Chapter:

Spectroscopy

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NMR Spectroscopy

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Chemistry with MJS

Chemistry Preparation by MJS

H-NMR

→ Interaction of Radiowaves with The matter.

Theory

- ★• Nucleous is understudy
- ★• This is the magnetic property of Nuclei.
- ★• Nucleous act as a tiny bar magnet.
- ★• All nuclei carry a charge & some show the spin about their axis.
- ★• Spinning of Nuclei depends upon the spin Quantum number value. (I) → depends upon No. of proton & Neutron.
- ★• Nuclei keeps on spinning → Rotation of Nuclei is known as precession
- ★• Here transitions occured in magnetic Energy levels.
- ★• When any nuclei start to spin → Thus magnetic moment is created (μ)
- ★• magnetic momement depends upon the no. of proton & neutron present in nuclei. so every nuclei has different magnetic moment(μ)

NMR Active/Inactive Nuclei:

- ★ The nuclei whose Quantum No. value is zero They are inactive.
- ★ The nuclei whose Q.N is present → All are active. Any nuclei will become active when it has resultant Nuclear spin

There is no energy gap so no excitation & dexcitation of nuclei so NMR inactive ↶ $I = 0$ ⟶ NMR inactive

$I = 1/2$
$I = 1$
$I = 3/2$
→ NMR active

* when Both p & n ⇒ even ⇒ $I = 0$ → no spin

e.g ^{12}C p=6, n=6

e.g ^{16}O

e.g ^{32}S ⇒ They are NMR inactive

* when either proton or neutron is odd ⇒ $I = \frac{1}{2}$ → Fractional spin

e.g ^{1}H, ^{13}C, ^{19}F, ^{31}P

If $I = 3/2$ e.g ^{127}I, ^{79}Br

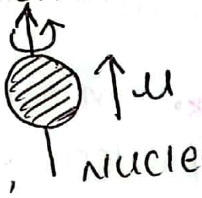
* when both p & n ⇒ odd then $I = 1$ → integral spin

e.g ^{14}N, ^{10}B, ^{2}D

* ~~when~~

* Spinning charge generates magnetic field- which boost up the magnetic moment. (μ)

$\mu \propto M.F (H_0)$



- In the absense of external magnetic field, Nuclei are oriented randomly-
- In the presence of M.F → Nuclei orientate either they will allign (+½) or opposed (−½)
- No. of possible orientations depends upon the value of spin Quantum No. value

Orientations OF Nuclei:

- In the presence of external M.F Nuclei orientate itself either allign or oppose.

* orientations

→ Allign (+½) → Low E → poor Nuclei
↳ α-spin

→ oppose (−½) → High E → Rich Nuclei
↳ β-spin

★ DifferencE in (ΔE) energy b/w two spins depends upon the strength of M·Field·(H_o)

⇒ No· of orientations can be calculated by the Following Formula; $(2I+1)$

★ $I=0$ ⇒ $2(0)+1=①$ No energy gap so inactive

★ $I=\frac{1}{2}$ ⇒ $2(\frac{1}{2})+1=②$ two orientations are allowed

one along the applied M·F

other against the M·F

★ $I=1$ ⇒ $2(1)+1=③$ → three orientations

one along the M·F

other against the M·F

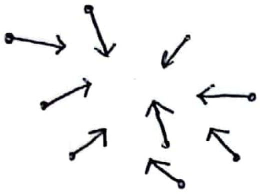
3rd is perpendicular to the M·F

⇒ AS No· of orientations increasES thus excitation & de-excitation will become complex and we can not study the Nucleous easily. So we usE $I=\frac{1}{2}$ = ② orientations

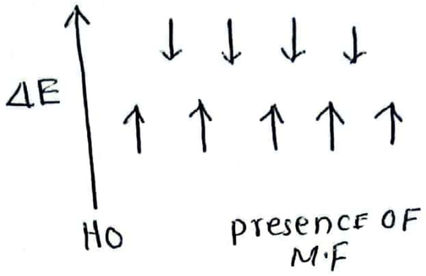
So ^1H proton NMR & ^{13}C-NMR can be interpret easily → so we study Both these b/c present in every structure.

⇒ in the absence of M·F ⇒ these two orientations have no energy gap and these are degenerate. when the nuclei are placED in external M·F the nuclei orientate & Energy gap is created b/w These two α & β- levels.

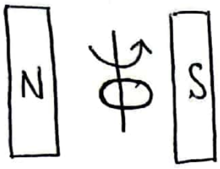
$$\Delta E \propto H_o$$



ABSENISE OF M·F



presence OF M·F



$$\Delta E = \frac{h\gamma H_o}{2\pi}$$

$$\frac{\Delta E}{h} = \frac{\gamma H_o}{2\pi}$$

$\because \Delta E = h\nu$

$\therefore \nu = \Delta E/h$

$$\boxed{\nu = \frac{\gamma H_o}{2\pi}}$$

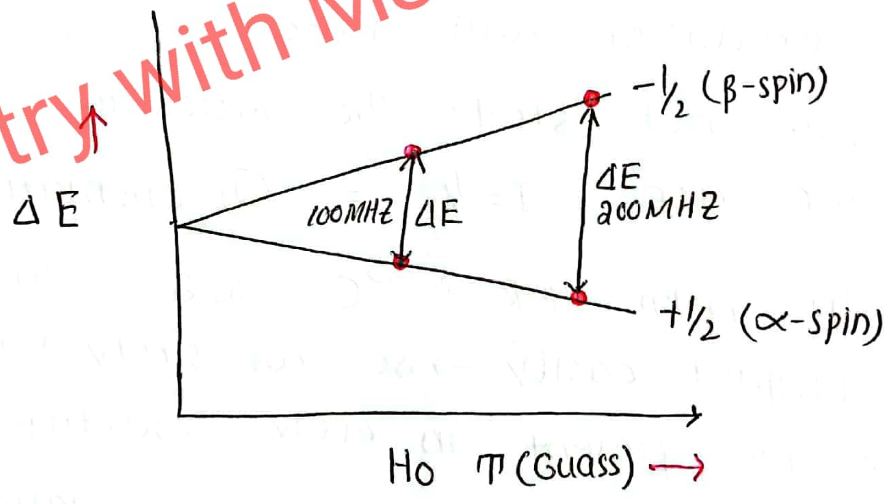
$$\boxed{\gamma = \frac{2\pi\nu}{H_o}}$$

ν → Radio frequency (MHZ) $\boxed{1 HZ = 1 ppm}$

H_o → M. Field (Testla, T) $\boxed{1 T = 10^4 \text{ Guass}}$

γ → Gyromagnetic Ratio → tells about the mag. strength of the nuclear magnet.

⇒ Ratio of Radiofrequency & strength of magnetic Field is known as Gyromagnetic Ratio /OR/ Gyromagnetic moment.



⇒ in case of ^1H For 60 MHZ ⇒ $H_o = 1.41\ T$

$$\gamma = \frac{60\ \cancel{1.41\,T}}{1.41\ \cancel{60}} = \boxed{42.58}$$

⇒ in case of ^{13}C For 60 MHZ ⇒ $H_o = 5.6\ T$

$$\gamma = \frac{60\ \cancel{5.6}\ T}{5.6\ \cancel{60}} = \boxed{10.71}$$

✓Principle:

Absorption of Radiowaves by a Nucleous to induce the spin-Flipping will take place when Frequency of Electromagnetic Radiation is exactly equal to the precessional frequency of Nucleous, thus two frequencies matched thus Nuclei start spinning. Known as (NMR)

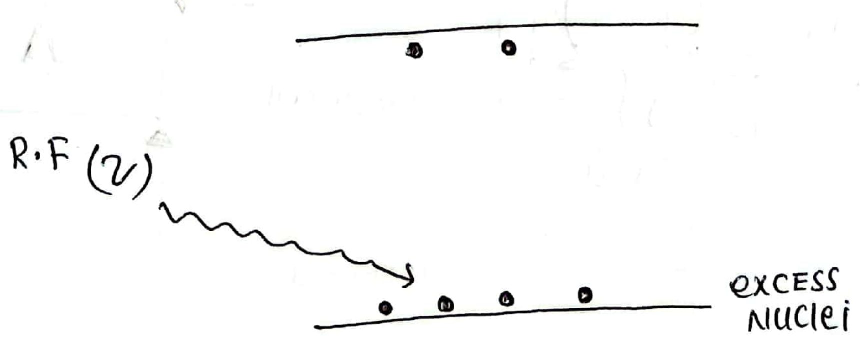
Spin Flipping:

★ When Nuclei are placed b/w the two poles of magnet thus Energy levels split and Energy gap is produced and thus Rf waves Required to excite & dexcite the Nuclei known as spin-Flipping

★ If powerful magnet Ho ↑ High energy gap is created thus Higher R.F will Required to excite & dexcite the Nuclei

Spin-Flipping → two modes of inducing the spin Flipping

- **Magnetic Sweep**
  - → M.F varies
  - → R.F constant
  - ↓ This Mode is convenient, technically as compared to the Frequency sweep.
- **Frequency Sweep**
  - → R.F varies
  - → M.F kept constant



★ Strong will be the Ho thus Higher will be the Energy gap thus Nuclei will excess at ground state
↓
thus greator will be signal

★ **For Better Signal/Results**

(i) excess of Nuclei At ground state
(ii) Minimization of Saturation

Spin relaxation: / Relaxation:

This phenomena is unlike the UV-Visible principle. Here, The Nuclei in the Higher energy spin state can not return to the lower energy spin state by the emission of radiation. (Heat is released so Radiationless emission occur)

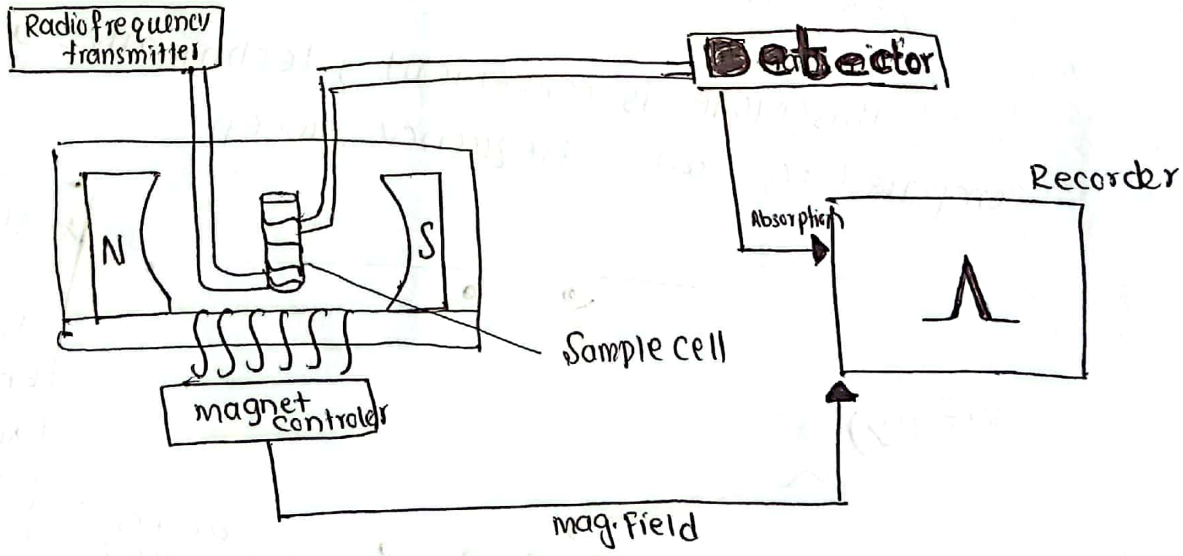
In this, Nuclei returns to the lower energy state and Nuclei become excess by losing the excess energy - in the form of heat this process is known as Relaxation

Relaxation (Energy transfer phenomena)

(t_1) spin-Lattice Relaxation
↓
- ⋆ Energy is transfer from one Nuclei (proton) to surrounding
- ⋆ This is longitudnal
- ⋆ Mostly used process in NMR

Spin-spin Relaxation (t_2)
↓
- ⋆ Energy is transfer from one nuclei to another Nuclei
- ⋆ This is transverse
- ⋆ less common

✓INSTRUMENTATION:



NMR → continuous wave NMR → classical → M.F varies, R.F constant

NMR → pulsed NMR → modern → M.F constant, R.F varies

Components:

(i) Magnet
(ii) R.F transmitter
(iii) Sample tube (probe)
(iv) Detector
(v) Amplifier
(vi) Recorder

NMR-mode:

* Today's Continuous wave NMR is used b/c It is very easy to handle than ~~continuous~~ pulsed wave mode of instrumentation

Magnetic Field:

* NMR spectrophotometers are available in wide range of M.F strength. e.g 60 MHZ, 90 MHZ, 100 MHZ, 200 MHZ & 900 MHZ.

900 MHZ ↓
* more E gap
* more excess Nuclei
* less saturation
* Better Results
* More cost

60 MHZ ↓
* less E gap ↓
* Less excess Nuclei
* More Saturation
* Thus Not better Results than 900 MHZ
* so less cost.

* Strength of M.F that passes through the sample can be varied by varying the current in the sweep coil.

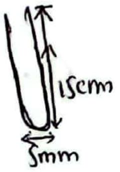
Magnet:

This is the most important part - total cost of NMR depends upon this component.

Magnet can be used permanent magnet, electromagnet or super conducting magnet.

Sampleprobe: → Sample is prepared with appropertiate solvent. There is No transparency Limit but Deuterated Solvent should used.

* Sample tube usually 15cm long & 5 mm diameter.



* It is made up of Borosilicate glass.
* It is placed b/w the poles of magnet.
  * For Sampling, Deuterated solvent should be used.

R.F transmitter:

* It provides the Radiowaves → interact with Sample
* R.f is provided perpendicular to the M.F through a coil wrapped around Sample tube

Detector:

Detector Detect the Signal.

Interpretation:
→ chemical shift
→ integiation
→ spin-spin splitting
→ J coupling (coupling constant)

①chemical shift: → Qualitative information
what type of proton?

Scale = PNMR

0 ← 14 ppm chemical shift

0 ↓ More shielded (upfield) ↓ less energy gap

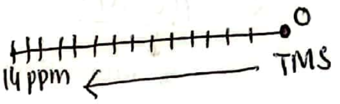
14 ppm ↓ more deshielded (dow Field) ↓ More energy gap

—OH, —CHO, —COOH, —CH_3, —CH_2

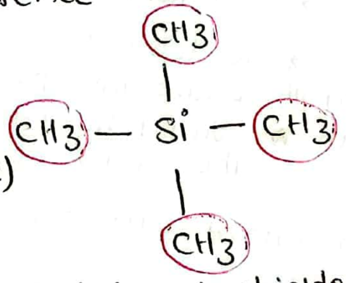
each proton has different energy gap so different frequency of Radiowaves is required to fill the gap.

* CH_3 → more shielded more toward zero
* —COOH → most deshielded system → value near to 14

→ chemical shift is a chemical property
→ shift is from certain reference point.



* The Reference is choosen (TMS)



(tetramethyle silane)

* TMS is reference for both ^1HNMR & ^{13}C-NMR

* 12 protons ↓ having equivalent (Most shielded system) enviroment at 0 ppm

why more shielded system show lower ppm (upfield)?

Higher the $\bar{e}$ density around the nucleous, the higher the opposing M.F to external M.F (B_0) From electrons, the greator the shielding. B/C the proton experieng low Ext. M.F, it needs a lower frequency to achieve Resonance therefore C-shift shifts at upfield (lower ppm)
⇒ so vise versa.

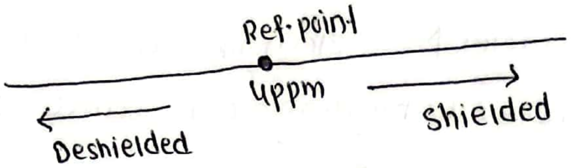
Q: Why we choose TMS as standard?

① containing 12 proton with strong signal
② Most shielded system
③ Here No electronegativity phenomena
④ chemical innert, so we add TMS while preparing sample

$$\boxed{\text{Sample + Solvent + TMS}}$$

⑤ low Boiling liquid, So eve easiey Recover the sample.

We can Also used chloroform as a Standard. 9ts proton value at 4ppm



⇒ Solvent choice for ^{1}H-NMR:

- Solvent should be used Neat.
- Aprotic solvent should be used e-g CCl_4, CS_2, D_2O

Also $CHCl_3$ can be used. but This solvent can not be used for Aromatic compounds b/c 9ts value overlap at ~7.3 ppm with Aromatic compound. But we can differentiate b/c $CHCl_3$ peak → large sharp peak but Aromatic → small multiple peaks.

$$\text{Chemical shift} = \frac{\overset{\text{Absorption of Protons Relative to TMS}}{\text{Shift in (HZ)}}}{\underset{\text{Radio}}{\text{operating frequency (MHZ)}}} \times 10^{6}$$

⇓

∴ $\frac{1\ \text{HZ}}{1\ \text{MHZ}} = 1$ ppm

9ts Answer is v.v.v.low so we Multiply 10^6 factor so Answer should be considerable

★ chemical shift is Also Known as Dalta-shift/scale OR Also called τ- scale → Rarely used

↓

0——10 ppm

⇒ Factors Affecting on chemical shift:-

① Inductive Effect:

−I Effect attract ēu electronic cloud toward itself thus proton containing carbon become less shielded & ppm value increases.

−I-Effect ∝ ppm value

$$+I \text{ Effect} \propto \frac{1}{\text{Chemical shift}}$$

② Mesomeric Effect:

$$+M \propto \frac{1}{\text{C.shift}}$$

$$-M \propto \text{Chem. shift}$$

③ Hybridisation:

sp^3, sp^2, sp

Generally S-character ↑ electronic cloud around H become less thus more deshielding occur value of chem-shift increases

× $sp > sp^2 > sp^3$ should follow this trend

But sometimes due to unsual behaviour / Non uniform behaviour Anisotropy occur & this trend is not followed.

✓ $sp^2 > sp > sp^3$ correct
↳ due to Anisotropy

Q: Why sp show lesser value than sp^2?

two factors

(i) S-character (ii) π-ē circulation

★ π-ē circulation ⟶ shielded the ≡ bond system & value decrease but deshielded the = bond system.

★ Aromatic = bond is more deshielded system
↓
4–7 ppm

④ Solvent:

Generally substances in Aromatic solvent give signal at lower chemical shift than Alephatic solvent.

e.g $CHCl_3$
↓
give high c.shift

Benzene
↓
give low c.shift.

⑤ H-Bonding:

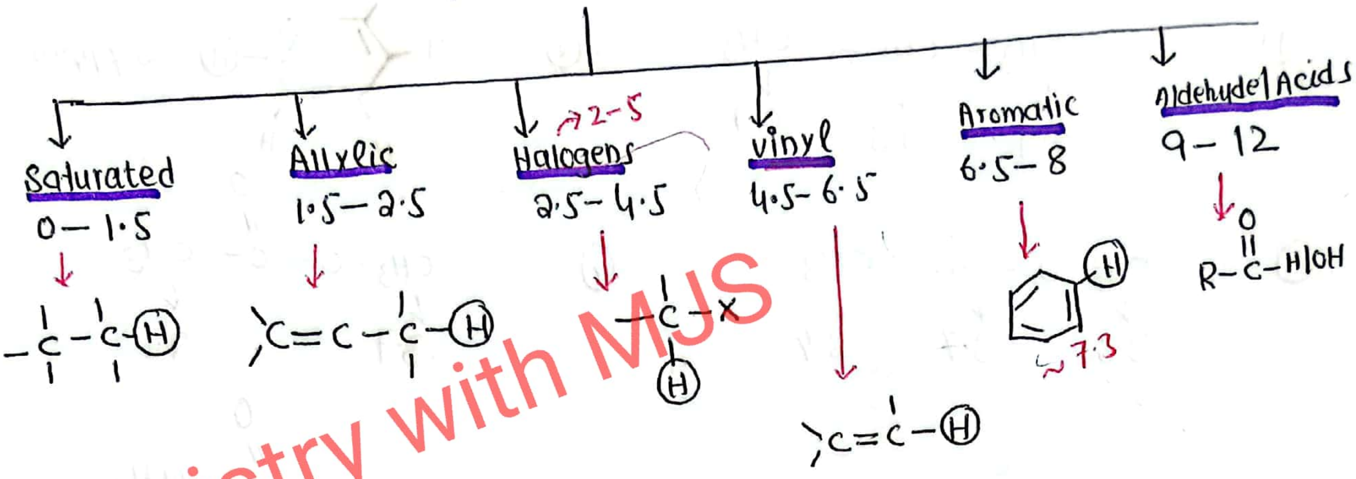
★ At low conc ⟶ low H-bonding
★ At high conc. ⟶ strong H-bonding

⇒ H-bonding increase the chemical shift value

✳ ———————— ✳

Regions

Chemical shift is Divided into six-major Regions



★ $-C-H$ (sp^3) 0 – 2 ppm ⟹
- ★ $-CH_3$ ~ 0.9 ✓
- ★ $-CH_2$ ~ 1.2 ✓
- ★ $>CH$ ~ ~~1.7~~ ✓

$\boxed{\sim 2.5}$ ★ $\equiv C-H$ (sp) 2 – 3 ppm

★ $Ar-CH_3$ ~ 2.3

★ $\overset{O}{\overset{\|}{C}}-CH_3$ ~ 2.1

★ $=C-H$ vinyl ↓ sp^2 4 – 7 ppm

★ $Ar-H$ ~ 7.3

CH_3-C	~0.9
CH_3-N	~2.3
CH_3-O	~3.3

Halogens

CH_3-F	~ 4.25
CH_3-Cl	~ 3.05
CH_3-Br	~ 2.7
CH_3-I	~ 2.1

★ O–H 0.~~8~~–5 varied

★ N–H 0.~~5~~–5 varied
↳ Bread peak
∩ –NH_2

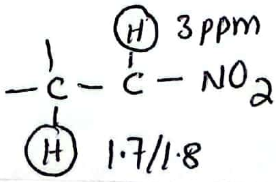
★ $R-NH_2 \rightarrow 0.5-5$ varied

★ $R-OH \rightarrow 0.5-5$

★ $Ar-NH_2 \rightarrow 3-6$

Aldehyde $\overset{O}{\overset{\|}{C}}-H$ 9 – 10 , $\overset{O}{\overset{\|}{C}}-NH_2$ ~ 5ppm ★ $Ar-OH \rightarrow 4-7$

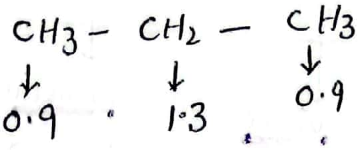
C.Acids $\overset{O}{\overset{\|}{C}}-OH$ 10 – 12 ,



$-\underset{H}{\overset{|}{C}}-\overset{H}{\overset{|}{C}}-NO_2$ ~

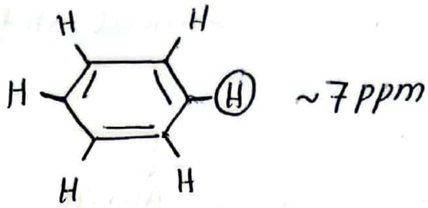
Examples;

①

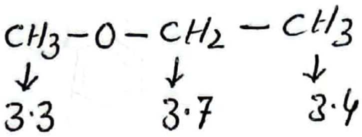


$CH_3-CH_2-CH_3$

②

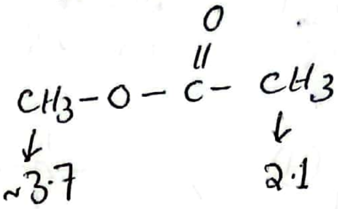


③



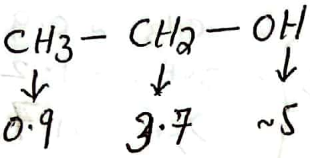
$CH_3-O-CH_2-CH_3$

④



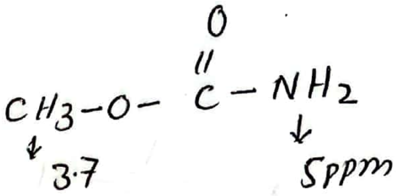
$CH_3-O-\overset{O}{\overset{\|}{C}}-CH_3$

⑤



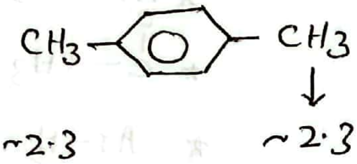
CH_3-CH_2-OH

⑥

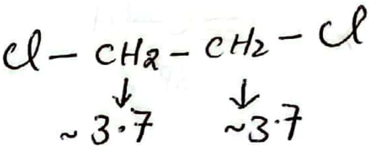


$CH_3-O-\overset{O}{\overset{\|}{C}}-NH_2$

⑦

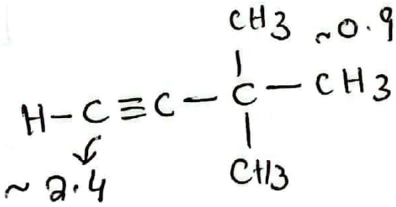


⑧



$Cl-CH_2-CH_2-Cl$

⑨



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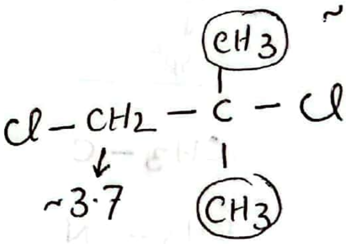
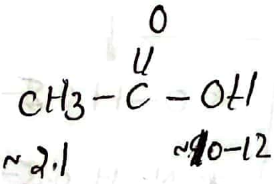


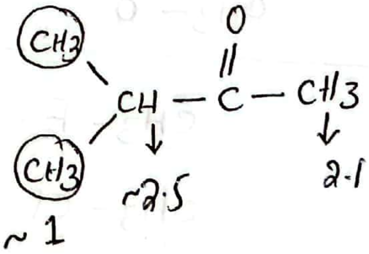
~2ppm increase due to E.W.D.G

⑪



$CH_3-\overset{O}{\overset{\|}{C}}-OH$

⑫



★ chemical shift value affected till 3→bond distance

2) Integration: ⟶ Quantitative information

- ⋆ It tells about the no. of protons present in each environment.
- ⋆ The peak intensity/Height depends upon the no. of protons. We can check by the scale but today's digitally measured.

$$\begin{array}{ccc} CH_3- & CH_2- & OH \\ \downarrow & \downarrow & \downarrow \\ 3 & : 2 & : 1 \end{array}$$

3) Spin-Spin Splitting:

splitting of proton is due to the neighbouring proton.

How much splitting?

$$\Rightarrow 2nI + 1$$

in case of ^1H & ^{13}C $I = \frac{1}{2}$

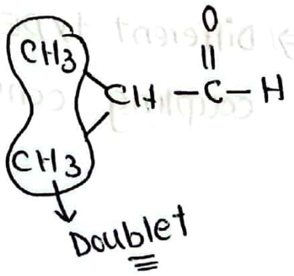
$$\cancel{2} n \times \frac{1}{\cancel{2}} + 1 = \underset{\substack{\downarrow \\ \text{no. of neighbouring protons.}}}{n+1}$$

⋆ If one proton in neighbourhood:

= 1+1 = ② → Doublet peak

Example

$$\begin{array}{ccc} CH_3 & - CH_2 & - Cl \\ \downarrow & \downarrow & \\ \text{Triplet} & \text{Quadret} & \end{array}$$



⋆ If two protons in neighbourhood

2+1 = ③ → Triplet

Pascal tringle OF Splitting peaks

n		
0	singlet →	1
1	Doublet →	1 1
2	triplet	1 2 1
3	quartet	1 3 3 1
4	quintet	1 4 6 4 1
5	sextet	1 5 10 10 5 1
6	Septet	1 6 15 20 15 6 1
7	octet	1 7 21 35 35 21 7 1

peaks


singlet


Doublet


Triplet


Quartet


quintet


sextet


septet


octet

Chemically Equivalent nuclei/proton:

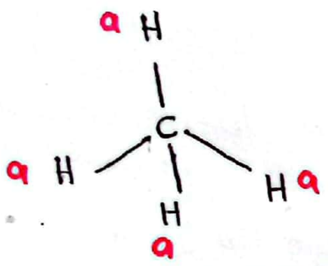
- ★ A group of Nuclei having same chemical shift.
- ★ These Nuclei have identital ē environment.

Magnetically Equivalent Nuclei:

- ★ chemically Equivalent Nuclei that couple Equally to any Nucleous in the same spin system.
- ★ All the magnetically equivalent Nuclei are chemically Equivalent but not All the chemically equavelent are magnetically Equivalent.

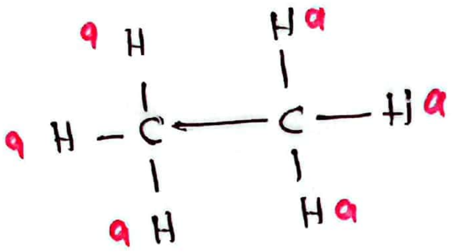
Examples;

1)



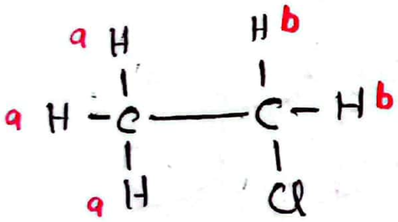
- ★ All 4-H give only one signal so, chemicall equivalent
- ★ Here no spin-spin coupling so info about Mag-Equivaleny

2)



- ★ All 6-H give only one signal - same environment chemically equivalent
- ★ No-spin-spin coupling so No info about mag-Equivalency

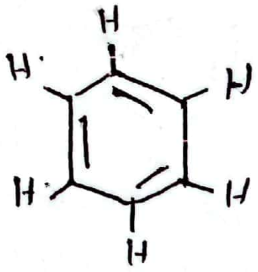
3)



2-signal in H-NMR

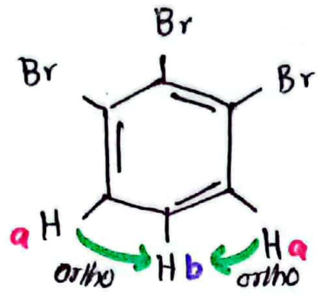
- ★ All 3-H (a) → Chemically Equivalent
- ★ Both 2H(b) → chemicall Eq-
- ★ All the 3-H (a) → Mag-Equivalent
- ★ Both 2-H (b) → magnetically Equivalent
- ★ CH_3 & CH_2 → chem-non-Equivalent

4)



6-H gives 1-signal in H-NMR so chemically Equivalent.

⑤



2-signals in H-NMR

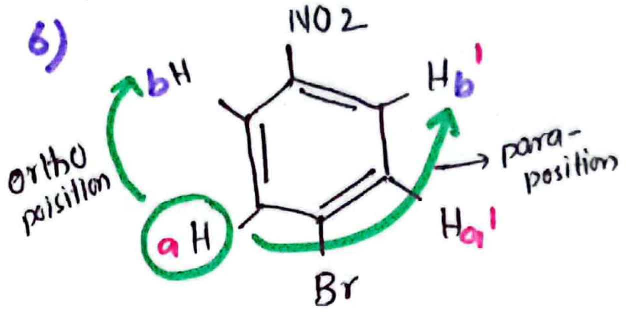
★
- a-H Doublet
- b-H Triplet

★ Both Ha → chemically Equivalent

★ Both Ha → magnetically Equivalent

★ Ha & Hb → chemically Non-Equivalent

6)



2 → signals

- a-H Doublet
- b-H Doublet

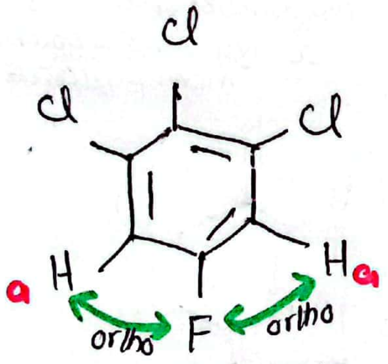
★ Both Ha & Hb chemically non-Equivalent

★ Both Ha → chemicall Equivalent

★ Both Hb → chemically Equivalent

★ Both Hb & Ha ↳ magnetically non-Equvalent so Represented by prime ~~by~~

7)

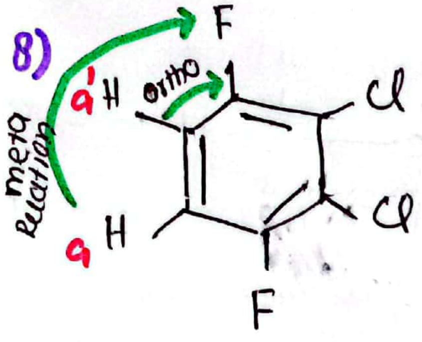


1-signal H-NMR

★ Both $_a$H chemically Equivalent

★ Both aH → have Same relation with F → So magnetically Equivalent

8)



1-signal H-NMR

★ Both aH → chemically Equivalent

★ Both aH → magnetically Non-Equivalent

* If no proton in neighbour → Singlet peak

0+1= ①

⊛ 3+1 ⇒ ④ Quadret

4) J-coupling (coupling constant)

↳ Represented by Jax

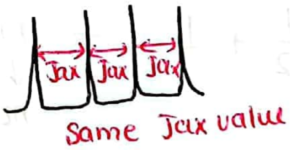
⇒ It tells about, how much bond distance interaction.

⇒ It tells about the gap b/w ~~in~~splitting peaks.

⇒ More will be the value of coupling constant more will be the gap b/w peaks of splitting proton.

⇒ Same type of proton show equal gap b/w Signals b/c of same no. of value of J-constant.

Quadret/Quartet



Quadret/ Quartet

$CH_3 - CH_2 - Cl$

↓ Triplet ↓ Quadret/Quartet

⇒ Different type of protons have different values of coupling constant -

Quadret

Triplet

⇒ unit of coupling constant is Hz. It max value is Generally 20Hz. Rarely J value exceed 20 Hz.

$CH_3 - CH_2 - OH$ (Neat solution)
↓
(pure Ethanol)

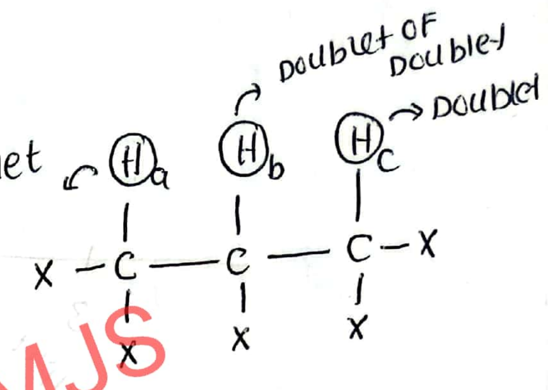
CH_3 ↓ Triplet
CH_2 ↓ penlet/Quintet (Quadret of Doublet)
OH ↓ Triplet

n+1
6+1 = ⑦
Septet

$CH_3 - CH_2 - CH_3$ (two signals)

1.2 ~0.9

CH_3 ↓ ~~Quadret~~ Triplet
CH_2 ↓ septet ~~Quadret of Quadret~~
CH_3 ↓ Triplet



⇒ J-value Also used to differentiate the cis & trans structure. J-value OF trans is higher than the cis-

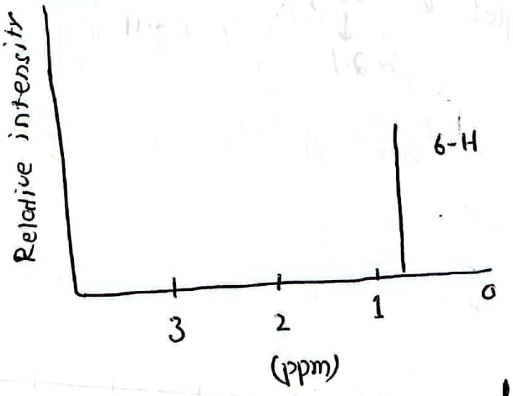
⇒ J-value does not depend upon the magnetic-Field. It only depends upon the Structure & Geometry OF molecule.

✓ INTERPRETATION OF H-NMR SPECTRA

Practice Examples;

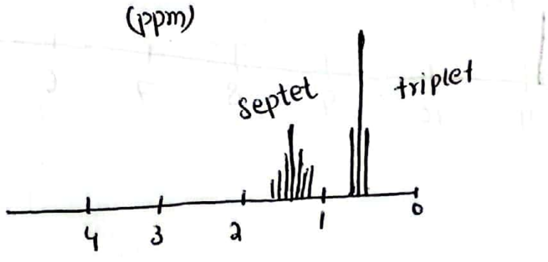
Ethane

$CH_3 - CH_3$
(Single peak)



propane

$CH_3 - CH_2 - CH_3$
0.9 1.2 0.9



butane

$CH_3 - CH_2 - CH_2 - CH_3$ ~ 0.9

1.2

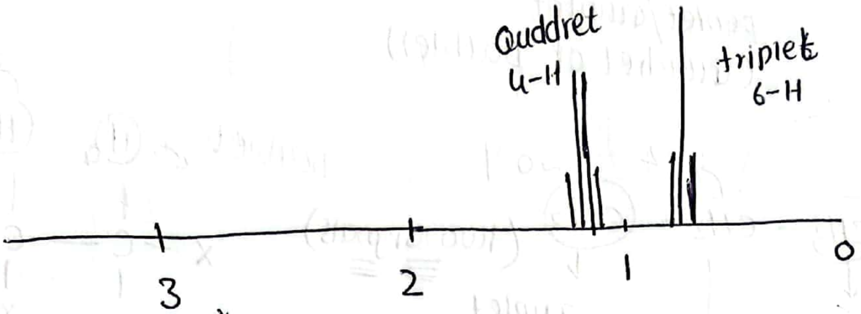
two peaks occured

6-proton

4proton

Quartet

Triplet

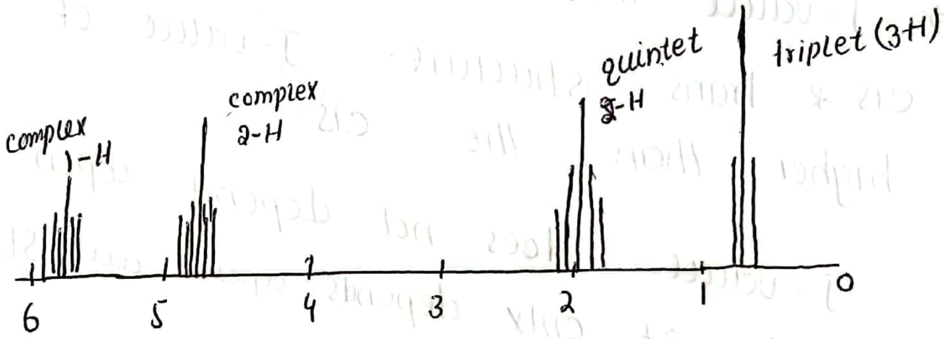


1-butene

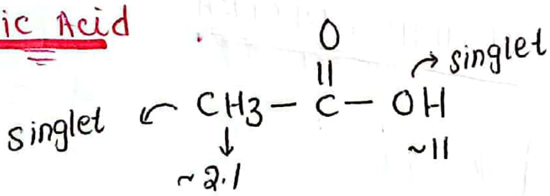
multiplet, multiplet, quinlet (5), triplet

$H_2C = CH - CH_2 - CH_3$

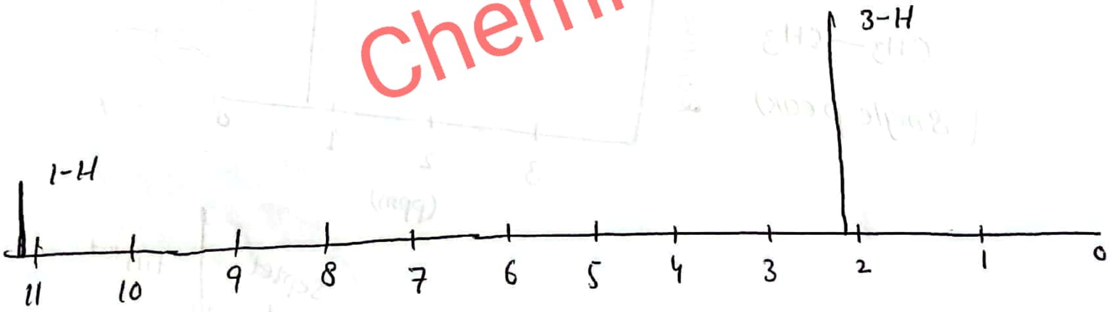
~4.95 ~5.8 ~2 ~0.9



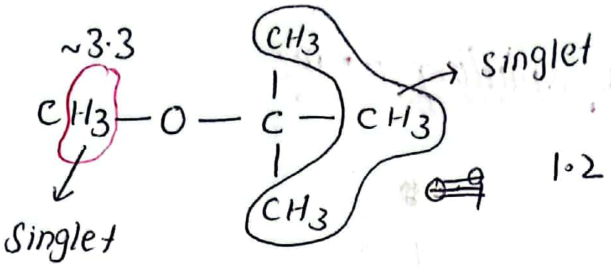
Acetic Acid

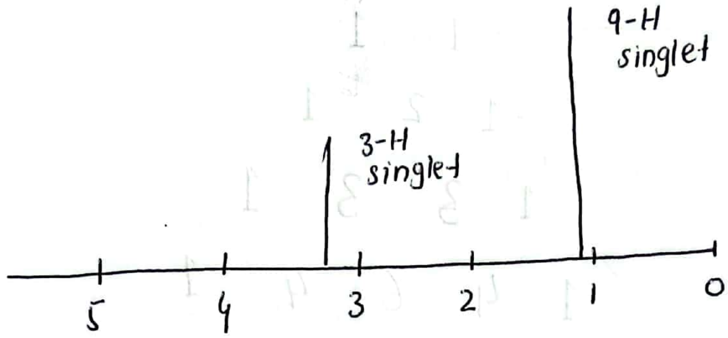


$CH_3 - \overset{\overset{O}{\|}}{C} - OH$

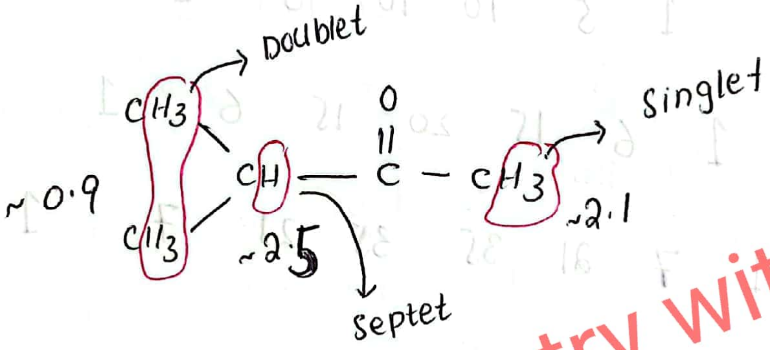


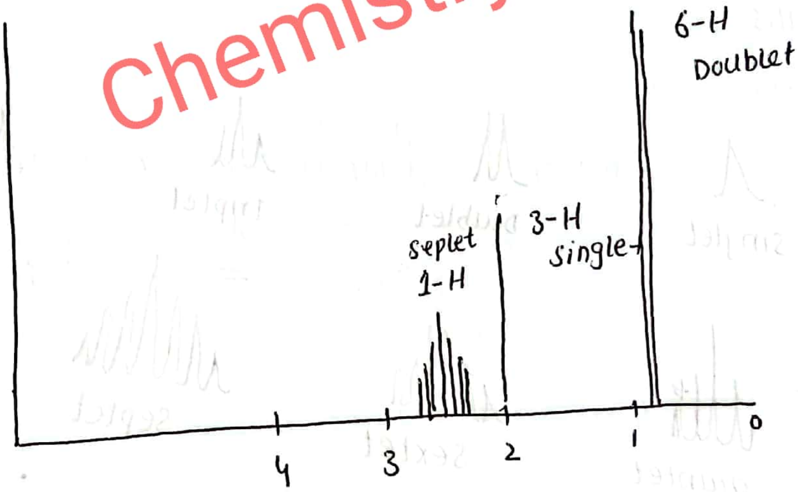
Ethers



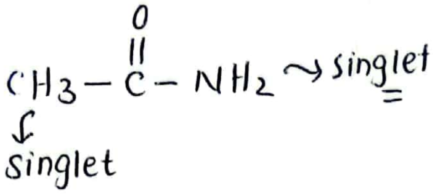


Ketones

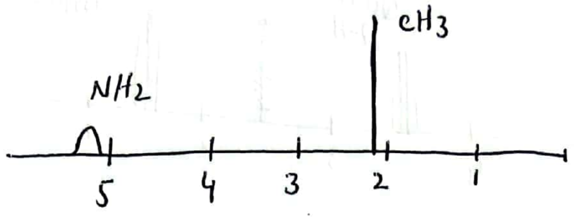




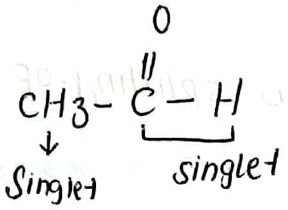
⇒ **Acetamide**



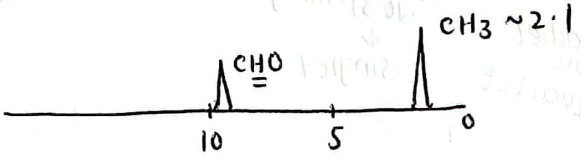
$CH_3-\overset{\overset{O}{\|}}{C}-NH_2$



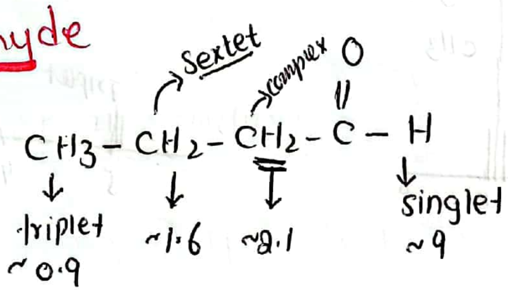
⇒ **Acetaldehyde**



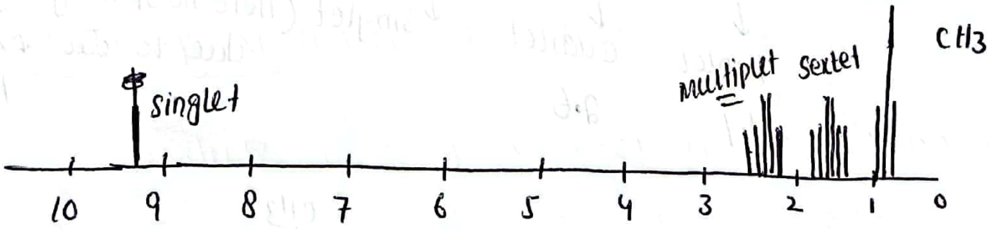
$CH_3-\overset{\overset{O}{\|}}{C}-H$



⇒ **Butyraldehyde**



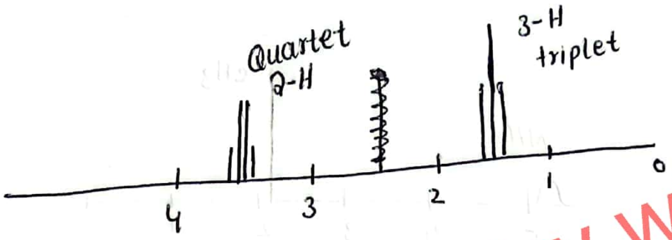
$CH_3-CH_2-CH_2-\overset{\overset{O}{\|}}{C}-H$



⇒ $CH_3 - CH_2 - Cl$

CH_3 → triplet → ~1.5

CH_2 → quartet → ~3.5



Alcohols → Neat
→ Dilute

ultra pure Sample of ethanol show splitting of O-H peak

Dilute → Here exchange of proton occur.

$CH_3 - CH_2 - OH$

CH_3 → triplet → ~1.1

CH_2 → Quadret OR quartet → ~3.6

OH → ~5 ppm No splitting → singlet

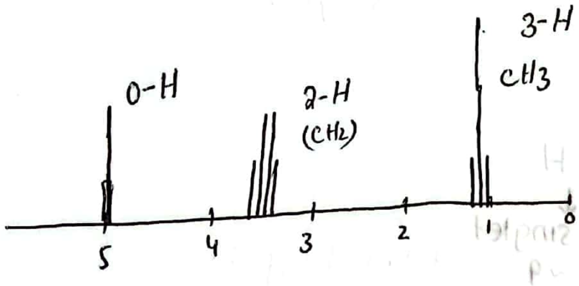
ultrapure

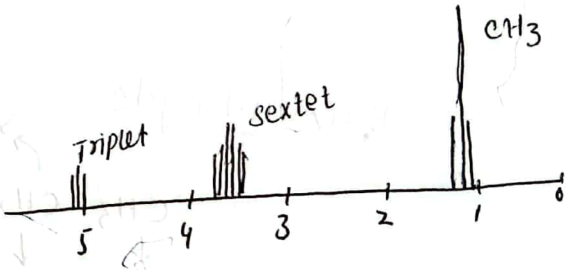
$CH_3 - CH_2 - OH$

CH_3 → triplet

CH_2 → ~~Quartet~~ quartet of Doublet OR sextet

OH → triplet





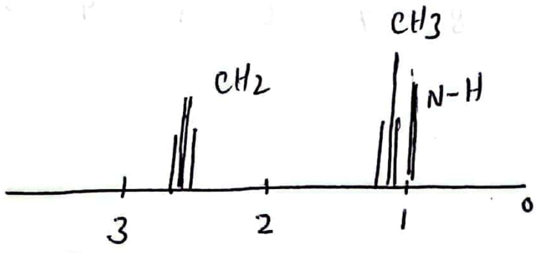
Ethye Amine

$CH_3 - CH_2 - NH_2$

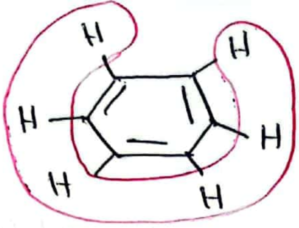
CH_3 → triplet → ~1.1

CH_2 → quartet → 2.6

NH_2 → ~1 → Singlet (Here no splitting by CH_2 group due to c̄eu exchange of proton

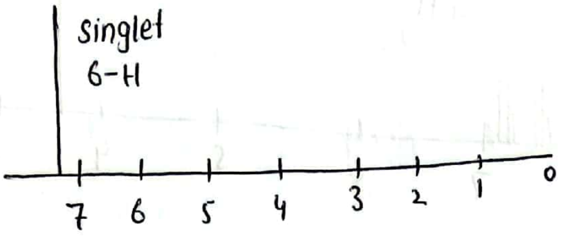


⇒ Benzene

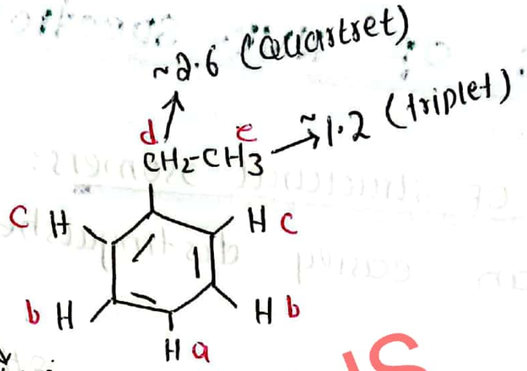


All six protons are chemically Equivalent ⟶ so give only one strong signal

6-H ~7.3



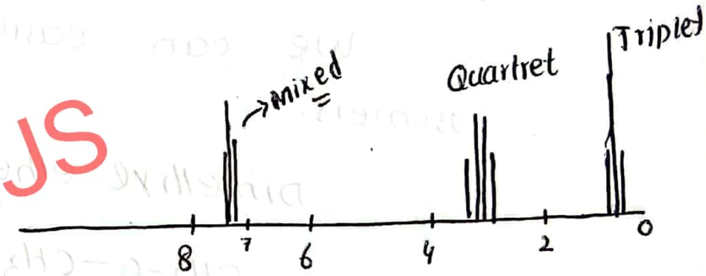
⇒ Ethyl benzene:



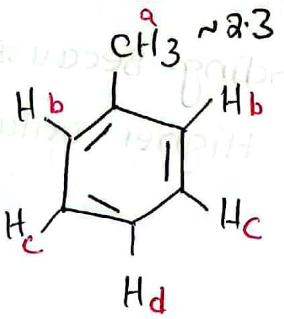
5-different proton environment

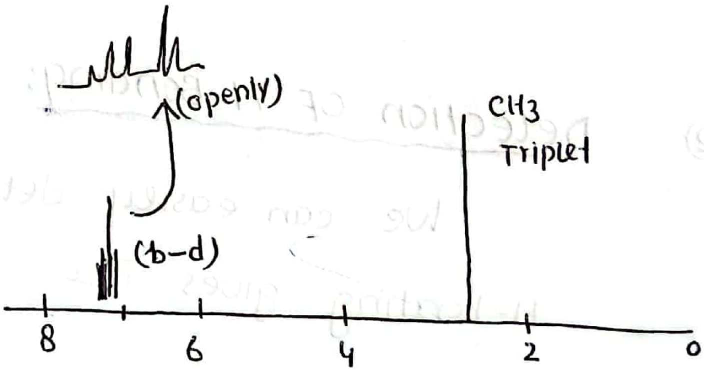
but a→c protons (5-H) ↘ 1:2:2 have almost v. closed ppm value 7→7.4

so merges in the same Region



⇒ Toluene





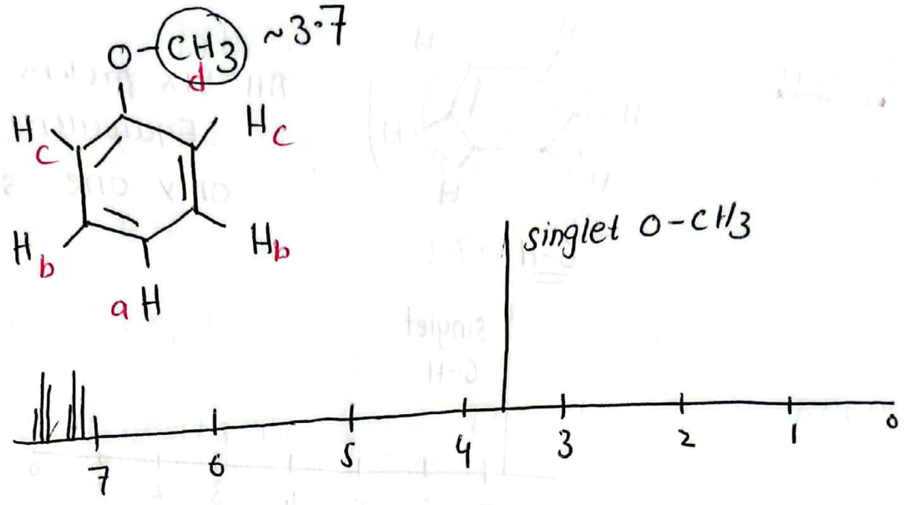
4- different Signals

* a → CH_3 ~ 2.7

* b → d ~ 7–7.3

Anisole

a→c ~7–7.3



:Applications of NMR- Spectroscopy:

① identification of structural isomers:

We can easily distinguished the structural isomers.

Dimethyle ether	Ethanol
CH_3-O-CH_3	CH_3-CH_2-OH
↓	↓
only one signal	3→signals

② Detection of H-Bonding:

We can easily detect the H-bonding. Because H-bonding gives the shift toward Higher value.

③ Study of Natural products:

Study of complex molecules, polymers, proteins, lipids, Nucleic Acids etc.

④ **Geometrical Isomers**

cis & trans structures can be distinguished B/c both have diff chemical shift & J-values. trans has higher J-value than cis.

⑤ **Detection of Aromaticity:**

Aromatic compound show Higher shift e.g at ~7.3 ppm.

⑥ **Quality Control:**

NMR is Also used to check the quality of substances. e.g Food products. Different compounds gives the Flavour & taste to Foods. These compounds can be identified by H-NMR.

e.g HMF in Food products e.g Honey & Beverages.

⑦ **Detection of impurity:**

impurity can be detected by the NMR. Additional signals at different chemical shift value indicate the impurity.

e.g Di-ethyl ether is a solvent - if Benzene as an impurity is added thus Additional peak of Aromatic-proton is observed at ~7 ppm.

⑧ Structure elucidation:

Different Nature OF protons give signals at. different chemical shift's value so we can identify the structure.

⑨ Oil & Fats industry

Study OF Fats & oils done by NMR-spectroscopy.

⑩ Forensic science:

To identify The poisnous & toxic compounds. This is done by NMR.

Good Luck

MJS