

Chemguide – answers

H-1 NMR: LOW RESOLUTION

1. a) A molecule with the molecular formula $C_3H_6O_2$ which gave this pattern of peaks:

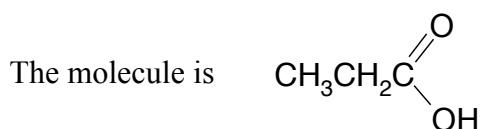
chemical shift (ppm)	11.73	2.380	1.159
ratio of areas under the peaks	1	2	3

The ratio 1:2:3 gives you the ratio of the number of hydrogen atoms in each environment. Adding $1 + 2 + 3$ gives you 6, which is the same as the number of hydrogens in $C_3H_6O_2$. (Always check this! The actual numbers of the different sorts of hydrogen could be 2:4:6 or any other multiple.)

Looking at the chemical shifts, the 11.73 value corresponds to a hydrogen in $-COOH$.

The 2.380 value comes from a CH_2 group (because of the 2 hydrogens) and is in the range for that group attached to a $C=O$ bond.

The 1.159 value is obviously a CH_3 group just attached to another carbon atom.



- b) A molecule with the molecular formula C_4H_8O which gave this pattern of peaks:

chemical shift (ppm)	9.764	2.37	1.64	0.97
ratio of areas under the peaks	1	2	2	3

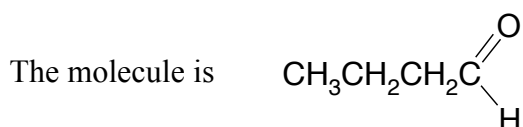
The ratio 1:2:2:3 is consistent with the 8 hydrogens in the molecule.

The peak at 9.764 falls within the range of a hydrogen in an aldehyde group, where you would obviously find a single hydrogen.

The other peaks look like two CH_2 groups and a CH_3 group. The peak at 2.37 would be a CH_2 group next door to the $C=O$ group in the aldehyde.

The peak at 1.64 is just about within the range of a CH_2 group in the middle of a chain. It is probably slightly high because of the effect of the $C=O$ bond not that far away.

The remaining peak is right for a CH_3 group at the end of a chain.



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c) A molecule with the molecular formula $C_5H_{10}O_2$ which gave this pattern of peaks:

chemical shift (ppm)	4.132	2.319	1.259	1.140
ratio of areas under the peaks	2	2	3	3

The ratio 2:2:3:3 is consistent with the 10 hydrogens in the molecule.

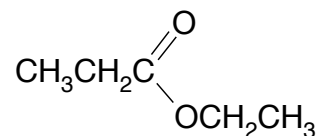
This suggests two CH_2 groups and two CH_3 groups. Lets start with the CH_2 groups.

The peak at 4.132 will be a CH_2 group attached to an oxygen atom.

The peak at 2.319 will be a CH_2 attached to a $C=O$ bond.

The CH_3 peaks are just CH_3 groups at the end of a chain.

If you play around with this information, you will get the molecule



Important: Don't leave this until you are sure about it all. These examples were designed to be fairly easy. When you come to look at high resolution NMR spectra, you must be confident about this simple stuff, because you will have an extra layer of complication to worry about.

It is essential that you can see how the ratios of the areas under the peaks are used, and how to use simple chemical shift tables to help decide what sort of environments the various groups are to be found in.