

Exercise walk-through

Carbon-13 NMR spectroscopy ■ 37.3

eXercise

You must be able to

- state what the number of peaks in a ^{13}C NMR spectrum tells you
- use chemical shift to suggest the type of carbon
- deduce possible structures from a ^{13}C spectrum

Method — Counting carbon environments

- in ^{13}C NMR, each different **carbon environment** gives **one peak** (equivalent carbons share a peak).
- **number of peaks** = number of different carbon environments.
- **chemical shift** (peak position) suggests the type of carbon (e.g. $\text{C}=\text{O}$ is far downfield).

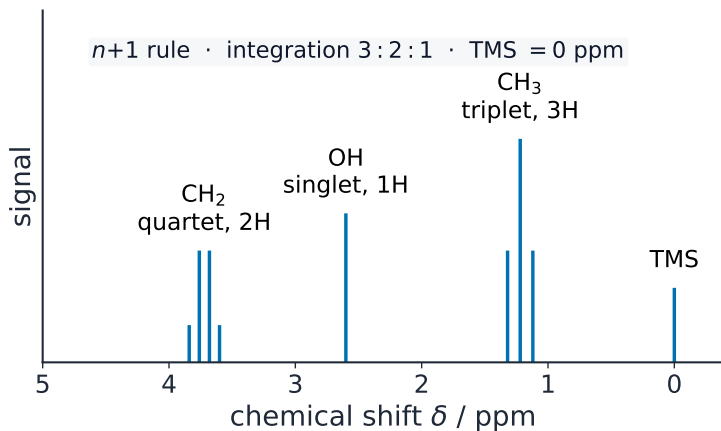
Example: ethanol $\text{CH}_3\text{CH}_2\text{OH}$ has 2 carbon environments $\rightarrow$ **2 peaks**.

Method — Counting carbon environments



A tall cylindrical NMR spectrometer with a strong magnetic field warning

Method — Counting carbon environments



An NMR spectrum from a carbon environment count

Practice 2.1 ■ 1 mark

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

Solution 2.1

Method: Counting carbon environments

Worked steps

the number of different carbon (chemical) environments in the molecule **B1**.

Practice 2.2 ■ 1 mark

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

Solution 2.2

Method: Counting carbon environments

Worked steps

2 peaks (the two CH_3 carbons are equivalent; the $\text{C}=\text{O}$ is the second) **B1**.

Exam-style 3.1 ■ 1 mark

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

A two separate peaks

B a single peak

C no peak

D a split peak

Solution 3.1

Method: Counting carbon environments

A two separate peaks

B a single peak



C no peak

D a split peak

Worked steps

B. Equivalent carbons in the same environment give a single peak.

Exam-style 3.2 ■ 1 mark

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

A 1

B 2

C 3

D 4

Solution 3.2

Method: Counting carbon environments

A 1

B 2

C 3



D 4

Worked steps

C. Propan-1-ol has three different carbon environments → 3 peaks.

Exam-style 3.3 ■ 2 marks

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

Solution 3.3

Method: Counting carbon environments

Worked steps

- (a) propanone, CH_3COCH_3 **M1** **A1** — the $\text{C}=\text{O}$ gives the downfield peak and the two equivalent CH_3 give the other.
- (b) the two equivalent methyl carbons share one peak and the $\text{C}=\text{O}$ gives the second, so two peaks fit **B1**.

Exam-style 3.4 ■ 2 marks

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

Solution 3.4

Method: Counting carbon environments

Worked steps

ethanoic acid has two different carbon environments — the CH_3 carbon and the COOH carbon (M1); each gives one peak, so there are two peaks (A1).