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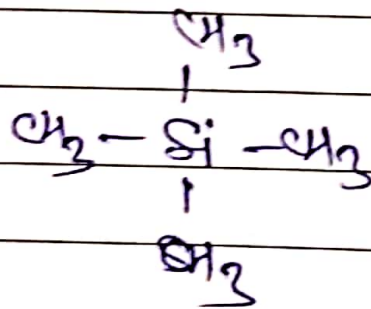
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Positions of signals (chemical shift)

The positions of the signals in the spectrum helps us to know the nature of proton viz. aromatic, aliphatic, acetylenic, vinylic etc. Each type of proton will have different electronic environments and thus they absorb at different applied field strength.

For measuring chemical shift of various protons in a molecule, the signal for TMS (tetramethyl silane) is taken as a reference.



The difference in the absorption position of the protons with ~~reference~~ respect to TMS signal is called chemical shift. It is denoted by δ -value.

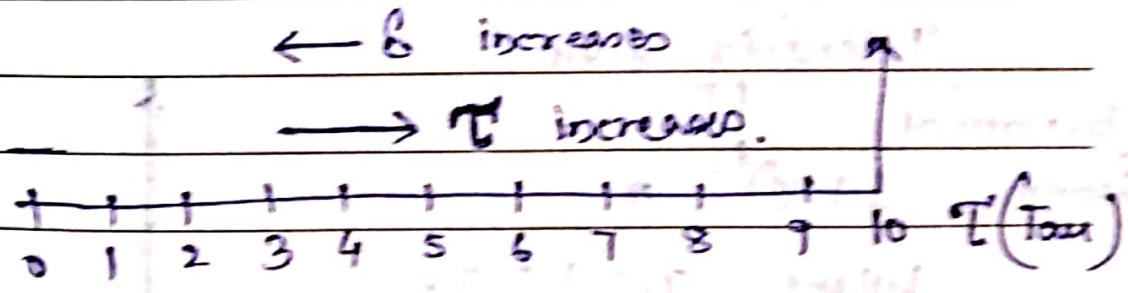
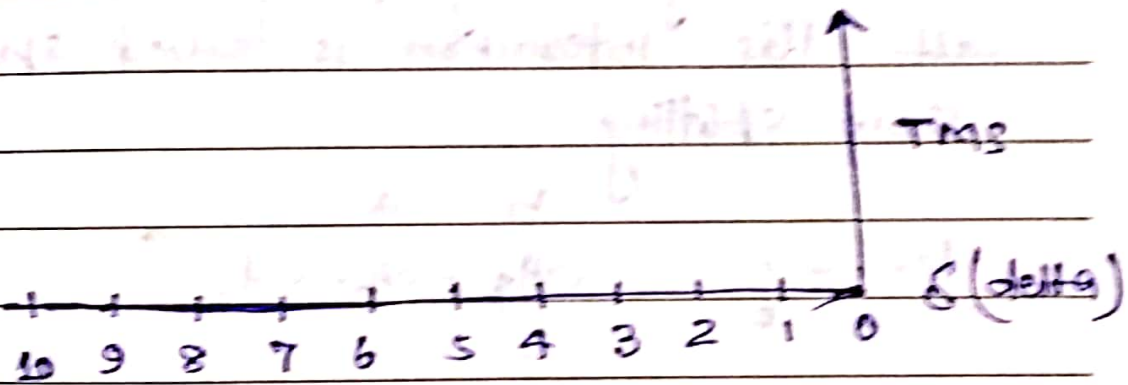
Thus .

$$\delta = \frac{H_s - H_r}{H_0} \times 10^6 \text{ ppm.}$$

where, H_s = magnetic field strength

H_r = field strength at which absorption occurs.

H_0 = applied field strength.



$$\tau = 10 - \delta$$



TITLE _____

Date: / /

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High resolution NMR - spectra - spin-spin splitting

In a molecule, there may be groups of equivalent protons, each group producing one NMR peak. In most NMR spectra, however, under high resolution, the no. of lines observed.

The splitting of the NMR peaks arises due to interaction between neighbouring protons. ~~which are~~ This interaction is called spin-spin splitting.

for eg. $\overset{b}{\text{CH}_3} - \overset{a}{\text{CH}_2} - \text{Cl}$

Intensity ratio -

Binomial

Theorem. $(1+x)^n$

where, $n = 1, 2, 3, \dots$

no. of protons. (neighbouring)

CH₂

$n = 3$. (neighbouring protons)

$$(1+x)^3 = 1 + 3x + 3x^2 + x^3$$

(1 : 3 : 3 : 1) (Quartet)



TITLE _____

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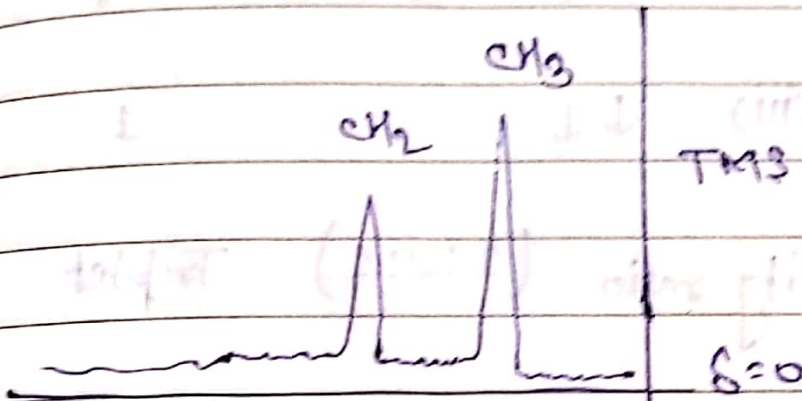
CH₂

$n = 2$. (neighbouring protons.)

$$(1+x)^2 = 1 + 2x + x^2$$

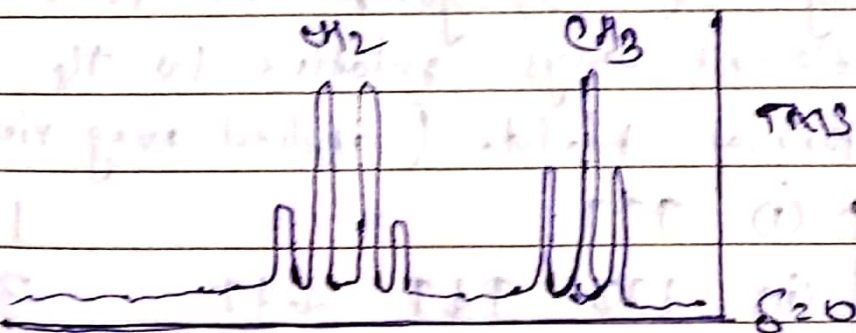
= 1 : 2 : 1 (Triplet)

Low resolution



← (δ in ppm)

High resolution



← (δ in ppm)



TITLE

Date: / /

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-CH₂

The spin of two protons (-CH₂-) can couple with the adjacent methyl group (-CH₃) in three different ways relative to the external field. (applied mag. field)

Applied mag. field (H ₀)	(i)	↑↑	1
	(ii)	↑↓ ↓↑	2
	(iii)	↓↓	1

Intensity ratio (1:2:1) Triplet

-CH₃

The spin of three protons (-CH₃) can couple with the adjacent methylene (-CH₂) group in four different ways relative to the external field. (applied mag. field)

Applied Mag. field (H ₀)	(i)	↑↑↑	1
	(ii)	↑↑↓ ↓↑↑ ↓↑↑	3
	(iii)	↓↑↑ ↓↑↓ ↑↓↓	3
	(iv)	↓↓↓	1

Intensity ratio (1:3:3:1) Quartet