Spectroscopy and Chromatography Map

Edexcel International A Level Chemistry · Unit 4 · Topic 15D Spectroscopy and Chromatography

1 High resolution MS

15.17

- M^+ to **4 decimal places**
- ^1H 1.0078, ^{12}C 12.0000, ^{16}O 15.9949
- Add up each candidate formula
- Closest value: **molecular formula**



2 ^{13}C NMR

15.18, 15.19

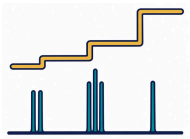
- One peak per **carbon environment**
- **Symmetry**: equivalent carbons share a peak
- δ from TMS (0 ppm)
- C=O 160–220; C–O 50–90

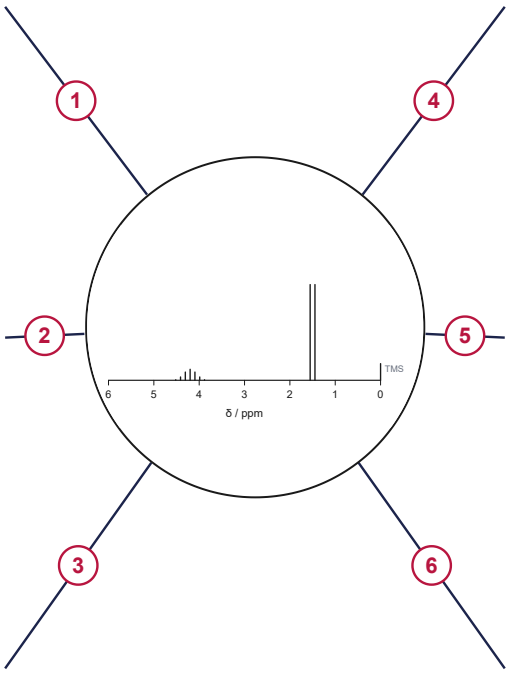


3 ^1H shifts and areas

15.20

- Peaks: **hydrogen environments**
- δ: what the H is near (O, C=O, ring)
- **Peak areas**: ratio of H
- Solvent $CDCl_3$; TMS at δ = 0

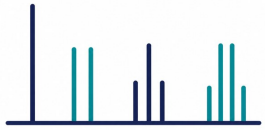




4 Splitting

15.20

- **n + 1 rule**: n H on adjacent C
- Singlet, doublet, triplet, quartet
- CH_2CH_3: quartet + triplet
- O–H: usually a singlet



5 Paper and TLC

15.21, 15.22

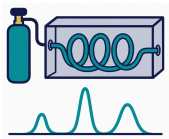
- Stationary: **silica** or water in paper
- Mobile: the **solvent**
- **Rf** = spot ÷ solvent front
- Same Rf, same solvent: same compound?



6 GC and HPLC

15.23

- GC: inert gas, liquid on a support
- **Retention time**; **peak area** ∝ amount
- HPLC: liquid at **high pressure**
- **GC–MS** identifies each peak



Which technique tells you what

use them together: each answers a different question

Technique	What you read	What it tells you
High resolution MS	M^+ to 4 d.p.	the molecular formula
^{13}C NMR	number of peaks, δ	carbon environments, C=O or C–O
^1H NMR	peaks, δ, areas	hydrogen environments and how many H
^1H NMR splitting	n + 1 lines	H on the adjacent carbon
TLC / paper	Rf	compare with a standard
GC, HPLC	retention time, peak area	identity (with MS) and amount

Worked examples

Accurate mass

- M^+ = 70.0419
- C_4H_6O 70.0417; C_5H_{10} 70.0780
- **C_4H_6O**

Read the splitting

- CH_3CHCl_2
- CH_3: doublet; CH: quartet
- **areas 3 : 1**

Rf value

- spot 2.7 cm; front 6.0 cm
- 2.7 ÷ 6.0
- **Rf = 0.45**

Spectra return in Topic 19 (amines, amides, amino acids) and Topic 20 (confirming a synthesis).

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