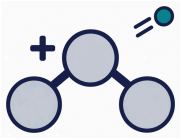
Spectra Summary Map

Edexcel International A Level Chemistry · Unit 2 · Topic 10D Mass Spectra and Infrared

1 The molecular ion

10.21

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



2 The M+1 peak

10.21

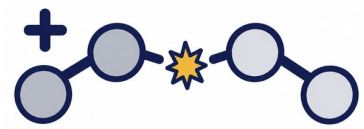
- ^{13}C is about **1.1%** of carbon
- n ≈ (M+1 ÷ M) × 100 ÷ 1.1
- More carbons: taller M+1
- Fits the formula to Mr

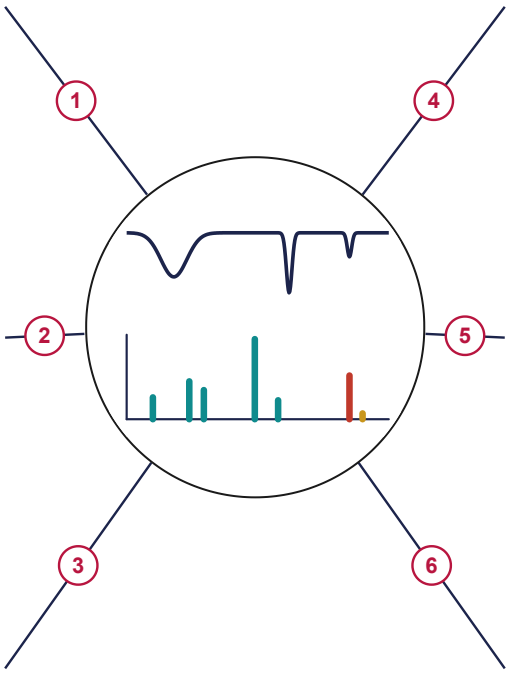


3 Fragmentation

10.21

- M⁺ → **X**⁺ + •**Y**
- Only the **ion** is detected
- Gap from M: the group lost
- Isomers: different fragments





4 Infrared absorption

10.22

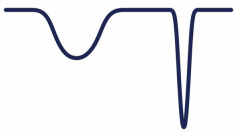
- Bonds **stretch and bend**
- Same frequency IR: absorbed
- Dip = low **transmittance**
- Below 1500: **fingerprint**



5 Reading IR spectra

10.22

- C=O 1740–1700 (by group)
- O–H alcohol 3550–3230
- O–H acid 3300–2500, very broad
- Absent bands count too



6 Core Practical 8

10.23

- Bromine water: **C=C**
- Dichromate: 1°/2° alcohol, CHO
- Benedict's: **CHO**; $NaHCO_3$: **COOH**
- PCl_5: –OH; $AgNO_3$: C–X



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 (alkane)	2962–2853
29	$C_2H_5^+$ or CHO^+	C=C	1669–1645
31	CH_2OH^+	O–H (alcohol)	3550–3230
43	$C_3H_7^+$ or CH_3CO^+	C=O (ketone)	1720–1700
45	$COOH^+$	O–H (acid)	3300–2500
57	$C_4H_9^+$ or $C_2H_5CO^+$	N–H (amine)	3500–3300

Worked examples

Counting carbons

- peak heights: M⁺ 30, M+1 1.3
- (1.3 ÷ 30) × 100 ÷ 1.1
- **4 carbons**: C_4H_8O

Which propanol?

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

An unknown

- Benedict's brick red; M⁺ 58
- IR 1730, 2720; no O–H
- **propanal**

NMR spectroscopy and chromatography follow at A2; mass spectra of elements were met in Topic 2.

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