Edexcel Chemistry A-level

Topic 7: Modern Analytical Techniques I

Detailed Notes

Topic 7A: Mass Spectrometry

Mass spectrometry 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 (they are 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 the path is dependent on the charge and mass of the ion.

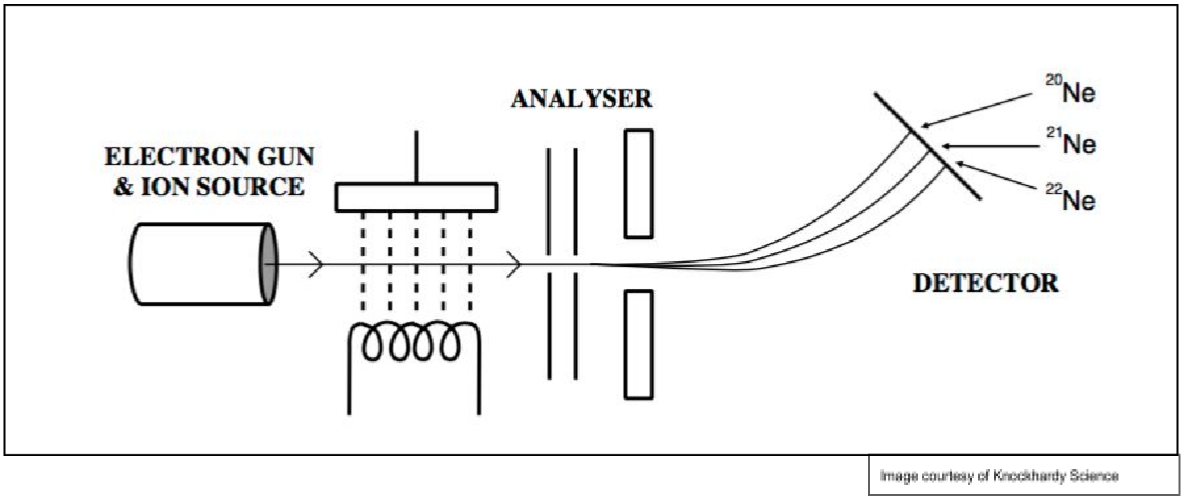


Image courtesy of Knockhardy Science

4. **Detection** - When the positive ions hit the negatively charged detection plate, they **gain an electron,** producing a **flow of charge**. The greater the current produced, the greater the abundance of that particular ion.

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:

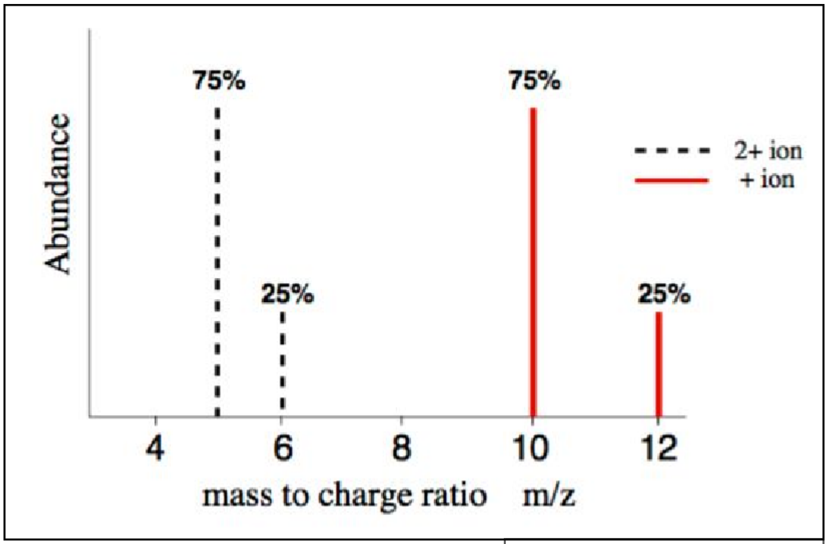


Image courtesy of Knockhardy Science

Using this print-out spectra, the ***Ar*** (relative atomic mass) **can be calculated** by multiplying each m/z value by its abundance and adding each of these together, before dividing by the total abundance of all species present.

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

Example: Using the above mass spectrum,

$$\mathbf{Ar = \frac{\underline{(10x75) + (12x25)}}{(75 + 25)} = 10.5}$$

Using this calculated value of Ar, the element can be identified by referring to the Periodic Table.

Predicting Mass Spectra

If you know the **abundances** of an isotope you can generate the mass spectra for its molecules, including **relative peak heights**.

Example:

The relative abundance of ^{35}Cl atoms is 75% and ^{37}Cl atoms is 25%. In other words, for every 100 atoms of chlorine, 25 would be ^{35}Cl and 75 would be ^{37}Cl.

Spectra produced by the mass spectrometry of chlorine display a **characteristic pattern** in a **3:1 ratio for Cl^+ ions** and a **3:6:9 ratio for Cl_2^+ ions**. This is because one isotope is more common than the other and the chlorine molecule can form in different combinations:

$^{70}Cl_2^+$ = 35 + 35
$^{72}Cl_2^+$ = 35 + 37 OR = 37 + 35
$^{74}Cl_2^+$ = 37 + 37

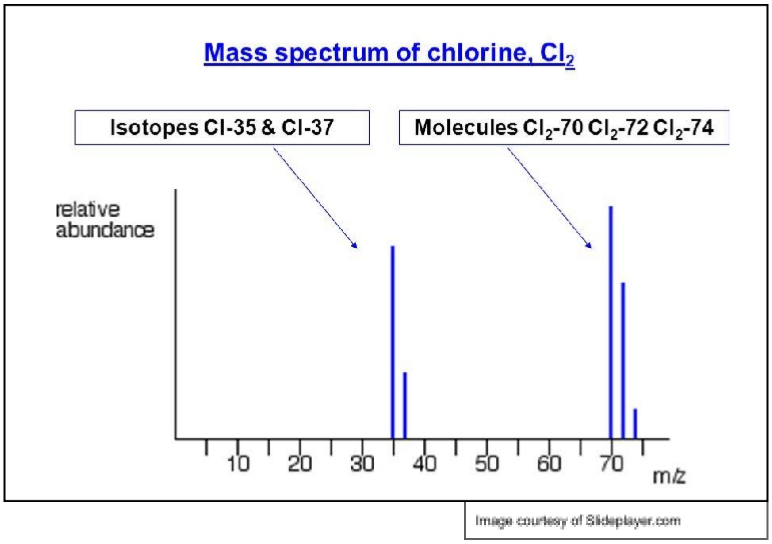


Image courtesy of Slideplayer.com

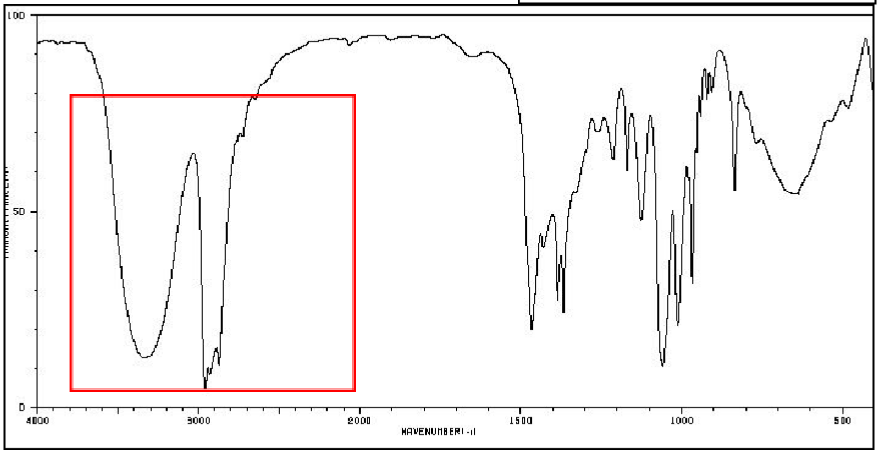
Topic 7B: Infrared (IR) Spectrometry

Infrared spectroscopy is an analytical technique that uses **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 thus functional groups, to be identified.

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

-O-H Alcohol Group

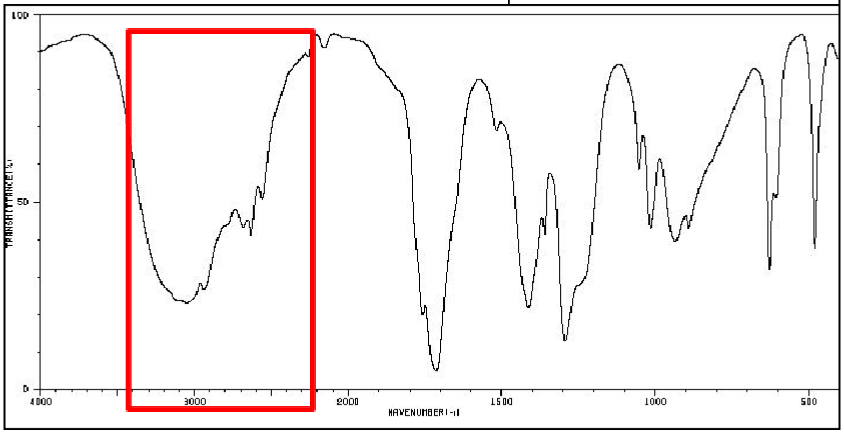
Image courtesy of Chemistry Stack Exchange



The characteristic -O-H alcohol group peak is in the range 3230 - 3550 cm^{-1}

-O-H Acid Group

Image courtesy of Chemistry Stack Exchange



The characteristic -O-H acid group peak is in the range 2500 - 3300 cm^{-1}

C=C Unsaturated Group

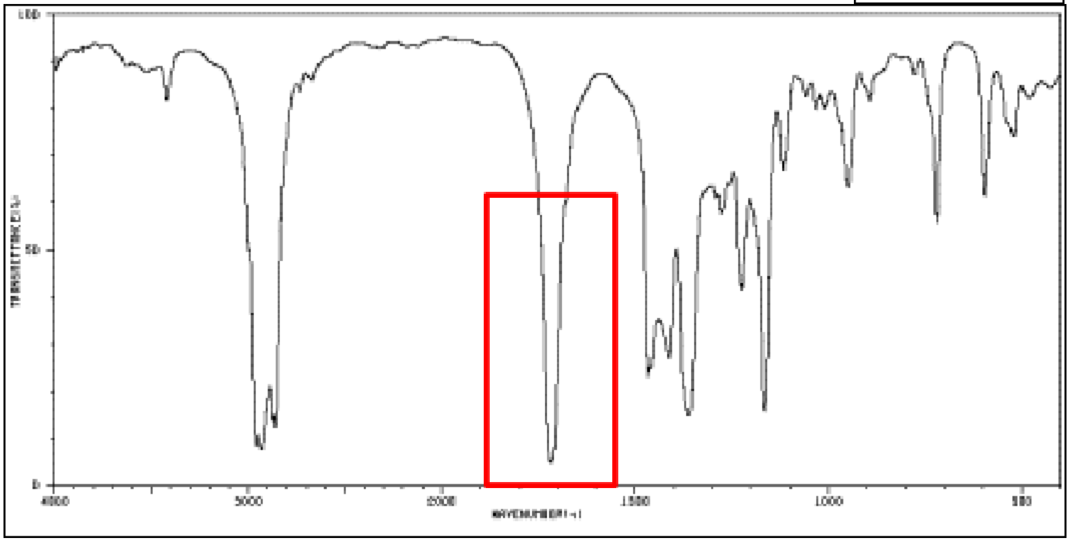


Image courtesy of csbsju

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

C=O Carbonyl Group

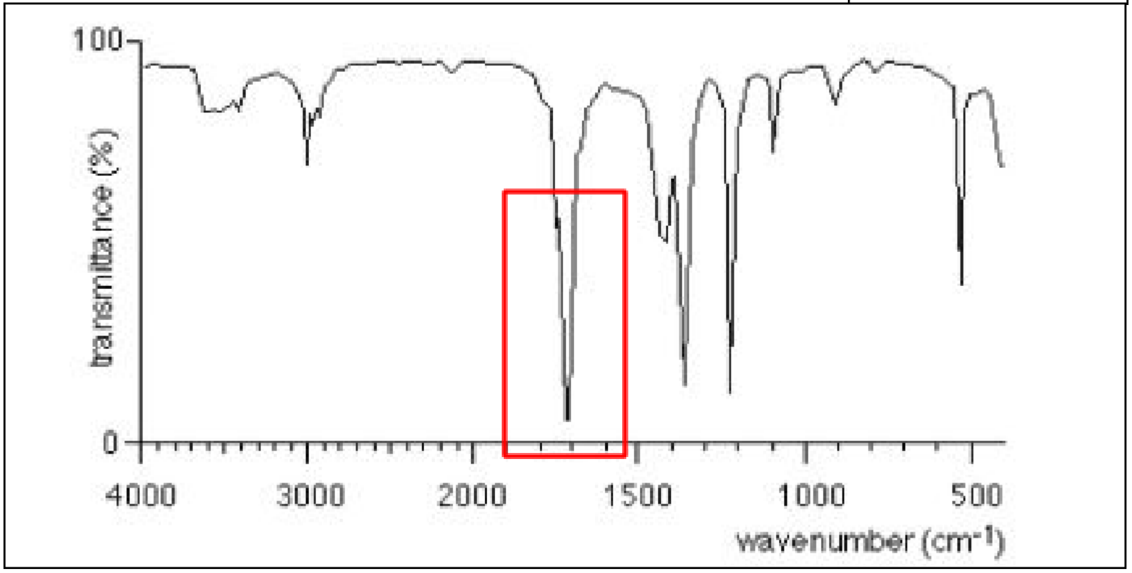


Image courtesy of Salters Chemistry

The characteristic C=O peak is in the range 1680 - 1750 cm^{-1}

Fingerprint Region

Each IR spectrum has a **fingerprint region** on the right-hand side, from 500-1500 cm^{-1}. This is unique for each species, containing **tiny differences** between each species. This means it acts as a molecules' 'fingerprint', allowing it to be **identified**.