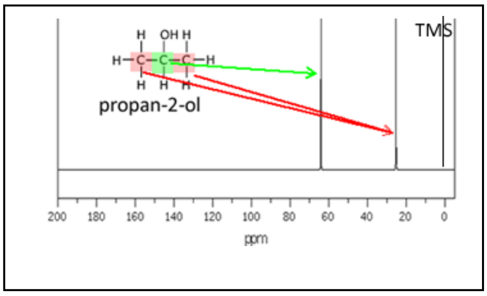
Lesson 1 $^{13}$CNMR

The phenomenon that causes chemical shifts of hydrogens also causes chemical shifts in carbon atoms ($^{13}$C). That is, electrons in the molecule generate small magnetic fields that shield carbon nuclei from the applied magnetic field. For example, the carbon atom in a carbonyl group (C = O) has a relatively low electron density around it due to the highly electronegative oxygen atom, hence, is relatively "deshielded" and so has a higher chemical shift than most other types of carbons.

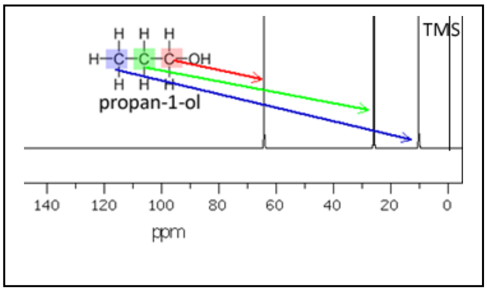
Carbon-12 atoms do not have a nuclear spin, and hence don't show up in the NMR. Remember, only atoms with an odd number of nucleons have a nuclear spin and can show up in NMR. Since only 1% of naturally occuring carbon atoms are carbon-13, we don't normally observe splitting patterns caused by adjacent carbon atoms, like we do between adjacent protons in $^{1}$H-NMR. The rare chance of two $^{13}$C atoms being next to each other is rare.

- A signal is created for every non-equivalent carbon atom
- Integration is not used in $^{13}$CNMR.



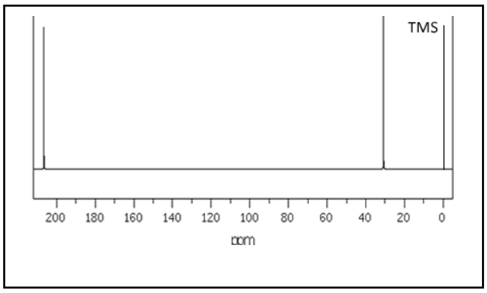

Lets look at some examples

Consider the $^{13}$CNMR of propan-2-ol shown on the right. Propan-2-ol has two signals. This is due to the fact that it has 2 non-equivalent carbons, the two $CH_3$ groups at each end of the molecule are identical and so produce one signal. Notice how the carbon attached to the oxygen atom is not as shielded from the applied magnetic field as are the other two equivalent carbons, so it is chemically shifted more than the other carbons




The $^{13}$CNMR shown on the right is of propan-1-ol. Three non-equivalent carbons exist so three signals are observed.

Identifying molecular structure using $^{13}$CNMR can also be achieved using the chemical shift data from the VCAA data sheet.




Consider the $^{13}$CNMR spectrum shown on the right a compound with the molecular formula $C_3H_6O$. Identify the molecule.

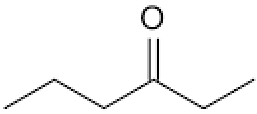
From the spectrum we immediately see :

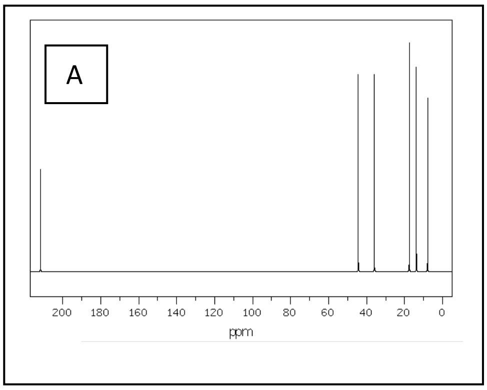
- there are two non-equivalent carbons.

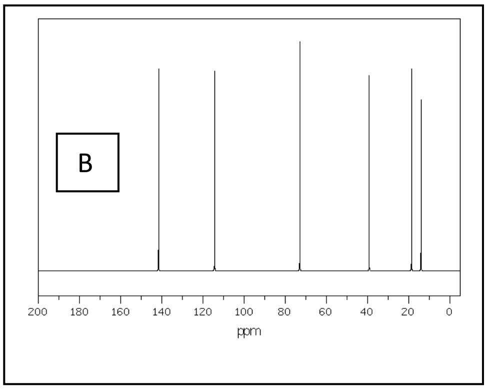
- the signal at 210ppm is probably of a carbonyl group ($R_2C = O$)

The compound is most likely $CH_3COCH_3$ (acetone)

1) Consider the two $^{13}$CNMR spectra shown on the right. Which one belongs to the compound with the structural formula shown below. Explain



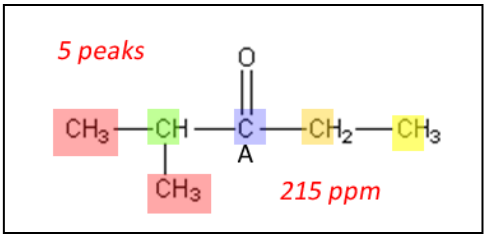



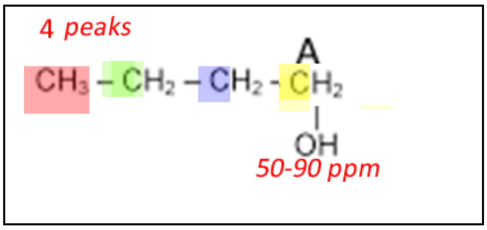



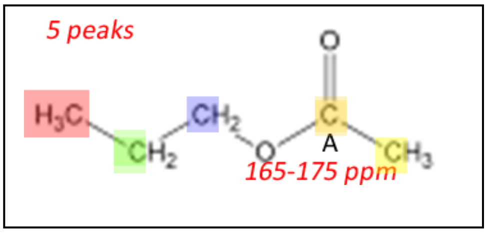

*A*

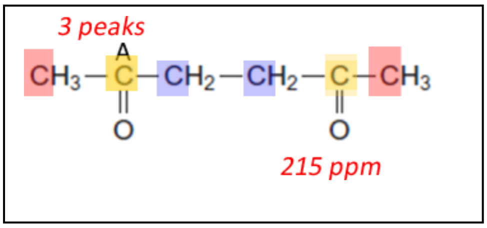
*It has a peak at 210-215ppm indicating a carbonyl group (C = O).*

2) Consider the molecules shown on the right. How many peaks are expected on the $^{13}$CNMR spectra of each. For each molecule predict the chemical shift of the atom labelled "A". Refer to you data sheet.



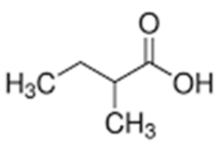




3) Explain why splitting patterns appear in $^{1}$HNMR but not in $^{13}$CNMR.

*$^{13}$C is very rare in nature and the chance of having two $^{13}$C atoms next to each other is very low. So the signals are not split by neighbouring carbon atoms. $^{1}$H on the other hand is very common and neighbouring hydrogens do split each other's signal.*

4) Give the structural formula of an optically active organic acid with five peaks in its $^{13}$CNMR spectrum.




*2-methylbutanoic acid*