

NMR Spectroscopy

How does NMR reveal the carbon–hydrogen framework of a molecule?

●●○ Intermediate

Analytical Chemistry

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Before you start: it helps to understand [Infrared Spectroscopy](#) and [Mass Spectrometry](#) and [Functional Groups](#).

What is it?

Nuclear magnetic resonance (NMR) spectroscopy places a sample in a strong magnetic field and probes it with radio waves. Hydrogen nuclei (protons) in **different chemical environments** absorb at slightly different frequencies, so a ^1H NMR spectrum shows how the hydrogen atoms in a molecule are arranged.

A ^1H NMR spectrum gives **four** pieces of information:

1. **Number of signals:** how many different hydrogen environments there are.
2. **Chemical shift**, δ (in ppm): what kind of environment each one is.
3. **Integration** (relative area): how many hydrogens are in each environment.
4. **Splitting** (multiplicity): how many hydrogens are on the **neighbouring** carbons.

Hydrogens are in the **same environment** if they are interchangeable by symmetry: the six H atoms in propanone, CH_3COCH_3 , are all equivalent, so propanone gives **one** signal.

KEY IDEA

Each signal is a group of equivalent hydrogens. Its **position** tells you what is nearby (an oxygen, a C=O, a benzene ring), its **area** tells you how many H atoms it represents, and its **splitting** tells you how many H atoms sit on the next carbon along.

Why does it matter?

- **Structure determination.** NMR is the most powerful tool chemists have for working out how atoms are connected in a new molecule.
- **Medicine.** MRI (magnetic resonance imaging) is NMR of the hydrogen nuclei in water and fat in the body.
- **Industry and research.** NMR checks the purity of medicines and follows reactions as they happen.

How does it work?

1. Chemical shift

Shifts are measured relative to a reference, **TMS** (tetramethylsilane, set at $\delta = 0$), and are given in **parts per million** so that they are the same on every spectrometer:

$$\delta \text{ (ppm)} = \frac{\text{shift from TMS (Hz)}}{\text{spectrometer frequency (MHz)}}$$

Nearby **electronegative atoms** and **C=O** or aromatic rings pull electron density away from a hydrogen (“deshielding”), moving its signal to a **higher** δ :

Type of hydrogen	Typical δ (ppm)
alkyl, $\text{R}-\text{CH}_3$, $\text{R}-\text{CH}_2-\text{R}$	0.9–1.7
next to $\text{C}=\text{O}$, $-\text{CO}-\text{CH}_3$	2.0–2.7
on carbon next to O, $-\text{O}-\text{CH}_2-$, $-\text{O}-\text{CH}_3$	3.3–4.3
alkene, $\text{C}=\text{C}-\text{H}$	4.5–6.5
aromatic, on a benzene ring	6.5–8.0
aldehyde, $-\text{CHO}$	9–10
carboxylic acid, $-\text{COOH}$	10–12
alcohol $-\text{OH}$	1–5 (variable)

2. Integration

The area under each signal is proportional to the number of hydrogens it represents. Spectrometers print the areas as a **ratio**, such as 3 : 2 : 1 for ethanol.

3. Splitting: the $n + 1$ rule

A signal from hydrogens with **n** equivalent hydrogens on **adjacent** carbons is split into **n + 1** peaks:

H on neighbouring carbons (n)	0	1	2	3
Peaks (n + 1)	1, singlet	2, doublet	3, triplet	4, quartet

So an ethyl group, $-\text{CH}_2\text{CH}_3$, always shows a **quartet** (the CH_2 , split by 3 H) and a **triplet** (the CH_3 , split by 2 H). An **O–H** hydrogen usually appears as a **singlet** and is not split by, nor does it split, its neighbours.

4. ^{13}C NMR in brief

^{13}C NMR shows one signal for each **carbon environment** (without splitting in the usual spectra). Typical ranges: alkyl carbons 0–50 ppm, carbons bonded to O 50–90 ppm, alkene and aromatic carbons 110–160 ppm, and C=O carbons 160–220 ppm.

∞ THINK OF IT LIKE THIS

Reading an NMR spectrum is like working out where people live from a list of neighbours. Each signal is a household; its shift says which part of town it is in (near an oxygen, near a ring); its area says how many people live there; and its splitting says how many people live next door.

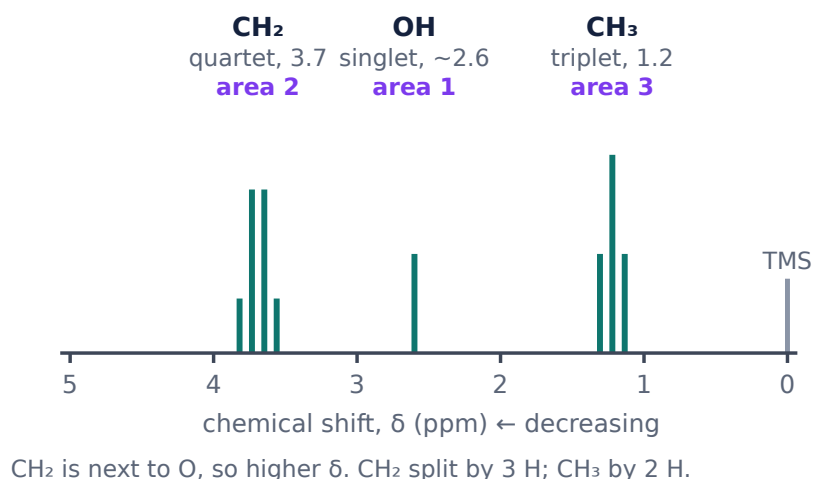
Q MORE PRECISELY

The $n + 1$ rule works when the neighbouring hydrogens are all equivalent and couple equally; more complex molecules give multiplets. Adding a drop of D_2O makes an O–H or N–H signal disappear, because deuterium replaces the hydrogen and does not show in ^1H NMR; this is a useful way to identify them. Spectrometers are described by their proton frequency (300 MHz, 400 MHz...); a higher frequency spreads the signals out more in Hz, but δ in ppm stays the same.

Visualise it

^1H NMR spectrum of ethanol, $\text{CH}_3\text{CH}_2\text{OH}$

Schematic: three environments, areas 2 : 1 : 3



^1H NMR spectrum of ethanol (schematic): three environments in a 2 : 1 : 3 ratio.

Worked example

WORKED EXAMPLE: Counting environments

Question: How many ^1H NMR signals do these give: (a) propanone, CH_3COCH_3 (b) ethanol, $\text{CH}_3\text{CH}_2\text{OH}$ (c) methyl ethanoate, $\text{CH}_3\text{COOCH}_3$?

Step 1 (a) Both CH_3 groups are equivalent: **1 signal** (6H).

Step 2 (b) CH_3 , CH_2 and OH : **3 signals** (3 : 2 : 1).

Step 3 (c) The CH_3 next to $\text{C}=\text{O}$ and the CH_3 on O are different: **2 signals**, at about 2.0 and 3.7 ppm, both singlets (no neighbouring H).

WORKED EXAMPLE: Chemical shift in ppm

Question: On a 400 MHz spectrometer, a signal appears 1092 Hz from TMS. Calculate δ , and say what kind of hydrogen it might be.

$$\begin{aligned}\delta &= \frac{1092 \text{ Hz}}{400 \text{ MHz}} \\ &= 2.73 \text{ ppm}\end{aligned}$$

(1 Hz per MHz = 1 ppm.) At 2.73 ppm, it is probably a hydrogen on a carbon **next to a $\text{C}=\text{O}$** group.

WORKED EXAMPLE: Predicting a spectrum: ethyl ethanoate

Question: Predict the ^1H NMR spectrum of ethyl ethanoate, $\text{CH}_3\text{COOCH}_2\text{CH}_3$.

Group	δ (ppm)	Area	Neighbours (n)	Splitting
CH_3-CO	about 2.0	3	0	singlet
$\text{O}-\text{CH}_2$	about 4.1	2	3	quartet
CH_2-CH_3	about 1.3	3	2	triplet

 WORKED EXAMPLE: Solving a structure

Question: A compound $C_4H_8O_2$ shows a strong IR absorption at 1740 cm^{-1} (no O–H). Its 1H NMR spectrum has a triplet at 1.2 ppm (3H), a quartet at 2.3 ppm (2H) and a singlet at 3.7 ppm (3H). Identify it.

Step 1 IR: C=O with no O–H, and two O atoms: an **ester**.

Step 2 Triplet (3H) + quartet (2H): an **ethyl group**. The quartet at 2.3 ppm means the CH_2 is next to C=O: $CH_3CH_2-CO^-$.

Step 3 Singlet at 3.7 ppm (3H): a CH_3 on **oxygen** with no neighbours: $-O-CH_3$.

Step 4 The compound is **methyl propanoate**, $CH_3CH_2COOCH_3$ (4 C, 8 H, 2 O ✓).

Common mistake

 COMMON MISTAKE: Counting the hydrogens on the same carbon

Splitting comes from hydrogens on the **neighbouring** carbons, not on the same carbon. The CH_3 in an ethyl group is a triplet because its neighbour, CH_2 , has 2 H.

 COMMON MISTAKE: Treating integration as an exact count

Integration gives a **ratio**. If the areas are 1 : 1.5, the actual numbers could be 2 : 3 or 4 : 6. Use the molecular formula to fix the totals.

 COMMON MISTAKE: Expecting O–H to be split

In most spectra the O–H hydrogen appears as a **singlet** and does not split neighbouring signals, because it exchanges rapidly between molecules.

 NOTATION NOTE

- δ is read “delta”; NMR spectra are drawn with δ **decreasing** from left to right (like IR).
- s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

Remember this

REMEMBER THIS

- Number of signals = number of H environments. Integration = relative number of H in each.
- δ (ppm) = shift (Hz) $\div$ spectrometer frequency (MHz); TMS = 0 ppm.
- Higher δ near electronegative atoms, C=O and rings: about 1 (alkyl), 2–2.7 (next to C=O), 3.3–4.3 (on C–O), 6.5–8 (aromatic), 9–10 (CHO), 10–12 (COOH).
- $n + 1$ rule: n neighbouring H give $n + 1$ peaks; ethyl = quartet + triplet.
- Combine MS (mass), IR (functional groups) and NMR (C–H framework) to solve a structure.

References

1. Brown, T. L.; LeMay, H. E., Jr.; Bursten, B. E.; Murphy, C. J.; Woodward, P. M.; Stoltzfus, M. W. Chemistry: The Central Science, 15th ed.; Pearson, 2022.

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