Fourier Transform N.M.R (F.T NMR) :-

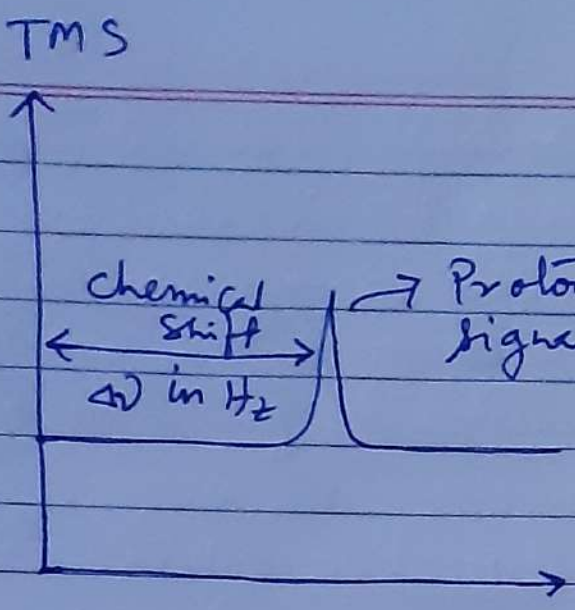
The modern F.T spectrometer operating with a pulse technique. When a R.F. puke of short duration excite all the nuclei of all the signals are collected in the same time with the help of a computer. The individual methods allows several 100 runs to be collected within a sec. The data are mathematically converted (Fourier Transform) to a spectrum.

The advantages of F.T NMR spectra over continuous wave spectra are given below:

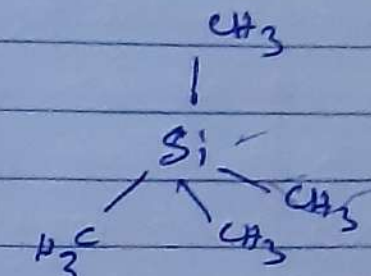
(i) F.T NMR is much faster and more sensitive.
(ii) F.T NMR can be obtained with less than 5 mg of compound.
(iii) The signals stand out clearly with almost no electronic background noise.

Chemical Shift :-

Absolute resonance frequency of protons is difficult to measure with an accuracy. However, relative proton resonance frequencies can be readily determined with an accuracy of ± 1 cps. The separation of resonance frequencies of the nuclei in different structural environments from some arbitrarily chosen standard, whose resonance frequencies are ~~arbitrarily~~ taken as Zero is term as the 'chemical shift' or 'relative resonance frquency'.



Tetramethyl Silane



(TMS)

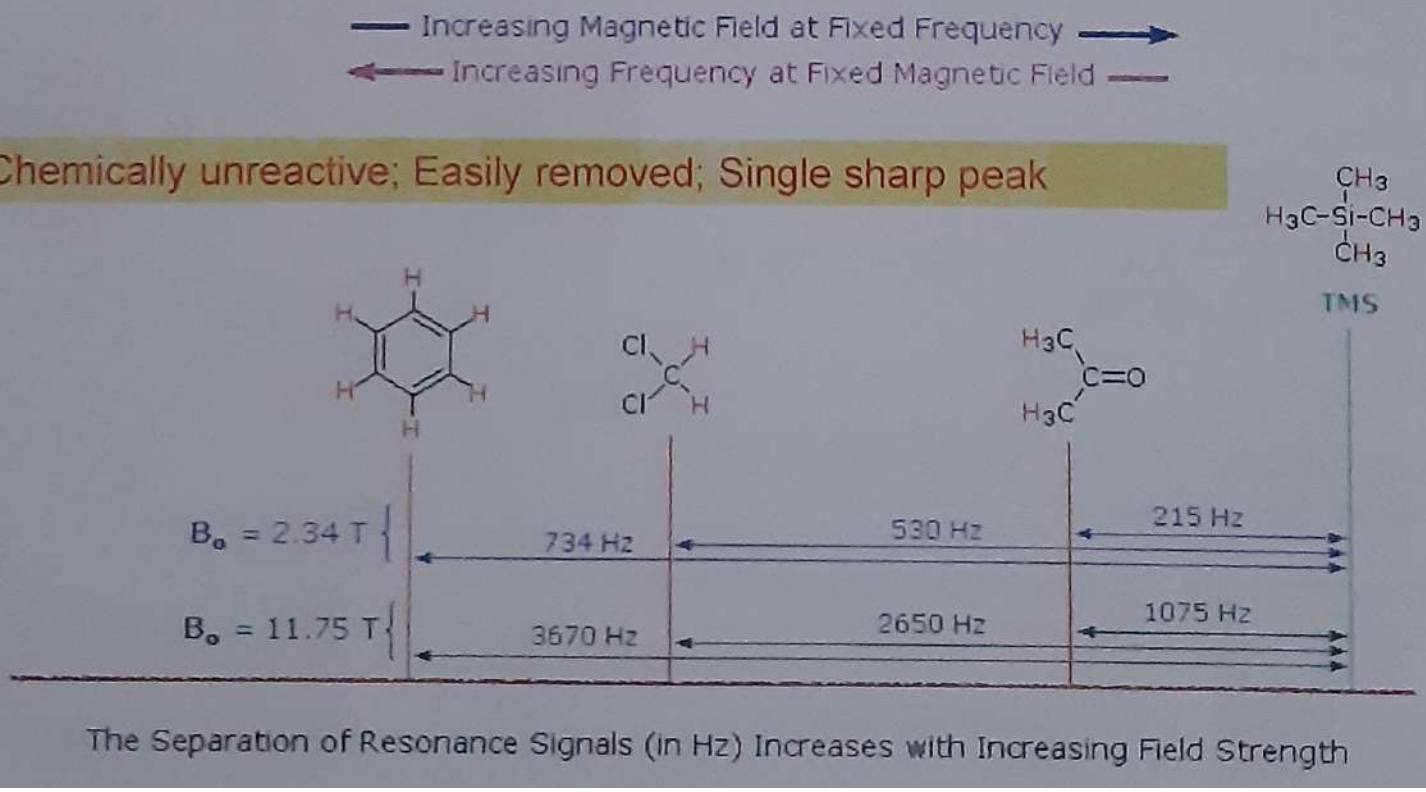
(Standard used in NMR)

Reconance frequency of TMS is used as an internal standard and is arbitarily taken as zero. The chemical shift of a proton of an organic Compound is given by the separation of a signal from that of the TMS signal ($\Delta\nu$ in Hz) run in a particular NMR experiment.

* Why TMS is used as an internal standard ?

(i) It is chemically inert.
(ii) It is magnetically isotopic in nature.
(iii) It is highly volatile, b.p → 27°c, so that sample materials can be recovered after taking the NMR spectra.
(iv) It is miscible with most organic solvent.
(v) It gives a sharp single spectral line.
(vi) The protons of the reference Compound resonate at higher field than most other types of protons of the organic Compound.

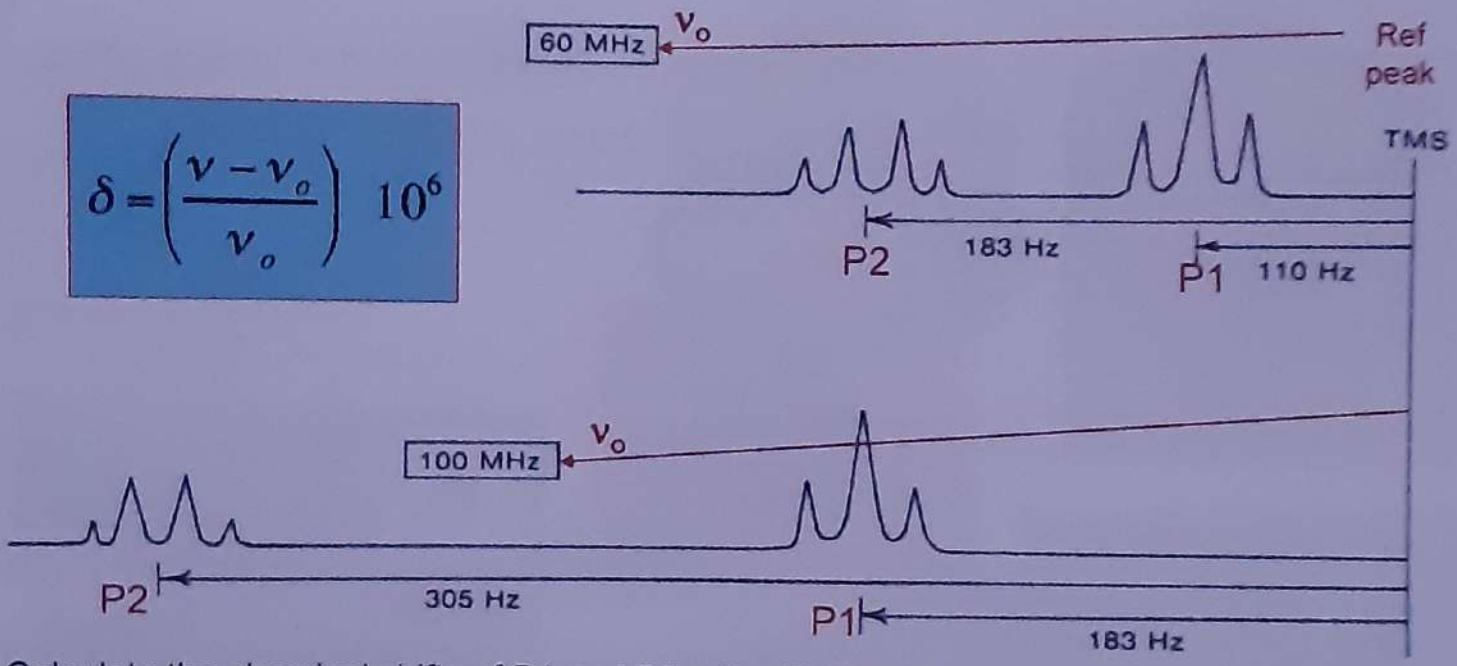
TMS as Reference in NMR



The Separation of Resonance Signals (in Hz) Increases with Increasing Field Strength

Chemical Shift Practice

$$\delta = \left(\frac{\nu - \nu_o}{\nu_o}\right) 10^6$$



Calculate the chemical shifts of P1 and P2 using TMS as 0 ppm

1. For 60 MHz system (i.e. υ_o=60 MHz)

$$\delta(\mathrm{P1}) = \frac{110}{60} = 1.83\,ppm \qquad \delta(\mathrm{P2}) = \frac{183}{60} = 3.05\,ppm$$

2. For 100 MHz system (i.e. υ_o=100 MHz)

$$\delta(\mathrm{P1}) = \frac{183}{100} = 1.83\,ppm \qquad \delta(\mathrm{P2}) = \frac{305}{100} = 3.05\,ppm$$