SUBJECT - CHEMISTRY
CLASS - B.Sc (Hons) PART - III
PAPER - V
TOPIC - Chemical Shift in nmr Spectroscopy

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Q Explain chemical shift in nmr spectroscopy.

Ans Chemical Shift(δ): we know that shielding of protons by electrons shifts the absorption in nmr spectrum upfield and deshielding shifts the absorption downfield to get an effective field necessary for absorption. Such shifts Compared with a reference Compound (usually TMS) in the position of nmr absorption are called chemical shifts. Due to low electronegativity of Si (1.8) shielding of equivalent proton of TMS is greater than most of the organic Compounds, So the nmr Signal of TMS is taken as reference and Chemical shifts of different Sets of protons are measured relative to it. The nmr Signal for TMS (highly shielded) appears at the extreme right in the spectrum with $\delta = 0$. Keeping the radio frequency Constant, nmr Signals for different Sets of protons appear at different field strengths Compared with the nmr Signal of TMS. This difference in absorption positions of protons with respect to TMS Signal is called Chemical shift(δ) Since operating frequency of the instrument is directly proportional to field strength hence -

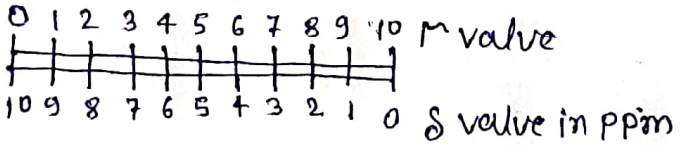
$$\delta \text{ (in ppm)} = \frac{V_s - V_{TMS} \text{ or } \Delta V}{(V_o) \text{ operating frequency (in MHz)}}$$

where $V_s$ & $V_{TMS}$ are the frequency (in Hz) of the signals in sample and TMS respectively and $\Delta V$ is the frequency shift. The $\delta$ value is expressed in ppm (parts per million). Most chemical shifts have $\delta$ values between zero to ten. The same signal at an applied frequency of 60MHz would be at $\nu 60$ but will be at $\delta = 1.00$ppm

$$\frac{60 \times 10^6}{60 \times 10^6} = \delta 1.00$$

· It is also expressed in $\tau$ scale -

$$\tau = 10 - \delta$$




$H_0$ ——— Increases ———→

Greater the shielding lower will be $\delta$ values and greater the deshielding, larger will be $\delta$ values.