

Exercise walk-through

37.3

Carbon-13 NMR spectroscopy

A-Level Chemistry

NMR basics

carbon-13 NMR

each carbon **environment** gives one peak

proton NMR

chemical shift &
peak areas give the proton ratio

NMR

studies nuclei in a strong magnetic field; the number of peaks = the number of environments.

Splitting and the $n + 1$ rule

**singlet**

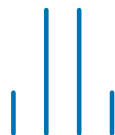
$$n = 0$$

**doublet**

$$n = 1$$

**triplet**

$$n = 2$$

**quartet**

$$n = 3$$

n equivalent neighbours split a peak into $n + 1$ lines

Splitting : n equivalent neighbouring protons split a peak into $n + 1$ lines.

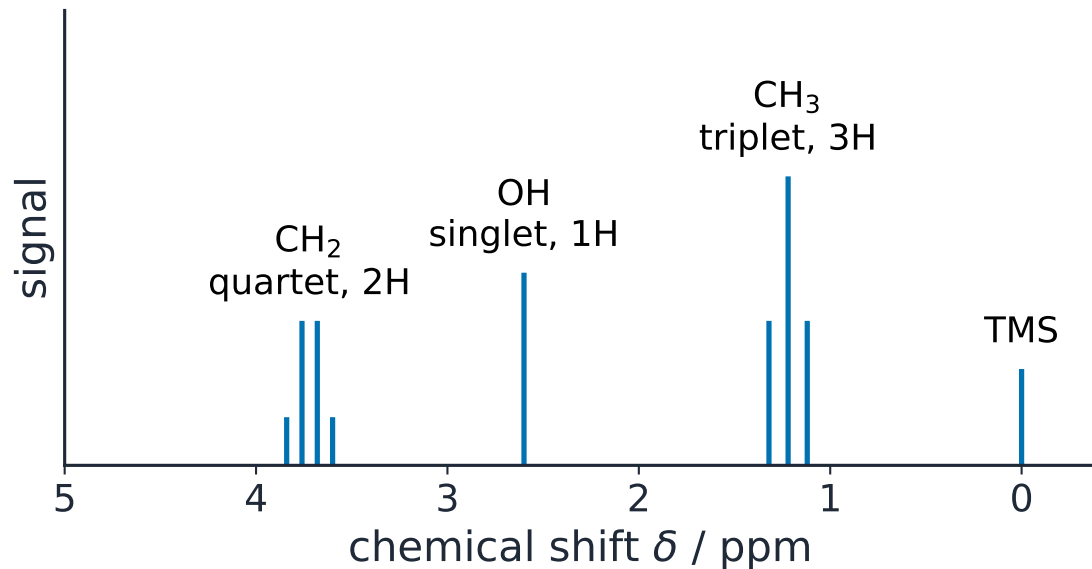
- $0 \rightarrow$ **singlet** ; $1 \rightarrow$ doublet
- $2 \rightarrow$ triplet; $3 \rightarrow$ quartet

A proton NMR spectrum

Ethanol: a CH_3 triplet, a CH_2 quartet & an OH singlet (areas 3:2:1).

- **TMS** is the zero reference
- a **deuterated solvent** gives no signal
- D_2O removes the O–H/N–H peak

A proton NMR spectrum, in detail



$n+1$ rule · integration 3 : 2 : 1 · TMS = 0 ppm

Ethanol: a CH_3 triplet, a CH_2 quartet & an OH singlet (areas 3:2:1).

Practical points

- **tetramethylsilane** (TMS) is the standard, set at a chemical shift of 0.
- a **deuterated solvent** (such as CDCl_3) is used so that the solvent itself gives no proton signal.
- shaking the sample with D_2O makes the O–H and N–H peaks disappear (their hydrogen is swapped for deuterium), which identifies those protons.

Exercises 2.1·2.2

2.1 State what the number of peaks in a ^{13}C NMR spectrum tells you. [1]

2.2 State how many peaks propanone, CH_3COCH_3 , gives in its ^{13}C spectrum. [1]

Exercises 2.1·2.2

2.1 State what the number of peaks in a ^{13}C NMR spectrum tells you. [1]

2.1

- the number of different carbon (chemical) environments in the molecule
-

2.2 State how many peaks propanone, CH_3COCH_3 , gives in its ^{13}C spectrum. [1]

2.2

- 2 peaks (the two CH_3 carbons are equivalent; the $\text{C}=\text{O}$ is the second)

Exercises 3.1·3.2

3.1 In ^{13}C NMR, two carbon atoms in the **same** environment give: [1]

☐

A two separate peaks

B a single peak

C no peak

D a split peak

3.2 How many peaks does propan-1-ol, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$, give in its ^{13}C spectrum? [1]

☐

A 1

B 2

C 3

D 4

Exercises 3.1-3.2

3.1 In ^{13}C NMR, two carbon atoms in the **same** environment give: [1]

☐

A two separate peaks

B a single peak

C no peak

D a split peak

3.1 B

- Equivalent carbons in the same environment give a single peak

3.2 How many peaks does propan-1-ol, $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$, give in its ^{13}C spectrum? [1]

☐

A 1

B 2

C 3

D 4

3.2 C

- Propan-1-ol has three different carbon environments
- 3 peaks

Exercise 3.3 (a)

3.3 A compound $\text{C}_3\text{H}_6\text{O}$ gives **two** peaks in its ^{13}C NMR spectrum, one far downfield (a $\text{C}=\text{O}$).

(a) Deduce a possible structure.

[2]

Exercise 3.3 (a)

3.3 A compound $\text{C}_3\text{H}_6\text{O}$ gives **two** peaks in its ^{13}C NMR spectrum, one far downfield (a $\text{C}=\text{O}$).

(a) Deduce a possible structure.

[2]

(a)

- propanone, CH_3COCH_3 – the $\text{C}=\text{O}$ gives the downfield peak and the two equivalent CH_3 give the other

Exercise 3.3 (b)

3.3 A compound $\text{C}_3\text{H}_6\text{O}$ gives **two** peaks in its ^{13}C NMR spectrum, one far downfield (a $\text{C}=\text{O}$).

(b) Explain how the number of peaks supports your structure.

[1]

Exercise 3.3 (b)

3.3 A compound $\text{C}_3\text{H}_6\text{O}$ gives **two** peaks in its ^{13}C NMR spectrum, one far downfield (a $\text{C}=\text{O}$).

(b) Explain how the number of peaks supports your structure. [1]

(b)

- the two equivalent methyl carbons share one peak and the $\text{C}=\text{O}$ gives the second, so two peaks fit

Exercise 3.4

3.4 Explain why ethanoic acid, CH_3COOH , gives **two** peaks in its ^{13}C NMR spectrum.[2]

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3.4

- ethanoic acid has two different carbon environments – the CH_3 carbon and the COOH carbon; each gives one peak, so there are two peaks