Analytical techniques

A-Level Chemistry

Infrared spectroscopy

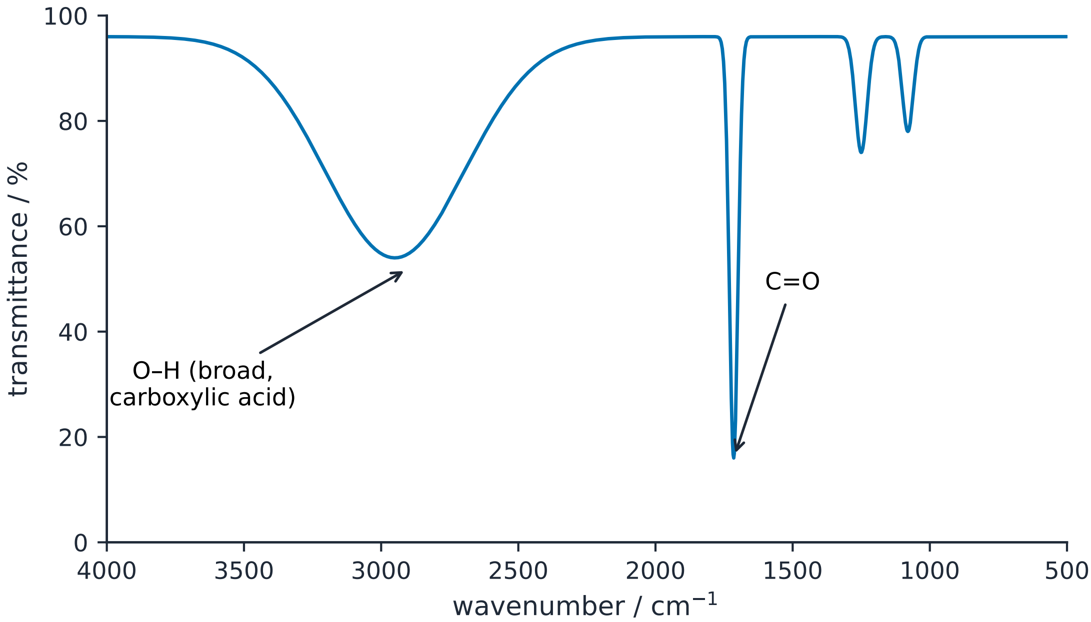
Infrared spectroscopy 红外光谱 helps you find the **functional group** 官能团 in a molecule. Each kind of bond soaks up (absorbs) infrared radiation at its own range of frequencies. Where the bond shows strong **absorption** 吸收, the spectrum has a dip.

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

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 3200–3650 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 2500–3000 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:

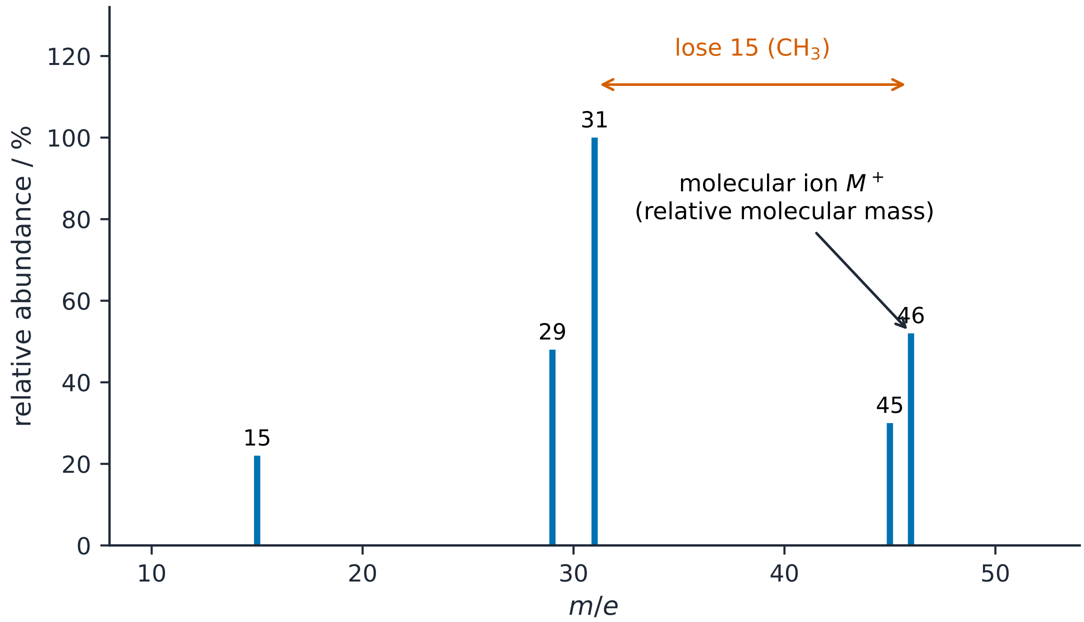
$$A_r = \frac{\sum(\text{isotope mass} \times \text{abundance})}{\sum \text{abundance}}$$

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.



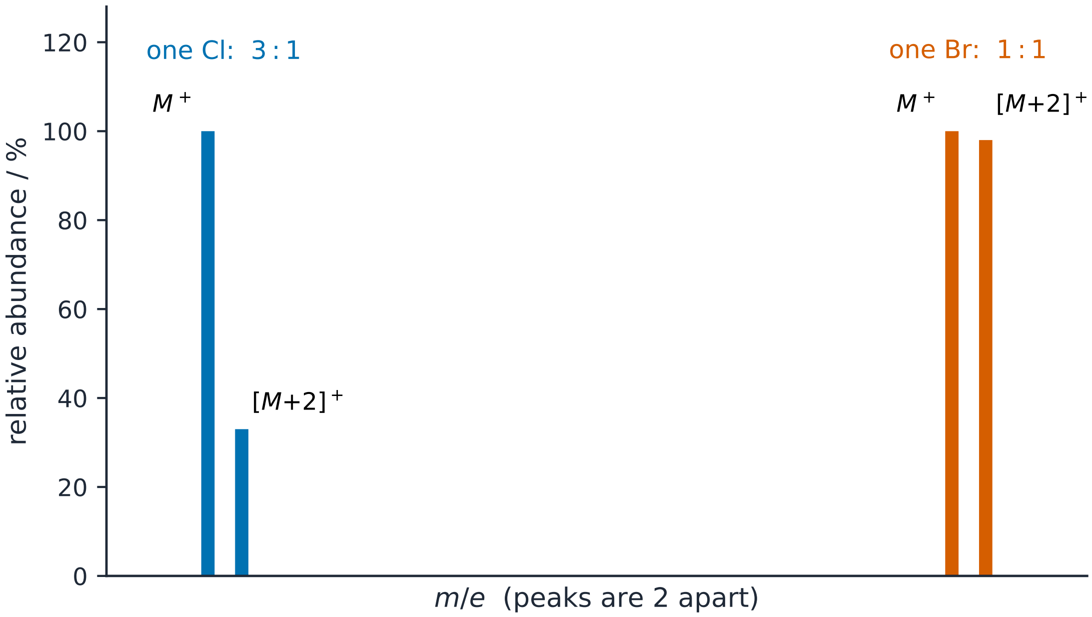
A mass spectrum: the highest-m/e peak is the molecular ion (M^+, the M_r); the gaps between peaks give the masses of the lost fragments

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