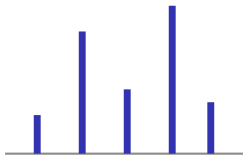
Analytical Techniques

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

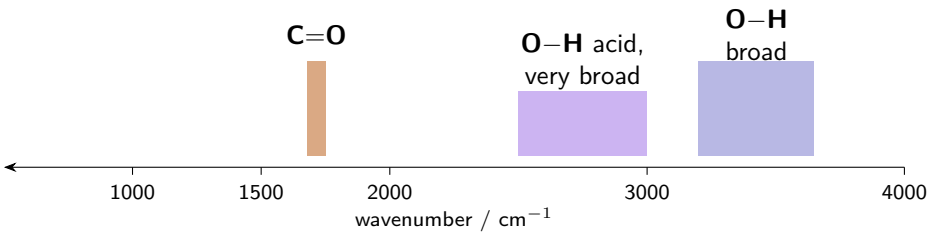


sorts ions by mass

1 Spectroscopy

Infrared spectroscopy

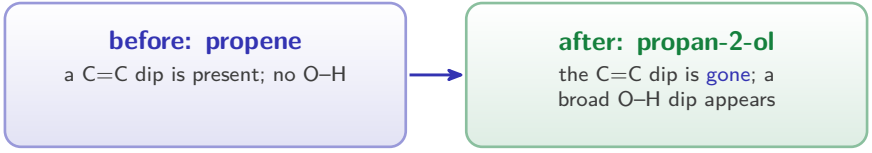
Infrared spectroscopy 红外光谱 finds the **functional group** 官能团: each bond absorbs at its own **wavenumber** 波数.



Very broad 2500–3000 **plus** C=O near 1700 $\Rightarrow$ a **carboxylic acid**.

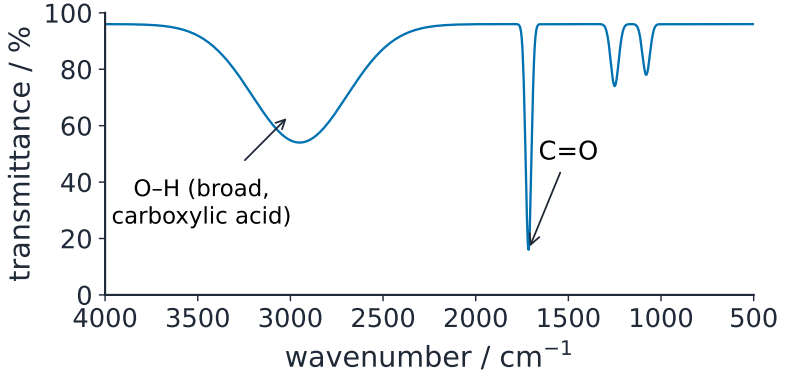
Using an IR spectrum to check a reaction

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



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



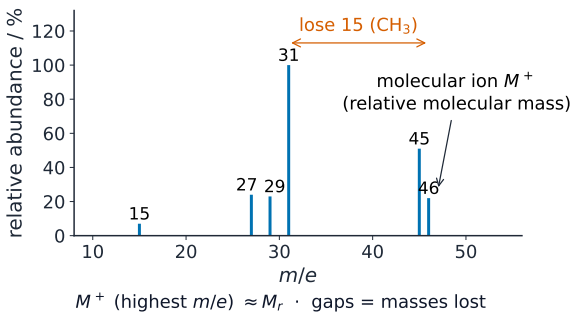
IR: dips at characteristic wavenumbers identify functional groups (e.g. C=O, O–H)

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 质谱 sorts ions by **mass-to-charge ratio** 质荷比 (m/e).

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



Relative atomic mass from isotopes

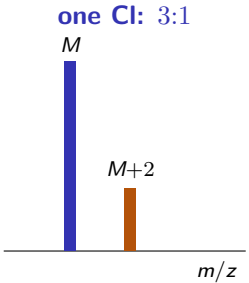
$$A_r = \frac{\sum(\text{isotope mass} \times \text{abundance})}{\sum \text{abundance}}$$

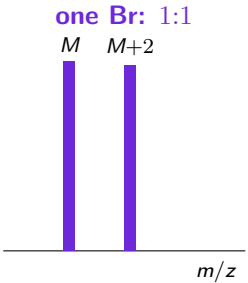
Chlorine: 75% ^{35}Cl, 25% ^{37}Cl

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

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

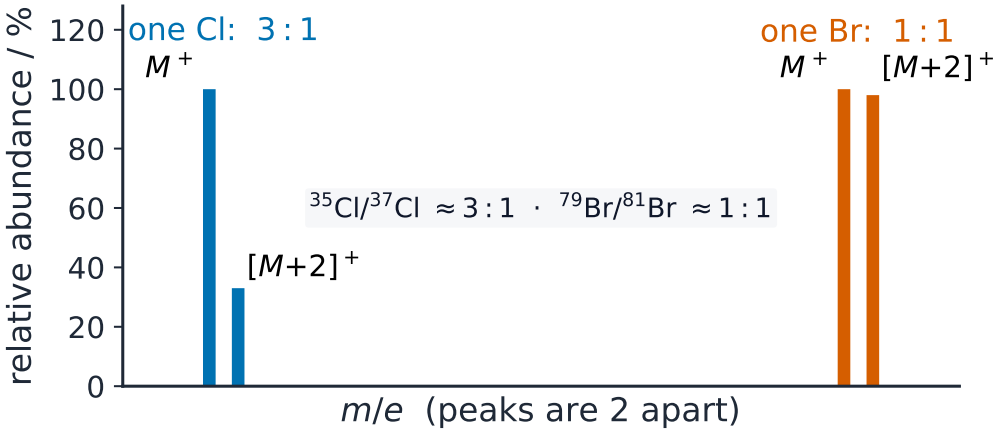
[M+1] and [M+2] peaks





- **[M+2]** M+2 峰 shows a **halogen**: the isotopes $^{35}Cl/^{37}Cl$ or $^{79}Br/^{81}Br$
- **[M+1]** M+1 峰 comes from ^{13}C: its height gives the **number of carbons**

[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 分子离子峰	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** 同位素丰度 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.

How an infrared spectrometer works



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** 吸收 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 3200–3600 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).

2 Recap

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

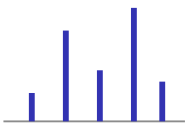
peak gaps give the lost masses

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