# NMR Spectroscopy Map

AQA A-level Chemistry · 3.3.15 Nuclear magnetic resonance spectroscopy

## 1 $^{13}$C NMR

3.3.15

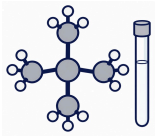
- One peak per **carbon environment**
- **Symmetry**: equivalent carbons share a peak
- Simpler than $^{1}$H: **no splitting**
- C=O 160–220; C–O 50–90



## 2 TMS and solvents

3.3.15

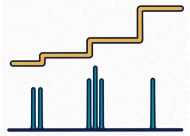
- **TMS**, $Si(CH_3)_4$: the δ = 0 standard
- One sharp peak, inert, volatile
- Solvents: **$CDCl_3$** or **$CCl_4$**
- No $^{1}$H: no solvent peak

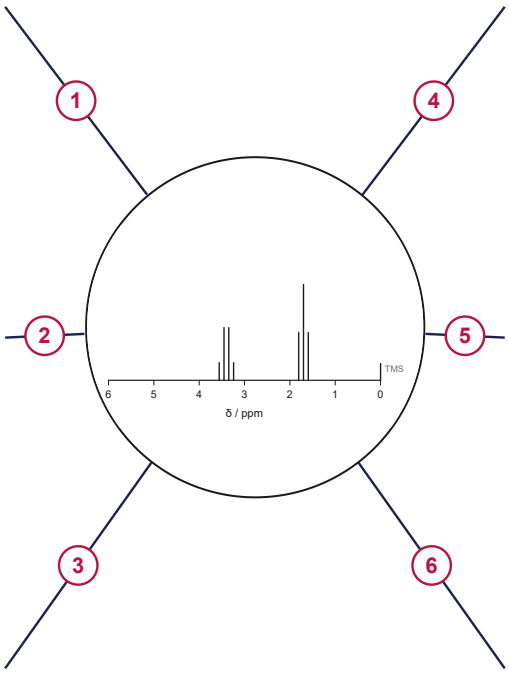


## 3 $^{1}$H shifts and areas

3.3.15

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

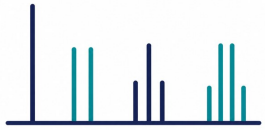





## 4 Splitting

3.3.15

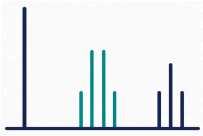
- **n + 1 rule**: n H on adjacent C
- Doublet, triplet, **quartet**
- Equivalent H do not split
- No H next door: **singlet**



## 5 Common patterns

3.3.15

- Quartet + triplet, 2 : 3: **ethyl**
- Singlet 3H, δ 2.1: **$CH_3C{=}O$**
- Singlet 3H, δ 3.7: **$OCH_3$**
- Singlet 9H: **$C(CH_3)_3$**



## 6 Deducing a structure

3.3.15

- Count the peaks; read the **areas**
- Use δ to place O and C=O
- Splitting: H next door
- Fit the fragments to the **formula**



## What each feature tells you

read a spectrum in this order

| Feature | What you read | What it tells you |
|---|---|---|
| $^{13}$C peaks | how many | carbon environments |
| $^{13}$C shift | δ in ppm | C=O, C–O or C–C |
| $^{1}$H peaks | how many | hydrogen environments |
| $^{1}$H areas | integration ratio | how many H in each |
| $^{1}$H shift | δ in ppm | what each H is near |
| $^{1}$H splitting | n + 1 lines | H on the adjacent carbon |

## Worked examples

### Count the carbons

- propan-2-ol, $CH_3CH(OH)CH_3$
- two $CH_3$ are equivalent
- **2 peaks**

### Read the splitting

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

### Integration

- heights 1.2 : 0.8 : 1.2 cm
- $C_4H_8O_2$: 8 H
- **3H, 2H, 3H**

Spectra return in 3.3.10 to 3.3.13 and in confirming the products of a synthesis (3.3.14).

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