

Analytical techniques

A-Level Chemistry

Infrared spectroscopy

Infrared spectroscopy 红外光谱 helps you find the **functional group** 官能团 in a molecule. Each kind of bond soaks up (absorbs) infrared radiation at its own range of frequencies. Where the bond shows strong **absorption** 吸收, the spectrum has a dip.



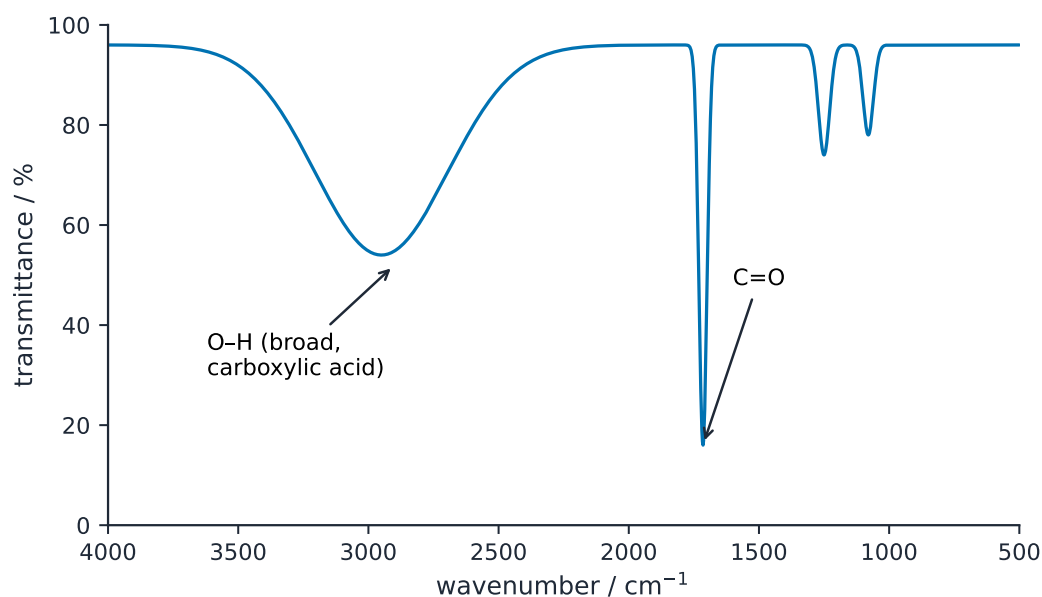
An infrared spectrometer shines infrared through a sample and records which wavenumbers its bonds absorb

Image: Wang, F., Zhang, L., Zhang, X., Li, H. and Wu, S, CC BY 4.0 (commons.wikimedia.org)

The position is measured in **wavenumber** 波数 (in cm^{-1}). You are given a data table, so you do not memorise the numbers. You just match the dips to bonds:

- a broad dip around $3200\text{--}3650\text{ cm}^{-1}$ → an O–H bond in an alcohol.
- a dip around 1700 cm^{-1} → a C=O bond (aldehyde, ketone, acid or ester).
- a broad dip $2500\text{--}3000\text{ cm}^{-1}$ together with a C=O dip → a carboxylic acid.

This is useful for checking a reaction. For example, if propene has been turned into propan-2-ol, the C=C dip should be gone and an O–H dip should appear.



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

In **mass spectrometry** 质谱, a molecule is turned into ions and sorted by its **mass-to-charge ratio** 质荷比 (m/e). The spectrum is a set of peaks at different m/e values.



A modern mass spectrometer: the sample is loaded at the front, then the machine ionises it and sorts the ions by their mass-to-charge ratio to give the spectrum

Image: Mike25 Michael Willett, Public domain (commons.wikimedia.org)

Relative atomic mass from isotopes

An element's **isotope** 同位素 mixture gives several peaks. From the **isotopic abundance** 同位素丰度 (how common each isotope is) you can find the **relative atomic mass** 相对原子质量—a weighted average:

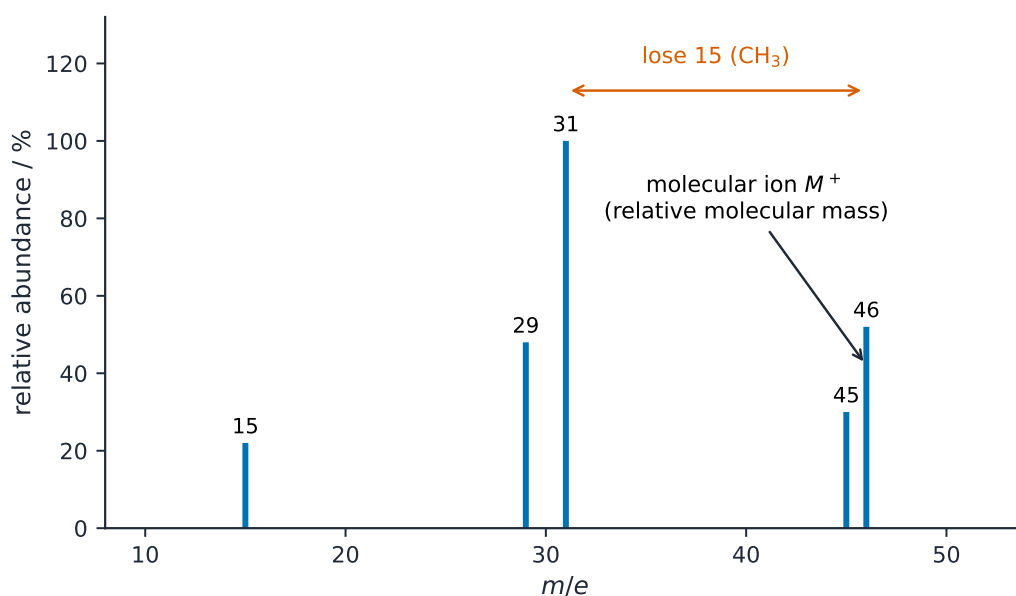
$$A_r = \frac{\sum(\text{isotope mass} \times \text{abundance})}{\sum \text{abundance}}$$

For example, chlorine is 75% ^{35}Cl and 25% ^{37}Cl , giving $A_r = \frac{35 \times 75 + 37 \times 25}{100} = 35.5$.

The molecular ion and fragmentation

The peak at the highest m/e (the **molecular ion** 分子离子 peak, or **molecular ion peak** 分子离子峰, M^+) gives the relative molecular mass of the whole molecule.

The molecule also breaks into smaller pieces —this is **fragmentation** 碎裂. The gap between two peaks tells you the mass of the lost piece, so you can suggest each **fragment** 碎片. For example, a loss of 15 means a CH_3 group was lost, and a loss of 29 means CHO or C_2H_5 .



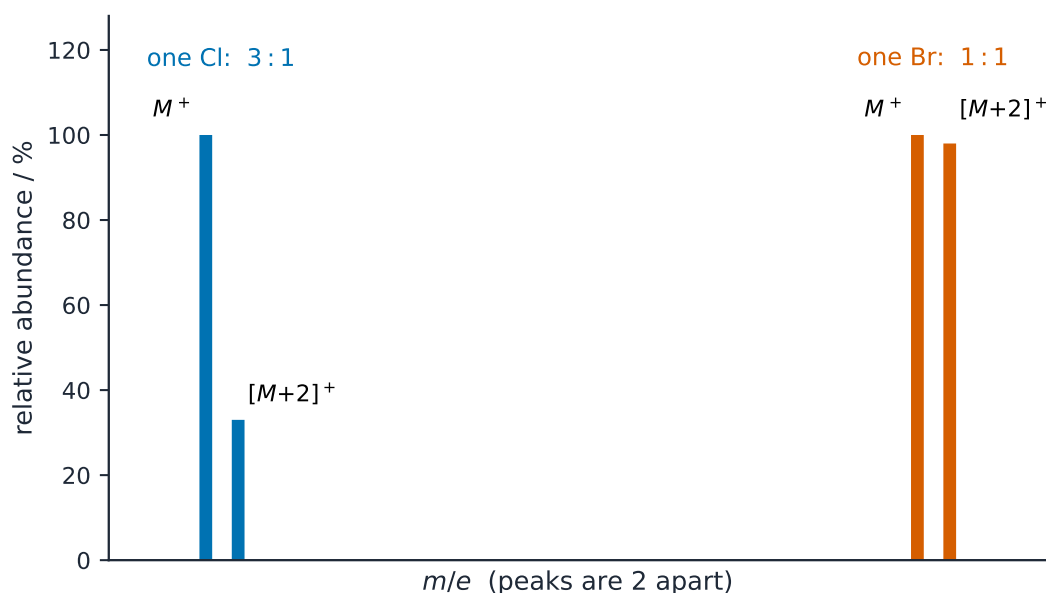
A mass spectrum: the highest- m/e peak is the molecular ion (M^+ , the M_r); the gaps between peaks give the masses of the lost fragments

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

- a small $[M + 1]$ peak comes from the ^{13}C isotope. The number of carbon atoms n is:

$$n = \frac{100 \times \text{abundance of } [M + 1]^+}{1.1 \times \text{abundance of } M^+}$$

- an $[M + 2]$ peak shows chlorine or bromine. One chlorine gives an $[M + 2]$ peak about one third the height of M^+ (from ^{37}Cl); one bromine gives an $[M + 2]$ peak about the **same** height as M^+ (from ^{81}Br).



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

Worked example. A compound shows a molecular ion at $m/e = 108$ and a peak of almost equal height at $m/e = 110$. Its infrared spectrum shows **no** broad absorption near 3300 cm^{-1} . Deduce its identity. Two peaks **two units apart with roughly equal heights** are the 1 : 1 signature of **one bromine** atom (from ^{79}Br and ^{81}Br); one chlorine would have given a 3 : 1 ratio instead. Take the bromine away from the molecular ion: $108 - 79 = 29$, which fits a C_2H_5 fragment. The absence of a broad peak near 3300 cm^{-1} rules out an O-H, so there is no alcohol group. The compound is **bromoethane**, $\text{C}_2\text{H}_5\text{Br}$. Read the $[M + 2]$ **ratio** rather than merely noting the peak: 1 : 1 means bromine, 3 : 1 means chlorine.

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).