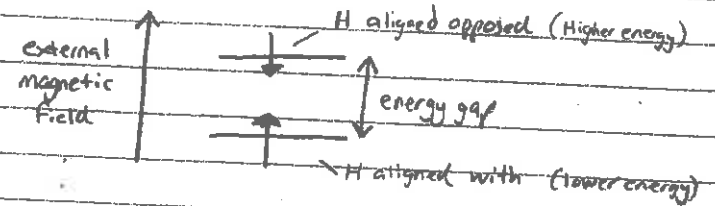
NMR

· Nuclear Magnetic Resonance
(nuclei)

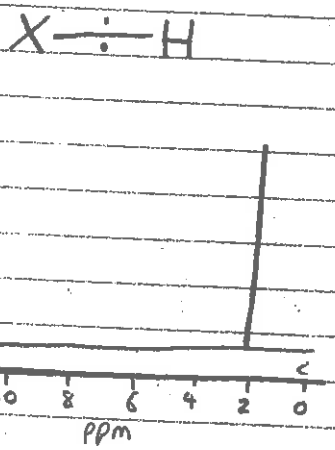
· Hydrogen atoms will line up with an external magnetic field. It is possible to line up the hydrogen atom into the more unstable position if supplied with exactly the right energy



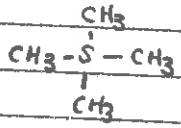
(usually in 60–100MHz range) (radio)

→ the alignment flipping is called resonance condition.

· environment makes huge difference to the needed energy



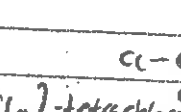
To use the ppm scale you need to compare to a standard TMS (tetramethylsilane).



Sometimes TMS is shown at zero (sometimes not at all), will produce strong peak, single peak.

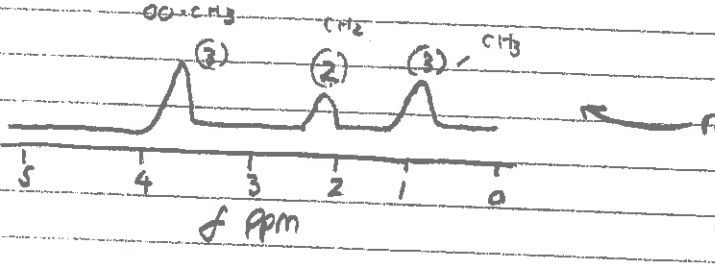
· The higher the number, less energy needed to produce resonance. We call this downfield of TMS.

· Samples usually dissolved in solvents that contain no hydrogens (CCl_4)-tetrachloromethane. Or use solvent with deuterium ($CDCl_3$) instead of $CHCl_3$. - Deuterium does not show peaks in same areas!



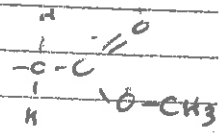
Low Resolution

does not distinguish between individual peaks in various groups.



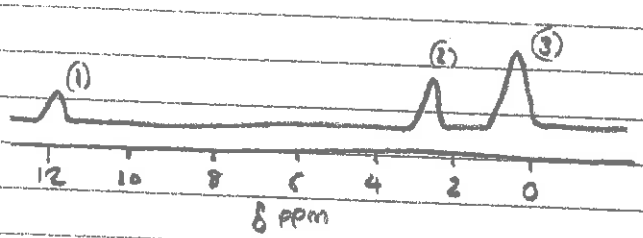
← relative areas under the peak.

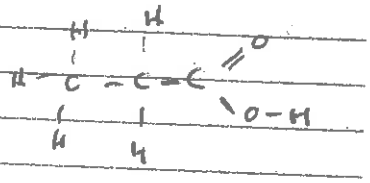
$CH_3CH_2COOCH_3$



→ might be given integrator trace to help find areas under peaks.

→ Chemical shifts also give clues to their identification.





High Resolution

• In a high resolution spectrum - many what you thought were single peaks are actually clusters of peaks.

1 peak = Singlet
2 peaks = doublet
3 peaks = triplet
4 peaks = quartet

n+1 rule: Splitting tells you about the number of hydrogens attached to the carbon atoms next door. ALSO the number of peaks is actually one more than the number of hydrogens attached next door.

Singlet = next door to a carbon with NO hydrogens

doublet = next door to a CH group

triplet = next door to a CH_2 group

quartet = next door to a CH_3 group.

- The OH group is a strange exception where -OH produces a singlet & has no effect on neighbouring groups. So even when next to a CH_2 it would **NOT** be a triplet!

- Easy way to remove OH is to add D_2O!

- You can also get equivalent hydrogens.

$$Cl - CH_2 - CH_2 - Cl$$

equivalent as same environment.

They would produce a single peak with no splitting.