PRINCIPLE OF PROTON NMR SPECTROSCOPY

BY

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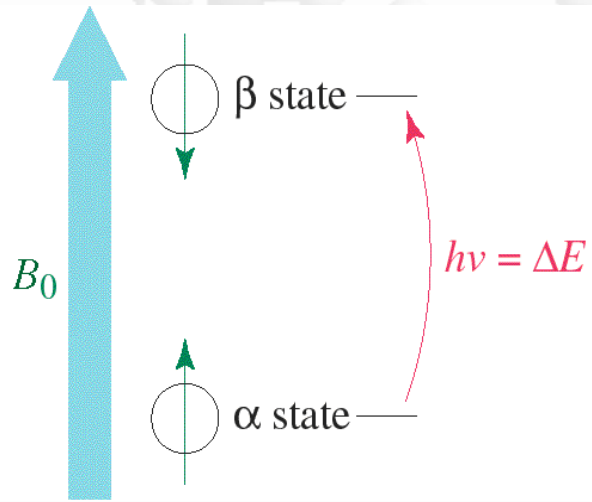
INTRODUCTION

- *Proton NMR is the most powerful tool to determine structure of organic comp.*
- *Developed based on Purcel & Bloch Phenomenon of NMR.*
- *When magnetic nuclei exposed to m. f. absorb Rf radiation at unique combination of field strength & freq. of light is called as Nuclear Magnetic Resonance.*
- *The phenomenon of absorption Rf radiation by proton when sample exposed to strong m. f. is called as Proton Magnetic resonance.*

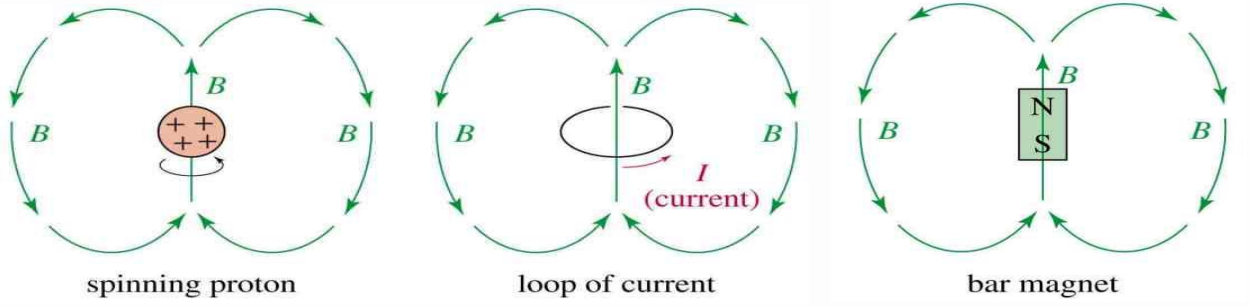


Spinning Nuclei & Magnetic moment

- *The nuclei of some atoms have a property called "SPIN". (degenerate)*
- *This nuclei is called as NMR active nuclei*

Sr. No.	Proton	Neutron	Spin quantum Number	Examples	NMR Active/Inactive
1	**Even**	**Even**	**0**	**^{12}C, ^{16}O**	**Inactive**
2	Even	Odd	½, 3/2	^{13}C	Active
3	Odd	Even	½,	^{1}H	Active
4	Odd	Odd	1,2,3	^{2}H, ^{14}N	Active

- *Due to spin, proton generates angular magnetic momentum along spin axis (i.e. magnetic field)*
- *Spinning nuclei acts like a tiny bar magnets, vector property*



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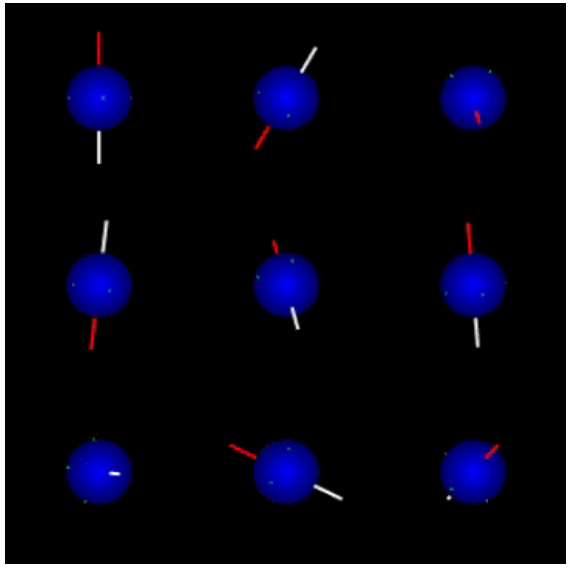
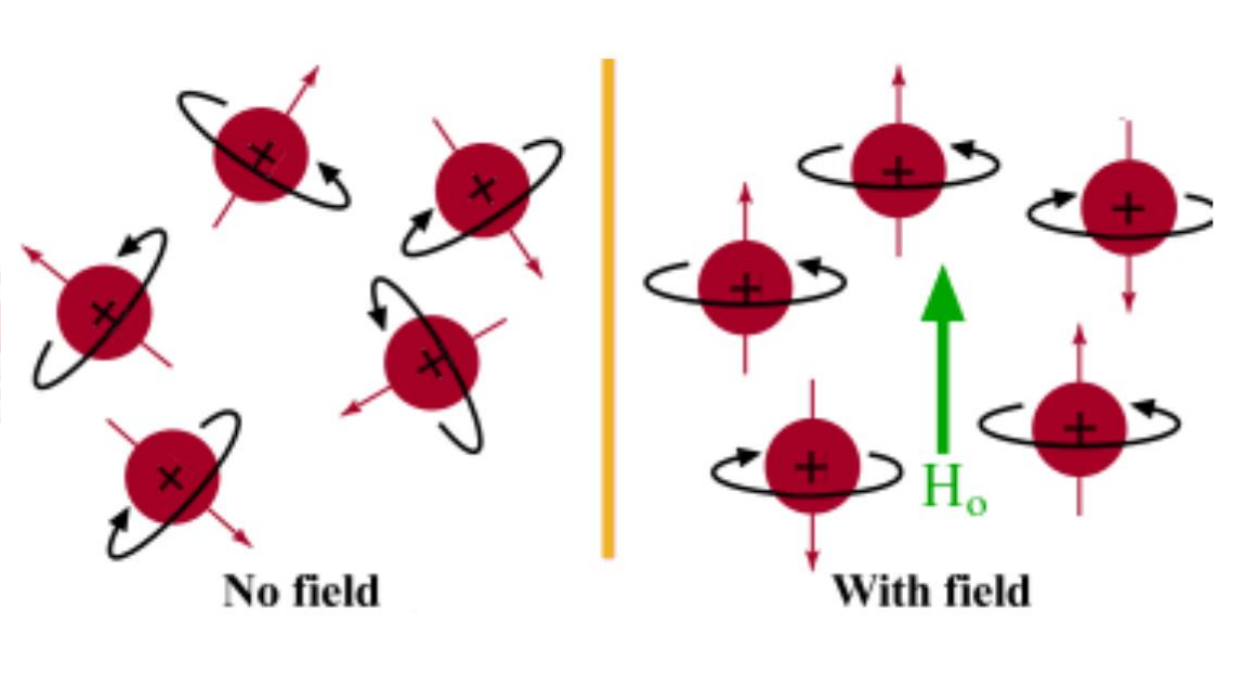
Spinning Nuclei

Nuclear Spins in the Absence and Presence of a Magnetic Field



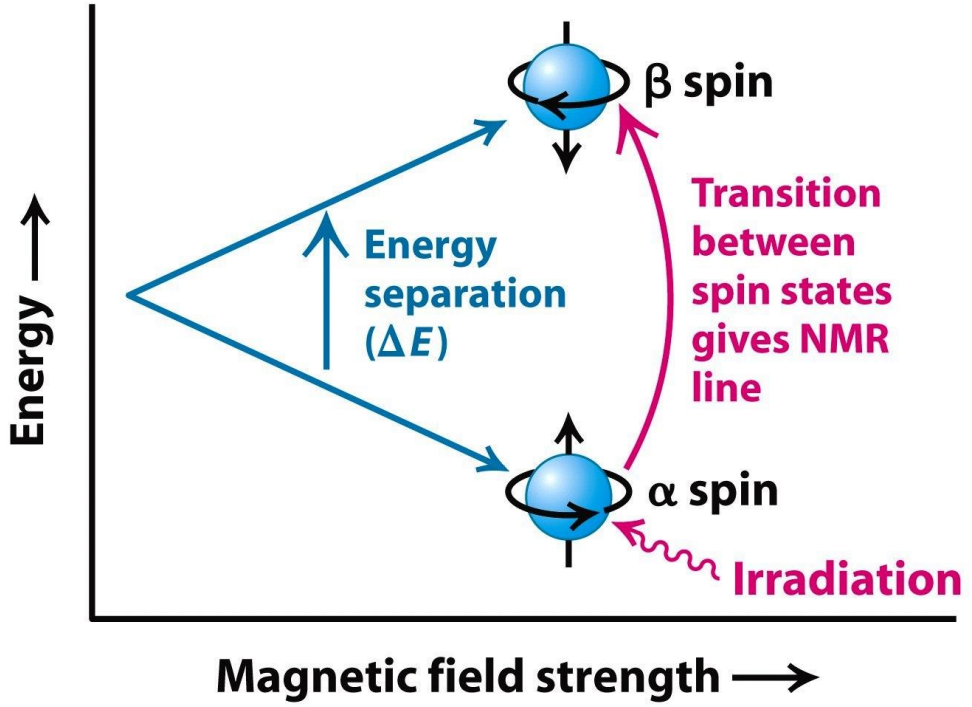


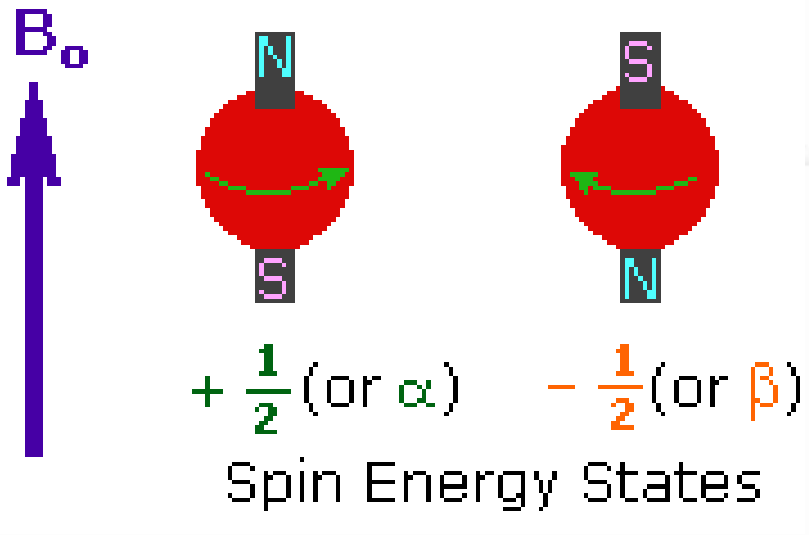
Randomly Arrangement of magnetic momentum vectors

Parallel & Anti parallel Arrangement of magnetic momentum vectors

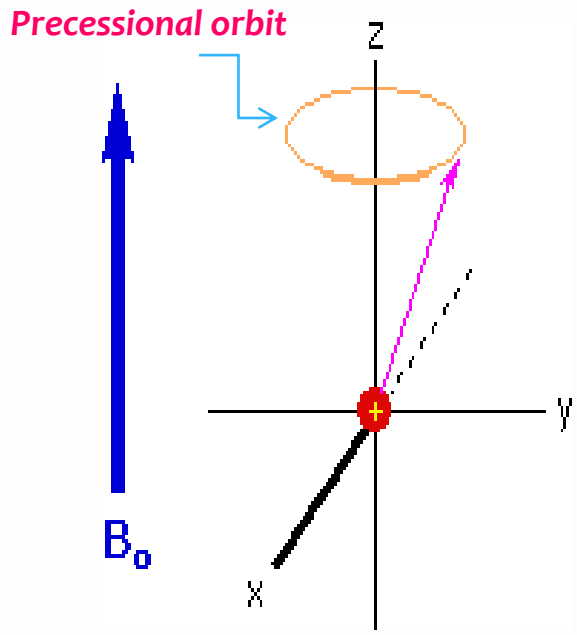
No. of orientations= 2I+1 ***(I is spin quantum number for H)***

Each alignment is quantized & its energy varies w. r. t. applied m. f.

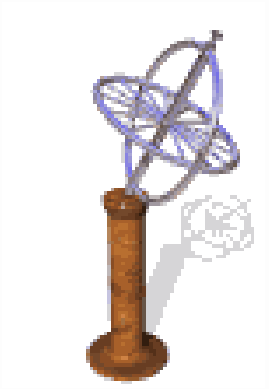




Processional Motion



Processional motion



- *Rotational motion of magnetic nucleus exposed to an applied field called Processional or Gyroscopic motion.*
- *When nucleus spins in an applied magnetic field, it draws out a circle perpendicular to applied m. f. called as Precessional orbit*
- *Number of revolutions per sec. made by magnetic moment vector (u) of nucleus under applied field called Precessional or Larmer frequency (ν).*
- *Processional frequency of an isolated proton is,*

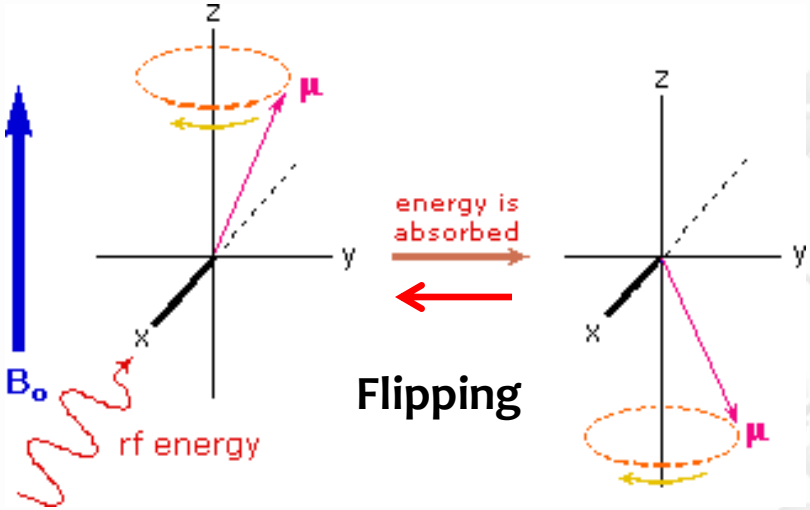
$$\nu = \gamma H_o / 2\pi \quad \ldots\ldots\ldots\ldots (1)$$

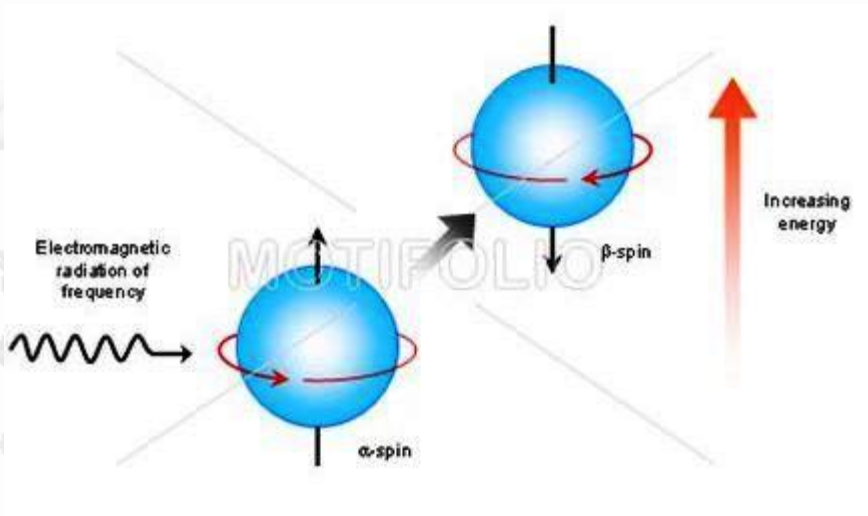
- *ν is directly proportional to applied m. f. strength*

Nuclear Resonance

A state where, frequency of irradiated Rf waves matches to the processional frequency of magnetic nuclei, then spinning magnetic nuclei absorbs Rf waves and changes spin from alpha to beta.

(Frequency absorbed during resonance called as Resonance frequency)





Flipping

Under special condition called resonance, the spin state of proton can change by exchanging energy this is called flipping.

- But, protons in an organic compound are not isolated, they are covalently bonded with C, N, O, S, etc.
- So equation (1) is not applicable. (i.e. $\nu = \gamma H_o / 2\pi$)
- Because electrons of covalent bond surrounding to H affects on precessional frequency.
- But electrons of covalent bond normally have paired spin & no net m. f.
- But under applied m. f. , additional modes of circulations are generated by these electrons.
- This circulations generates a small but its own m. f. called Secondary or Induced m. f.
- If induced field align to applied m. f. then actual m. f. felt by proton is greater than applied m. f.
- If induced field align opposite to applied m. f. then actual m. f. felt by proton is lesser than applied m. f.

- *Therefore actual field experienced by proton in a molecule, slightly different from that of applied called as Local or effective field (H).*

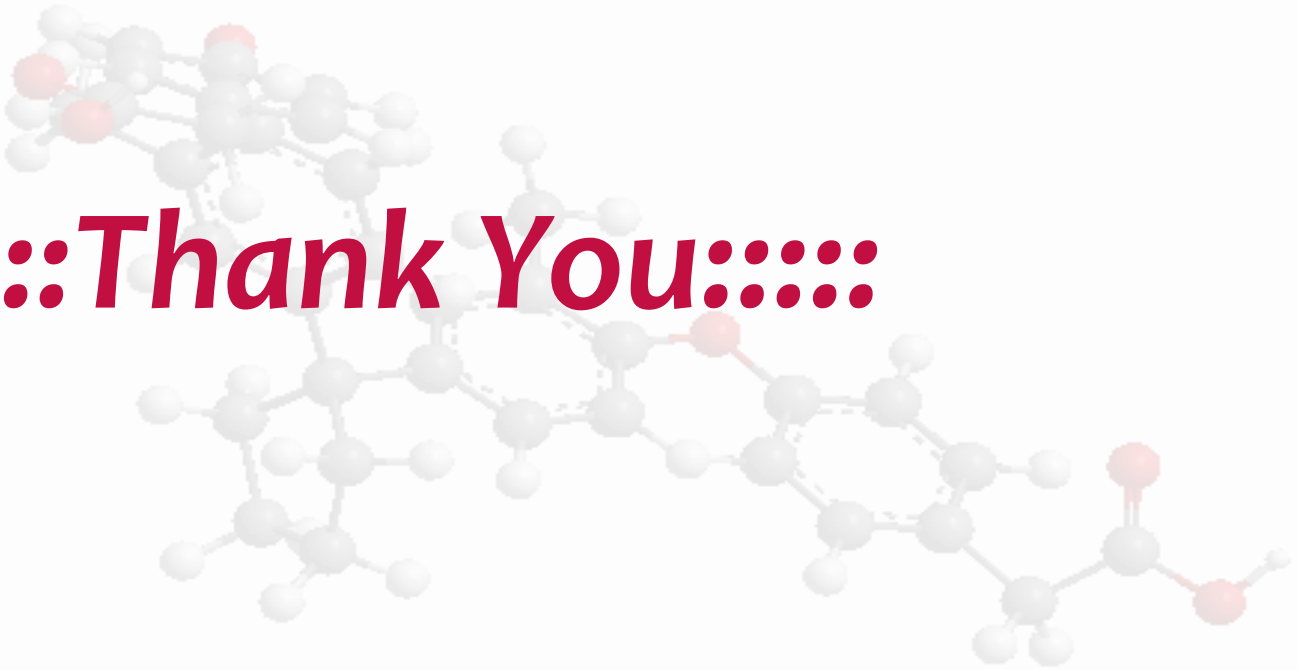
  $H = H_o - H_{ind}$ *(Applied field-induced field) ……(2)*

- *Again strength induced field depend on strength of applied field.*
- $H_{ind} \propto H_o$
- $H_{ind} = \sigma H_o$ *……..(3)* *[σ = shielding parameter constant]*
- *By putting value of eq-3 in eq-2, we get*

  $H = H_o - \sigma H_o$

  $H = H_o (1 - \sigma)$
- *So, finally corrected precessional frequency for H surrounded by electrons is*

  $[\nu = \gamma H_o (1 - \sigma)/2\pi]$ *……(4)*
- *When this precessional frequency matches to Rf waves then nuclei undergoes resonance and absorbs energy and signal appears in the spectrum.*



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