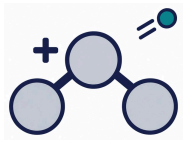
Analysis Summary Map

Cambridge International AS & A Level Chemistry · Topic 22 Analytical techniques

1 The molecular ion

22.2.1, 22.2.3

- $M \rightarrow M^+ + e^-$
- Highest major peak: m/z = **Mr**
- Base peak: the tallest (100%)
- Mr alone may fit several formulas



2 M+1 and M+2

22.2.5, 22.2.6

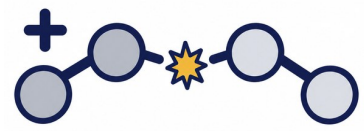
- ^{13}C is about **1.1%** of carbon
- $n = 100 \times [M+1] \div (1.1 \times [M^+])$
- **M+2**: Cl 3 : 1; Br 1 : 1
- Fits the formula to Mr

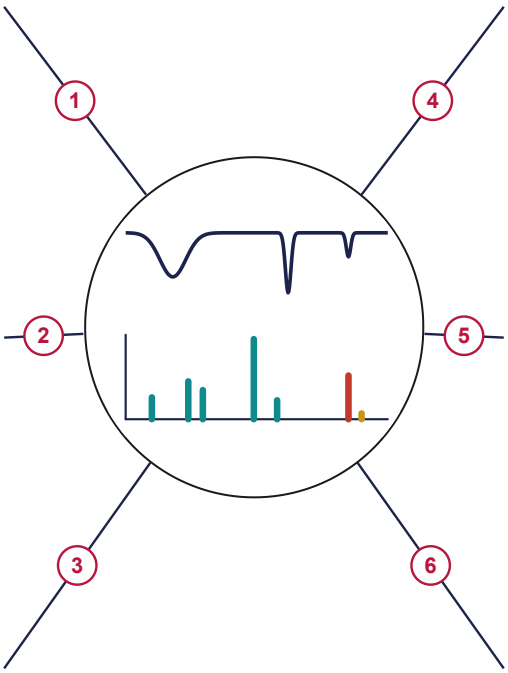


3 Fragmentation

22.2.4

- $M^+ \rightarrow X^+ + \bullet Y$
- Only the **ion** is detected
- Gap from M: the group lost
- Isomers: different fragments





4 Infrared absorption

22.1.1

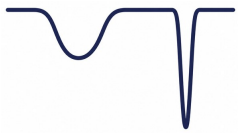
- Bonds **stretch and bend**
- Same frequency IR: absorbed
- Dip = low **transmittance**
- Below 1500: **fingerprint**



5 Reading IR spectra

22.1.1

- C=O 1670–1740 (ester 1710–1750)
- O–H hydroxy 3200–3600
- O–H carboxyl 2500–3000, very broad
- Absent bands count too



6 Qualitative analysis

Paper 3

- Bromine water: **C=C**
- Dichromate: 1°/2° alcohol, CHO
- Fehling's, Tollens': **CHO**; I_2/OH^-: CHI_3
- NaOH, NH_3, Ba^{2+}, Ag^+: **ions**



Fragments and absorptions

m/z values from the mass spectrum; IR ranges from the Data booklet (cm^{-1})

m/z	Ion	Bond	Range / cm^{-1}
15	CH_3^+	C–H	2850–2950
29	$C_2H_5^+$ or CHO^+	C=C	1500–1680
31	CH_2OH^+	O–H (hydroxy)	3200–3600
43	$C_3H_7^+$ or CH_3CO^+	C=O	1670–1740
45	$COOH^+$	O–H (carboxyl)	2500–3000
57	$C_4H_9^+$ or $C_2H_5CO^+$	N–H	3300–3500

Worked examples

Counting carbons

- peak heights: M^+ 30, M+1 1.3
- $100 \times 1.3 \div (1.1 \times 30) = 3.9$
- **4 carbons**: C_4H_8O

Which propanol?

- both Mr 60
- base peak 31: CH_2OH^+
- **propan-1-ol**

An unknown

- Fehling's orange-red; M^+ 58
- IR 1730; no O–H
- **propanal**

NMR spectroscopy and chromatography follow at A Level (Topic 37); the mass spectra of elements were met in Topic 2.

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