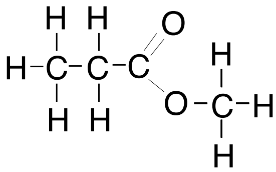
Chemguide – answers

C-13 NMR: INTERPRETING SPECTRA

(The table of chemical shifts is repeated at the end of this file if you want to refer to it.)

1. The ethanol spectrum would have two lines because of the two carbons in different environments. The line for the carbon with the oxygen attached would be in the region 50 - 90 ppm, and the other one due to the CH_3 group in the 10 - 15 region. (In fact, it is slightly higher than this. The effect of the oxygen atom is still felt slightly.)

   The methoxymethane spectrum will consist of a single line, because both CH_3 groups are in exactly identical environments. The presence of the C-O single bond would mean the line would be in the 50 - 90 ppm region.

2. Methyl propanoate is 

   The line at 174 is due to the carbon attached to the C=O bond (range 160 - 185 in an ester).

   The line at 51 is due to the methyl group attached to the oxygen (range 50 - 90).

   The line at 27 will be the CH_2 group attached to the C=O bond. The table gives this as CH_3CO-, but replacing one of the hydrogens by another carbon doesn't make much difference.

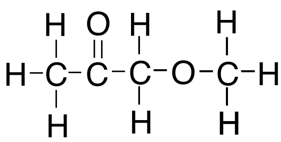
   The line at about 10 is the CH_3 group at the left-hand side of the molecule (range 10 - 15). (The SDBS actually gives the line at 9.22. You mustn't take the figures in the table too literally!)

3. An isomer of methyl propanoate will have the molecular formula $C_4H_8O_2$. Start at the left-hand side of the spectrum.

   The line at 207 is likely to be a carbon in the C=O bond in a ketone. So this isn't an acid or an ester. Ketones have the C=O bond in the middle of a chain.

   The lines at 59 and 78 are both due to carbons singly bonded to an oxygen, but that oxygen can't be joined to the C=O bond otherwise it would be an acid or an ester.

   The line at 26 is most likely to be a CH_3 group attached to a C=O bond.

   Putting that together will lead you to 

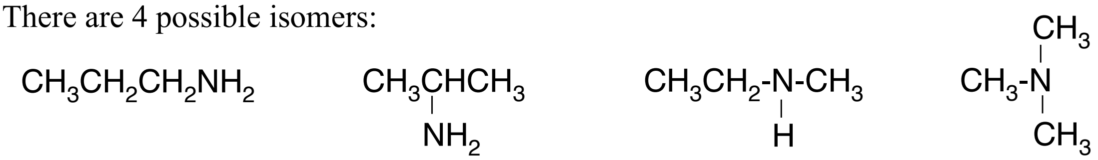
4. Start with the relative molecular mass of 59. How many carbons are there in the molecule? Looking at the spectrum, there must be at least 3, because you have got 3 lines. It is possible that there could be 4 if there were two carbons in identical environments.

So lets get rid of that possibility first. 4 carbons adds to a relative formula mass of 48 - leaving 11 presumably made up of hydrogens. That would give a formula C_4H_{11}. It is impossible. C_4H_8, yes; C_4H_{10}, yes; C_4H_{11}, no!

So if there are 3 carbons, that leaves a missing mass of 23. That's far too many to be accounted for by hydrogens alone, so there must be some other small atom in the molecule. The only possibilities that might make sense are oxygen or nitrogen. Fluorine is too heavy, only leaving room in the RMM for 4 hydrogens.

There are no lines in the region of the spectrum where you would expect carbons attached to oxygen to show up. That leaves nitrogen as a possibility. A formula of C_3H_9N adds to 59.

There are 4 possible isomers:



A B C D

Two of these will have the wrong number of lines. In B, both CH_3 groups are in exactly the same environment, and so you would only get two lines - one for the CH_3 groups and one for the carbon with the nitrogen attached. In D, all of the CH_3 groups are in the same environment, and so you will only get one line.

Of A and C, notice that in C there are two carbons attached to nitrogen, and so you would expect two lines in the 30 - 65 region with similar (although not identical) values. But in the spectrum there is only one. So it is probably A.

We need to confirm that by accounting for all three lines.

The line at 44 is due to the carbon with the NH_2 group on it.

The line at 27 is fractionally higher than the range given for the R_2CH_2 group. This will be the CH_2 carbon in the middle of the chain. The value is probably raised a bit because of a small amount of influence from the nearby nitrogen.

The line at 11 is nicely in the range for a CH_3 group at the end of a chain.

So the molecule is $CH_3CH_2CH_2NH_2$.

carbon environment	chemical shift (ppm)
C=O (in ketones)	205 - 220
C=O (in aldehydes)	190 - 200
C=O (in acids and esters)	160 - 185
C in aromatic rings	125 - 150
C=C (in alkenes)	115 - 140
RCH_2O-	50 - 90
RCH_2Cl	30 - 60
RCH_2NH_2	30 - 65
R_3CH	25 - 35
CH_3CO-	20 - 50
R_2CH_2	16 - 25
RCH_3	10 - 15