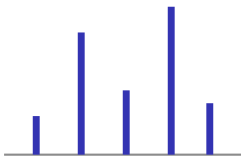


Analytical Techniques

A-Level Chemistry ■ Topic 22

A-Level Chemistry



What we will cover

- 1 Infrared spectroscopy
- 2 Mass spectrometry
- 3 Molecular ion & fragments
- 4 $[M+1]$ & $[M+2]$ peaks



sorts ions by mass



Infrared spectroscopy

Infrared spectroscopy finds the **functional group** : each bond absorbs at its own **wavenumber** .

- broad O—H $\sim$ 3200–3650
- C=O $\sim$ 1700
- broad 2500–3000 + C=O $\rightarrow$ acid

Using an IR spectrum to check a reaction

Each bond absorbs infrared at its own range of **wavenumber** (cm^{-1}). You are **given** the data table – the skill is matching dips to bonds, not memorising numbers.

before: propene

a C=C dip is present; no O–H

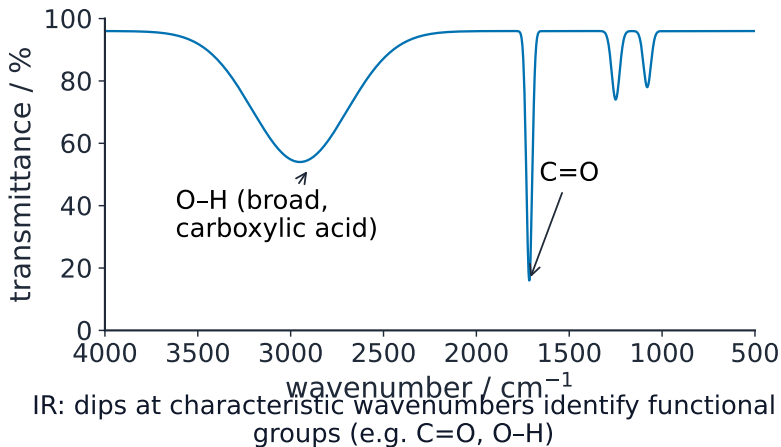


after: propan-2-ol

the C=C dip is **gone**; a broad O–H dip appears

That pair of changes – one dip gone, one appeared – is how the exam asks you to prove a reaction happened. Name the bond, not just the number.

Infrared spectroscopy, in detail



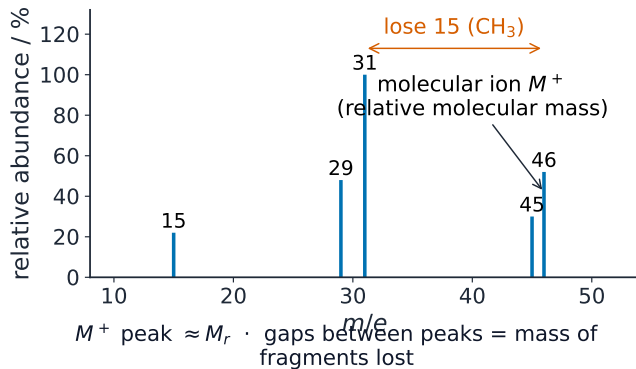
An infrared spectrum: each bond gives a dip at its own wavenumber. A broad O-H dip together with a C=O dip identifies a carboxylic acid

Mass spectrometry

Mass spectrometry sorts ions by **mass-to-charge ratio** (m/e).

The highest- m/e peak is the **molecular ion** M^+ ($= M_r$); the gaps between peaks give the masses of the lost **fragments** (loss of 15 = CH_3).

Mass spectrometry, in detail



A mass spectrum: the highest- m/e peak is the molecular ion (M^+ , the M_r); the gaps between peaks give the masses of the lost fragments

Relative atomic mass from isotopes

$$A_r = \frac{\sum(\text{isotope mass} \times \text{abundance})}{\sum \text{abundance}}$$

Chlorine: 75% ^{35}Cl , 25% ^{37}Cl

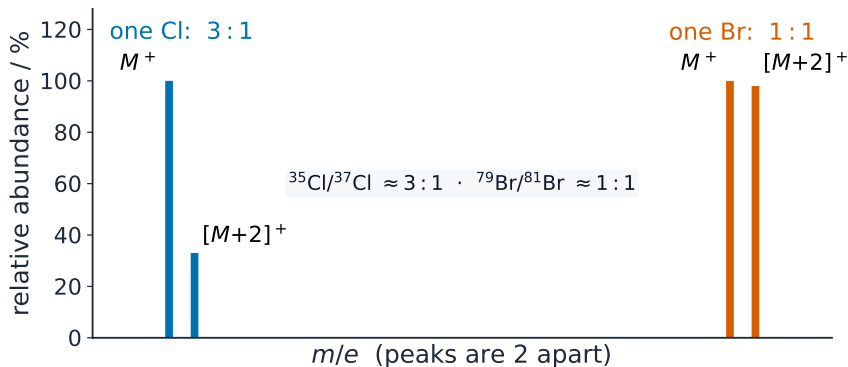
$$A_r = \frac{35 \times 75 + 37 \times 25}{100} = 35.5$$

An element's **isotopes** give several peaks; the **abundance** of each gives the weighted-average A_r .

[M+1] and [M+2] peaks

- **[M+1]** M+1 comes from ^{13}C – its height gives the number of carbons
- **[M+2]** M+2 shows a halogen: Cl gives 3:1, Br gives 1:1

[M+1] and [M+2] peaks, in detail



An $[M+2]$ peak two mass units above M^+ shows a halogen: one chlorine gives a 3 : 1 ratio, one bromine a 1 : 1 ratio

Reading the molecular ion and its neighbours

the molecular ion peak

the highest m/e of significance – it gives the **relative molecular mass**

the $[M + 1]$ peak

small, from the 1.1% of carbon that is ^{13}C – its **height relative to M** gives the number of carbons

the $[M + 2]$ peak

from **isotopic abundance** in chlorine or bromine

chlorine

^{35}Cl and ^{37}Cl in a 3 : 1 ratio – so M and $M + 2$ appear in a 3 : 1 ratio

bromine

^{79}Br and ^{81}Br in a 1 : 1 ratio – so M and $M + 2$ are of **almost equal height**

A molecular ion at 108 with an almost equal peak at 110 says **bromine**, immediately. The IR then tells you what the rest of the molecule is.

Infrared spectroscopy, continued



An infrared spectrometer shines infrared through a sample and records which wavenumbers its bonds absorb

Using IR to check a reaction happened

what IR shows

absorption at characteristic wavenumbers, one per bond type

the useful test

a **disappearing** peak is as informative as a new one

the standard example

propene $\rightarrow$ propan-2-ol: the **C=C dip should be gone** and a broad **O-H** peak should appear

the O-H peak

broad, around $3200\text{--}3600\text{ cm}^{-1}$ – unmistakable

the C=O peak

sharp and strong, around 1700 cm^{-1}

the fingerprint region

below 1500 cm^{-1} : too complex to read bond by bond, but **unique** to the compound

Say which peak **went** and which **arrived**. Naming only the new one leaves half the evidence unused.

Exam tips

- On an **IR spectrum** quote the **wavenumber and the bond** (O-H broad $\sim 3200 - 3600$, C=O ~ 1700); use the data booklet.
- The peak at the **highest** m/z is the molecular ion M^+ and gives the M_r .
- Explain **fragmentation**: the gap between peaks is the lost fragment (loss of 15 = CH_3 , 29 = C_2H_5 or CHO).
- Learn common **isotope patterns** (Cl gives M and M+2 in about 3:1; M+1 from ^{13}C).



Topic 22 – key takeaways

1

Infrared

each bond absorbs at its own wavenumber

2

Molecular ion

the highest- m/e peak gives M_r

3

Fragments

peak gaps give the lost masses

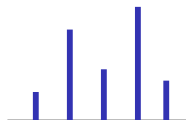
4

Isotope peaks

$[M+1]$ counts C; $[M+2]$ shows Cl or Br

Check yourself

- 1 Which bond absorbs around 1700 cm^{-1} ?
- 2 What does the highest- m/e peak give?
- 3 A loss of 15 means which fragment was lost?
- 4 An $[M+2]$ peak in a 1:1 ratio shows which halogen?



Answers 1. C=O 2. the relative molecular mass 3. CH_3 4. bromine