Exercise walk-through

Proton (1H) NMR spectroscopy ▪ 37.4

eXercise

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

Method — Splitting and areas

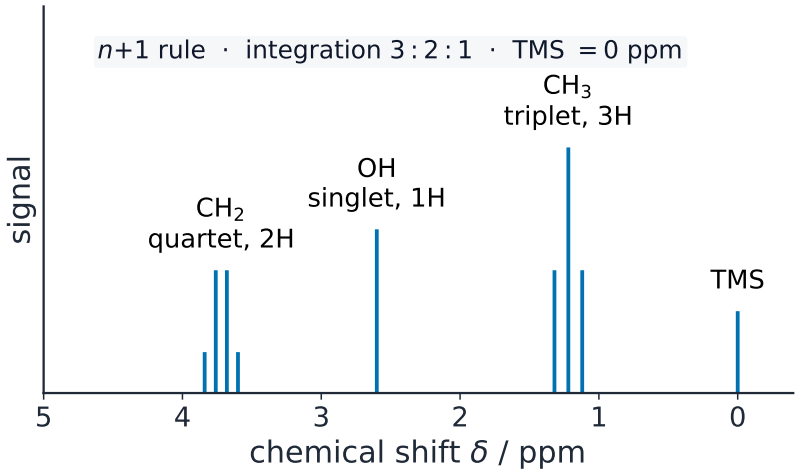
- **number of peaks** = number of proton environments; **area ratio** = ratio of protons.
- $n+1$ **rule:** n equivalent neighbours $\rightarrow$ $n+1$ lines (0$\rightarrow$singlet, 1$\rightarrow$doublet, 2$\rightarrow$triplet, 3$\rightarrow$quartet).
- **TMS** sets the shift = 0; a **deuterated solvent**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

Method — Splitting and areas

singlet	**doublet**	**triplet**	**quartet**
$n = 0$	$n = 1$	$n = 2$	$n = 3$

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

Method — Splitting and areas



Practice 2.1 ▪ 1 mark

State what the relative **areas** of ^{1}H NMR peaks tell you.

Solution 2.1

Method: Splitting and areas

Worked steps

the ratio of the numbers of protons in each environment **B1**.

Practice 2.2 ▪ 1 mark

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

Solution 2.2

Method: Splitting and areas

Worked steps

a triplet ($n = 2$ neighbours $\rightarrow 2 + 1 = 3$ lines) B1.

Exam-style 3.1 ▪ 1 mark

A proton with **two** equivalent neighbours appears as a:

A singlet

B doublet

C triplet

D quartet

Solution 3.1

Method: Splitting and areas

A singlet

B doublet

C triplet ✓

D quartet

Worked steps

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

Exam-style 3.2 ▪ 1 mark

Shaking a sample with D_2O causes a peak to **disappear**. This peak is due to:

A a CH_3 group

B an O–H or N–H proton

C a CH_2 group

D the TMS reference

Solution 3.2

Method: Splitting and areas

A a CH_3 group

B an O–H or N–H proton ✓

C a CH_2 group

D the TMS reference

Worked steps

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

Exam-style 3.3 ▪ 2 marks

The ^{1}H 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.
(b) State the ratio of the peak areas.

Solution 3.3

Method: Splitting and areas

Worked steps

(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 $3+1=4$) M1 A1.
(b) $CH_3 : CH_2 : OH = 3 : 2 : 1$ B1.

Exam-style 3.4 ▪ 3 marks

A compound has two ^{1}H 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.

Solution 3.4

Method: Splitting and areas

Worked steps

the triplet (area 3) is a CH_3 with 2 neighbours, and the quartet (area 2) is a CH_2 with 3 neighbours **M1**; so the groups are CH_3 and CH_2 next to each other, i.e. an ethyl group **M1**; each splits the other by the $n + 1$ rule **A1**.