A-LEVEL CHEMISTRY • EXERCISE SHEET

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.

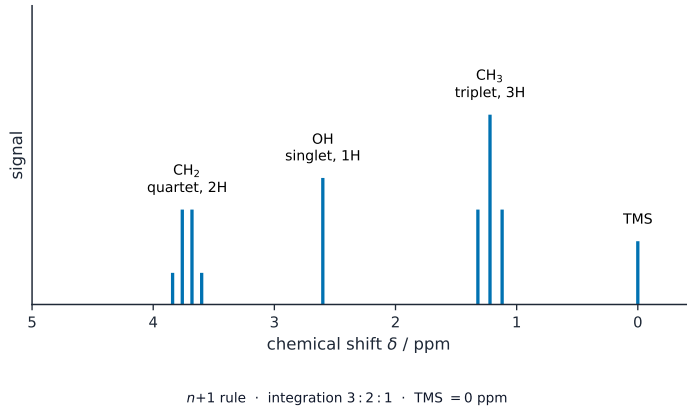
You must be able to:

- 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. C=O is far downfield).

Example: ethanol CH_3CH_2OH 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

3.2 How many peaks does propan-1-ol, $CH_3CH_2CH_2OH$, give in its ^{13}C spectrum? [1]

- **A** 1
- **B** 2
- **C** 3
- **D** 4

3.3 A compound C_3H_6O gives **two** peaks in its ^{13}C NMR spectrum, one far downfield (a C=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 C=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 → 3 peaks.

3.3 (a) propanone, CH_3COCH_3 — the C=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 C=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.