# DEPARTMENT OF CHEMISTRY

## Udai Pratap Autonomous College
## Varanasi -221002

### E-content

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**Topic** : Spectroscopy
**Sub-topic** : Nuclear Magnetic Resonance Spectroscopy

**Key words** : Basic principle of NMR, Chemical Shift, Shielding Deshielding mechanism, Coupling constant, Application of NMR

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# B. Sc. IV semester

## Unit VI

## Nuclear Magnetic Resonance Spectroscopy

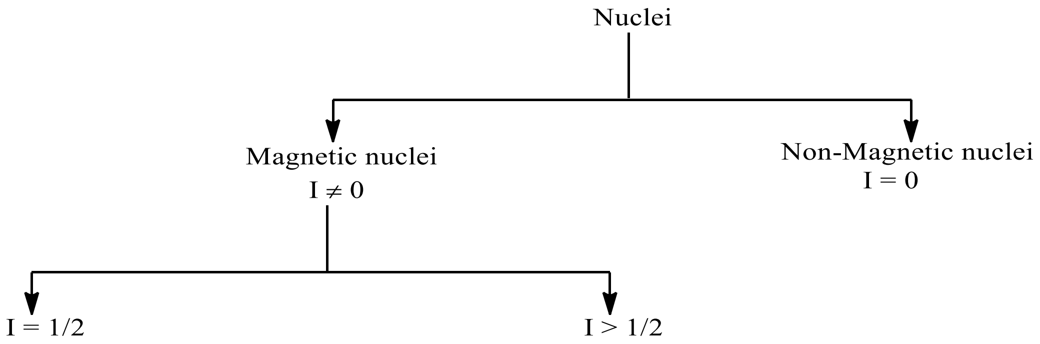
NMR spectroscopy was developed by physical chemists to study the properties of atomic nuclei. NMR signals were first observed in 1945 independently by Purcell at Harvard university and Bloch at standford university. Ethanol was the first compound to be studied.

It is example of absorption spectroscopy and observes in radiofrequency region. It gives information about the different kinds of protons (CH, $-CH_2$, $-CH_3$) in the molecule. The nuclear spin quantum number (I) of a nucleus is related to mass number and atomic number of the nucleus. I value of some nuclei are given below.

| Mass Number | Atomic Number | I-Value | Examples |
|---|---|---|---|
| odd | odd or even | $n + \frac{1}{2}$<br>Where $n = 0, 1, 2 ...$<br>$\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2} \dots\dots\dots$ | $^{1}_{1}H$, $^{13}_{6}C$, $^{15}_{7}N$<br>$^{19}_{9}F$<br>$\left(I = \frac{1}{2}\right)$ |
| Even | Even | 0 | $^{16}_{8}O$, $^{12}_{6}C$ |
| Even | odd | Where I= 1, 3, … | $^{14}_{7}N$, $^{2}_{1}D$ (I = 1)<br>$^{10}_{5}B$, (I = 3) |

i. If the mass number of nuclei is divisible by 4 then nuclear spin will be zero. I = 0 Examples: $C^{12}$, $O^{16}$, $Si^{28}$ etc.

ii. If the mass number of nuclei is not divisible by 4 then nuclear spin will not be zero. $I \neq 0$ Examples: $N^{14} = 1$, $C^{13} = 1/2$, $N^{15} = 1/2$, $B^{10} = 3$ etc.



On the basis of the value of (I), the nucleus can be classified into three categories.

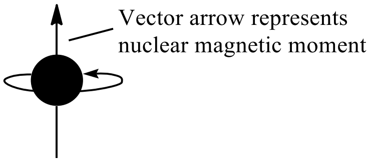
**Type-I:** Nucleus with I = 0, these nuclei do not interact with an applied magnetic field (Ho or Bo) and are not NMR active. It has even number of protons and even number of spin is property characteristic of certain isotopes rather than of certain elements.

**Type-II:** Nucleus with I = 1/2, these are spherical nuclei and have a non-zero magnetic moment and NMR active and have no nuclear electric quadrupole (Q). It gives sharp signal very easily because it has large relaxation time.

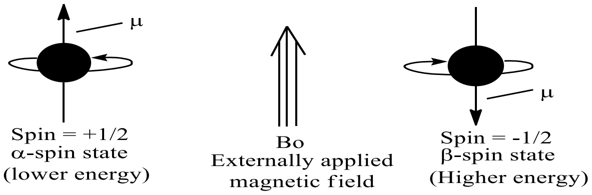
**Type-III:** Nucleus with I > 1/2, these are non-spherical nuclei and have both a magnetic moment and nuclear electric quadrupole (Q). It gives broad signal very difficultly because it has small relaxation time.

**Theory of 1H-NMR spectroscopy:**

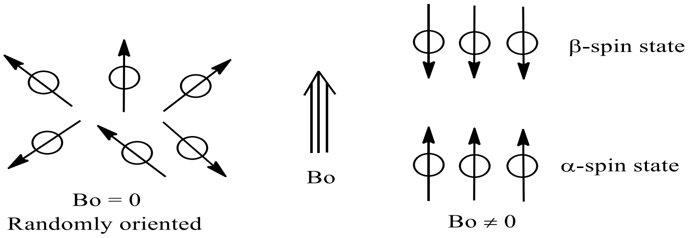
**(a) Spinning nuclei-Magnetic Moments:** Some nuclei were spinning about an axis much like Earth or a child's top. The spinning of charged particles generates a magnetic field of its own axis, whose magnitude and direction can be described by a vector called magnetic moment. Consequently, the spinning nuclei behave as tiny bar magnets with North Pole and a South Pole.



**(b) Nuclear Magnetic Moments:** Spin states are equal in absence of applied magnetic field. However spin states are not equal in presence of applied magnetic field because the nucleus is a charged particle and any moving charge generates a magnetic field of its own axis. Thus, the nucleus has a μ generated by its charge and spin. In an applied magnetic field, all protons have their magnetic moments either aligned with the field or oppose to it.



In the absence of a magnetic field the spins of magnetic nuclei are oriented randomly but under the influence of a strong magnetic field Bo, these nuclei adopt specific orientation.



**(c) Origin of the signal in 1H-NMR: The Mechanism of Absorption (Resonance):** Protons absorb energy because they begin to precess in an applied magnetic field. The phenomenon of precession is similar to that of a spinning top. Owing to the influence of the earth's gravitational field, the top begin to wobble or precess, about its axis. A spinning nucleus behaves in a similar fashion under the influence of an applied magnetic field.

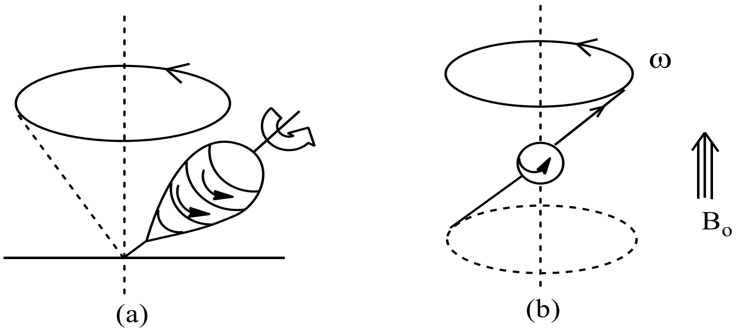


**Figure: (a) A top precessing in the earth's gravitional field, (b) the precession of a spinning nucleus resulting from the influence of an applied magnetic field.**

When the magnetic field is applied, the nucleus begins to precess about its own axis of spin with angular frequency(ω), which is called as Larmor frequency. The frequency at which a proton precesses is directly proportional to the strength of the applied magnetic field, the stronger the applied field, the higher the rate of precession.

Since the nucleus has a charge, the precession generates an oscillating electric field of the same frequency. If radiofrequency waves of this frequency are supplied to the precessing proton, the energy can be absorbed. That is, when the frequency of the oscillating electric field component of the incoming radiation just matches the frequency of the electric field generated by the precessing nucleus, the two fields can couple, and energy can be transferred from incoming radiation to the nucleus, thus causing a spin change. This condition is called resonance.

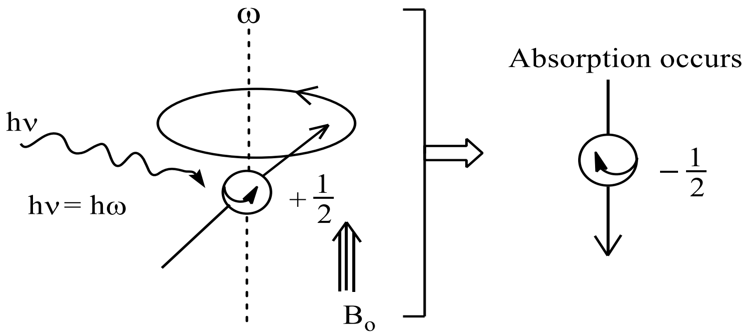
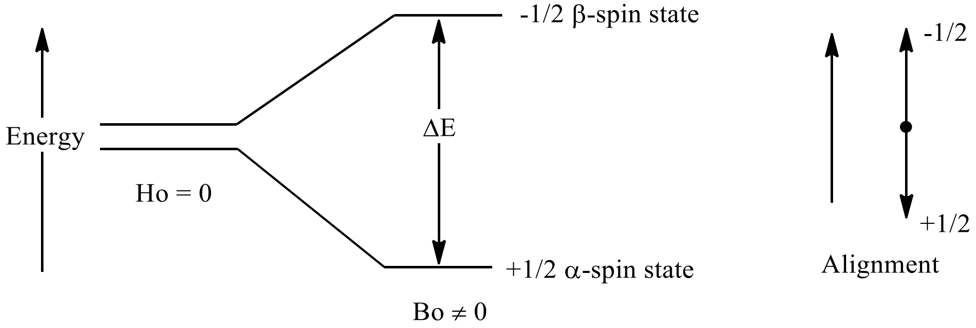


**Figure: The nuclear magnetic resonance process, absorption occurs when h = ω**

When a proton is placed in a strong magnetic field, the energies of the two nuclear spin states become unequal and proton starts to precess direction of applied magnetic field. Thus precessional motion is also known as gyroscopic. These energetically different states provide the necessary condition for 1H-NMR spectroscopy. Energy is needed to flip the proton from its lower energy state to higher energy state. In an NMR spectrometer this energy is provided by electromagnetic radiation in radio wave region.



$$\Delta E = E_{-1/2\text{ state}} - E_{+1/2\text{ state}}$$

The stronger the Bo, the greater the energy difference between the possible spin states.

According to quantum mechanics it is known that the energy of interaction of nuclear magnetic moment μ with an external magnetic field $B_o$ applied in z-direction, is given by

$$E = -\mu B_o \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (1)$$

$$\because \quad \mu = g_N \mu_N I \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

$$\therefore \quad E = -g_N \mu_N B_o I \quad \ldots\ldots\ldots\ldots (3)$$

$$E = -g_N \mu_N B_o m_l$$

For $^1H$ I = ½ so that $m_{l} = \pm ½$

$$E_{1/2} = -\frac{1}{2} g_N \mu_N H_z \text{ , } E_{-1/2} = \frac{1}{2} g_N \mu_N B_o$$

$$\Delta E = E_{-1/2} - E_{1/2} = g_N \mu_N B_o \ldots\ldots\ldots\ldots \quad (4)$$

Where, $g_N$ = nuclear g factor, $\mu_N$ = nuclear magnetic moment

$$\Delta E = h\nu$$

$$h\nu = g_N \mu_N B_o$$

$$\nu = \frac{g_N \mu_N H_z}{h} = \frac{\Delta E}{h} \ldots\ldots\ldots\ldots \quad (5)$$

The frequency of precessional motion will be directly proportional to applied magnetic field and precessional frequency is equal to $\gamma B_o$.

Angular precessional frequency or Larmor frequency is given by $\omega = \gamma B_o$

$$\gamma = \frac{\omega}{B_o}$$

$$\gamma = \frac{2\pi\nu}{B_o}$$

$$\nu = \left(\frac{\gamma}{2\pi}\right) B_o$$

Where $\gamma$ is magnetogyric ratio

The magnitude of the energy level separation also depends on the particular nucleus involved. Each nucleus (hydrogen, chlorine and so on) has a different ratio of magnetic moment to angular momentum since each has different charge and mass. This ratio, called the magnetogyric ratio, is constant for each nucleus.

**Proton Nuclear Magnetic resonance spectroscopy:** With help of 1H-NMR we can identified whether proton attached to aromatic, aliphatic, $sp^3$, $sp^2$, sp and electronegative atom etc.

**Shielding:** When magnetic field applied, the electron surrounding the nucleus starts to circulate perpendicular to the applied magnetic field (Bo) and so they generates a secondary magnetic field called induced magnetic field $\sigma$Bo. This field opposes the applied field in the region of nucleus. Thus, the nucleus experiences a weaker magnetic field $B_{eff}$ than Bo and it is said to shielded. This type shielding is termed as diamagnetic shielding and its effect is termed as shielding effect.

$$B_{eff} = Bo - \sigma Bo$$

Where $\sigma$ is screening constant

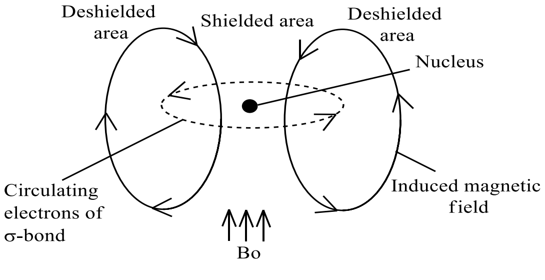


**Figure: Diamagnetic shielding of nucleus by circulating electrons**

**Deshielding:** If the induced field reinforce the applied magnetic field then the field experienced by proton is greater than the Bo. Such proton is said to be deshielded and this effect is termed as Deshielding effect. It is also called as paramagnetic Deshielding.

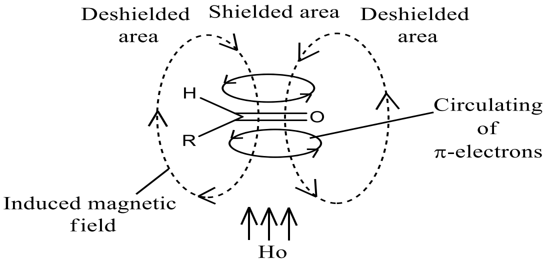


**Figure: Deshielding of aldehydic protons**

**Q: Explain why? Ethylenic proton is more deshielded than acetylenic proton but electronegativity of acetylenic proton is greater than ethylenic proton.**

When acetylene molecules are aligned parallel to the applied magnetic field, the acetylenic proton falls in the shielded region (Fig-1). However**,** when acetylene molecules are aligned perpendicular to the applied field. The acetylenic proton falls in the deshielded region (Fig-2). The magnitude of this deshielding is far less than that of the shielding because electrons are much more free to circulate in the direction shown in Fig-1 than the direction shown in Fig-2. This is understandable in the light of the fact that $\pi$ electrons of the triple bond are symmetrical about the bond axis, and the circulation as shown in Fig-2 will disturb the symmetry. Although only a small fraction of tumbling molecules are aligned parallel to the applied magnetic field, the overall average chemical shift is affected by them, i.e. the acetylenic protons are much more shielded than expected from the electronegativity of the acetylenic carbons and they absorb at higher field.

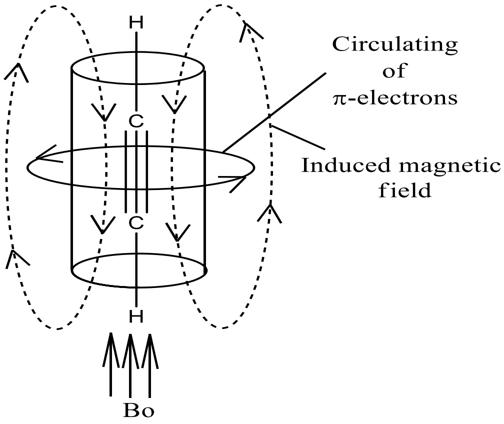


**Fig-1: Shielding of acetylenic protons**

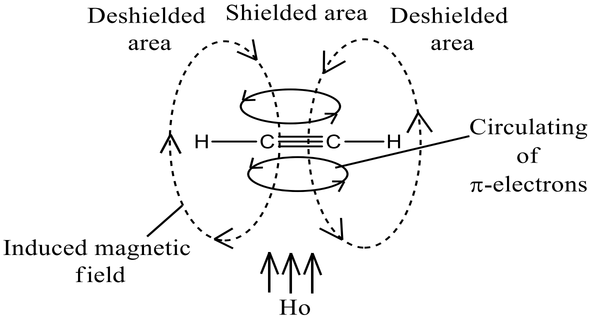


**Fig-2: Deshielding of acetylenic protons**

When an alkene molecule is oriented perpendicular to the applied magnetic field Ho, the induced magnetic field generated by circulating $\pi$-electrons has the same direction at the olefinic protons as the applied magnetic field (Fig. 5.13). Thus, the induced magnetic field reinforces the applied field resulting in deshielding of the olefinic protons. Consequently, they absorb at lower field than expected from the electronegativity of olefinic carbons.

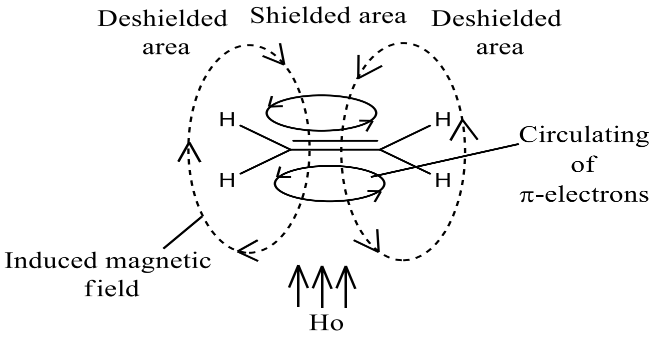


**Fig-3: Deshielding of ethylene protons**

**Chemical shift:** The shifting of signals either up field or down field with respect to TMS called as chemical shift.

The separation of signal with respect to TMS is called as chemical shift.

**Measurement of chemical shift:** The chemical shift is expressed in ppm which is dimensionless quantity.

$$\text{Suppose } B_{local} = Bo(1 - \sigma)$$

Where σ is dimensionless quantity

For two nuclei A & B the local fields are

$$B_A = Bo(1 - \sigma_A)$$

$$B_B = Bo(1 - \sigma_B)$$

Where $\sigma_A$ and $\sigma_B$ is the respective screening constant

Thus

$$B_B - B_A = Bo(1 - \sigma_B) - B_A - Bo(1 - \sigma_A)$$

$$B_B - B_A = Bo(\sigma_B - \sigma_A)$$

$$B_B - B_A = Bo\,\delta_{AB}$$

$$\delta_{AB} = \frac{B_B - B_A}{Bo}$$

Where $\delta_{AB}$ is called chemical shift

$$\delta = \frac{B_{sample} - B_{reference}}{Bo} \times 10^6$$

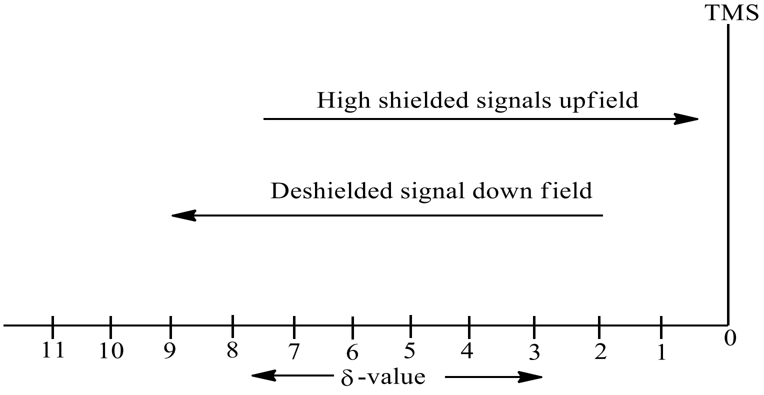
or

$$\delta = \frac{\nu_{sample} - \nu_{reference}}{\nu_o} \times 10^6$$

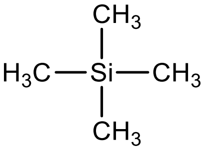
$$\tau\text{-value} = 10 - \delta\text{-value}$$

or

$$\delta\text{-value} = 10 - \tau\text{-value}$$



**Reference compound:**



Tetramethylsilane
(TMS)

$Me_4Si$ is used as reference compound due to following reasons.

1. It is easily miscible in all organic compounds
2. It is chemically inert and has symmetrical structure.
3. Its twelve protons are magnetically equivalent.
4. It is volatile; therefore it can be easily removed from the organic compounds.
5. Its boiling point is very high.

| **Organic compounds** | **Chemical shift ($\delta_{ppm}$)** |
|---|---|
| Alkane | 0.7-2.0 |
| Alkyne | 3.0-4.0 |
| Alkene | 5.0-6.0 |
| Benzene | 6.0-8.0 |
| Aldehyde | 9.0-10.0 |
| Acid | 11.0-12.0 |

Q: If the observed chemical shift of a proton is 200 Hz from TMS and instruments frequency 60 MHz. What is chemical shift in terms of δ and express in τ-value?

$$\delta = \frac{\text{Chemical shift in Hz}}{\nu_o} \times 10^6$$

$$\delta = \frac{200}{60 \times 10^6} \times 10^6$$

$$\delta = 3.3 \text{ ppm}$$

$$\tau\text{-value} = 10 - \delta\text{-value} = 10 - 3.3 = 6.7\text{ppm}$$

Q: Protons of a compound exhibit a NMR signal at δ 2.5. What will be the value of chemical shift of these protons in Hz? If the spectrum is recorded in 60 MHz spectrometer

$$\delta = \frac{\text{Chemical shift in Hz}}{\nu_o} \times 10^6$$

$$2.5 = \frac{\text{Chemical shift in Hz}}{60 \times 10^6} \times 10^6$$

$$\text{Chemical shift in Hz} = 60 \times 2.5 = 150\text{Hz}$$

Q: At 100MHz the shift of proton in $CH_3Br$ 270 Hz from TMS calculate chemical shift in terms of δ and express in τ-value.

$$\delta = \frac{\text{Chemical shift in Hz}}{\nu_o} \times 10^6$$

$$\delta = \frac{270}{100 \times 10^6} \times 10^6$$

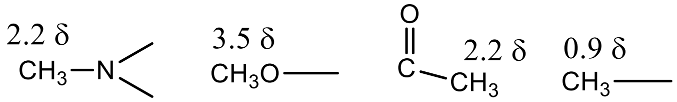
$$\delta = 2.7 \text{ ppm}$$

$$\tau\text{-value} = 10 - \delta\text{-value} = 10 - 2.7 = 7.3 \text{ ppm}$$

**Factors affecting the value of Chemical shift:**

1. **Electronegativity effects:** The degree of shielding depends on the electron density around the proton. The higher the electron density around a proton, the higher the shielding and higher is the field (lower the $\delta$-value) at which the proton absorbs. Electronegativity of substituents increases which increase the $\delta$-value due to –I effect. Example:

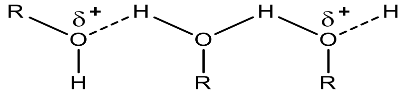
| $CH_3X$ | $CH_3F$ | $CH_3OH$ | $CH_3Cl$ | $CH_3Br$ | $CH_3I$ | $CH_4$ | $(CH_3)_4Si$ |
|---|---|---|---|---|---|---|---|
| Elements X | F | O | Cl | Br | I | H | Si |
| Electronegativity of X | 4.0 | 3.5 | 3.1 | 2.8 | 2.5 | 2.1 | 1.8 |
| $\delta$-value (ppm) | 4.26 | 3.4 | 3.05 | 2.68 | 2.16 | 0.23 | 0 |



**2.** **Hydrogen bonding:** Hydrogen bonded protons are absorbs lower field i.e. deshielded than the non-hydrogen bonded proton. This is because of electron density decreases around the proton during the hydrogen bonding.

**3.**

| **Organic compounds** | **Chemical shift ($\delta_{ppm}$)** |
|---|---|
| RCOOH | 10.5-12.0 |
| ArOH | 4.0-7.0 |
| ROH | 0.5-5.0 |
| $RCONH_2$ | 5.0-8.0 |
| $CH_2=CH-OH$ (Enols) | . 15 |



**Hydrogen bonded (Concentrated sol$^{n}$)**

4. **Anisotropic effects or Diamagnetic anisotropy:** The chemical shifts of some protons are not easily explained by simple considerations of the electronegativity of the attached groups. For instance, consider the protons of benzene and other aromatic systems. When benzene is placed in a magnetic field, the $\pi$-electrons in the aromatic ring system are induced to circulate around the ring. This circulation is called ring current. The benzene hydrogens are said to be deshielded by the diamagnetic anisotropy of the ring. Thus, a proton attached to a benzene ring is influenced by three magnetic fields; the strong magnetic field applied by the electromagnets of the NMR spectrophotometer and two weaker fields; one due to the usual shielding by valence electrons around the proton, and the other due to the anisotropy generated by the ring-system $\pi$-electrons. It is the anisotropic effect that gives the benzene protons a chemical shift that is greater than expected. These protons lie in a deshielding region of the anisotropic field. If proton were placed in the center of the ring rather than periphery, it would be found to be shielded since the field lines there would have the opposite direction from those at the periphery.

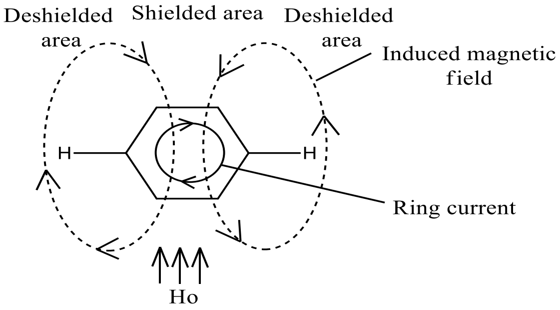
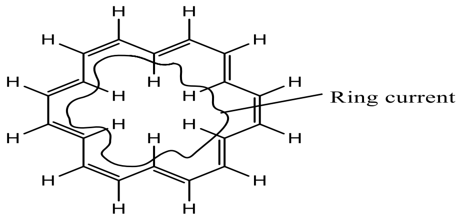


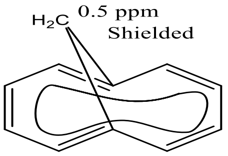
**Fig: Anisotropic effect of benzene ring**

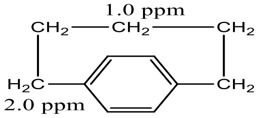


[18]-annulene

Inner hydrogen = 1.8 δppm

Outer hydrogen = 8.9 δppm



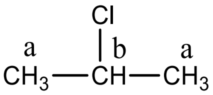


**Number of PMR signal:** Chemically equivalent proton gives same NMR signal and chemically non-equivalent proton gives different NMR signal.

Substitution method can be used to identify chemical equivalence and non-equivalence of proton.

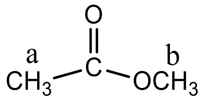
$\overset{a}{CH_3}\overset{b}{CH_2}\overset{c}{CH_2}Cl$

3-signal



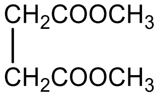
$\overset{a}{CH_3}-\overset{Cl}{\overset{|}{\overset{b}{CH}}}-\overset{a}{CH_3}$

2-signal

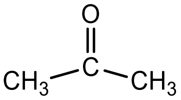


$\overset{a}{CH_3}-\overset{O}{\overset{\|}{C}}-\overset{b}{OCH_3}$

2-signal

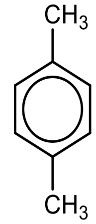


2-signal

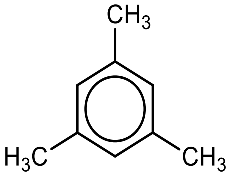


$CH_3-\overset{O}{\overset{\|}{C}}-CH_3$

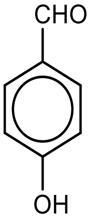
1-signal



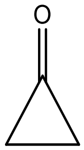
2-signal



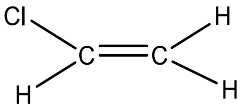
2-signal



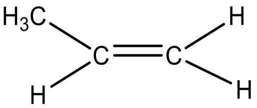
4-signal



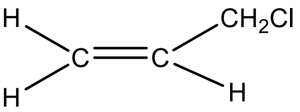
1-signal



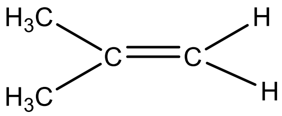
3-signal



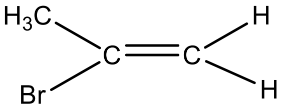
4-signal



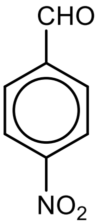
4-signal



2-signal



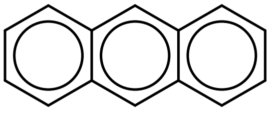
3-signal



3-signal

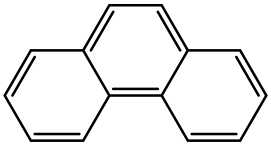
**Integration or Area ratio of signal:**

Area ratio ∝ No of proton ratio



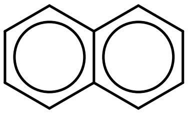
3-signal

Intensity ratio = 2:2:1



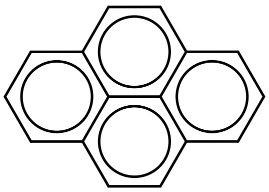
3-signal

Intensity ratio = 2:2:1



2-signal

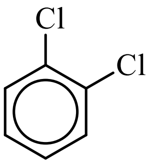
Intensity ratio = 1:1



3-signal

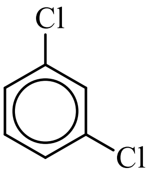
Intensity ratio = 2:2:1

2H:4H:4H



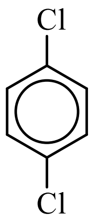
2-signal

Intensity ratio = 1:1



3-signal

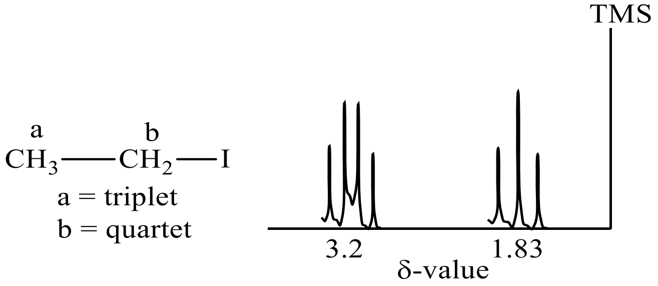
Intensity ratio =1:2:1

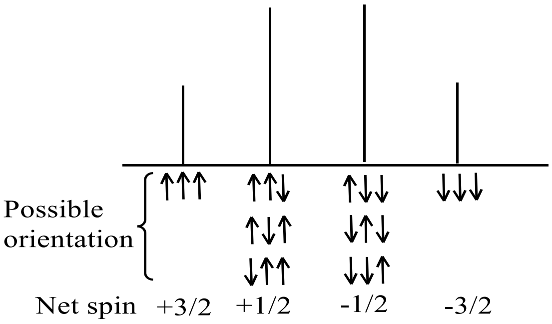


2-signal

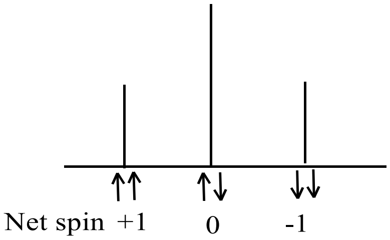
Intensity ratio = 1:1

**Spin-spin splitting or spin-spin coupling:** Spin-spin splitting provides nature and number of neighbour protons in a sample. The cleavage of NMR signal due to mutual influence of spin orientation of neighbourhood protons called spin-spin splitting. Spin-spin coupling very common in 3-bonds separation neighbours (vicinal bond). Generally spin-spin splitting follows n+1 rule.

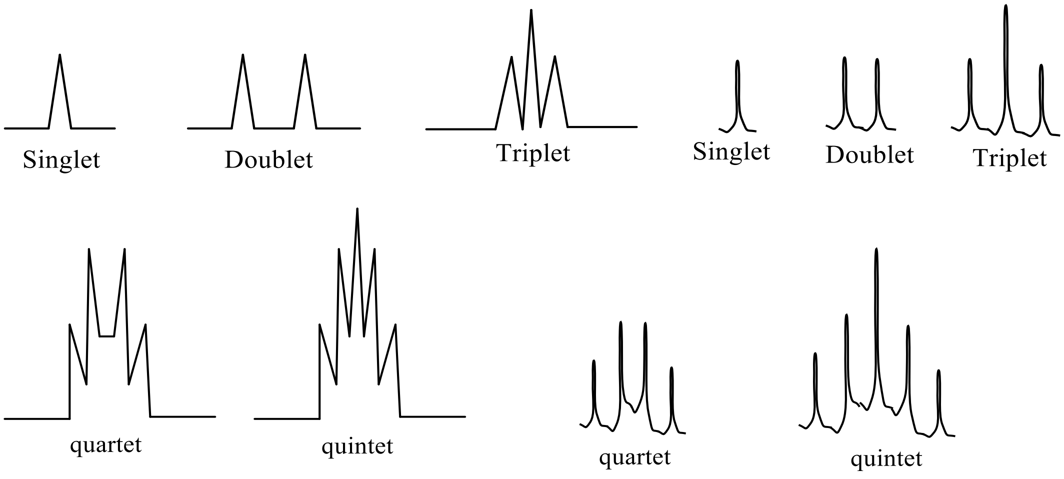


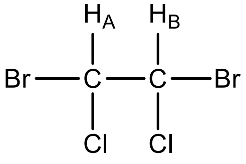


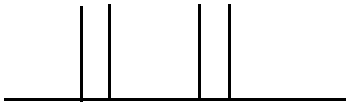
**The splitting pattern of methylene protons due to the presence of an adjacent methyl group**



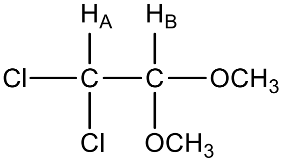
**The splitting pattern of methyl protons due to the presence of an adjacent methylene group**



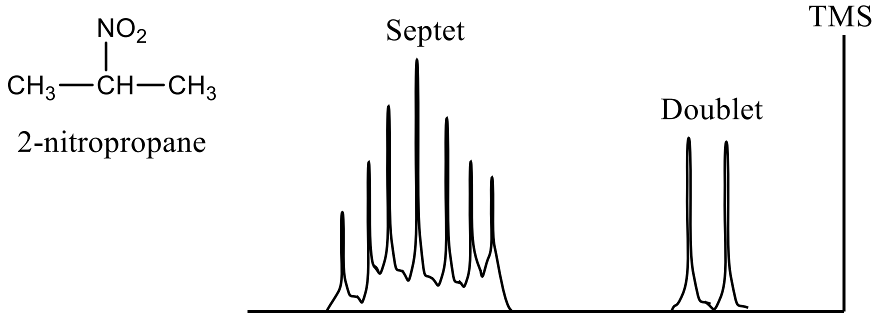




Two doublet



Two doublet and one siglet



**Relative intensity ratio of lines of $^1$H-NMR signal:**

Binomial theorem: $(1+x)^n$

$(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \frac{n(n-1)(n-2)}{3!}x^3 \ldots\ldots\ldots\ldots \frac{n(n-1)(n-2)\ldots\ldots\ldots(n-r+1)}{r!}x^n$

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

$(1+x)^2 = 1 + 2x + \frac{2(2-1)}{2!}x^2 = 1 + 2x + x^2$

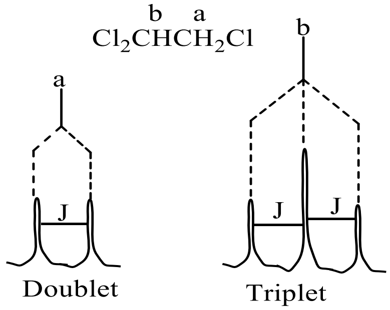
$(1+x)^3 = 1 + 3x + \frac{3(3-1)}{2!}x^2 + \frac{3(3-1)(3-2)}{3!}x^3 = 1 + 3x + 3x^2 + x^3$ and so on

**Pascal Triangles:**

Singlet 1
Doublet 1 : 1
Triplet 1 : 2 : 1
Quartet 1 : 3 : 3 : 1
Quintet 1 : 4 : 6 : 4 : 1
Sextet 1 : 5 : 10 : 10 : 5 : 1
Septet 1 : 6 : 15 : 20 : 15 : 6 : 1

**Coupling constant:** The separation between two adjacent peaks or lines in $^1$H-NMR spectrum (signal) called coupling constant. It is denoted by J and measured in cps or Hz. The value of *J* remains constant in different applied magnetic fields or radio frequencies used, whereas the values of chemical shifts (in Hz) are directly proportional to the applied magnetic fields or radio frequencies. The values of coupling constants J between protons generally lie between 0 and 20 Hz.

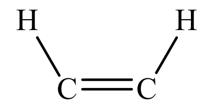
**Example:**



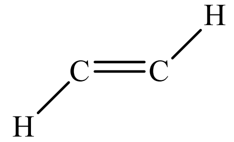
1 Cps = 1Hz

J-value = Distance between two adjacent peak × frequency of instruments

J-value = d × $\nu_{\text{instruments}}$



J-value = 6-12Hz

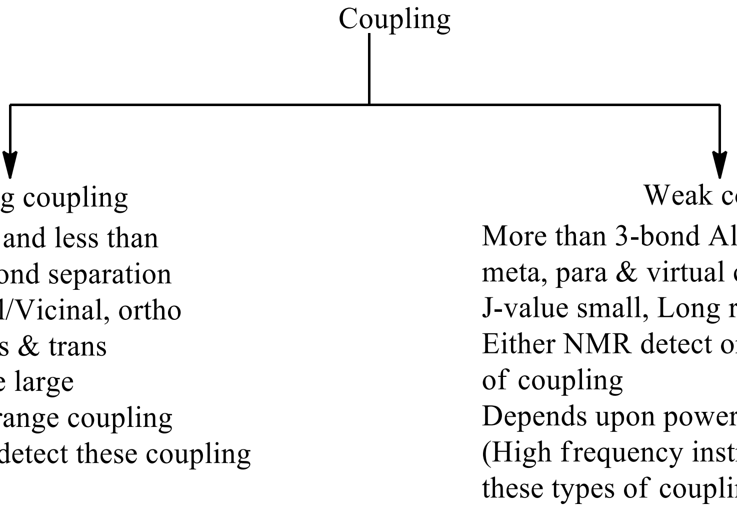


J-value = 12-18Hz

**Types of coupling:**

**Homonuclear coupling:** Coupling between two nuclei of the same type is called homonuclear coupling. Example: $^{1}H$-$^{1}H$, $^{13}C$-$^{13}C$, $^{19}F$-$^{19}F$, $^{31}P$-$^{31}P$ etc.

**Heteronuclear coupling:** Coupling between two different types of nuclei is called heteronuclear coupling. Example: $^{1}H-^{13}C$ = 110−270Hz, $^{13}C-^{19}F$ = -165−370Hz, $^{13}C-^{31}P$ = 48−56Hz, $^{13}C-D$ = 20−30Hz, $^{31}P-^{1}H$ = 190-700Hz etc.



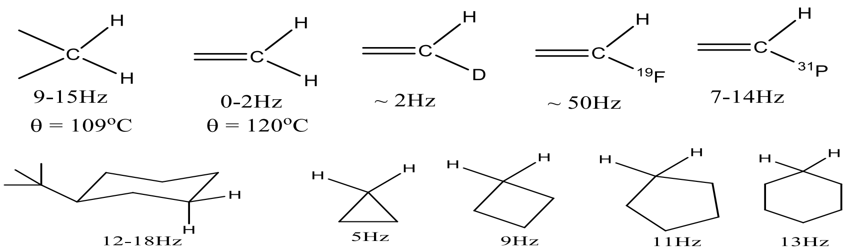
Coupling

Strong coupling
Three and less than three bond separation
Geminal/Vicinal, ortho cis & trans
J-value large
Short range coupling
NMR detect these coupling

Weak coupling
More than 3-bond Allylic, Homoallylic, meta, para & virtual coupling
J-value small, Long range coupling
Either NMR detect or not these types of coupling
Depends upon power of instruments (High frequency instruments detect these types of coupling)

**Strong Coupling:**

**(a) Geminal Coupling:** Protons attached to the same carbon atom are called geminal protons. These are separated by two bonds, and when they are nonequivalent, they show spin-spin splitting. Geminal coupling constant $^{2}J_{H-H}$ is usually negative and increases algebraically on increasing the angle θ between the coupling protons.

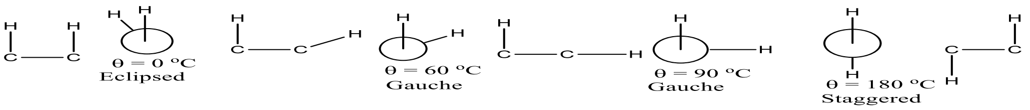


Note: Ring strain increases, s-character increases then coupling decrease.

Electronegativity group attached to the carbon, hybridization of carbon and angle strain in the molecule effect $^{2}J$ or $J_{gem}$ coupling.

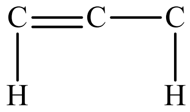
**(b) Vicinal Coupling:** Protons attached to adjacent atoms are called vicinal protons. These are separated by three bonds. Vicinal coupling constants $J_{Vic}$ depend on the dihedral angle.

$$J_{Vic} \propto \frac{1}{\text{E.N.and Bond length}} \propto \text{Bond angle}$$



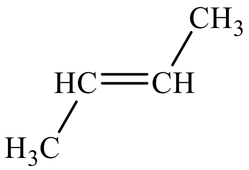
**Long range coupling:** The magnitude of J decreases sharply with distance. Such proton-proton couplings beyond three bonds are called long-range couplings. Some appreciable long range couplings are as follows:

i. **Allylic coupling:** The four bond coupling is called allylic coupling. Allylic coupling interaction assumes the maximum value ($^4J$ = 3-4Hz).

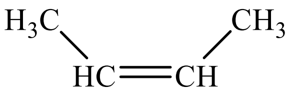


$^4J$ = 0-3Hz

ii. **Homo allylic coupling:** The five bond coupling is called homoallylic coupling ($^5J$) but is naturally weaker than allylic coupling ($^4J$) because it occurs a greater distance.

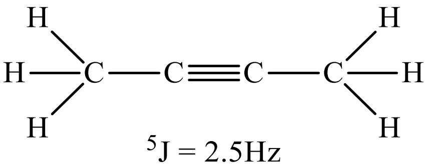


$^5J$ = 1.6Hz



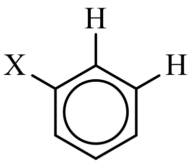
$^5J$ = 1.2Hz

iii. **Homo propargylic coupling:** Homopropargylic coupling is almost always observed in the $^1$H-NMR spectra of internal alkynes. This is also five bond coupling.

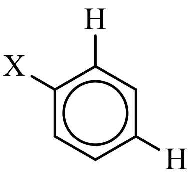


$^5J$ = 2.5Hz

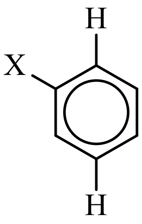
iv. **Aromatic protons:** Meta coupling in benzene ring is 1-3Hz, and para 0-1 Hz. Ortho coupling in benzene ring is 6-10Hz. It should be noted that the ortho coupling is not a long-range coupling because here the coupled protons are separated by only three bonds. However, Meta and para coupling is example of large range coupling.



$^3J$ = 7-10Hz



$^4J$ = 2-3Hz



$^5J$ = 0-1Hz

**Double bond equivalent (DBE):**

$$\mathrm{DBE} = \frac{2 \times \text{Total No of carbon} + 2 - \text{Total No of hydrogen} \pm z}{2}$$

If oxygen then z = 0

If halogen then z = -1

If nitrogen then z = 1

Note: If DBE is four or greater than four then the possibility of benzene ring in given molecular formula.

Q: Calculate the DBE for following molecular formula.

$C_9H_{12}$, $C_8H_{14}O_4$, $C_6H_{10}O_4$, $C_3H_7NO$, $C_6H_{12}O_3$, $C_6H_{12}O$, $C_5H_7NO_2$, $C_4H_9NO$

Q: Propose the structure for the compounds that fit the following $^1$H NMR data:

(i) $C_5H_{10}O$, δ 0.95, 6H, doublet, δ 2.10, 3H, singlet, δ 2.43, 1H, multiplet

(ii) $C_4H_7BrO$, δ 2.11, 3H, singlet, δ 3.52, 2H, triplet, J = 6 Hz, δ 4.40, 2H, triplet, J = 6 Hz

Answer:

(i) $(CH_3)_2CHCOCH_3$ (ii) $BrCH_2CH_2COCH_3$

Q: Give a structure consistent with the NMR data of the following two compounds

(i) $C_{10}H_{14}$, singlet δ 0.88 (9H), singlet δ 7.28 (5H)

(ii) $C_9H_{11}Br$ quartet δ 2.15 (2H), triplet δ 3.38 (2H), singlet δ 7.25 (5H)

Q: An organic compound, $C_9H_{10}O_2$ showed three singlet's in the NMR at δ 7.31 (2H), 5.08 (2H) and 2.06 (3H). Identify the organic compound.

Q: An organic compound having the molecular formula $C_9H_{11}Br$ exhibited in its NMR spectra a singlet (δ 7.25), two doublets (δ 2.75 and δ 1.45, 2H & 3H respectively) and a multiplet (δ 3.4, 1H). Assign a structure to this compound.