

Analytical Techniques

A-Level Chemistry ■ Topic 22

A-Level Chemistry



Analytical Techniques

What we will cover

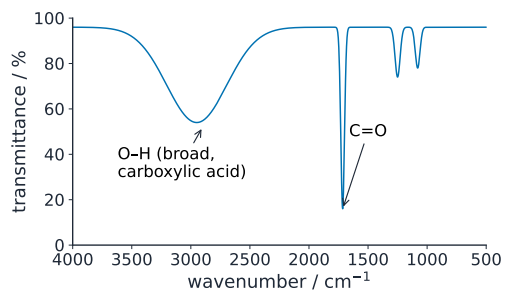
- 1 Infrared spectroscopy
- 2 Mass spectrometry
- 3 Molecular ion & fragments
- 4 $[M+1]$ & $[M+2]$ peaks



sorts ions by mass

1 Spectroscopy

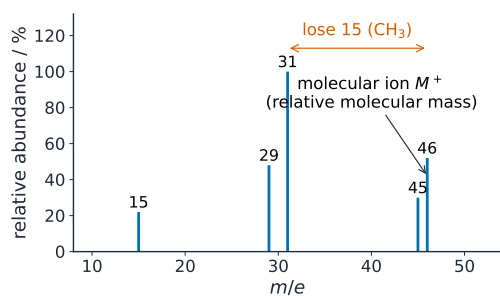
Infrared spectroscopy



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

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

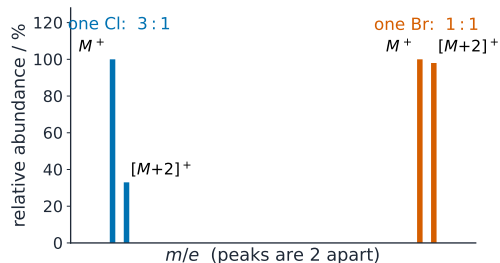
$$A_r = \frac{\sum(\text{isotope mass} \times \text{abundance})}{\sum \text{abundance}}$$

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+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

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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

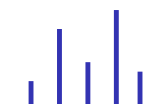
Check yourself

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