

37.3 Carbon-13 NMR spectroscopy

Name: _____ Class: _____ Date: _____

Total: 9 marks

KEY WORDS carbon-13 nmr 碳 • nmr 核磁共振 • chemical shift 化学位移 • chemical environment 化学环境

Objective

Build the skills to answer exam questions on **carbon-13 NMR** 碳-13 核磁共振 — using the number and position of peaks to count carbon **chemical environments** 化学环境 and suggest structures.

You must be able to:

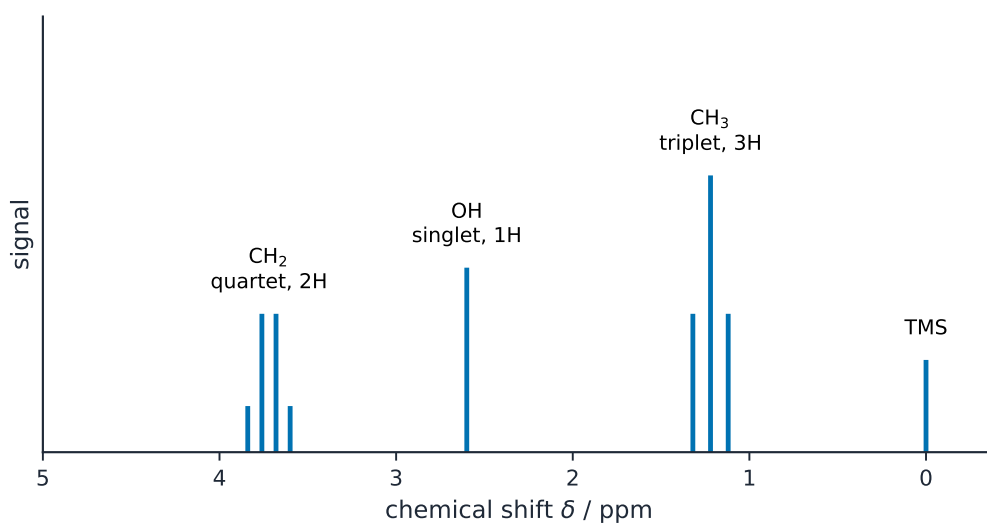
- state what the number of peaks in a ^{13}C NMR spectrum tells you
- use chemical shift to suggest the type of carbon
- deduce possible structures from a ^{13}C spectrum

1 Worked examples

■ Counting carbon environments



NMR uses a very strong magnetic field (from a superconducting magnet) to study how nuclei behave



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

An NMR spectrum from a carbon environment count

- 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 → **2 peaks**.

2 Practice

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]

3 Exam-style questions

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
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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
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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]

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

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

Solutions

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

2.2 2 peaks (the two CH_3 carbons are equivalent; the $\text{C}=\text{O}$ is the second).

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

3.2 C. Propan-1-ol has three different carbon environments $\rightarrow$ 3 peaks.

3.3 (a) propanone, CH_3COCH_3 — 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.

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.