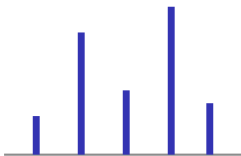


# Analytical Techniques

## A-Level Chemistry ■ Topic 22

A-Level Chemistry



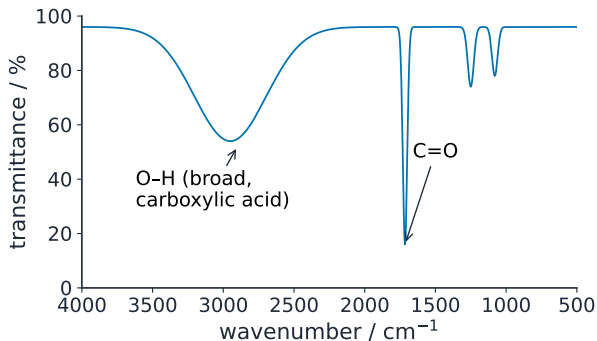
# What we will cover

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



*sorts ions by mass*

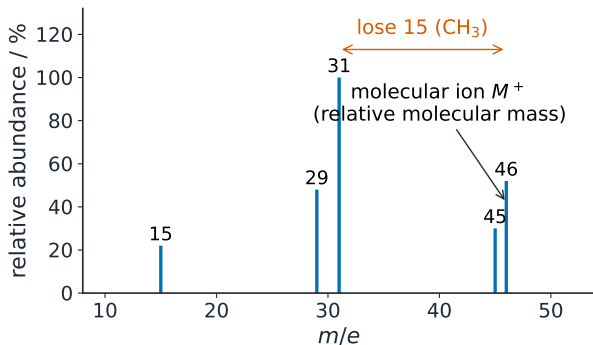
# Infrared spectroscopy



**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  $15 = \text{CH}_3$ ).

## Relative atomic mass from isotopes

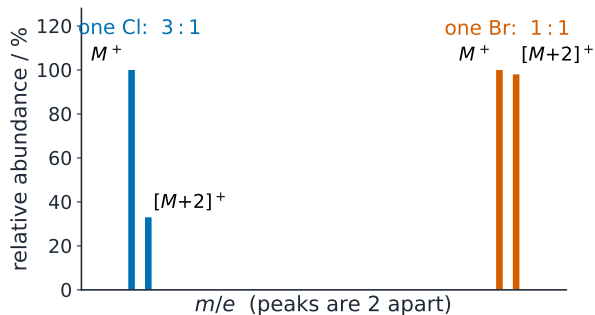
$$A_r = \frac{\sum(\text{isotope mass} \times \text{abundance})}{\sum \text{abundance}}$$

**Chlorine: 75%  $^{35}\text{Cl}$ , 25%  $^{37}\text{Cl}$**

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

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  $^{13}\text{C}$  – its height gives the number of carbons
- **[M+2]**  $M+2$  峰 shows a halogen: Cl gives 3:1, Br gives 1:1

## 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

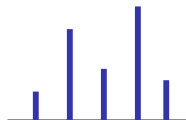
## Check yourself

1 Which bond absorbs around  $1700\text{ cm}^{-1}$ ?

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.  $\text{CH}_3$  4. bromine