Nuclear Magnetic Resonance

Ankita Ojha
Department of Chemistry
Maharaja College
Arrah

Nuclear Magnetic Resonance (NMR)

- NMR abbreviated for Nuclear Magnetic Resonance is a phenomenon which occurs when the nuclei of certain atoms are immersed in a static magnetic field and exposed to a second oscillating magnetic field. NMR spectroscopy is the use of the NMR phenomenon to study physical, chemical and biological properties of matter.

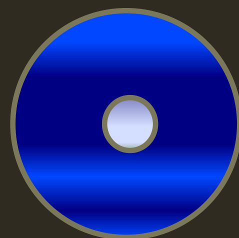
Which nuclei experience NMR?

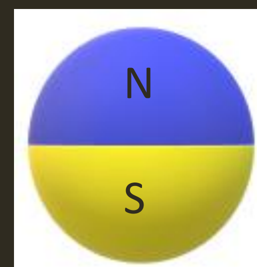
- Only nuclei possessing non-zero spin angular momentum or spin (I) show NMR. I can be half-integral e.g. ½ (1H, 13C, 15N, 19F, 31P…), 3/2 (23Na…) etc., or integral e.g. 1 (2H, 14N…) etc. The spin of such a nucleus can be thought of as a magnetic moment vector. Molecules possessing such nuclei can be examined with NMR. Of these NMR sensitive nuclei, 1H, 13C, 15N and 31P are most important for biological studies.

How do simplest such nuclei with I=1/2 behave?

- As a tiny bar magnet with a North and South Pole. It is the property of spin that causes the nucleus to produce an NMR signal.

There is no spin for nuclei with I=0





Spin Angular Momentum & Spin Magnetic Moment

A spinning charge behaves as a spin magnet. The spin-magnet has a magnetic moment (**μ**) proportional to the spin angular momentum $\mathbf{I}\,\hbar$:

$$\mu = \gamma\, \mathbf{I}\, \hbar$$

where γ is the gyromagnetic ratio, and it is a constant for a given nucleus

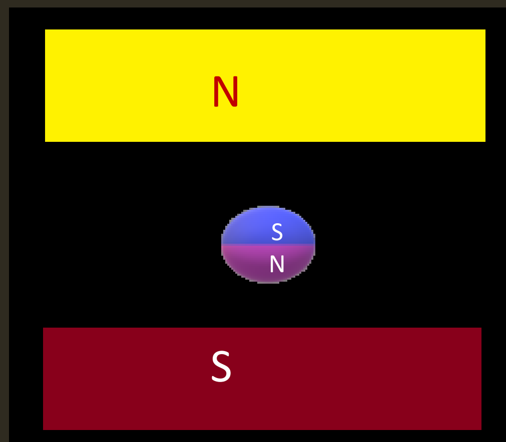
where the magnitude of **I** is $\{I\,(I+1)\}^{1/2}$, I = 0, ½, 1, 3/2….

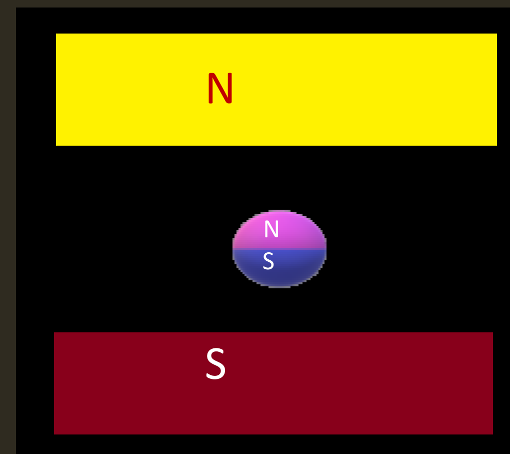
Some of the applications of NMR spectroscopy are listed below:

- **Solution structure :**The only method for atomic-resolution structure determination of biomacromolecules in aqueous solutions under near physiological conditions or membrane mimeric environments.
- **Molecular dynamics :**The most powerful technique for quantifying motional properties of biomacromolecules.
- **Protein folding** The most powerful tool for determining the residual structures of unfolded proteins and the structures of folding intermediates.
- **Ionization state** For determining the chemical properties of functional groups in biomacromolecules, such as the ionization states of ionizable groups at the active sites of enzymes.
- **Weak intermolecular interactions**
- **Protein hydration** A power tool for the detection of interior water and its interaction with biomacromolecules.

- **A** unique technique for the DIRECT detection of hydrogen bonding interactions.
- **Drug screening and design** Determining the conformations of the compounds bound to enzymes, receptors, and other proteins.
- Native membrane protein Solid state NMR has the potential for determining atomic-resolution structures of domains of membrane proteins in their native membrane environments, including those with bound ligands.
- Metabolite analysis A very powerful technology for metabolite analysis.
- Chemical analysis A matured technique for chemical identification and conformational analysis of chemicals whether synthetic or natural.
- Material science A powerful tool in the research of polymer chemistry and physics.

When an Isolated bare Spin (1/2) nucleus or particle when placed in an external magnetic field?





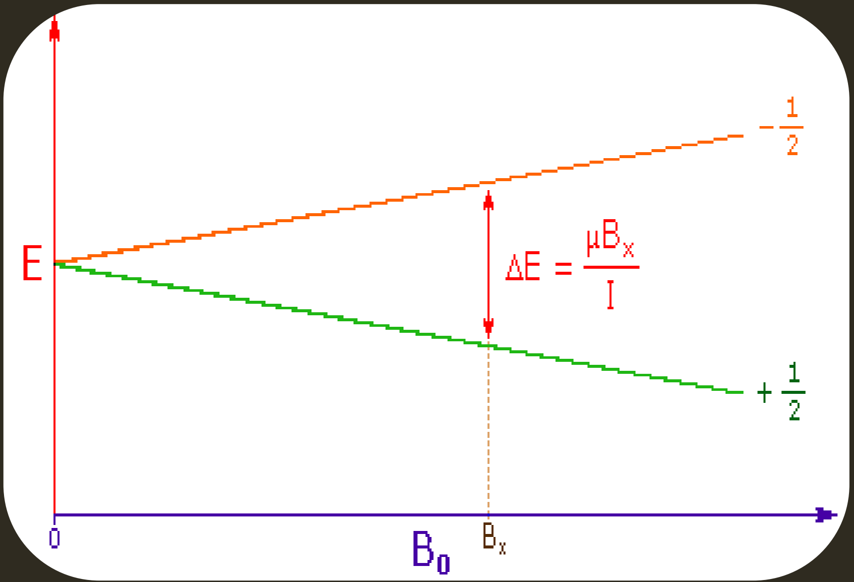
In the presence of an external magnetic field (**B**), the energy of interaction between the spin magnet and the magnetic field is :

$E = \mathbf{-\mu\ \hat{U}\ B = -}\ \gamma\ \hbar\ \mathbf{I\hat{U}B}.$

The magnetic field is applied along the +z direction, when the expression for E becomes = $\mathbf{-}\ \gamma\ \hbar\ \mathbf{I\hat{U}}B_0\ \mathbf{k = -}\ \gamma\ \hbar\ I_z\ B_0\ (B_0 = B_z)$.

The result of measurement of E will be = $\mathbf{-}\ \gamma\ \hbar\ m_I\ B_0$ (m_I = + ½ or – ½ for I = ½)

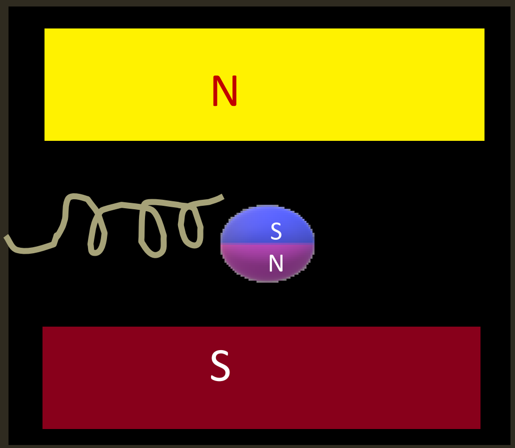
Thus two spin states exist, **+** ½ and **-** ½ (For I= ½).



Aligned with the applied field

Aligned against the applied field

On being exposed to electromagnetic radiation



The result $\boldsymbol{\omega_0} = \gamma B_0$ defines transition (+ ½ → - ½) frequency (ω_0) and underpins the whole of NMR

Thus, if a spin in + ½ state placed in a static magnetic field, B_0 is irradiated by electromagnetic radiation of frequency $\nu_0 = \gamma B_0 / 2\pi$, magnetic resonance absorption will occur flipping the spin into -½ state. Transition frequency ω_0 is therefore referred also as resonance frequency

Thank You

Contents will be updated further

For any subject related query

Mail : ankitaojha26@gmail.com