

Edexcel Chemistry A-Level

Topic 7: Modern Analytical Techniques I Detailed Notes





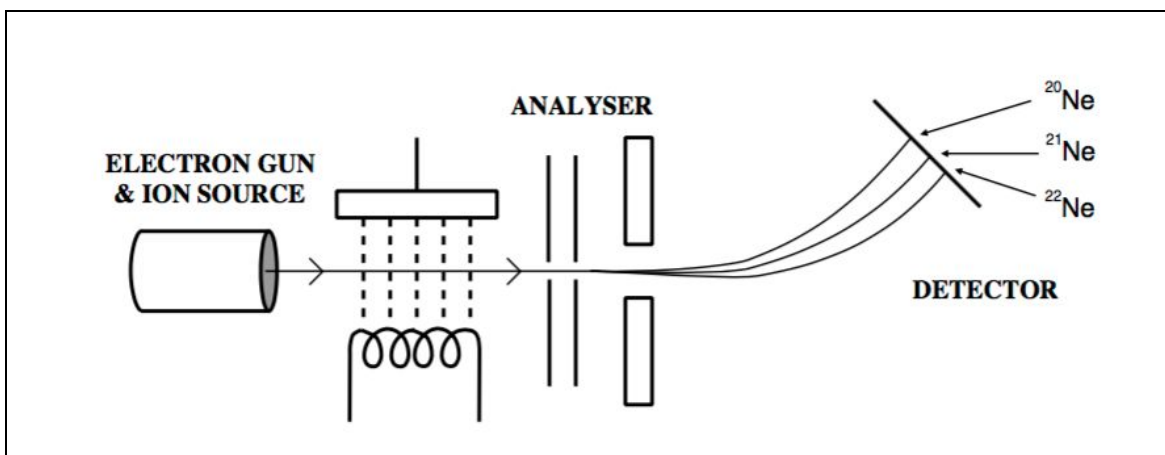
Topic 7A: Mass Spectrometry

This is an **analytical technique** used to identify different isotopes and find the overall relative atomic mass of an element.

Time of Flight (TOF) Mass Spectrometry

This form of mass spectrometry records the time it takes for ions of each isotope to reach a detector. Using this, **spectra** can be produced showing **each isotope present**.

1. **Ionisation** - A sample of an element is **vapourised** and injected into the mass spectrometer where a **high voltage** is passed over the chamber. This causes electrons to be removed from the atoms (it is ionised) leaving **+1 charged ions** in the chamber.
2. **Acceleration** - These positively charged ions are then **accelerated** towards a negatively charged **detection plate**.
3. **Ion Drift** - The ions are then deflected by a **magnetic field** into a **curved path**. The radius of their path is dependant on the charge and mass of the ion.



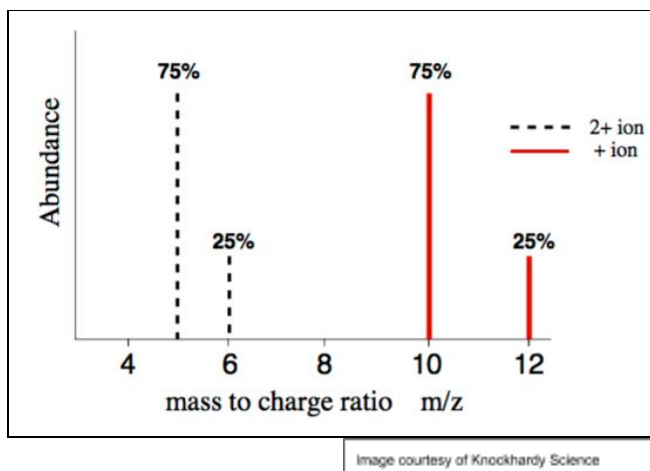
4. **Detection** - When the positive ions hit the negatively charged detection plate, they **gain an electron** producing a **flow of charge**. The greater the abundance, the greater the current produced.
5. **Analysis** - These current values are then used in combination with the **flight times** to produce a **spectra print-out** with the relative abundance of each isotope displayed.

During the ionisation process, a **2+ charged ion** may be produced. These ions are affected more by the magnetic field producing a curved path of **smaller radius**. As a result, its mass to charge ratio (m/z) is halved and this can be seen on spectra as a trace at **half the expected m/z value**.





Example:



Using this spectra, the **Ar** can be calculated:

$$\text{Ar} = \frac{m/z \times \text{abundance}}{\text{Total abundance}}$$

Example:

$$\text{Ar} = \frac{(10 \times 75) + (12 \times 25)}{(75 + 25)} = 10.5$$

High Resolution Mass Spectrometry

This is a much **more sensitive** form of mass spectrometry which allows the Mr of a substance to be determined to **several decimal places**. Precise atomic masses are always given and can then be used to calculate the molecular formula of the compound being tested.

Topic 7B: Infrared (IR) Spectrometry



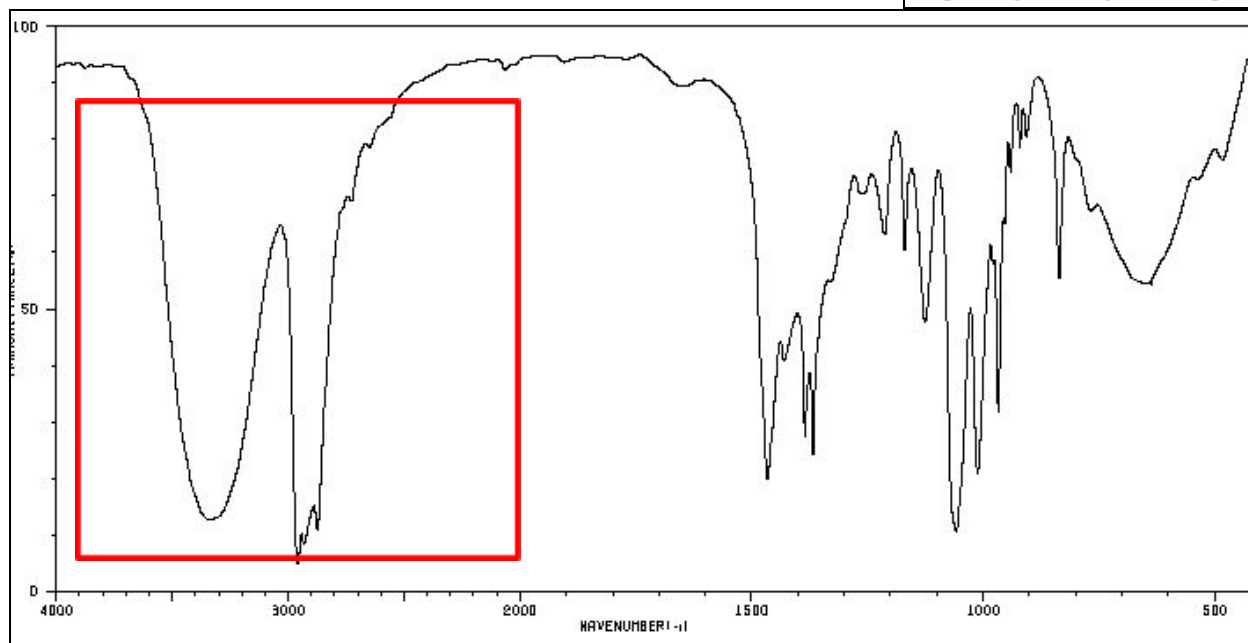


This analytical technique used **infrared (IR) radiation** to determine the **functional groups** present in organic compounds. The IR radiation is passed through a sample where the different types of bonds **absorb** the radiation in different amounts. These varying amounts of absorbance are **measured and recorded** allowing certain bonds and therefore functional groups to be identified.

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

-OH Alcohol Group

Image courtesy of Chemistry Stack Exchange

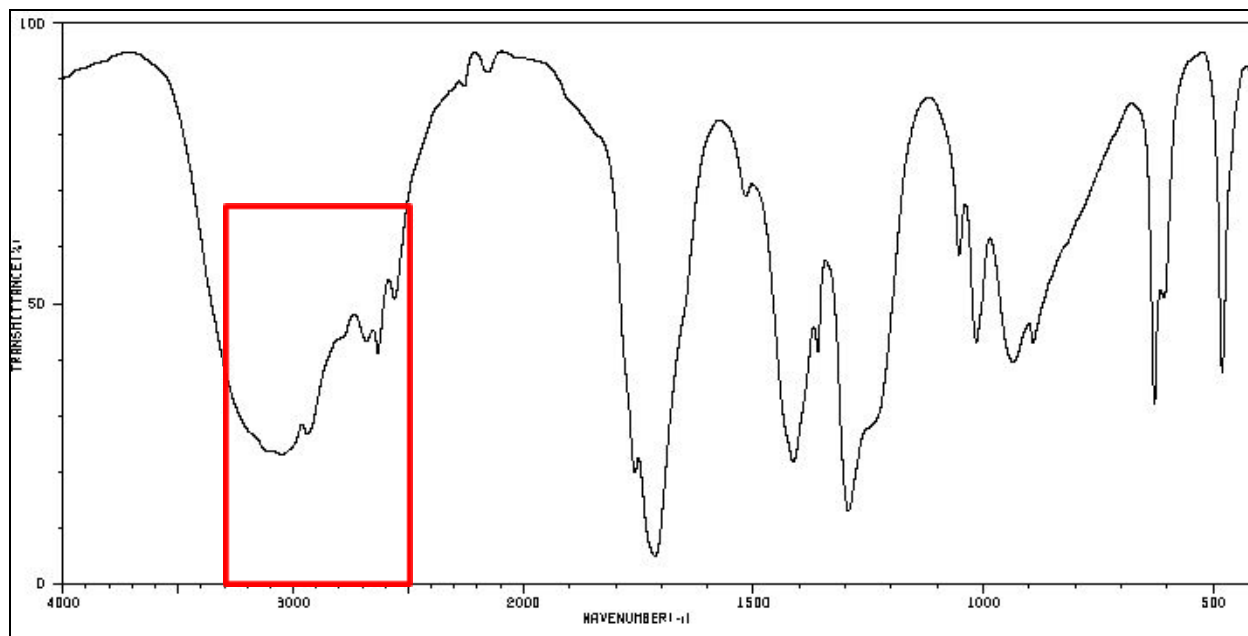


*The characteristic peak is in the range **3230 - 3550 cm⁻¹**.*

-OH Acid Group

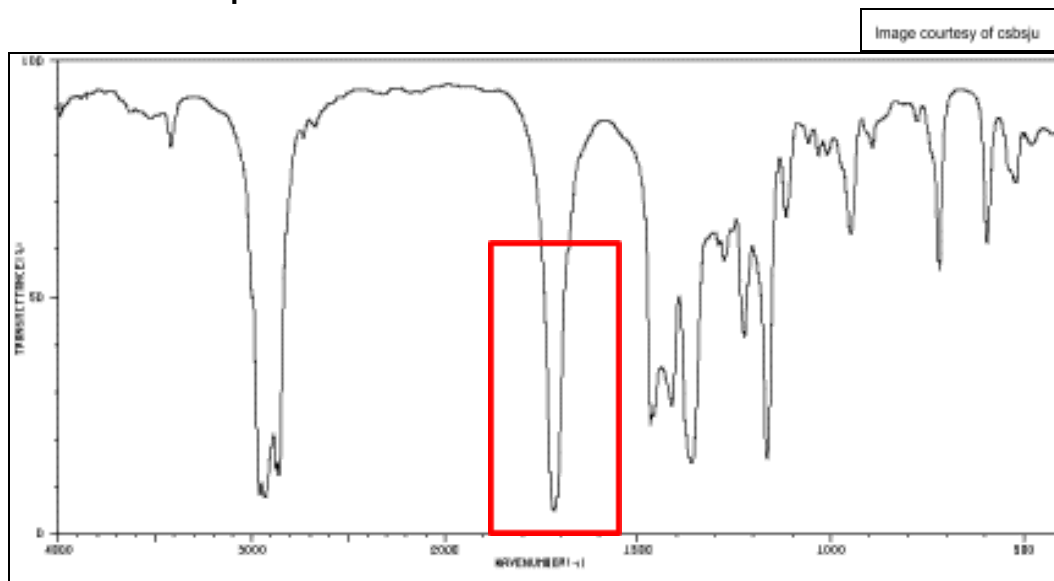
Image courtesy of Chemistry Stack Exchange





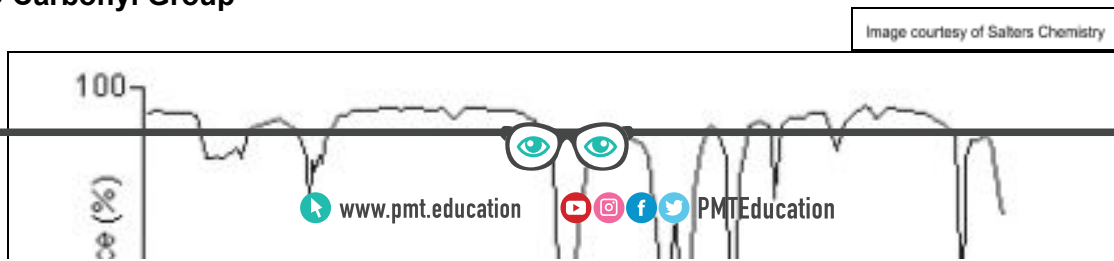
The characteristic peak is in the range $2500 - 3300 \text{ cm}^{-1}$.

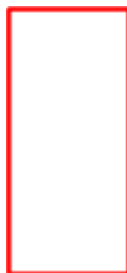
C=C Unsaturated Group



The characteristic peak is in the range $1620 - 1680 \text{ cm}^{-1}$.

C=O Carbonyl Group





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

Fingerprint Region

Each IR spectrum has a **fingerprint region** to the right-hand side. This contains **tiny differences** from species to species which act as a molecules 'fingerprint', allowing it to be **identified**.

