NMR SPECTROSCOPY

Dr. M. Ganapathi
Assistant Professor
Department of chemistry
Government arts college
Tiruvannamalai – 606 603

Spin – Spin Splitting

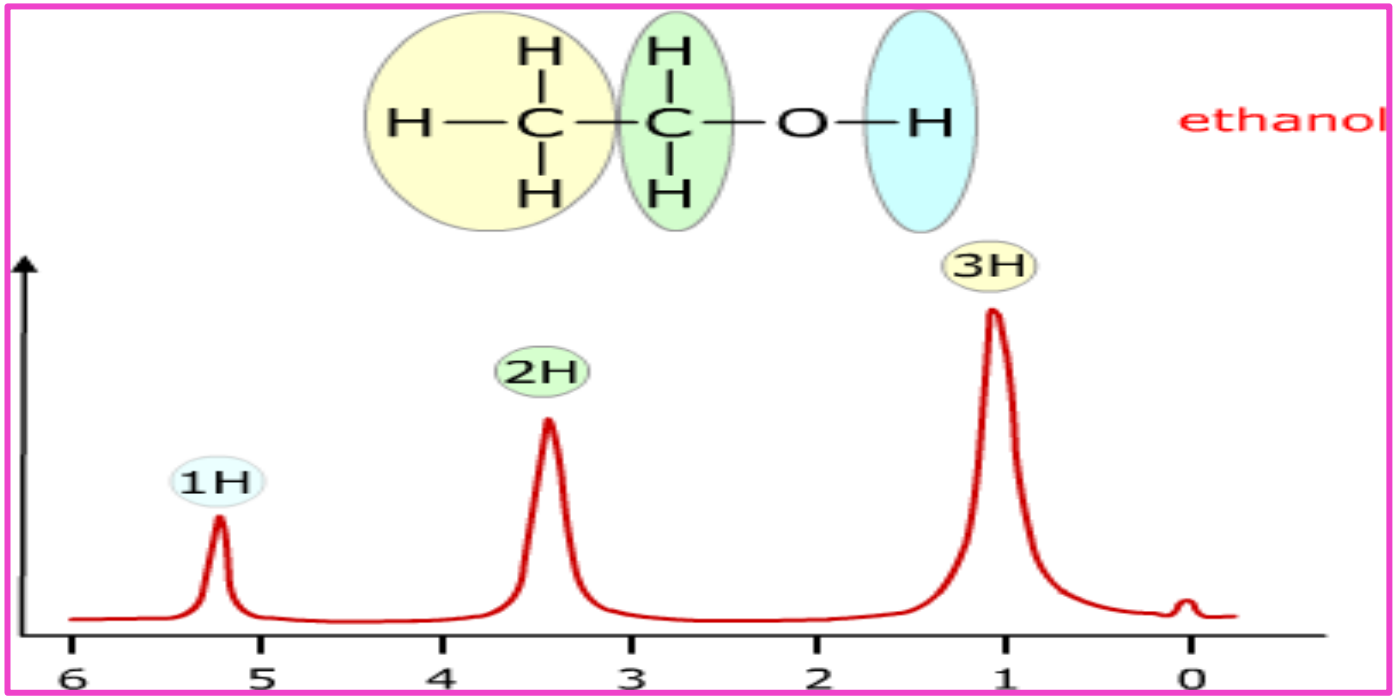
Spin – Spin Splitting

“The interaction between the spins of the neighbouring nuclei in a molecule may cause the splitting of the lines in the NMR spectra is called spin-spin splitting or spin – spin interaction”

Low resolution NMR Spectra of acidified ethanol

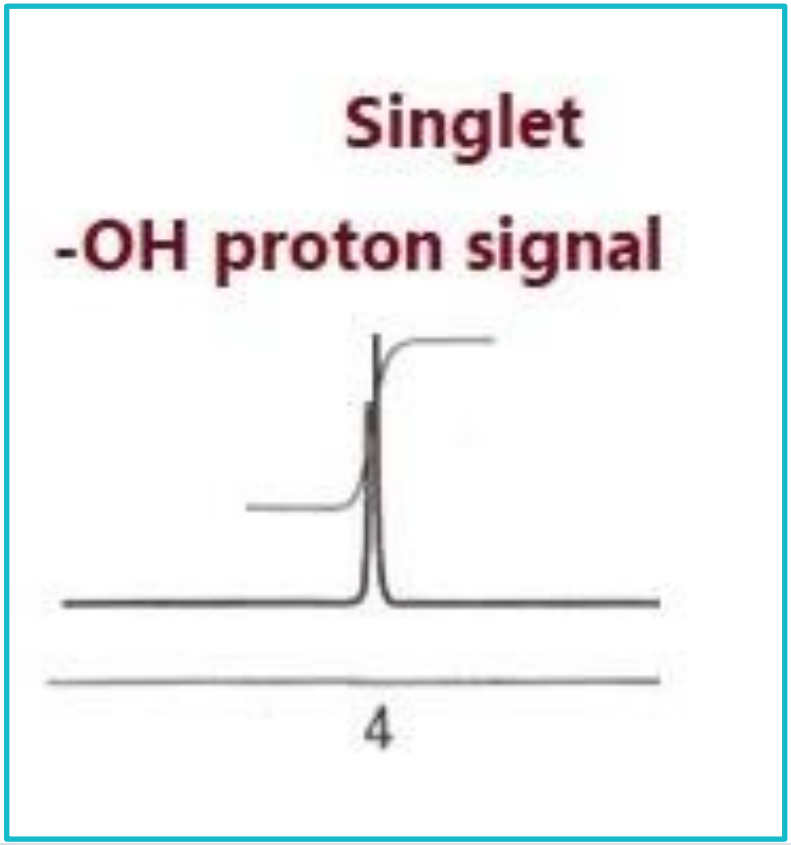
- In acidified Ethanol (CH_3-CH_2-OH) contains three different environmental Protons.
- Low resolution spectra of ethanol gives THREE peaks.

NMR Spectra of acidified ethanol



High resolution NMR Spectra of acidified ethanol

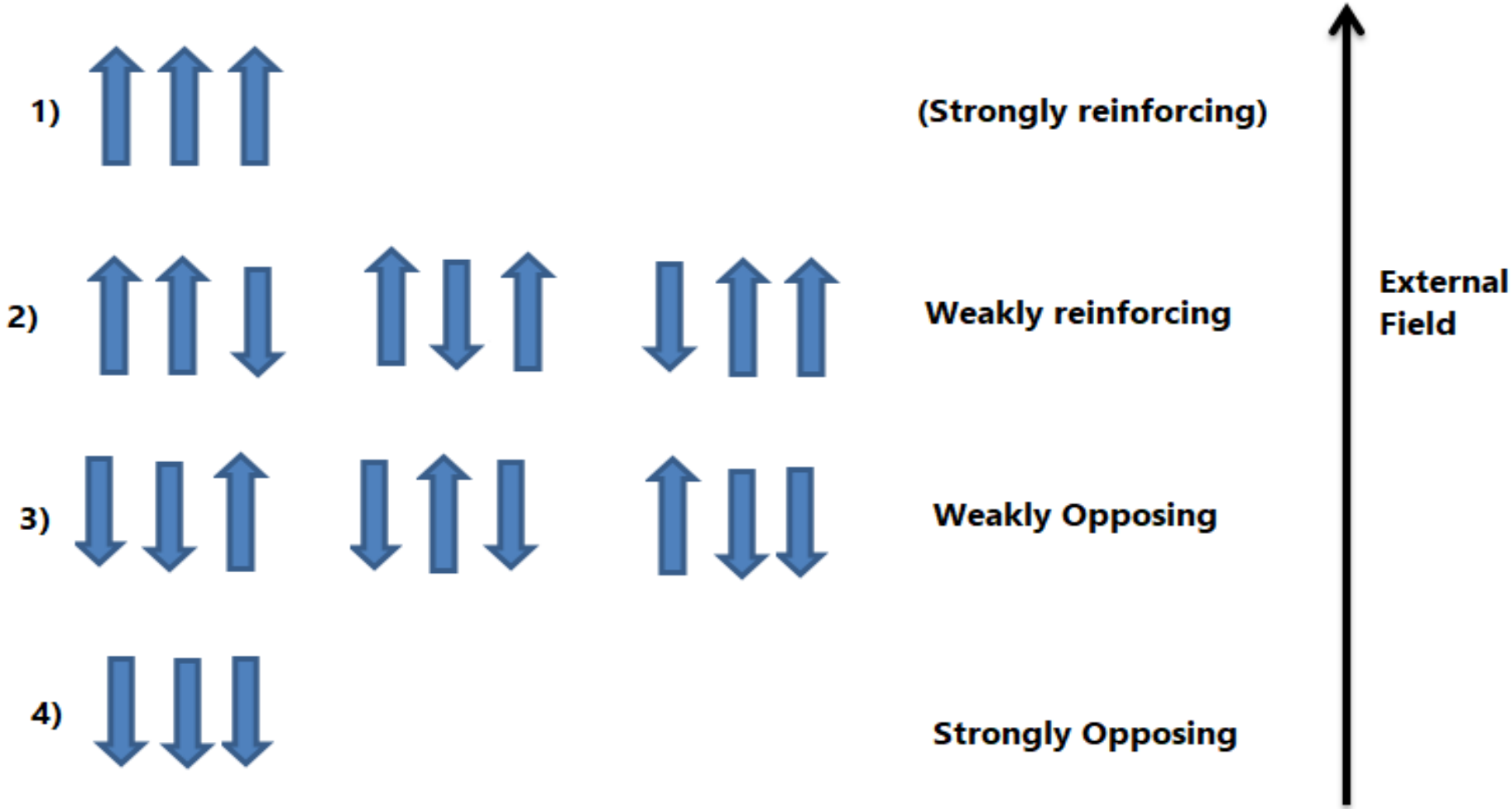
- -OH proton does not involve any split to the neighboring protons. Since –OH proton undergoes fast proton exchange with solvent.



No splitting OH proton signal

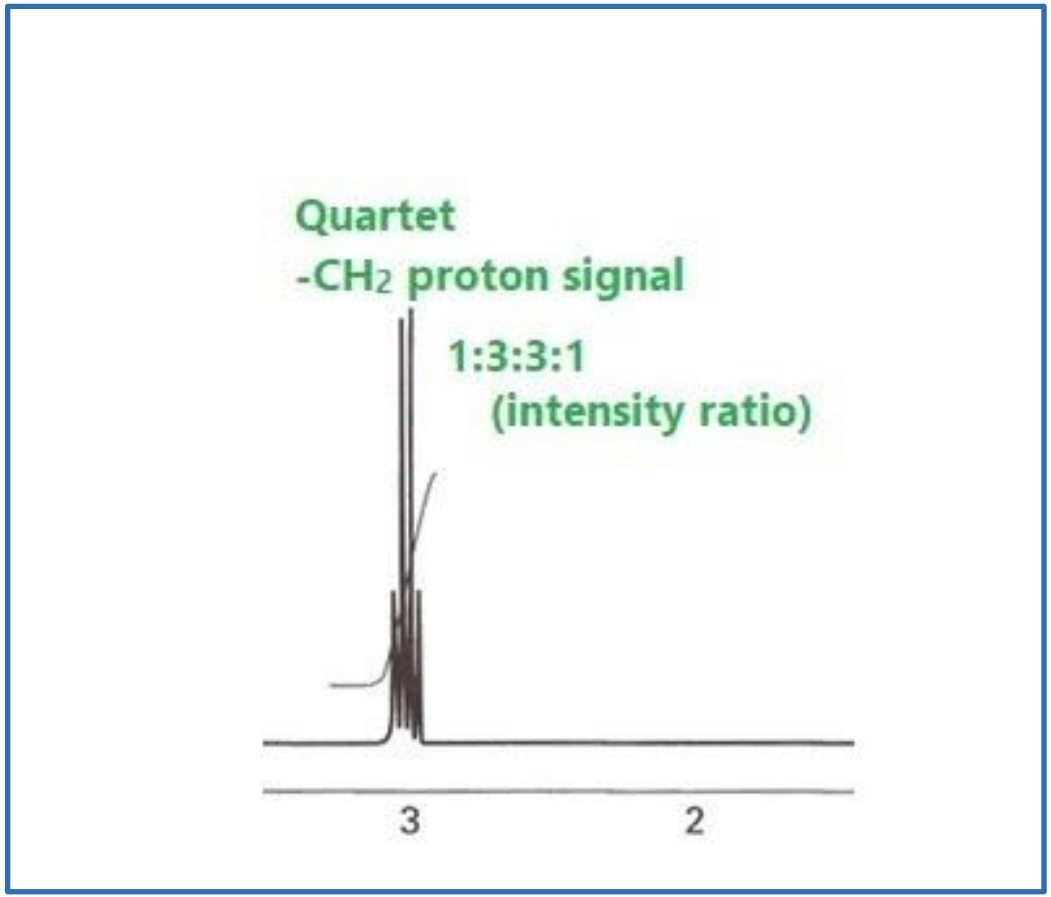
High resolution NMR Spectra of acidified ethanol

- Methylene($-CH_2$) proton peak is splitted only by the adjacent $-CH_3$ protons. The spin of three protons (CH_3) can couple with the adjacent methylene ($-CH_2$) group in four different ways relative to the external field.


1)
(Strongly reinforcing)
2)
Weakly reinforcing
3)
Weakly Opposing
4)
Strongly Opposing
External Field

High resolution NMR Spectra of acidified ethanol

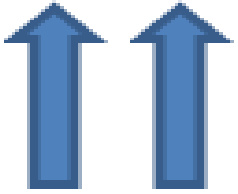
- Thus quartet of peaks results with an intensity ratio of 1:3:3:1 which corresponds to the distribution ratio of all the alignments.
- Based on (2I + 1) or (n + 1) no. of splitting occurs



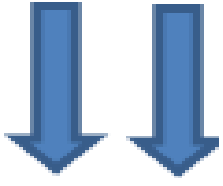
CH_2 proton signal can splitted neighbour methyl proton (3H)

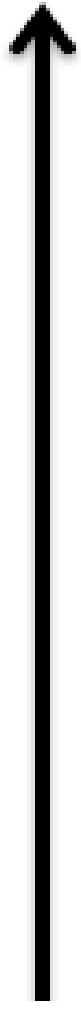
High resolution NMR Spectra of acidified ethanol

- Methyl proton ($-CH_3$) peak is splitted by the adjacent methylene ($-CH_2$) protons. ie., the spin of two protons can couple with the adjacent ($-CH_2$)methyl group in three different ways relative to the external field.

1)  (Reinforcing)

2)  (Not affecting)

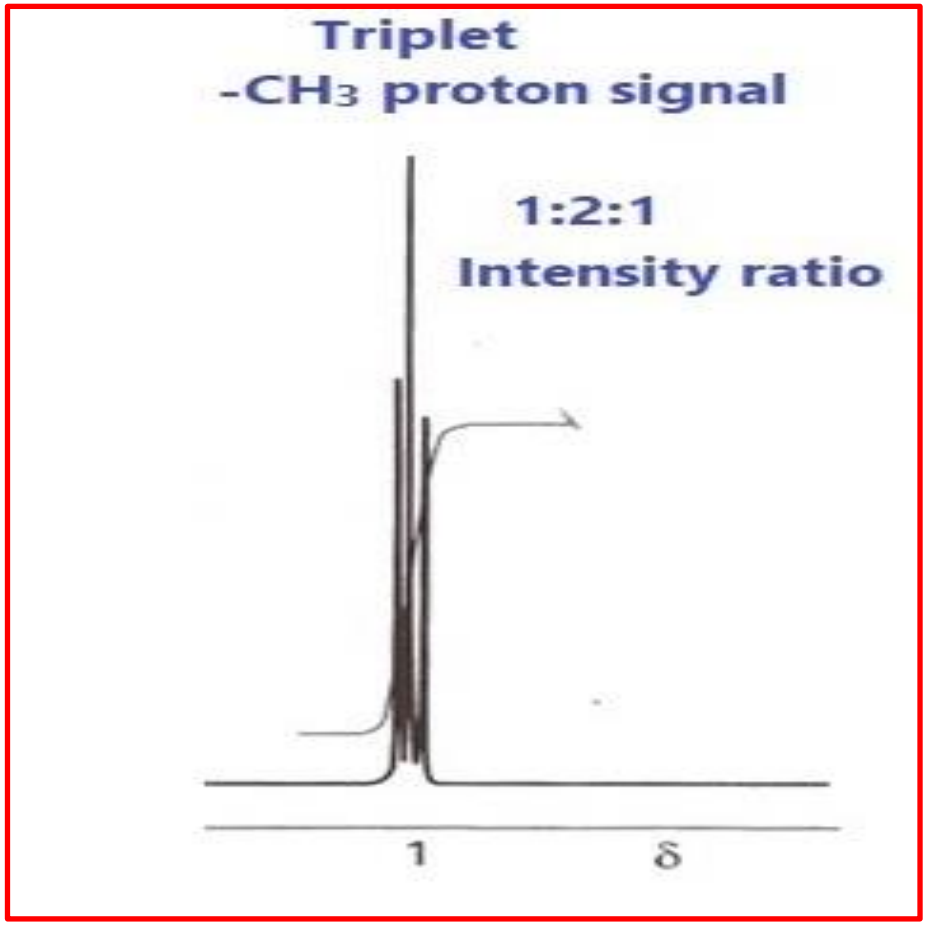
3)  Opposing



External Field

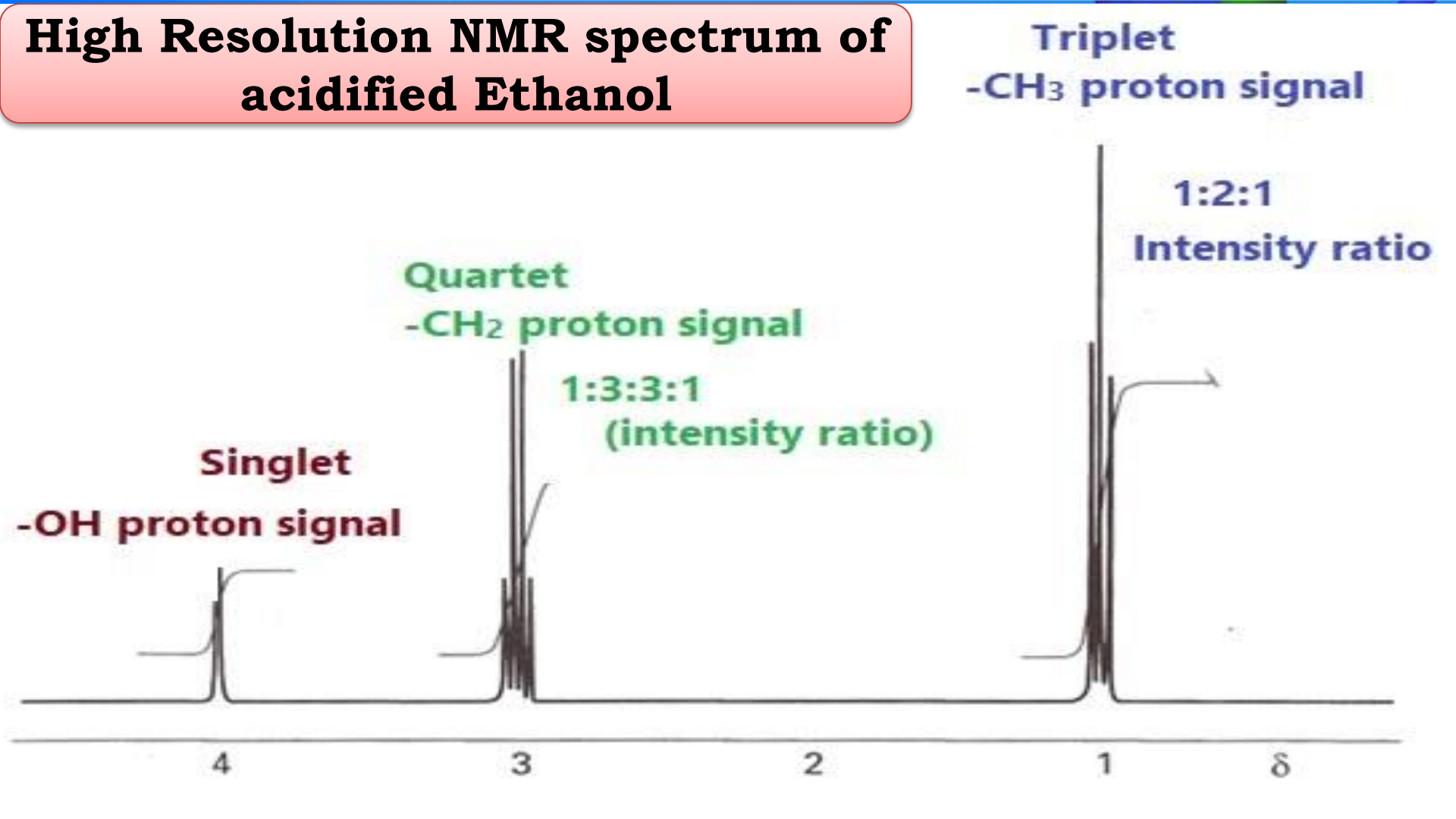
High resolution NMR Spectra of acidified ethanol

- Thus, a triplet of peaks results with the intensity ratio of 1:2:1 which corresponding to the distribution ratio alignment.
- According (n+1) = 2+1 = 3 triplet peak

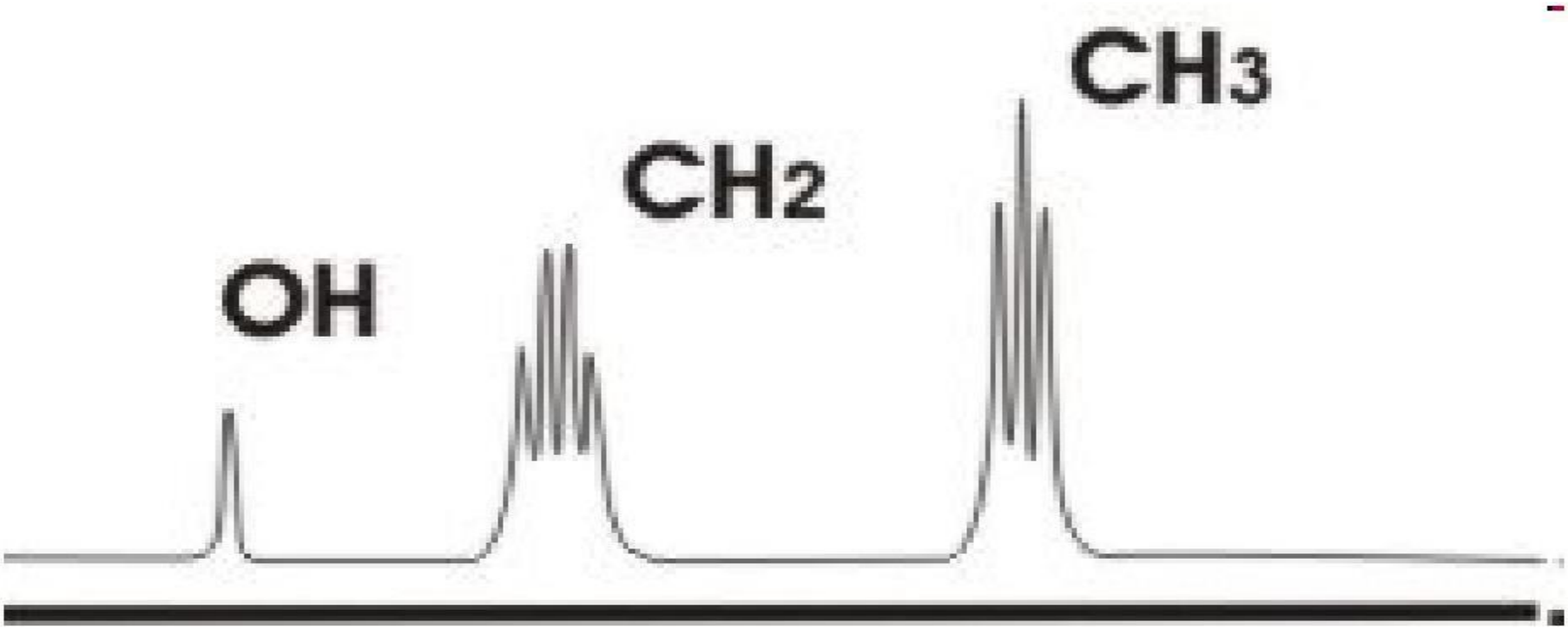


CH_3 proton signal splitted by neighbor CH_2 proton

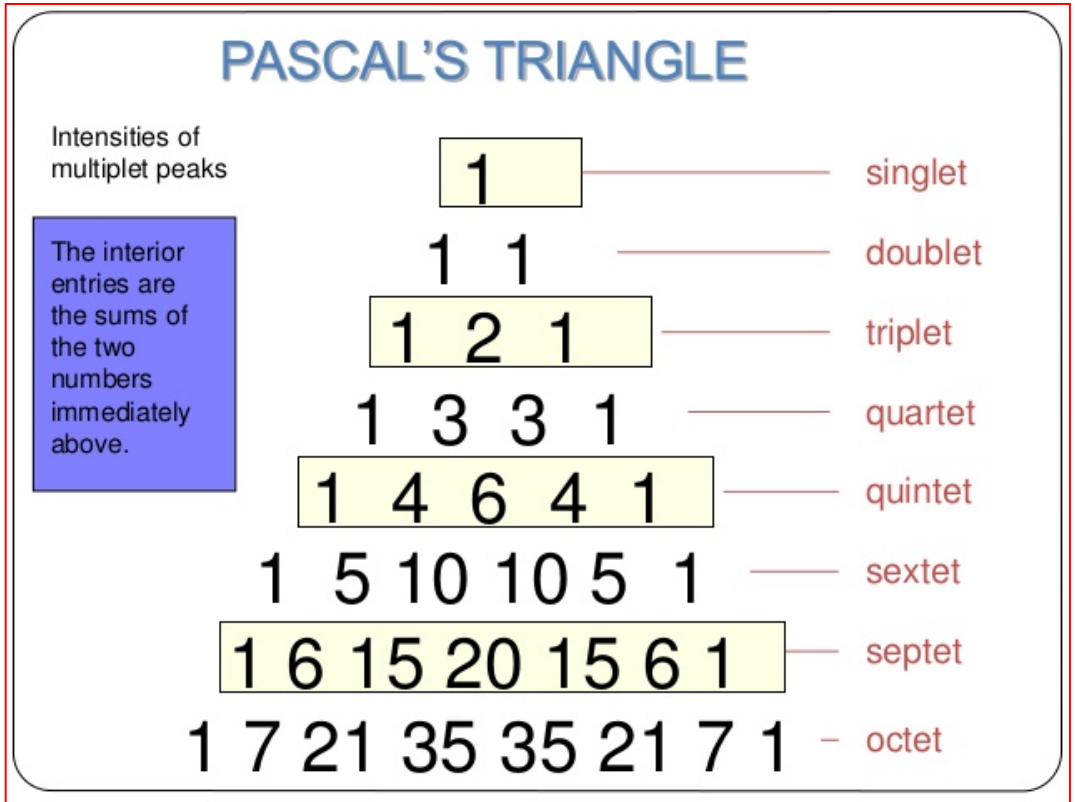
High Resolution NMR spectrum of acidified Ethanol



High Resolution NMR Spectrum Ethanol

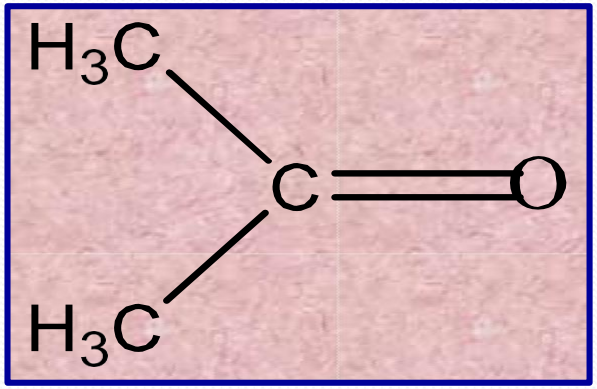


Intensity of NMR spectral lines – Pascal Triangle



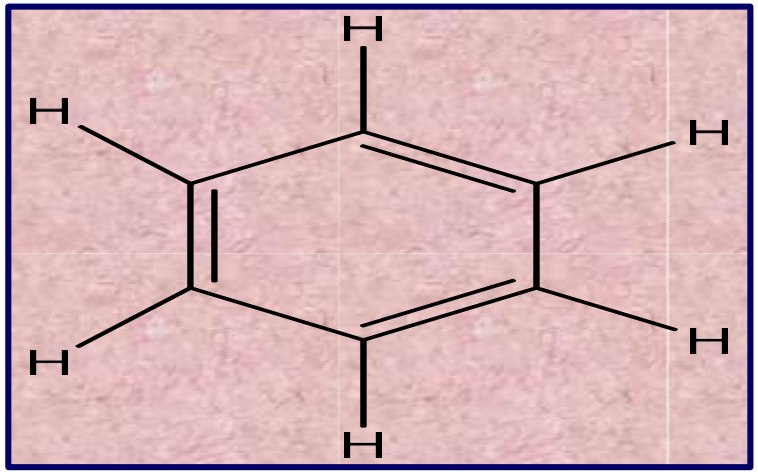
Prediction of Number of Signals

Acetone



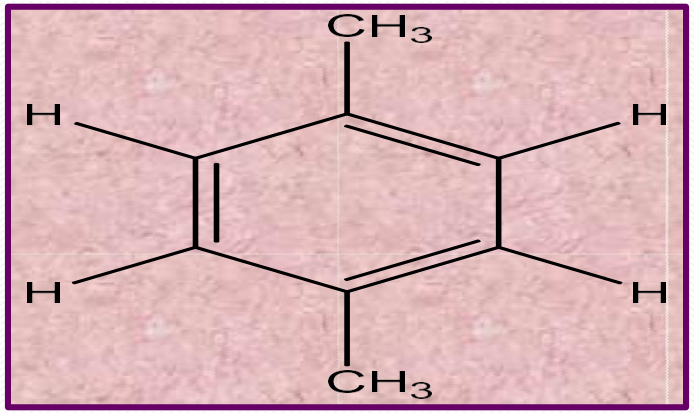
(one signal)

Benzene



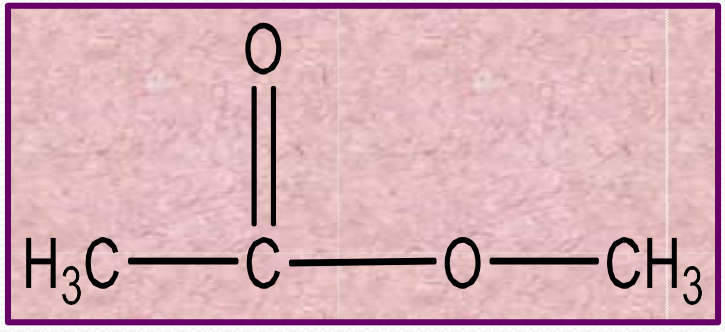
(one signal)

p- xylene



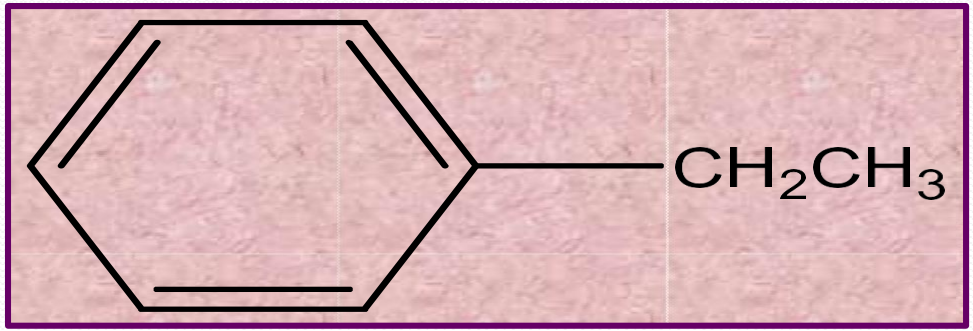
(Two NMR signals)

Methyl Acetate



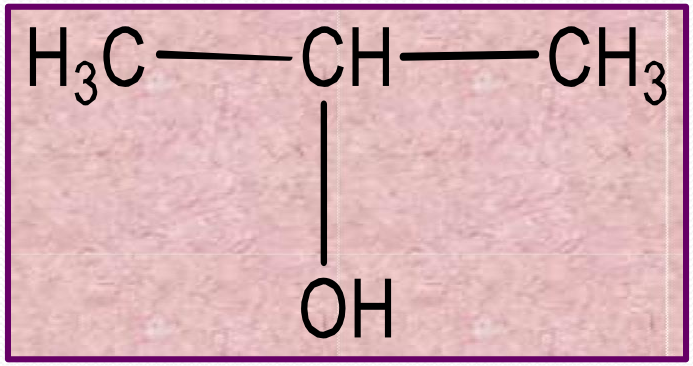
(Two NMR signals)

Ethyl benzene



(Three NMR signals)

Propane-2-ol



(3 NMR signals)


Thank You