Spectroscopy Map

OCR A Level Chemistry A · 6.3.2 Spectroscopy

1 ^{13}C NMR

6.3.2(a)

- One peak per **carbon environment**
- **Symmetry**: equivalent carbons share a peak
- Simpler than ^{1}H: **no splitting**
- C=O 160–220; C–O 50–90



2 TMS, solvents and D_2O

6.3.2(d)

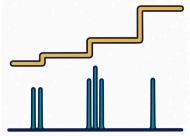
- **TMS**, $Si(CH_3)_4$: the δ = 0 standard
- Deuterated solvent: **$CDCl_3$**
- No ^{1}H: no solvent peak
- **D_2O**: O–H and N–H peaks vanish

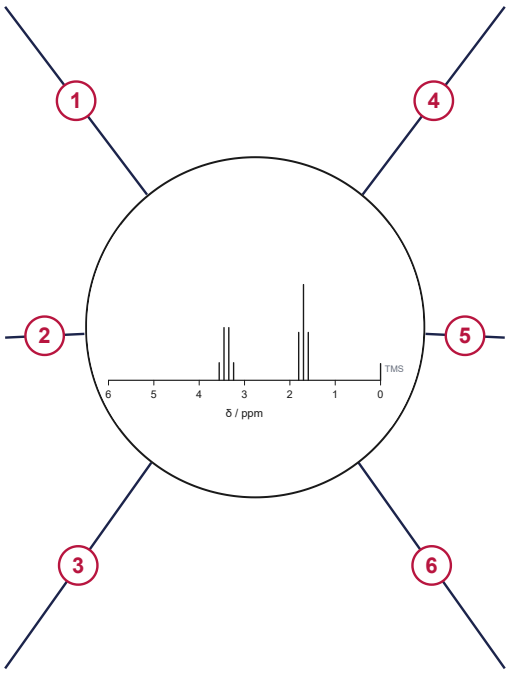


3 ^{1}H shifts and areas

6.3.2(b)

- Peaks: **proton environments**
- δ: what the H is near (O, C=O)
- **Integration**: ratio of H
- Shifts from the **Data Sheet**

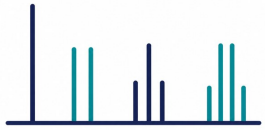




4 Splitting

6.3.2(b)

- **n + 1 rule**: n H on adjacent C
- Doublet, triplet, quartet … septet
- Equivalent H do not split
- No H next door: **singlet**



5 Combining techniques

6.3.2(e)

- **Elemental analysis**: empirical formula
- **M^+**: Mr, so molecular formula
- **IR**: O–H, C=O
- **Fragments**: pieces of the chain



6 Deducing a structure

6.3.2(c), (e)

- Formula first, then IR
- ^{13}C: carbon environments
- ^{1}H: areas, shifts, splitting
- Check **every** piece of data



What each technique tells you

use them together

Technique	What you read	What it tells you
Elemental analysis	% by mass	empirical formula
Mass spectrum	M^+; fragment m/z	Mr; pieces of the chain
Infrared	absorptions, cm^{-1}	bonds: O–H, C=O, N–H
^{13}C NMR	number of peaks; δ	carbon environments and types
^{1}H NMR	peaks, areas, δ, splitting	proton environments and neighbours
D_2O shake	a peak disappears	O–H or N–H protons

Worked examples

A molecular formula

- C 54.5%, H 9.1%, O 36.4%
- C_2H_4O; M^+ = 88
- **$C_4H_8O_2$**

Read the splitting

- $(CH_3)_2CHCl$
- CH_3: doublet; CH: septet
- **areas 6 : 1**

Spectra together

- C=O at 1740, no O–H
- quartet 4.1, singlet 2.0, triplet 1.2
- **ethyl ethanoate**

Mass spectra and IR were met in 4.2.4; spectra confirm the products of a synthesis in 6.2.5.

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