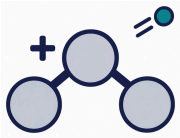
Analysis Summary Map

OCR A Level Chemistry A · 4.2.4 Analytical techniques

1 The molecular ion

4.2.4(f)

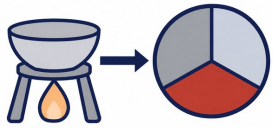
- M → **M**⁺ + e⁻
- Highest m/z: m/z = **Mr**
- Base peak: the tallest (100%)
- Cl: M, M+2 3 : 1; Br: 1 : 1



2 Elemental analysis

4.2.4(h)

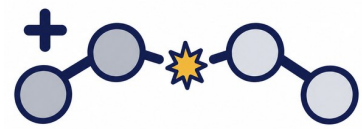
- **% by mass** of each element
- ÷ A_r, then ÷ the smallest
- Empirical formula, e.g. CH_2O
- Mr ÷ empirical mass: **molecular**

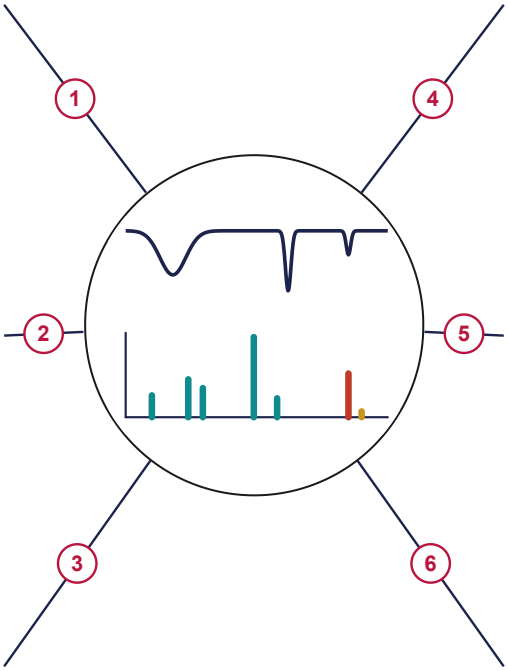


3 Fragmentation

4.2.4(g)

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





4 Infrared absorption

4.2.4(a), 4.2.4(b), 4.2.4(e)

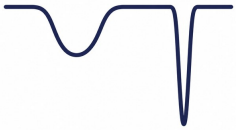
- Bonds **stretch and bend**
- Same frequency IR: absorbed
- **CO_2, CH_4, H_2O**: greenhouse
- Breathalysers: ethanol **C–H**



5 Reading IR spectra

4.2.4(c), 4.2.4(d)

- C=O 1630–1820
- O–H alcohol 3200–3600
- O–H acid 2500–3300, very broad
- Absent bands count too



6 PAG 4 and PAG 7

3.1.4(a), PAG 4, PAG 7

- Bromine water: **C=C**
- Dichromate: 1°/2° alcohol, CHO
- Tollens' mirror: **CHO**; $NaHCO_3$: **COOH**
- $AgNO_3$: C–X and **ions**



Fragments and absorptions

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

m/z	Ion	Bond	Range / cm^{-1}
15	CH_3^+	C–H	2850–3100
29	$C_2H_5^+$ or CHO^+	C=C	1620–1680
31	CH_2OH^+	O–H (alcohol)	3200–3600
43	$C_3H_7^+$ or CH_3CO^+	C=O	1630–1820
45	$COOH^+$	O–H (acid)	2500–3300
57	$C_4H_9^+$ or $C_2H_5CO^+$	N–H	3300–3500

Worked examples

From percentages

- 40.0% C, 6.7% H, 53.3% O
- ratio 1 : 2 : 1: CH_2O
- M^+ 60: **$C_2H_4O_2$**

Which propanol?

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

An unknown

- Tollens' mirror; M^+ 58
- IR 1730; no O–H
- **propanal**

NMR spectroscopy and chromatography follow at A level (6.3); the mass spectra of elements were met in 2.1.1.

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