A-LEVEL CHEMISTRY • EXERCISE SHEET

37.4 Proton (1H) NMR spectroscopy

Name: _____ Class: _____ Date: _____ **Total: 10 marks**

KEY WORDS splitting 裂分 • chemical environment 化学环境 • proton 质子 • singlet 单峰 • triplet 三峰

Objective

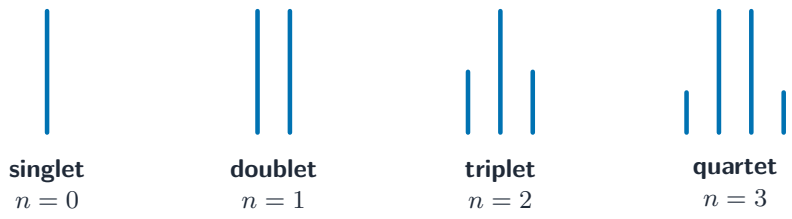
Build the skills to answer exam questions on **proton (^{1}H) NMR** 质子核磁共振 — chemical environments, peak **area** ratios, **splitting** 裂分 by the $n+1$ rule, and the use of TMS and D_2O.

You must be able to:

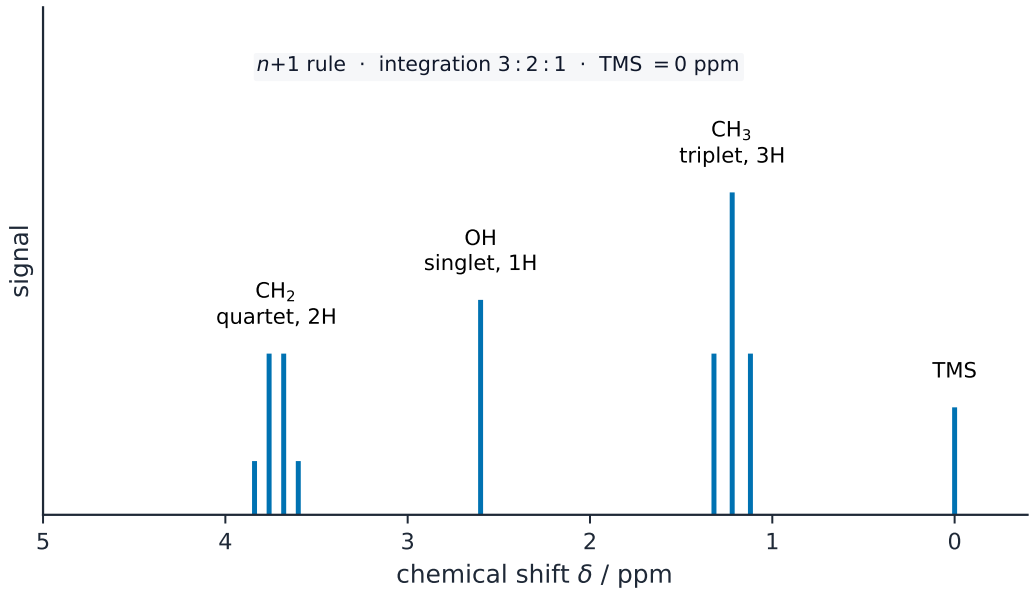
- count proton environments and use area ratios
- apply the $n+1$ rule to predict splitting patterns
- explain the roles of TMS, a deuterated solvent and D_2O

1 Worked examples

Splitting and areas



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



Ethanol: three environments give a CH_3 triplet, a CH_2 quartet and an OH singlet, areas in ratio 3:2:1

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

2 Practice

2.1 State what the relative **areas** of ^{1}H 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

3.3 The ^1H NMR spectrum of ethanol, CH_3CH_2OH, 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]

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) $CH_3 : CH_2 : OH = 3 : 2 : 1$.

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.