

37.4 Proton (^1H) NMR spectroscopy

Name: _____ Class: _____ Date: _____

Total: 10 marks

Objective

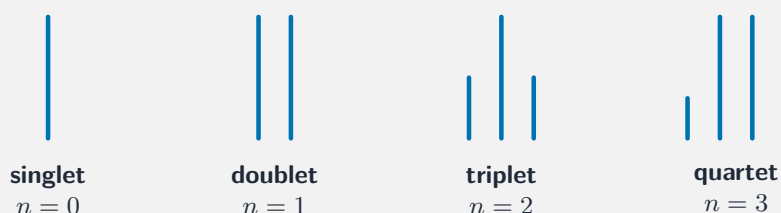
Build the skills to answer exam questions on **proton (^1H) NMR** 质子核磁共振—chemical environments, peak **area** ratios, **splitting** 裂分 by the $n + 1$ rule, and the use of TMS and D_2O .

You must be able to:

- count proton environments and use area ratios
- apply the $n + 1$ rule to predict splitting patterns
- explain the roles of TMS, a deuterated solvent and D_2O

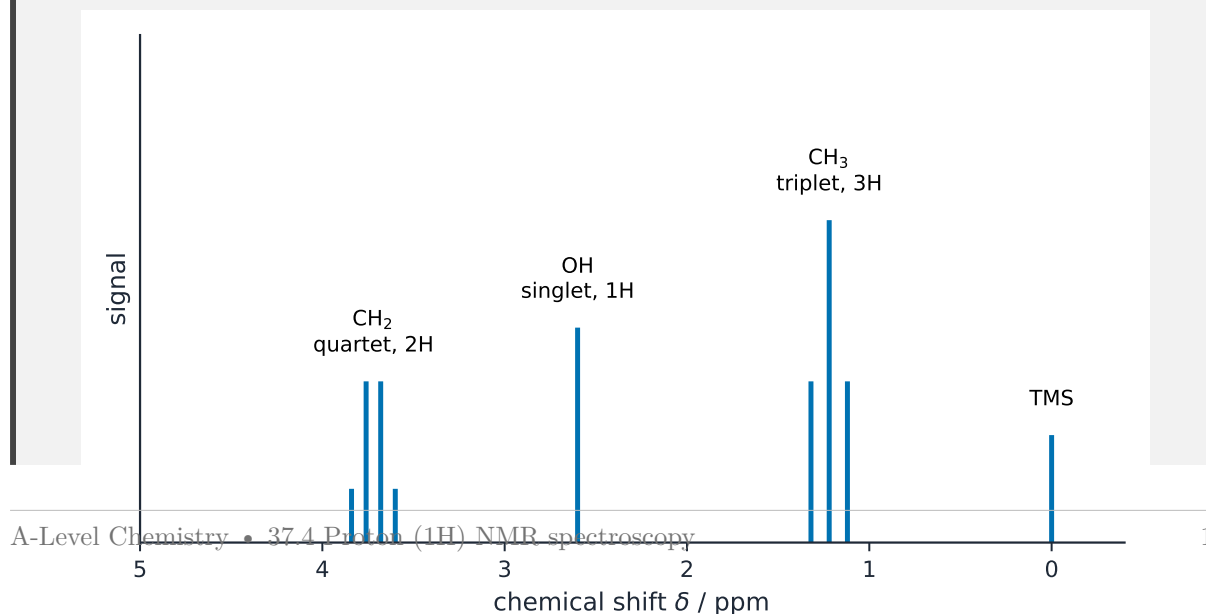
1 Worked examples

■ Splitting and areas



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

The $n + 1$ rule: n equivalent neighbouring protons split a peak into $n + 1$ lines



- **number of peaks** = number of proton environments; **area ratio** = ratio of protons.
- **$n + 1$ rule:** n equivalent neighbours $\rightarrow n + 1$ lines (0 $\rightarrow$ singlet, 1 $\rightarrow$ doublet, 2 $\rightarrow$ triplet, 3 $\rightarrow$ quartet).
- **TMS** sets the shift = 0; a **deuterated solvent** (CDCl_3) gives no signal; shaking with D_2O removes O–H/N–H peaks.

2 Practice

2.1 State what the relative **areas** of ^1H NMR peaks tell you. [1]

2.2 Using the $n + 1$ rule, state the splitting of a CH_3 next to a CH_2 . [1]

3 Exam-style questions

3.1 A proton with **two** equivalent neighbours appears as a: [1]

- **A** singlet
 - **B** doublet
 - **C** triplet
 - **D** quartet
-

3.2 Shaking a sample with D_2O causes a peak to **disappear**. This peak is due to: [1]

- **A** a CH_3 group
 - **B** an O–H or N–H proton
 - **C** a CH_2 group
 - **D** the TMS reference
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3.3 The ^1H NMR spectrum of ethanol, $\text{CH}_3\text{CH}_2\text{OH}$, has three groups of peaks.

(a) Give the splitting pattern of the CH_3 and the CH_2 peaks, with reasons. [2]

(b) State the ratio of the peak areas.

[1]

3.4 A compound has two ^1H environments with area ratio 3:2; the larger peak is a triplet and the smaller a quartet. Deduce the two groups present and explain the splitting. [3]

4 Go further

You are now ready for the real exam questions on this subtopic. Open the **37.4 Proton NMR** material in the Library, or try this in **Practice mode**:

- 9701/42 N25 —Q7 (proton NMR spectroscopy)

Solutions

2.1 the ratio of the numbers of protons in each environment.

2.2 a triplet ($n = 2$ neighbours $\rightarrow 2 + 1 = 3$ lines).

3.1 C. Two equivalent neighbours give $2 + 1 = 3$ lines —a triplet.

3.2 B. D_2O exchange removes the O–H / N–H peak.

3.3 (a) the CH_3 is a triplet (its 2 CH_2 neighbours give $2 + 1 = 3$); the CH_2 is a quartet (its 3 CH_3 neighbours give $3 + 1 = 4$).

(b) $\text{CH}_3 : \text{CH}_2 : \text{OH} = 3 : 2 : 1$.

3.4 the triplet (area 3) is a CH_3 with 2 neighbours, and the quartet (area 2) is a CH_2 with 3 neighbours; so the groups are CH_3 and CH_2 next to each other, i.e. an ethyl group; each splits the other by the $n + 1$ rule.