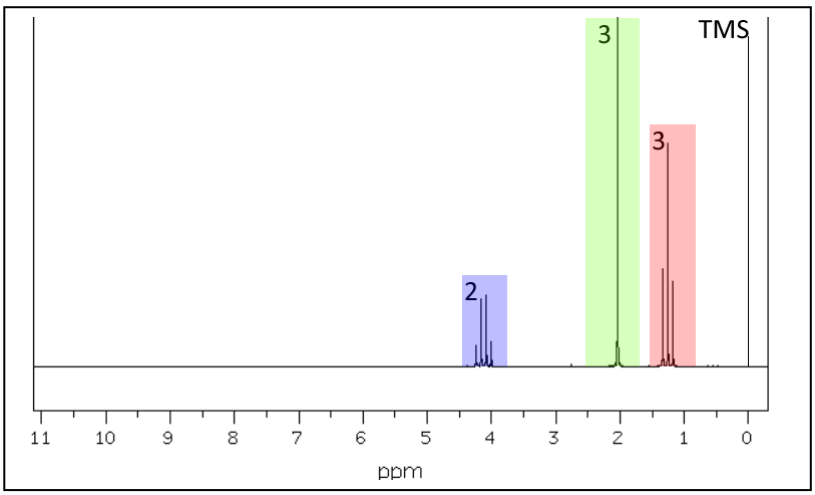
Lesson 4 ^{1}HNMR

When interpreting HNMR spectra don't forget>

- Each signal represents a non-equivalent hydrogen
- The integration tells us about the relative number of hydrogens that caused the signal
- The splitting pattern tells us something about the neighbouring non-equivalent hydrogens

A compound has the molecular formula $C_4H_8O_2$. Its ^{1}HNMR spectrum is shown on the right.



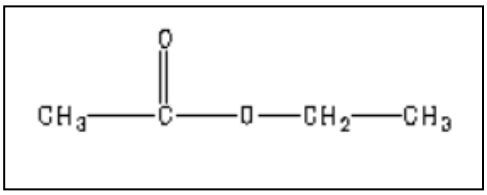
What can be deduced from the spectrum.

i. There are three non-equivalent hydrogens

ii. Most likely there is a:

- CH_3 next to a CH_2 group of hydrogens as indicated by the red shaded signal. Its integration is 3 so it represents, most likely 3 hydrogens being split by a neighbouring CH_2 according to the n+1 rule.
- CH_3 on its own represented by the green shaded hydrogens.
- CH_2 next to a CH_3 as indicated by the blue shaded hydrogens. It is most likely close to a electronegative atom, such as oxygen, as indicated by its chemical shift.

The most likely structure is shown on the right.



1) A compound has the molecular formula $C_5H_{10}O_2$. Its HNMR spectrum is shown below.

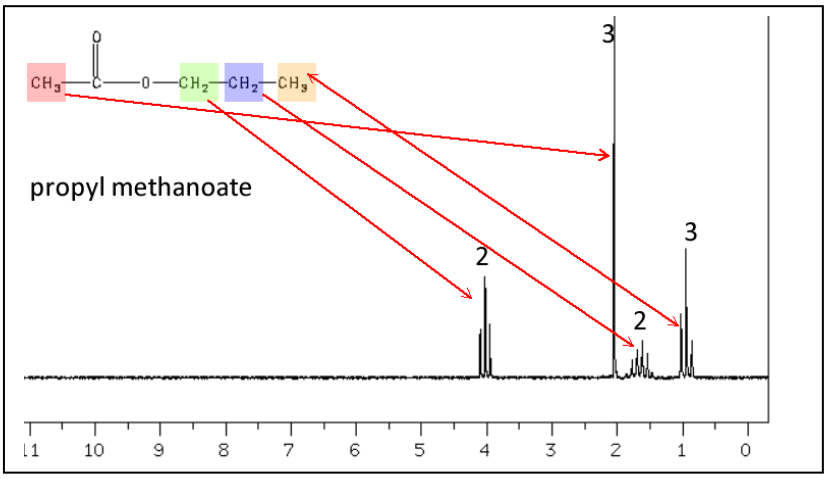
a) Draw its structural formula

b) Name the compound.

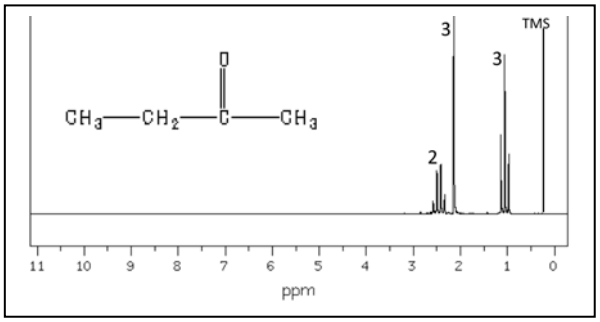
Students should use the data from the data sheet to identify the correct isomer.

Two possible isomers can give the splitting pattern shown.

Propyl ethanoate and methyl butanoate. Using the chemical shifts given in the data sheet students should be able to select the right one.



c) An unknown compound has the molecular formula C_4H_8O.



i. What can you say about the equivalent hydrogens that formed the signals at:

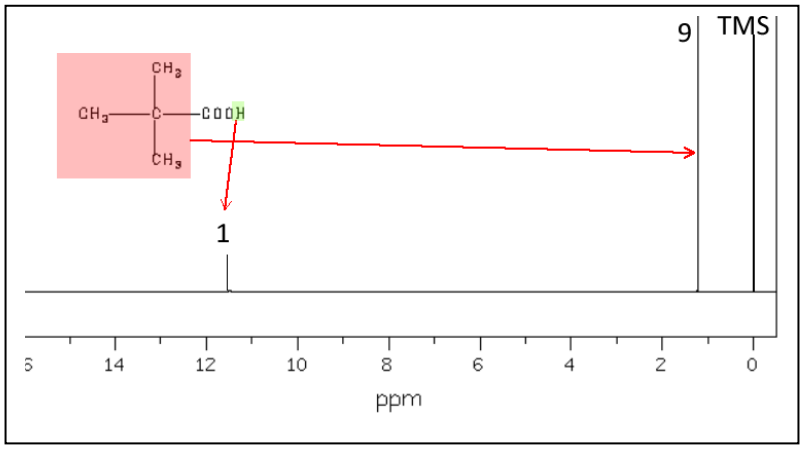
- 2.5 ppm *it is most likely a CH_2 group, with 3 non-equivalent hydrogens as neighbours. Since it is chemically shifted more to the right than any other hydrogen it is most likely closer to electronegative oxygen.*
- 2.1 ppm *it is most likely a CH_3 with no neighbouring hydrogens.*
- 1.0 ppm *it is most likely a CH_3 with two neighbouring non-equivalent hydrogens.*

ii. Draw the structural formula of the molecule.

2) Another compound also has the molecular formula $C_5H_{10}O_2$. Its HNMR spectrum is shown below.

a) Draw its structural formula

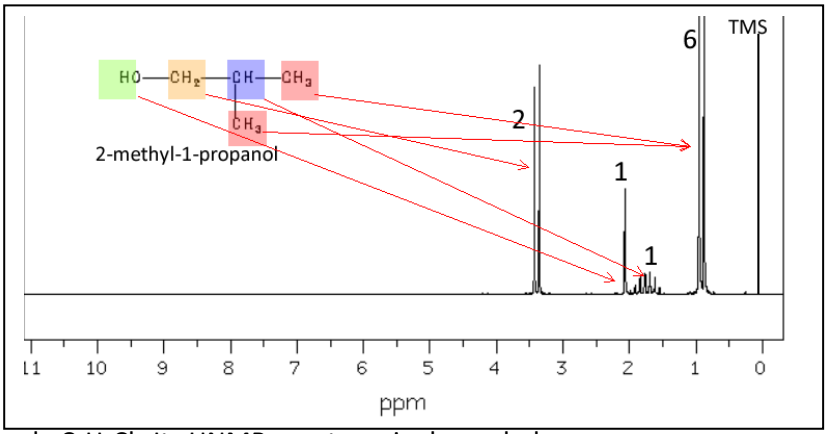
b) Name the compound.



3) A compound has the molecular formula $C_4H_{10}O$. Its HNMR spectrum is shown below. The peak signal at 1.75 ppm is split into a nonet (9).

a) Draw its structural formula

b) Name the compound.



4) A compound has the molecular formula $C_4H_8Cl_2$. Its HNMR spectrum is shown below.

a) Draw its structural formula

b) Name the compound.