* How Chemical Shift Can be expressed ?

Chemical Shift Can be expressed in Three different units.

① In CPS or Hz
② In δ (ppm)
③ $\tau = 10 - \delta$

When chemical shifts of protons are expressed in CPS or Hz one should have to maintain not only the internal reference Compound but also the instrument in which the spectrum is run.

To avoid this, the chemical shifts are now a days expressed in terms of δ ppm which is independent of the instrument in which the spectra are run.

$$\delta = \frac{\Delta\nu \text{ in Hz}}{\text{Oscillator frequency in Hz}} \times 10^6$$

$$= \frac{\Delta\nu \text{ in Hz}}{\text{Oscillator frequency in MHz}}$$

The chemical shifts in δ units express the amount by which a proton resonance is shifted from TMS, in parts per million (ppm) of the spectrometer's basic operating frequency.

Values of δ for a given proton are always the same irrespective of whether the measurement was made out 60 MHz ($H_0 = 1.41$ T) or at 100 MHz ($H_0 = 2.35$ T). For instance, a 60 MHz the shift of

The protons are in CH_3Br is 162 Hz from TMS, while at 100 MHz, the shift is 270 Hz. However, both of these correspond to the same value of δ (2.70 ppm)

$$\delta = \frac{162\ Hz}{60\ MHz} = \frac{270\ Hz}{100\ MHz} = 2.70\ ppm$$

Chemical shifts may also expressed in terms of J. When it is expressed in terms of J, the higher the J value of a proton higher the field at which the proton resonates.

Those compounds which are soluble only in H_2O NMR spectrum of the these compounds are to be run in D_2O. But TMS is insoluble in D_2O. it can not be used with this solvent.

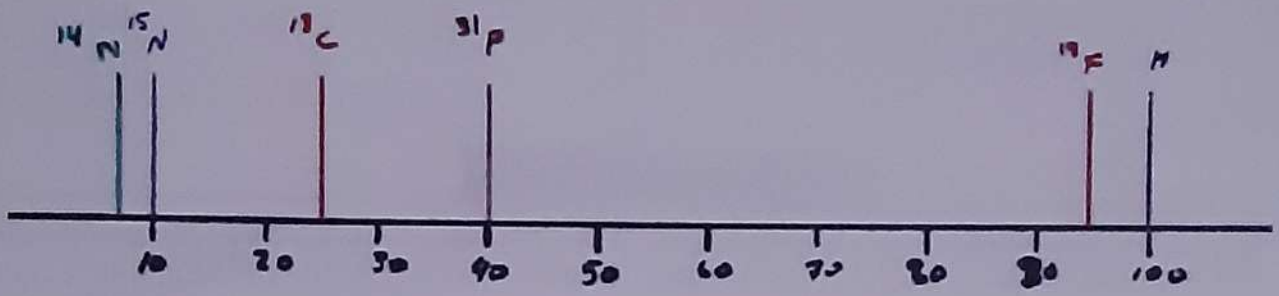
Multinuclear NMR

The table below shows the *resonance frequencies*, ν, of several nuclei at different magnetic field strengths (B_o).

B_o	Resonance Frequency (ν, MHz)				
(tesla)*	^{1}H	^{13}C	^{11}B	^{19}F	^{31}P
2.35	100	25.2	32.1	94.1	40.5
4.70	200	50.4	64.2	188.2	81.0

*a tesla is a unit describing magnetic field strength

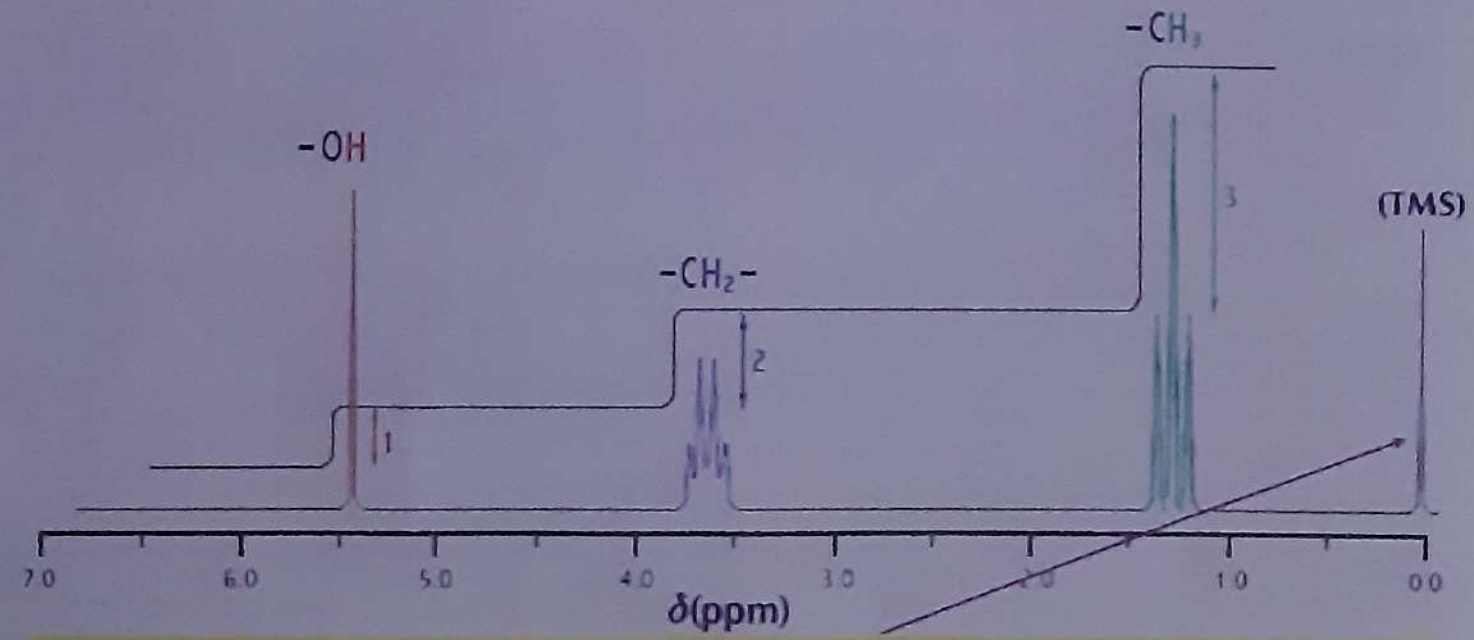
at 23.5 KGasss => 2.35 Tesla



CH_3CH_2OH

Example

- the three types of protons of ethanol appear at different chemical shifts (relative resonance frequency)
- the ratio of the integrated area under each peak is equal to the ratio of the number of each type of proton



TMS signal is used as a reference peak to set zero on the ppm scale of chemical shift (more discussion later).