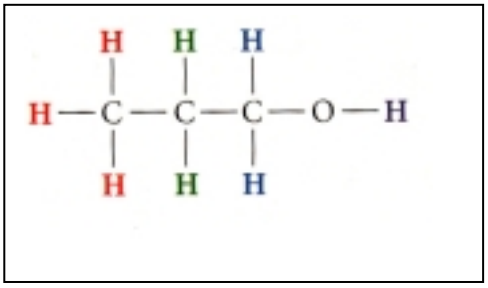
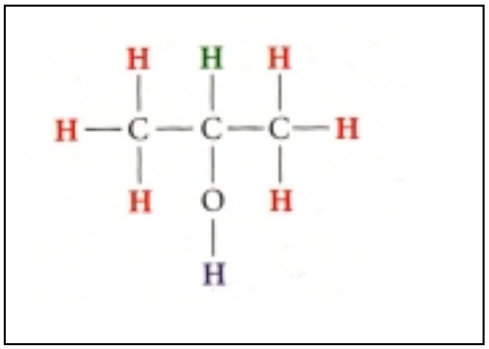
Lesson 2 HNMR

Click to revise ^{1}HNMR

Atoms with an odd number of nucleons are magnetically active.



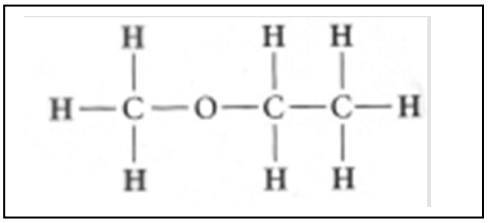
Hydrogen atoms on a particular molecule can find themselves surrounded by different neighbouring groups of atoms and hence are said to be chemically different.
Consider the molecule shown on the right of propanol. It has 4 chemically different hydrogen atoms.
The black hydrogen has a neighbouring oxygen atom.
The blue hydrogens have a neighbouring CH_2 and a neighbouring oxygen atom
The green hydrogens have neighbouring CH_3 and CH_2 groups
The red hydrgens have a CH_2 as a neighbour.



Consider the molecule of 2-propanol shown on the right. It has three chemically different hydrogens.
The red hydrogens are identical because they are both next to a CHOH group.
The green hydrogen has two CH_3 groups as neighbours and also an oxygen atom.
The balck hydrogen has an oxygen atom as a neighbour.

Consider the molecules shown on the right. How many chemically different hydrogens are present in each molecule. Identify each chemically different set of hydrogens.

a)



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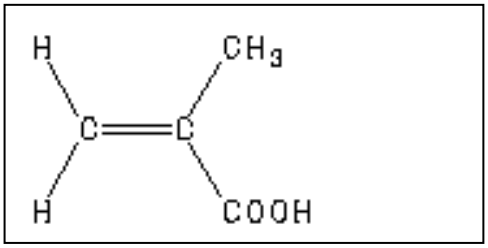
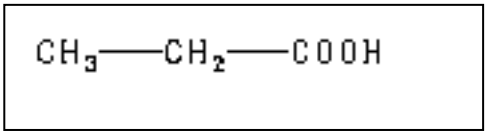
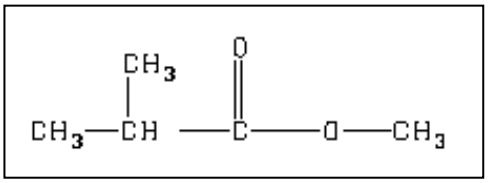


c)

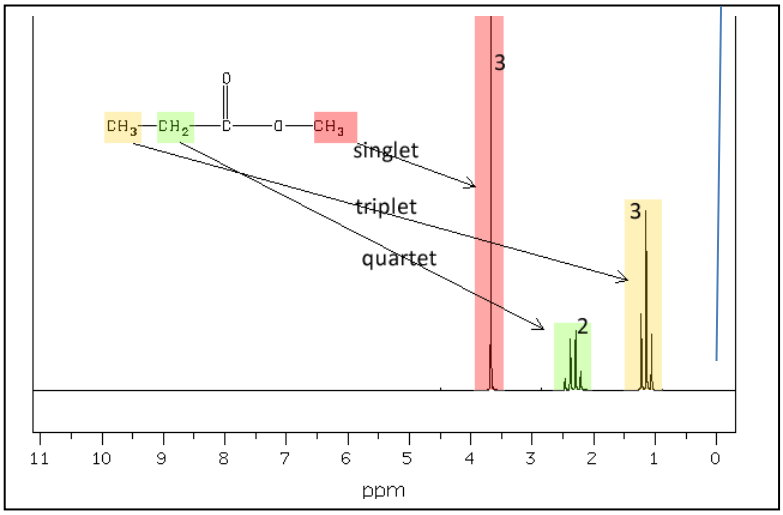


d)

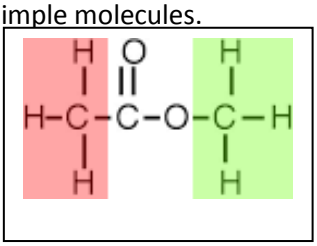


A ^{1}HNMR spectrum consists of a set of peaks. Three things are significant in an ^{1}HNMR spectrum.

-The number of set of peaks- which indicates the number of chemically different (non-equivalent) hydrogens in the molecule.
-The ***splitting*** pattern of the peaks- which tells us something about the neighbouring hydrogens
-The area under each peak, ***integration,*** which indicates the number of non-equivalent hydrogens involved.
Each non-equivalent group of hydrogens produces a signal which is split by neighbouring hydrogens according to the n+1 rule.



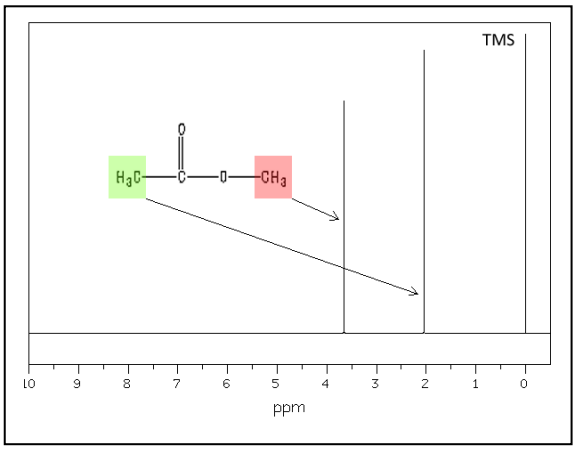
Consider the spectrum shown on the right.
It consists of three sets of peaks a singlet, a quartet and a triplet. From this information we can see that there are three chemically different hydrogen groups.
We can also see that there is a ***singlet*** with a peak area of three. This indicates three chemically similar hydrogens, most likely a CH_3 without neighbouring hydrogens.
The ***quartet*** has a peak area of two, this indicates that the signal belongs to possibly a CH_2 group. Since it splits into four peaks it must be next to three chemically different hydrogens, so applying the n+1 rule produces four peaks.
The ***triplet*** has a peak area of three indicating that it belongs to possibly a CH_3. This group of hydrogens is next to two hydrogens that are chemically different to the CH_3 hydrogens. It is possibly next to a CH_2 group.
Notice how the positioning of the groups of peaks is determined. Generally speaking if the group of hydrogens is next to an oxygen it is further to the left of the spectrum than other hydrogens which are further from the oxygen.
From this information we can build up a picture of the molecular structure and derive its structural formula.
Let's start with what we should be seen in ^{1}HNMR spectrum of some simple molecules.



example 1 Lets take methyl ethanoate, its structural formula is shown on the right.
1) It has two, chemically different hydrogens, shaded. We should, therefore, expect two signals on the ^{1}HNMR spectrum.
Both signals should have an equivalent area under each peak proportional to three hydrogens.

2) The signal from the CH_3 group on the right ,shaded in green, should be further to the left on the spectrum than the signal from the CH_3 group on the left, shaded in red. This is because the CH_3 on the left is next to an electronegative atom, such as oxygen, which tends to reduce the ***nuclear shielding*** of the three hydrogen nuclei. The signal from this CH_3 is therefore ***chemically shifted*** further to the left.

3) Each of the two signals will not have a splitting pattern as there are no neighbouring hydrogens next to each CH_3 group that are chemically different. Hence the 1HNMR spectrum of methyl ethanoate should look like that shown on the right.



Keep in mind that hydrogens close to an electronegative atom, such as oxygen, are shifted more to the left of the spectrum than hydrogens that are further from the electronegative atom.

1) Consider the following molecules.

a) ethyl methanoate

i. Draw the molecule
ii. How many signals appear on the ^{1}HNMR spectrum?
iii. What are the splitting patterns.
iv. Draw the spectrum as best you can.

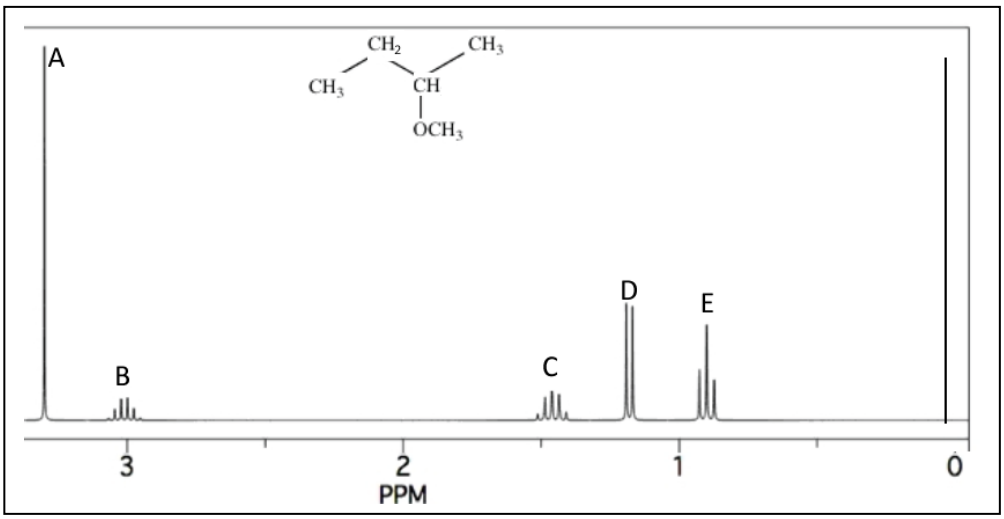
b) butanoic acid

i. Draw the molecule
ii. How many signals appear on the ^{1}HNMR spectrum?
iii. What are the splitting patterns.
iv. Draw the spectrum as best you can.

c) propan-2-ol

i. Draw the molecule
ii. How many signals appear on the ^{1}HNMR spectrum?
iii. What are the splitting patterns.
iv. Draw the spectrum as best you can.

d) Consider the molecule shown on the right with its ^{1}HNMR spectrum.



i. Identify the hydrogens that are represented by each peak in the ^{1}HNMR spectrum?

ii. What are the relative areas under each peak

e) Consider the compound butan-2-ol

i. Draw its structural formula in the space provided on the right.

ii. How many chemically different hydrogen environments exist?

iii. Draw the spectrum as best you can in the space below.