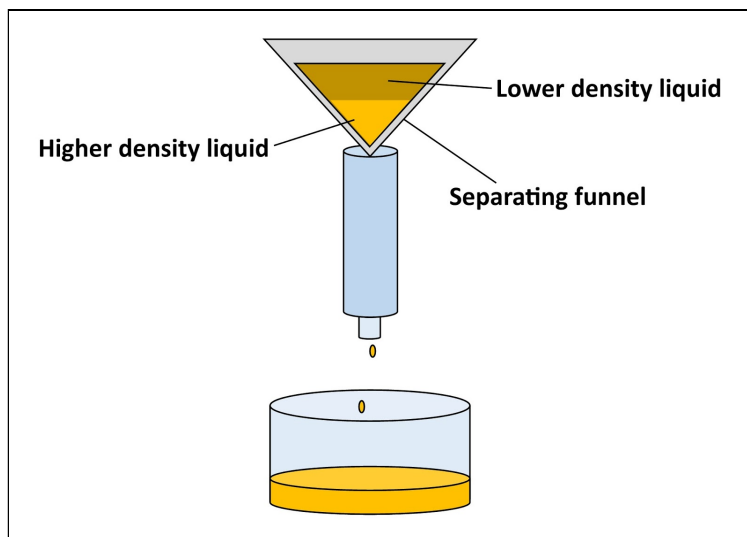
Diagrams: Reflux apparatus (left) and distillation apparatus (right)



Separating Funnel

A separating funnel is used to separate two liquids with **different densities**. The mixture is added to the flask, and then the flask is stoppered and inverted to mix the contents. The liquids are allowed to **separate** into **two layers**. The tap can then be opened to collect the bottom, denser liquid in one flask and the second, less dense liquid in a second flask. Usually, these layers will be distinguished to be an aqueous and an organic layer.

Diagram: Separating funnel



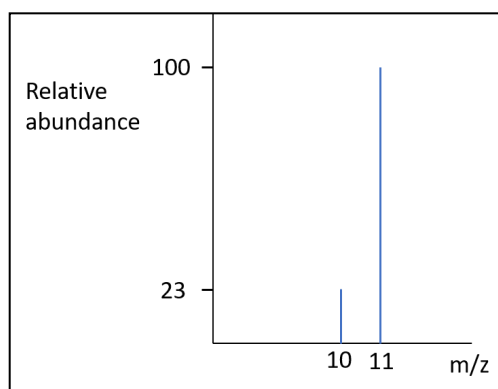
Green Chemistry

Green chemistry has the aim of reducing the impact of chemistry on human health and the environment by using alternative **environmentally-friendly** reactions, such as ones that require lower temperatures. They often try to follow the '**12 Principles of Green Chemistry**', for example choosing a reaction with an efficient **atom economy**, using a **catalyst** to reduce reaction temperatures and reducing the production of **pollutants**.

Modern Analytical Techniques - Mass Spectrometry

This is an **analytical technique** used to identify different molecules and find their **relative molecular mass**. During mass spectrometry, a **vaporised** sample (atoms or molecules) is ionised to form positive ions. The ions are then accelerated, deflected by a magnetic field and detected. A graph is produced with the **mass to charge ratio (m/z)** on the x-axis and **relative abundance** on the y-axis.

Example:



The M⁺ Peak

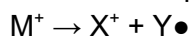
The molecular ion peak (**M⁺**) is the peak with the **greatest mass to charge ratio**. The molecular mass (**Mr**) of a compound is equal to the m/z value of this peak. This is the peak that is furthest to the right on the spectrum. Other techniques can be used to determine the **empirical formula**, then scaled up to the Mr value from mass spectrometry to give the **molecular formula**.

The M⁺¹ Peak

The M⁺¹ peak is a small peak which is 1 unit to the right of the molecular ion peak. This is **caused by the presence of the ¹³C isotope** (the relative abundance of ¹³C is 1.11%). ¹³C has one more neutron than ¹²C meaning that the relative formula mass is **increased by 1**.

Fragmentation

Fragment ions are formed when an **unstable molecular ion breaks** up into a positive ion and an uncharged **free radical** (a species which contains an unpaired electron):



Only charged particles are detected so the free radical ($Y\bullet$) will not produce a line on the spectrum. Each line on the mass spectrum represents a different fragment ion. Fragments can also help to deduce the structure of the compound.

Modern Analytical Techniques - Infra-red Spectroscopy

When infra-red radiation is directed at a compound, specific frequencies are absorbed by bonds in the molecule. The percentage transmittance of infra-red at each frequency is recorded by a detector and then plotted on a graph.

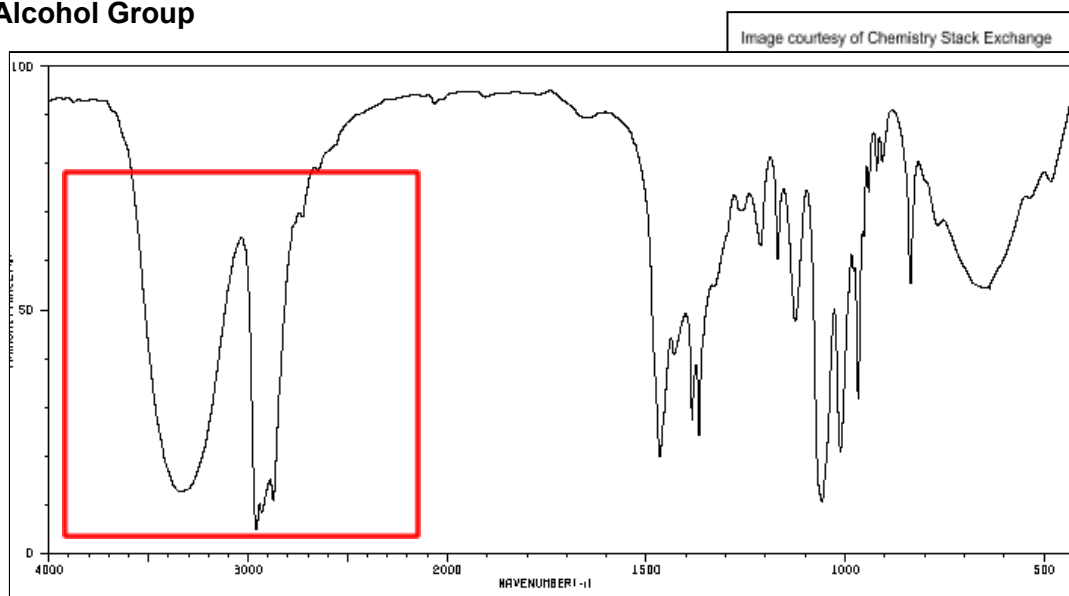
Energy that is absorbed by the compound causes bonds to vibrate, meaning the bond stretches or bends. The amount of vibration depends on the length of the bond and the mass of the atoms.

The peaks on an infra-red spectrum can be used to identify the functional groups present in a molecule, as each bond absorbs a specific frequency of IR radiation. A peak can be compared with known values from a databook to identify the bond.

The fingerprint region on an infra-red spectrum is the region (typically between 1500cm^{-1} and 500cm^{-1}) that contains a complicated series of absorptions. Every compound has a unique fingerprint region.

A spectrum is produced from the measurements which has characteristic curves for the different functional groups:

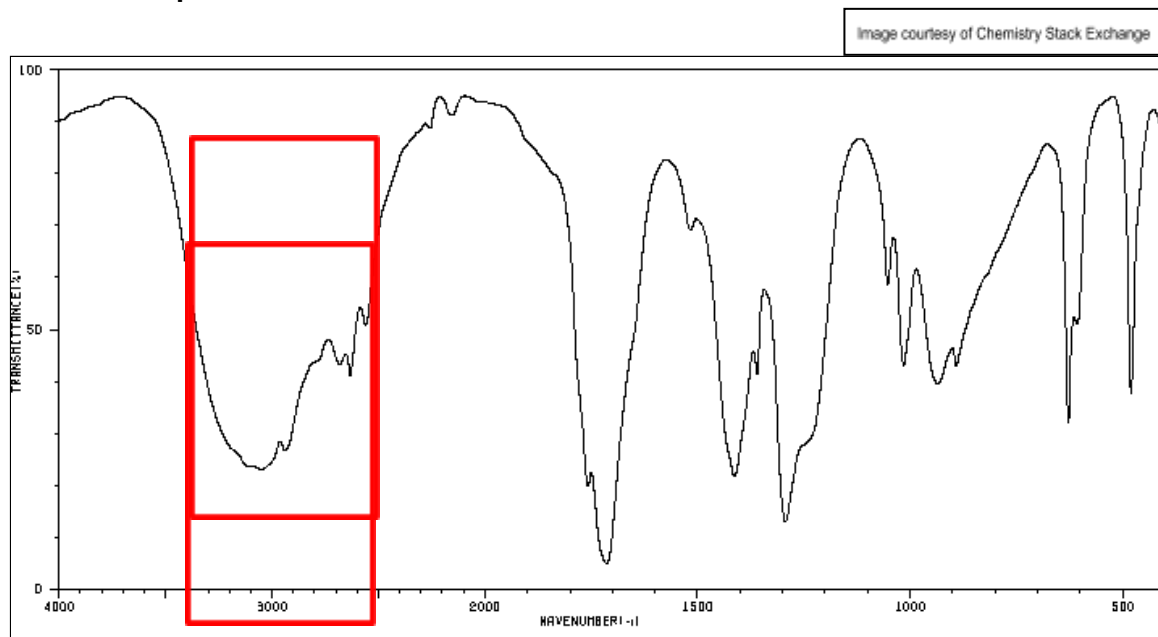
-OH Alcohol Group



The characteristic peak is in the range $3230\text{--}3550\text{ cm}^{-1}$

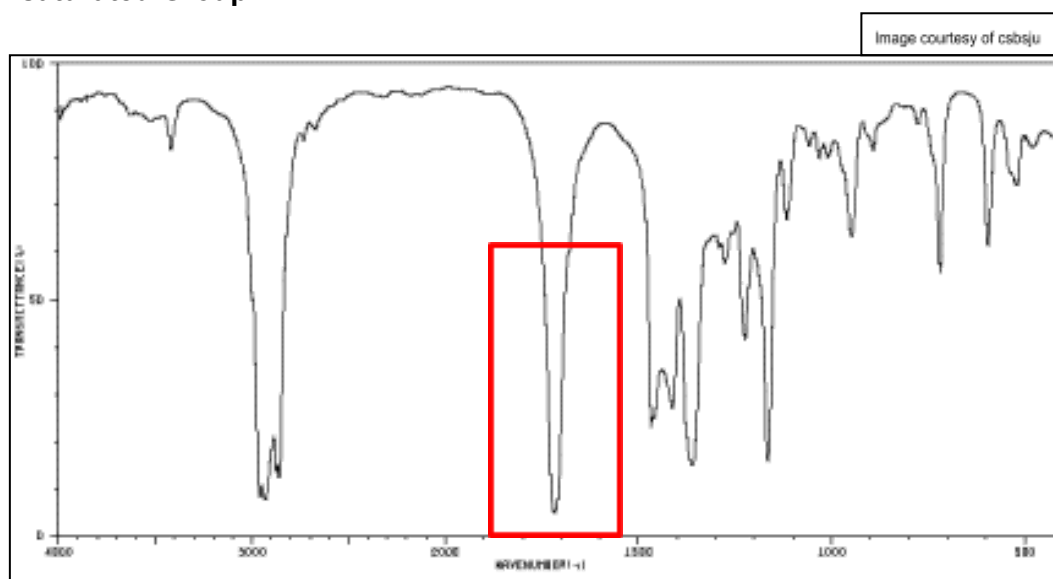


-OH Acid Group



The characteristic peak is in the range 2500-3300 cm^{-1}

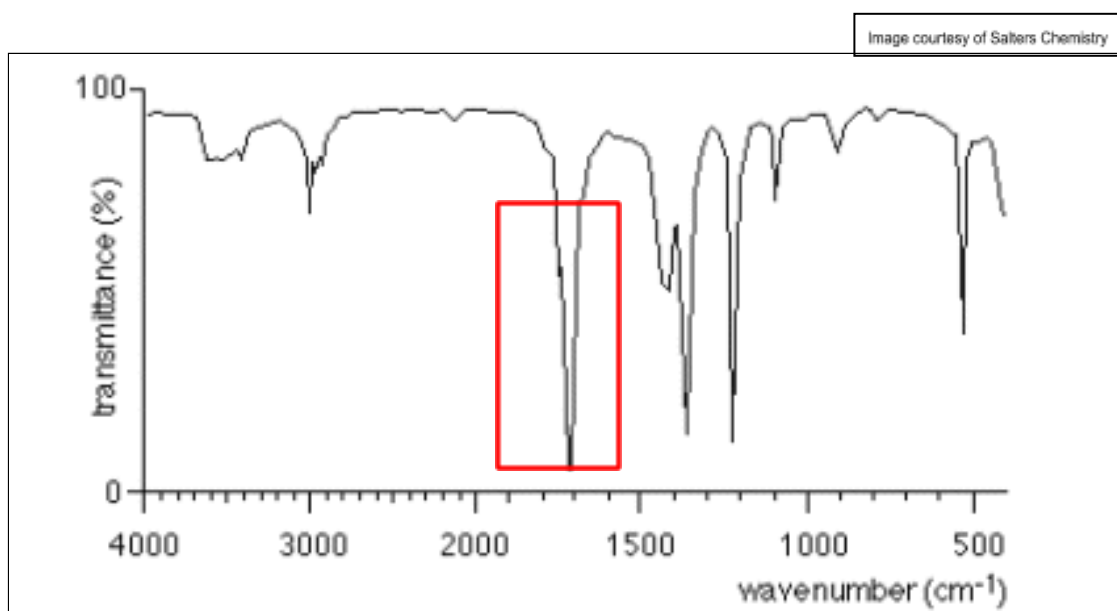
C=C Unsaturated Group



The characteristic peak is in the range 1620-1680 cm^{-1}



C=O Carbonyl Group



*The characteristic peak is in the range **1680-1750 cm⁻¹***

