

AQA Chemistry A-level

3.3.15: NMR Spectroscopy Detailed Notes

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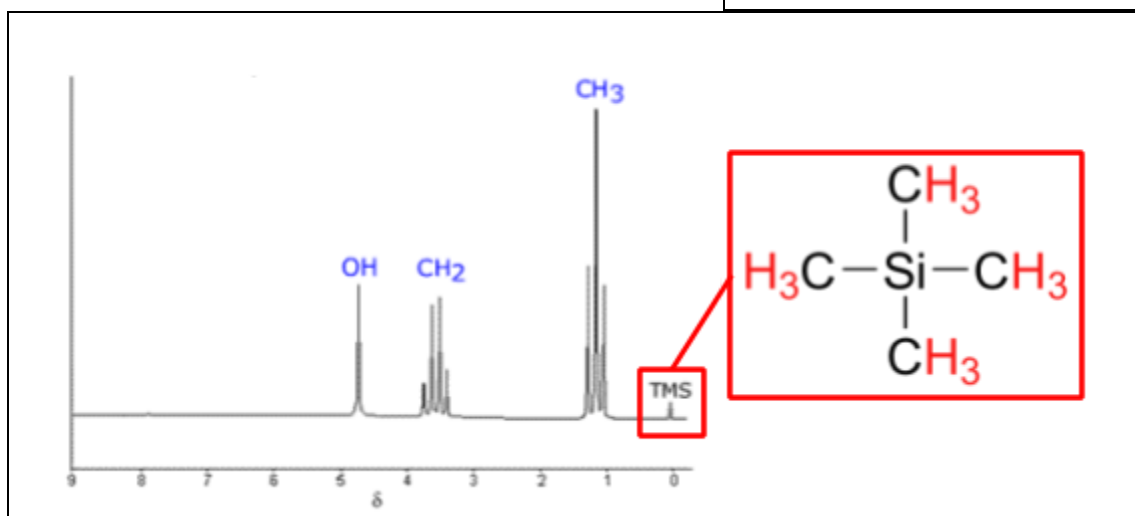


3.3.15.1 - NMR Spectroscopy

This is an **analytical technique** that allows the structure of a molecule to be determined by analysing the energy of each bond environment. Different bond environments within a molecule **absorb different amounts of energy** meaning they show as **different peaks** on a spectra print out.

The bond environment peaks are measured against a standard molecule, **tetramethylsilane (Si(CH₃)₄)** known as TMS. This is a standard molecule as it contains four **identical** carbon and hydrogen environments. It is seen as a peak at **δ=0 ppm** on the x-axis.

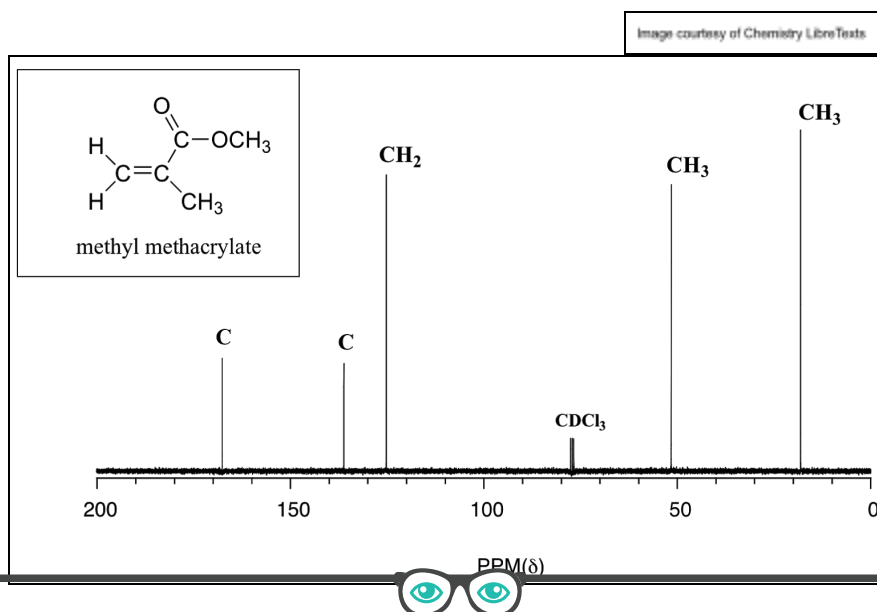
Example:



C¹³ NMR

This form of NMR spectroscopy analyses the different **carbon environments** in a molecule. The different environments are shown as peaks at different **δ** values.

Example:

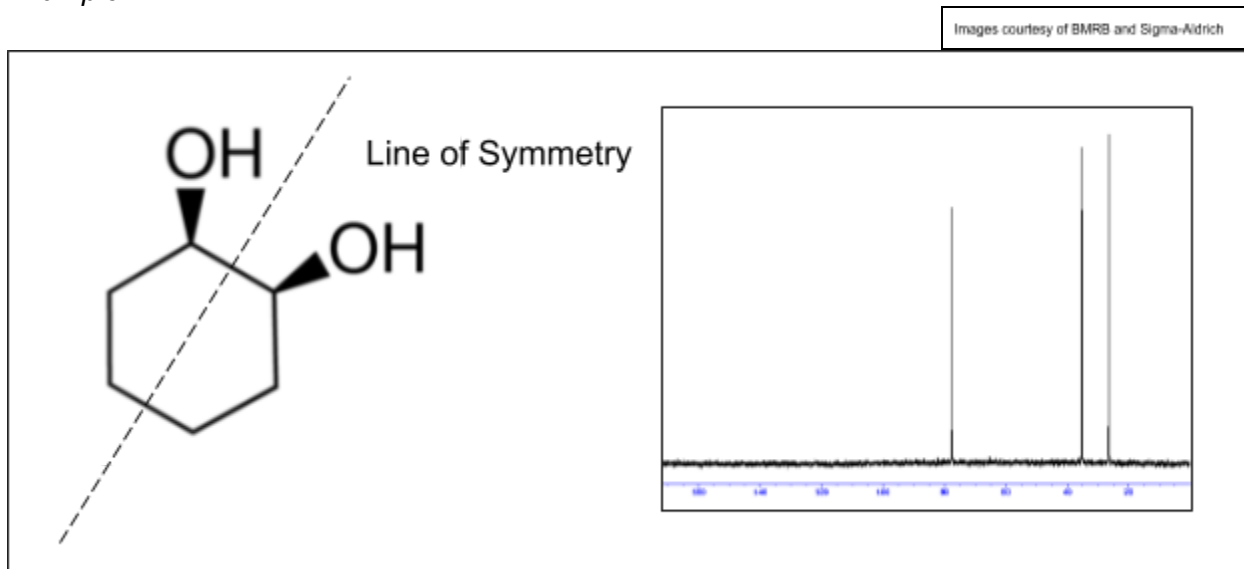




Carbon environments that are **near to an oxygen** have δ values that are **shifted to the right**. This is because oxygen is very **electronegative** and changes the bond environment and how it absorbs energy.

Molecules that have **symmetry** may display fewer δ peaks than the number of carbon atoms in the molecule. Therefore in these cases, it is important to look at the given molecular formula of the compound in order to decipher its displayed structure.

Example:



This molecule, 1,2-cyclohexanediol, contains six carbon atoms but the NMR spectrum only has three peaks due to the symmetry of the molecule.

All C^{13} NMR δ shift values are given on the 'AQA Chemistry Data Sheet'.

H¹ NMR (Proton NMR)

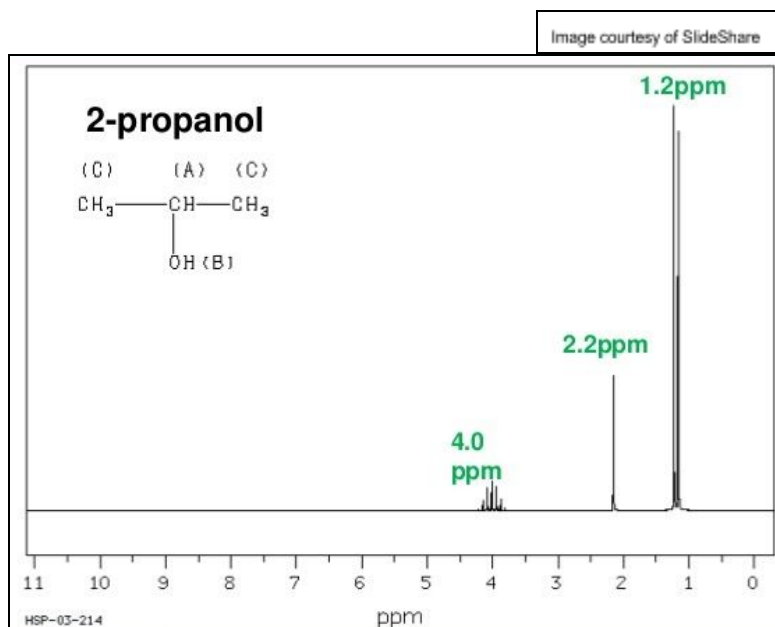
In this form of NMR, the different **hydrogen environments** in a molecule are analysed and displayed as peaks on a spectra. These peaks are also measured against the TMS standard.

The samples being analysed must be dissolved in a **non-hydrogen-containing solvent** so that it doesn't produce any δ peaks on the spectrum. CCl_4 is therefore a common solvent used along with **deuterated solvents** containing deuterium, an isotope of hydrogen.



H^1 NMR spectra are more complex than C^{13} spectra as the heights of the peaks show the **relative intensity** of each δ value. These relative intensities correspond to the number of hydrogen in that certain environment within a molecule, shown as a number above the peak.

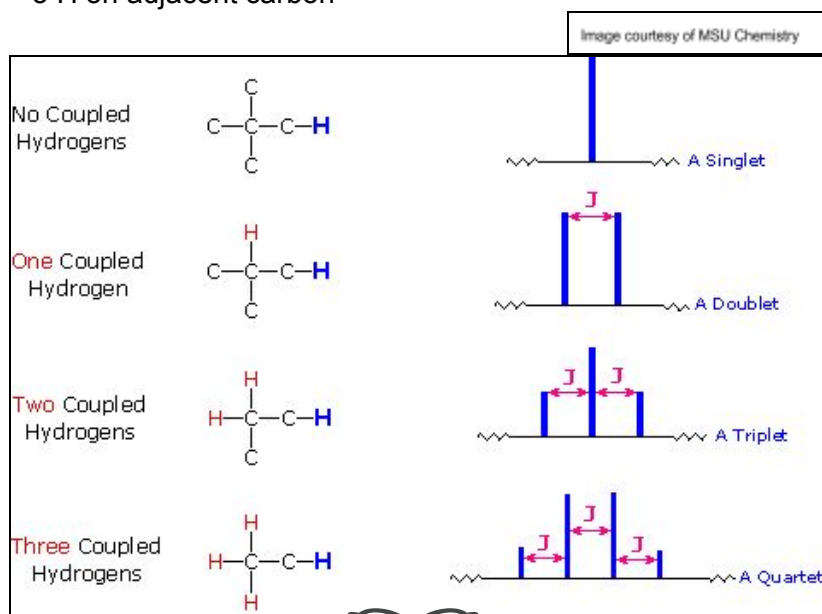
Example:



The peaks of a H^1 NMR spectra also inform **where each environment is positioned** within the molecule. Peaks are split into a **small cluster** with smaller peaks indicating how many hydrogens are on the **adjacent carbon atom** within the molecule. These smaller peaks are a **splitting pattern** and follow an '**n+1**' rule, where n is the number of hydrogen on the adjacent carbon.

- Singlet = no H on adjacent carbon
- Doublet = 1 H on adjacent carbon
- Triplet = 2 H on adjacent carbon
- Quartet = 3 H on adjacent carbon

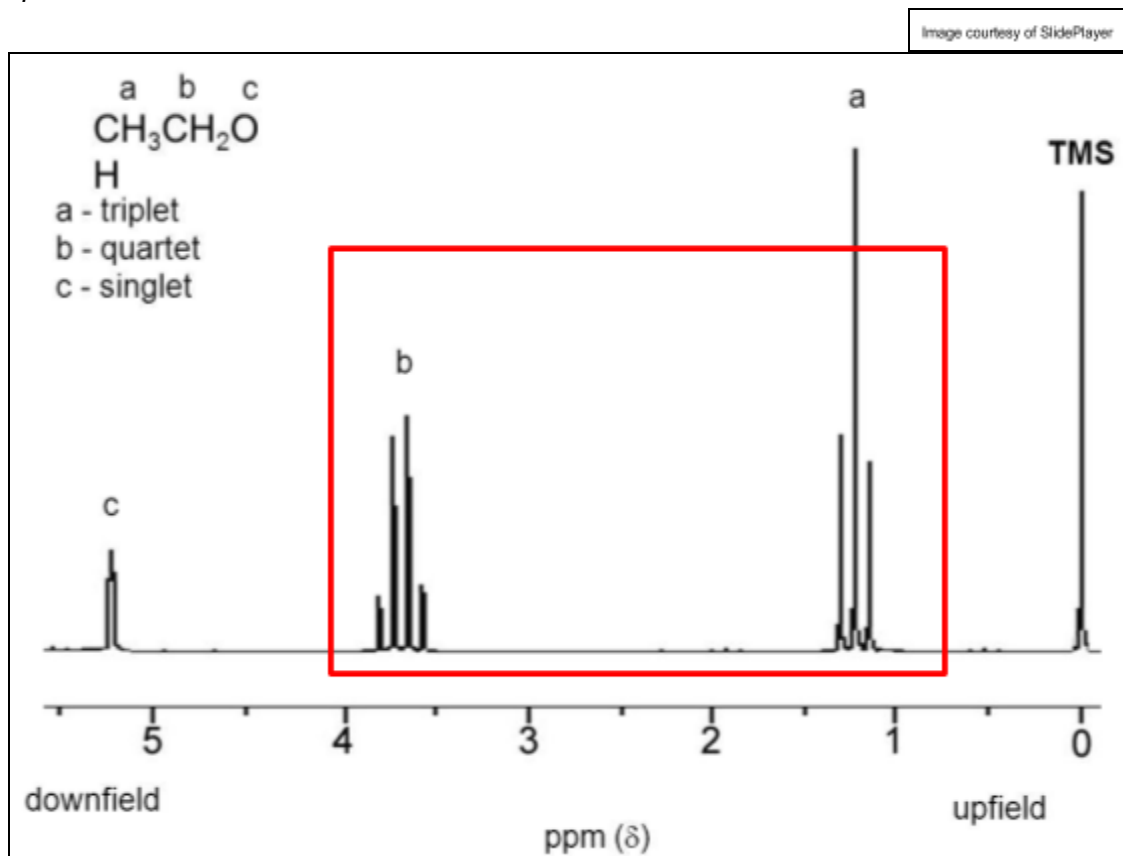
Example:





There are some common **combinations of peaks and splitting patterns** that make deciphering the structure of the molecule easier. A **triplet-quartet** splitting pattern is a common combination as it represents a **-CH₂-CH₃** fragment.

Example:



The boxed peaks are produced by the -CH₂-CH₃ fragment.

Multiple fragments can be worked out and **pieced together** to determine the **full molecule structure**.

