This page describes how you interpret simple high resolution nuclear magnetic resonance (NMR) spectra. It assumes that you have already read the background page on NMR so that you understand what an NMR spectrum looks like and the use of the term "chemical shift". It also assumes that you know how to interpret simple low resolution spectra.

The difference between high and low resolution spectra

What a low resolution NMR spectrum tells you

- The number of peaks tells you the number of different environments the hydrogen atoms are in.
- The ratio of the areas under the peaks tells you the ratio of the numbers of hydrogen atoms in each of these environments.
- The chemical shifts give you important information about the sort of environment the hydrogen atoms are in.

High resolution NMR spectra

In a high resolution spectrum, you find that many of what looked like single peaks in the low resolution spectrum are split into clusters of peaks.

1 peak a singlet
2 peaks in the cluster a doublet
3 peaks in the cluster a triplet
4 peaks in the cluster a quartet

You can get exactly the same information from a high resolution spectrum as from a low resolution one - you simply treat each cluster of peaks as if it were a single one in a low resolution spectrum. But in addition, the amount of splitting of the peaks gives you important extra information.

Interpreting a high resolution spectrum

The n+1 rule

The amount of splitting tells you about the number of hydrogens attached to the carbon atom or atoms next door to the one you are currently interested in. The number of sub-peaks in a cluster is one more than the number of hydrogens attached to the next door carbon(s). So - on the assumption that there is only one carbon atom with hydrogens on next door to the carbon we're interested in.

singlet next door to carbon with no hydrogens attached
doublet next door to a CH group
triplet next door to a CH\textsubscript{2} group
Using the n+1 rule

What information can you get from this NMR spectrum?

Assume that you know that the compound above has the molecular formula C₄H₈O₂.

Treating this as a low resolution spectrum to start with, there are three clusters of peaks and so three different environments for the hydrogens. The hydrogens in those three environments are in the ratio 2:3:3. Since there are 8 hydrogens altogether, this represents a CH₂ group and two CH₃ groups. What about the splitting?

- The CH₂ group at about 4.1 ppm is a quartet. That tells you that it is next door to a carbon with three hydrogens attached - a CH₃ group.
- The CH₃ group at about 1.3 ppm is a triplet. That must be next door to a CH₂ group. This combination of these two clusters of peaks - one a quartet and the other a triplet - is typical of an ethyl group, CH₃CH₂. It is very common.
- Finally, the CH₃ group at about 2.0 ppm is a singlet. That means that the carbon next door doesn't have any hydrogens attached.

So what is this compound? You would also use chemical shift data to help to identify the environment each group was in, and eventually you would come up with:
Alcohols

Where is the -O-H peak? This is very confusing! Different sources quote totally different chemical shifts for the hydrogen atom in the -OH group in alcohols - often inconsistently. For example:

- The Nuffield Data Book quotes 2.0 - 4.0, but the Nuffield text book shows a peak at about 5.4.
- The OCR Data Sheet for use in their exams quotes 3.5 - 5.5.
- A reliable degree level organic chemistry text book quotes 1.0 - 5.0, but then shows an NMR spectrum for ethanol with a peak at about 6.1.
- The SDBS database (used throughout this site) gives the -OH peak in ethanol at about 2.6.

The problem seems to be that the position of the -OH peak varies dramatically depending on the conditions - for example, what solvent is used, the concentration, and the purity of the alcohol - especially on whether or not it is totally dry.

A clever way of picking out the -OH peak

If you measure an NMR spectrum for an alcohol like ethanol, and then add a few drops of deuterium oxide, D₂O, to the solution, allow it to settle and then re-measure the spectrum, the -OH peak disappears! By comparing the two spectra, you can tell immediately which peak was due to the -OH group.

The reason for the loss of the peak lies in the interaction between the deuterium oxide and the alcohol. All alcohols, such as ethanol, are very, very slightly acidic. The hydrogen on the -OH group transfers to one of the lone pairs on the oxygen of the water molecule. The fact that here we’ve got “heavy water” makes no difference to that.

\[
\text{CH}_3\text{CH}_2\text{OH} + \text{D}_2\text{O} \rightarrow \text{CH}_3\text{CH}_2\text{OD} + \text{HCO}_2\text{D} \]

The negative ion formed is most likely to bump into a simple deuterium oxide molecule to regenerate the alcohol - except that now the -OH group has turned into an -OD group.
Deuterium atoms don't produce peaks in the same region of an NMR spectrum as ordinary hydrogen atoms, and so the peak disappears.

You might wonder what happens to the positive ion in the first equation and the OD\(^{-}\) in the second one. These get lost into the normal equilibrium which exists wherever you have water molecules - heavy or otherwise.

\[
\text{CH}_3\text{CH}_2\text{D}^+ + \text{D}_2\text{O} \rightarrow \text{CH}_3\text{CH}_2\text{OD}^- + \text{D}_2\text{O}
\]

The lack of splitting with -OH groups

Unless the alcohol is absolutely free of any water, the hydrogen on the -OH group and any hydrogens on the next door carbon don't interact to produce any splitting. The -OH peak is a singlet and you don't have to worry about its effect on the next door hydrogens.

Equivalent hydrogen atoms

Hydrogen atoms attached to the same carbon atom are said to be equivalent. Equivalent hydrogen atoms have no effect on each other - so that one hydrogen atom in a CH\(_2\) group doesn't cause any splitting in the spectrum of the other one.

But hydrogen atoms on neighboring carbon atoms can also be equivalent if they are in exactly the same environment. For example:
These four hydrogens are all exactly equivalent. You would get a single peak with no splitting at all. You only have to change the molecule very slightly for this no longer to be true.

Because the molecule now contains different atoms at each end, the hydrogens are no longer all in the same environment. This compound would give two separate peaks on a low resolution NMR spectrum. The high resolution spectrum would show that both peaks subdivided into triplets - because each is next door to a differently placed CH₂ group.

Contributors and Attributions

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