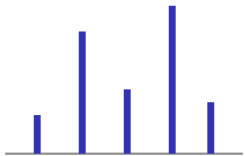
# Analytical Techniques

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

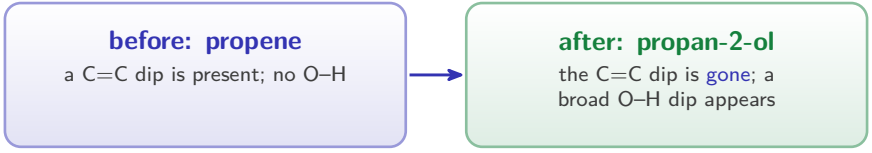
# Infrared spectroscopy

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

- broad O−H ∼3200–3650
- C=O ∼1700
- broad 2500–3000 + C=O → acid

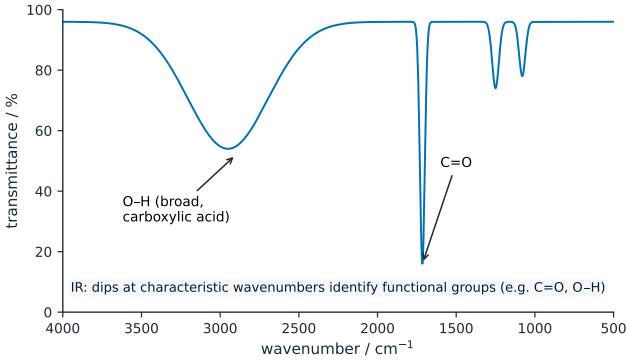
# Using an IR spectrum to check a reaction

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



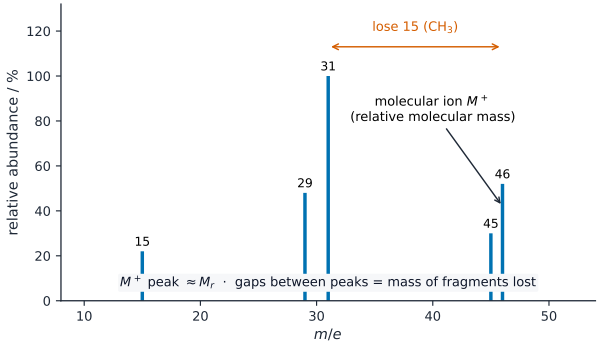

An infrared spectrum: each bond gives a dip at its own wavenumber. A broad O–H dip together with a C=O dip identifies a carboxylic acid

# 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 $15 = CH_3$).

# 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**

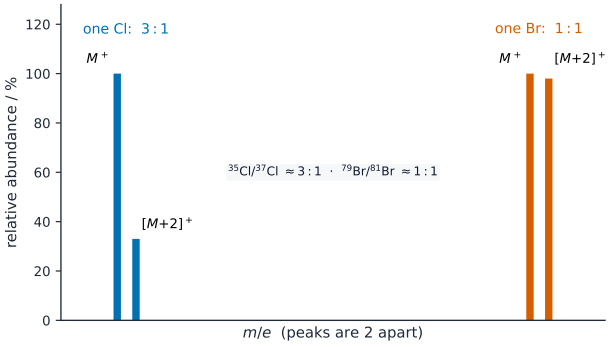
$$A_r = \frac{35 \times 75 + 37 \times 25}{100} = 35.5$$

An element's **isotopes** 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+1]** M+1 峰 comes from $^{13}$C – its height gives the number of carbons
- **[M+2]** M+2 峰 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 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.

# 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** 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 → 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 $\sim 1700$); 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**

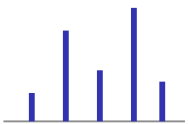
peak gaps give the lost masses

**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