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ORGANIC CHEMISTRY

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# Nuclear Magnetic Resonance ( NMR) Spectroscopy.

## INTRODUCTION :

**NMR Spectroscopy-** The magnetic nuclei exposed to magnetic field absorb light radiation under resonance. This phenomenon is called as *nuclear magnetic resonance, abbreviated as NMR.*

*It was soon developed into a powerful tool of chemical analysis called NMR Spectroscopy.*

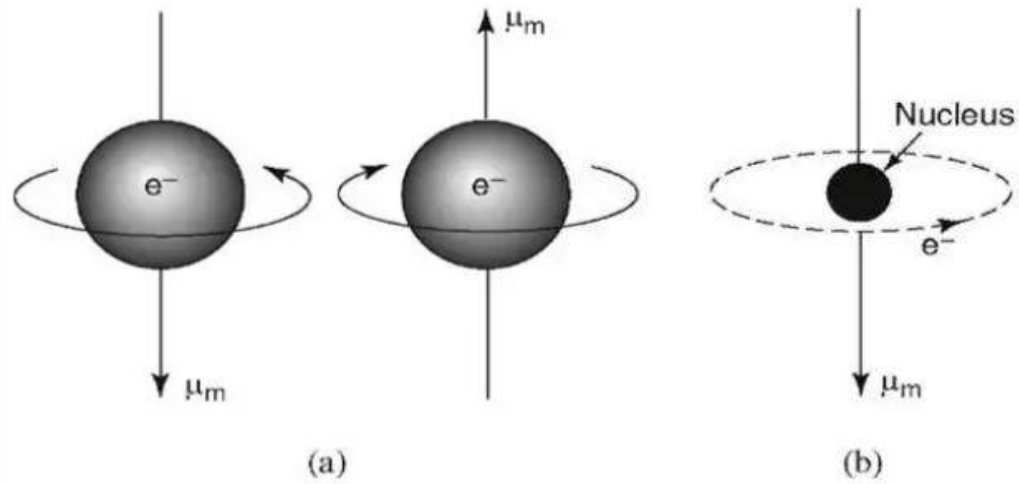
The hydrogen nucleus consists of single proton only so, it is magnetic so like any other magnetic nuclei, a proton absorbs radio frequency light radiation at unique combination of field strength and frequency of radiation.

This phenomenon of light absorption by proton is called proton magnetic resonance. Abbreviated as PMR. The analytical technique based on PMR called as PMR-spectroscopy.

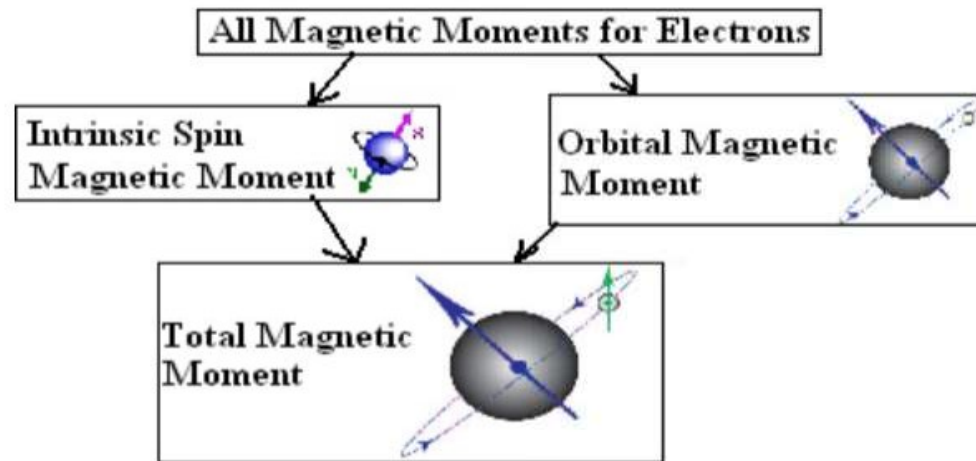
# Principle of PMR-SPECTROSCOPY.

- ▶ **PMR- spectroscopy is based on the net absorption of energy in the radio frequency range by hydrogen nucleus ( proton) exposed to a strong magnetic field . Absorption of energy by the nucleus occurs at unique combination of field strength and frequency of radiation irradiated(resonance). This leads to change in spin state (flipping). The frequency of radiation absorbed or the magnetic field strength at the time of absorption proton.**

- ▶ 1. Spinning nucleic and magnetic moment :
- ▶ The hydrogen nuclei ( proton) due to there spin axis and act as tiny bar magnets.In the absence of applied field the magnetic moment vector is oriented randomly in all possible directions.
- ▶ When the proton are placed in uniform applied field, the magnetic moment vector aligns in one of two *orientations* with respect to direction of applied magnetic field.Beacuse,
- ▶ Number of orientations = $2l+1$
- ▶ .  $=2 \times 1/2 + 1 = 2 \dots \dots \dots$  (for H , $l=1/2$ ).



### *Orbital Magnetic moment*



# Flipping of spin.

## Flipping :

Under a special condition called *resonance*, the spin state of proton changes by exchanging energy and is called flipping.

Transition from low energy state to high energy state occurs with emissions of energy.

However, the energy difference between the two spin state is extremely small and can be met by radio-frequency (60-1000 MHz) radiations.

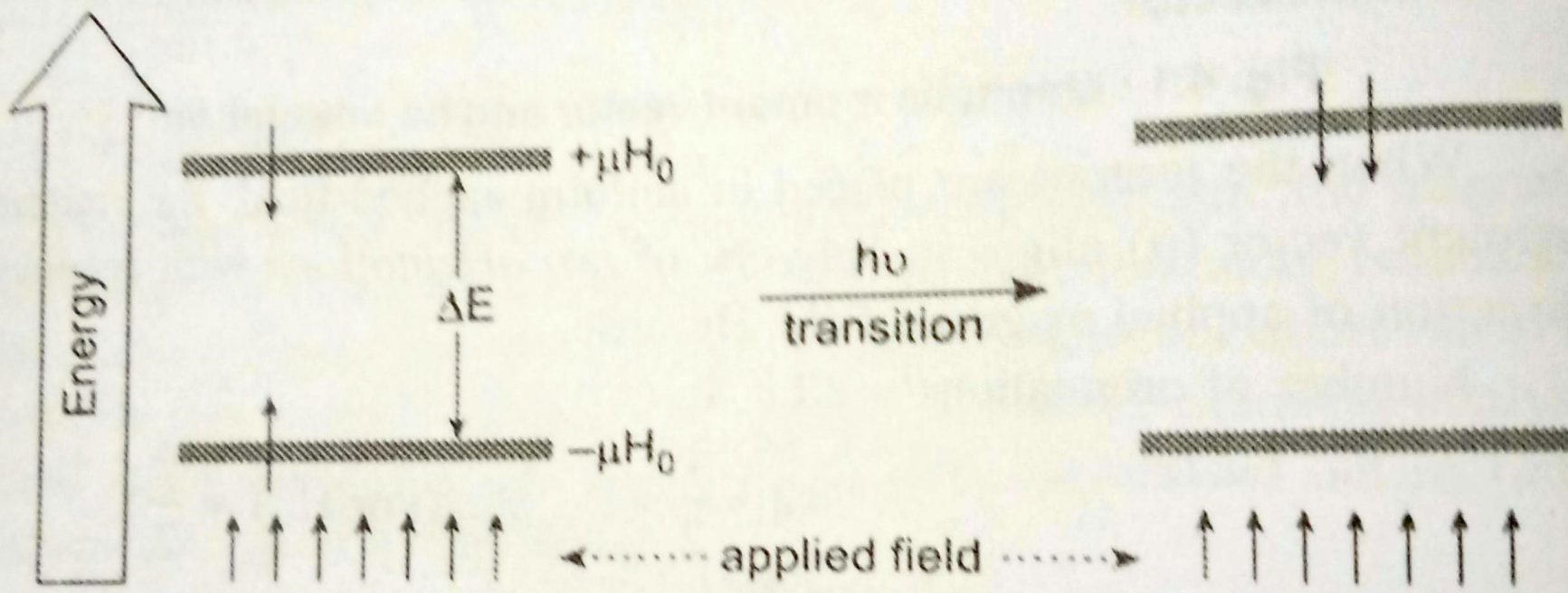


Fig. 4.3 : Flipping of spin state of proton under resonance

**Precessional motion :** A proton is a spinning magnet so, while it spin in an applied magnetic field , it's rotational axis draws out a circle perpendicular to applied.

The rotational motion of magnetic nucleus exposed to an applied field is called as *precessional or gyroscopic motion*. The precessional frequency of an isolated proton is

The *precessional frequency* is the number of revolutions per second made by magnetic moment vector of the nucleus applied external field



- ▶ The precessional frequency of proton in an organic compound cannot be calculated, as they are not isolated. That is, in an organic compound, the protons are covalently bonded to other atoms like, C, N, O, S. The electrons of a covalent bond normally have paired spins and have no net magnetic field. But under the influence of an applied magnetic field, additional modes of circulation are induced for these paired electrons. This circulation generates a small but its own magnetic field called as *secondary or induced magnetic field*.

# Magnetic and non- magnetic nuclei.

- ▶ **Magnetic nuclei :**

- ▶ They are the nuclei of atoms whose spin quantum number is greater than zero ( $I > 0$ ) . These nuclei act like a bar magnets and align in an applied magnetic field . Depending on their mass number (A) atomic number (z), integral or half integral value is assigned to 'I'

- ▶ **Non-magnetic nuclei :**

- ▶ They are the nuclei of atoms whose spin quantum number (I) is zero. Nuclei having even atomic number and even mass number have 'I' value equal to zero.so they are non –magnetic.

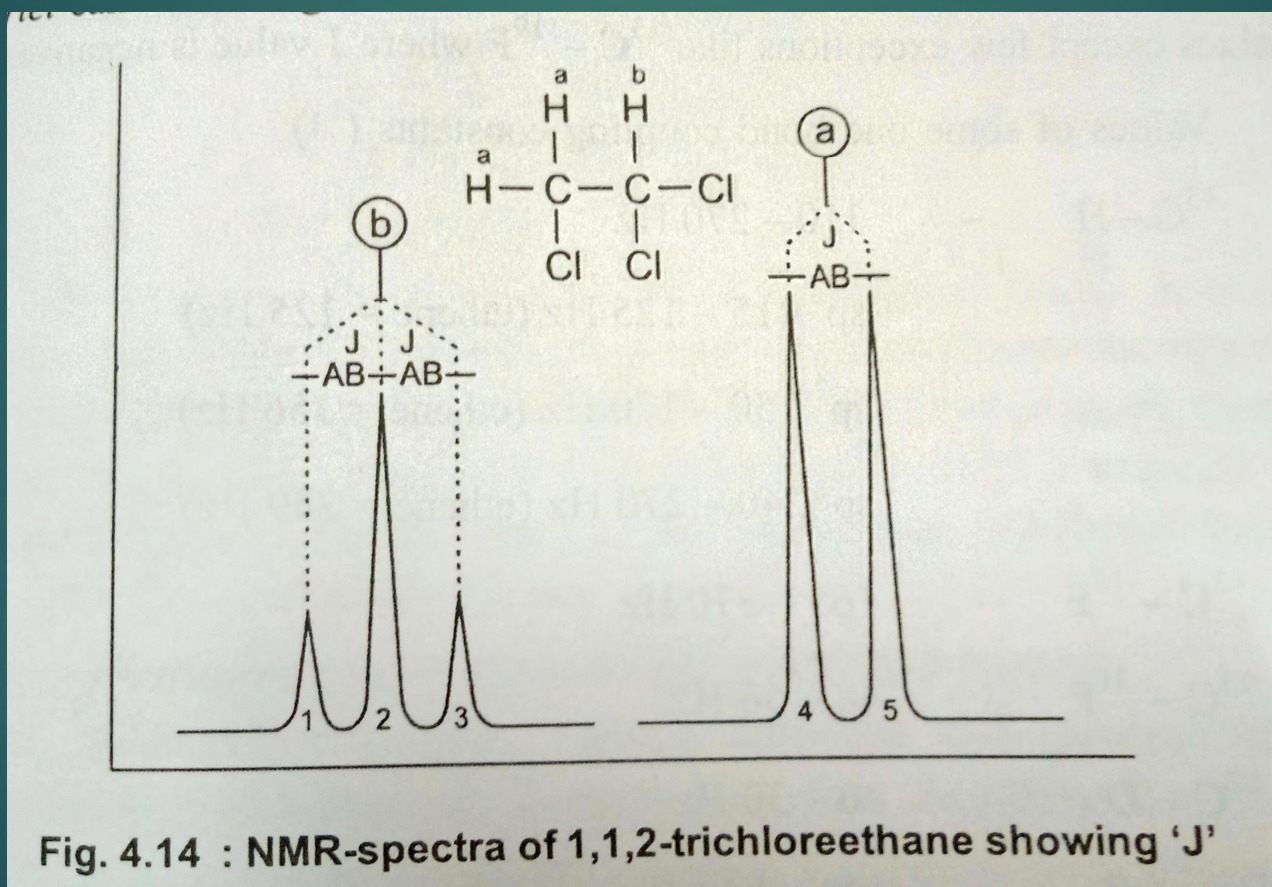
**Table 4.1 : Spin-quantum number of magnetic nuclei**

Atomic number	Mass number	'I' value	Examples
Odd	Odd	$1/2, 3/2, 5/2$	${}^7\text{N}^{15}, {}^9\text{F}^{19}, {}^{15}\text{P}^{31}$ etc.
Even	Odd	$1/2, 3/2, 5/2, 7/2 \dots$ etc.	${}^6\text{C}^{13}, {}^8\text{O}^{17}, {}^{16}\text{S}^{31}$ etc.
Odd	Even	$1, 2, 3 \dots$ etc.	${}^5\text{B}^{10}, {}^{15}\text{P}^{30}, {}^{17}\text{Cl}^{36}$ etc.

# Coupling Constant.

The *coupling Constant* is the distance between the center of two adjacent or successive peaks in a multiplet. It is denoted as  $J$ , expressed in units of Hertz or CPS and its value ranges from zero to twenty.

The  $J$  values depends partly on the number of covalant bonds through which proton may interact and also upon the strutural relationships between the coupled protons. The  $J$  value independent of applied field strength so remains constant .But Delta values change as they depend on field strength.this property is used to reorganize singlet peaks and the peaks of multiplets. For this we need to record the pmr-sprcra at two different field strength or frequencies. If  $J$  value from two Spectra remains same then the two peaks represent a doublet. If its value increase with increasing field strength (frequency), they represent two singlet peaks . Similarly a quartet can be distinguished from two doublets.





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THANK YOU.....

