Lec 1 **5th stage**

Advanced Pharmaceutical Chemistry
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Nuclear magnetic resonance

Nuclear magnetic resonance (NMR) spectroscopy: - is the study of molecular structure through measurement of the interaction of an oscillating radio-frequency (RF) electromagnetic field with atomic nucleus have magnetic properties are placed in a strong external magnetic

Typical Applications of NMR

1. Chemical structure analysis

2. Study of dynamic processes

3. Structural studies of soluble biomacromolecules

4- Drug design

5- Magnetic Resonance Imaging (MRI)

NMR spectroscopy:-

1. RF (radio frequency)→ low frequency $\nu = 10^6$-10^{10} Hz , long wavelength = 10^{11}- $3*10^7$ nm
2. External magnetic field.
3. Atomic nucleus.

The Fundamental basis of Magnetic resonance

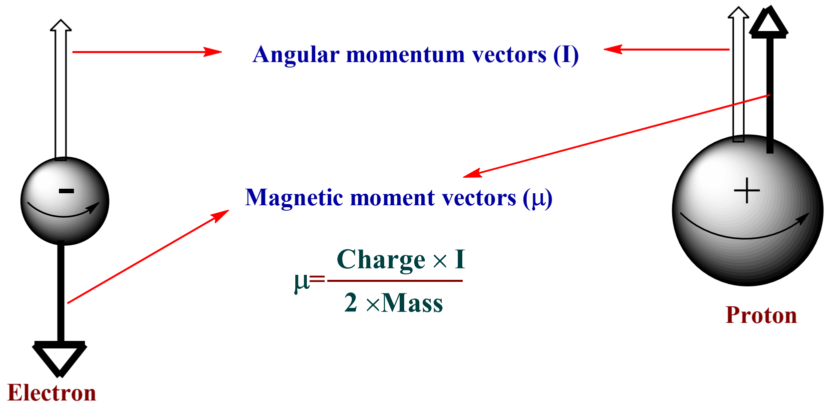
Nuclear spin

1. Atomic nuclei having spin →NMR
2. Atomic nuclei not having spin → no NMR

Spin:- **nuclei considered as rotating charges, then they have both**

1. Electrical properties
2. Angular momentum

The rotating charge is electric current flowing and behave as a magnetic dipole (**(μ)**.



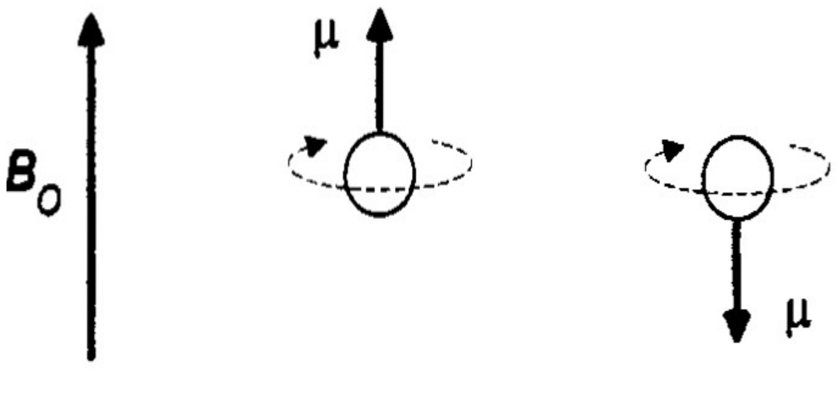
the spinning electron and the spinning proton both are shown with the same direction of spin thus their angular momentum vectors point in the same direction. the vectors representing their magnetic moments point in opposite direction. however the vector representing spin angular momentum for the proton is in the same sense (that is, of the same sign) as the vector representing its magnetic moment.

The proton is a spinning charged (Z=1), so it exhibits a magnetic moment. It is magnetic moment has only two possible orientations that are degenerate in the absence of an external magnetic field.

The electron spin quantum number labeling as *s, thus for electron, (s = +1/2 or -1/2)*

The nuclear spin quantum number labeling as *m, thus* for proton, (m = +1/2 or -1/2). Such nucleus was described as having a nuclear spin (spin quantum number) (*I*) of 1/2.

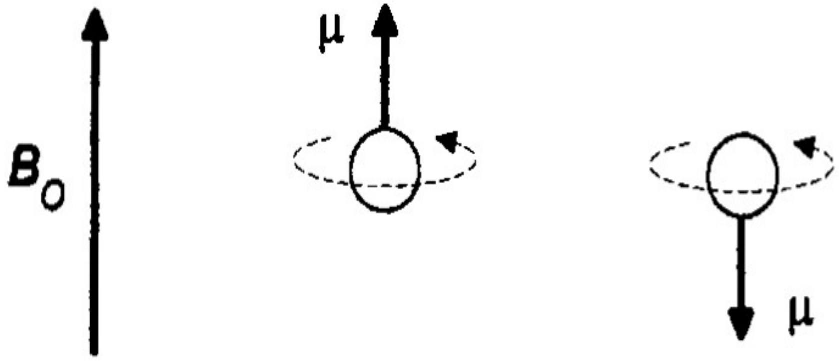
Because the nuclear charge is the opposite of electron charge, a nucleus whose magnetic moment is aligned with the magnetic field (m= +1/2) has the lower energy. So ^{1}H nuclei (i,e., protons) exhibit two possible magnetic spin orientations.



s=+1/2
Higher energy

s= -1/2
Lower energy

Two possible orientations of the magnetic moment (μ) of spining electron in an external magnetic field (B_0)



m=+1/2
Lower energy

m= -1/2
Higher energy

Two possible orientations of the magnetic moment (μ) of spining proton in an external magnetic field (B_0)

μ:- An NMR activity of isotope caused by μ (magnetic moment).

Nucleus has a positive charge and an angular momentum, it will have a magnetic moment, → local field.

The spin Quantum number I

Zeeman effect:- is the splitting of spin into specific group

Zeeman found only certain isotopes gives rise to multiple nuclear spin states when immersed in an external magnetic field.

The dimension of spin angular moment(I) for all nuclei are quantized and can be characterized by spin Quantum number(*I*), The allowed values of *I* may be zero, integer, or half integer.

a. **If protons and neutron are both even number → *I* =0 such nuclei are invisible to NMR**

Example: - ^{12}C, ^{16}O, ^{18}O and ^{32}S→ have no spin property.

a. **If(protons + neutron) is an odd number→ *I* = half integer. Such nuclei are detectable by NMR.**

Example $^{1}H(I=1/2)$, $^{13}C(I=1/2)$, $^{15}N(I=1/2)$, $^{17}O(I=5/2)$, $^{19}F(I=1/2)$, $^{29}Si(I=1/2)$, and $^{31}P(I=1/2)$.

a. **If both protons and neutron are odd number → *I* =integer. Such nuclei are detectable by NMR**

Example:- $^{2}H(I=1)$, $^{14}N(I=1)$.

The magnitude of the spin angular momentum (I) is given by Eqn.1.

Spin quantum number

Spin angular momentum

$$I = \hbar\sqrt{I(I+1)} \quad \text{.................} \quad 1$$

h/2π (h = 6.626×10^{-34} J.s is planck's constant)

The direction of spin angular momentum

nuclear angular momentum spin angular momentum(I) has quantized limits to its direction.

•The number of allowed orientations for I is restricted and defined by a formula (2*I*+1)

Thus for nuclei *I*=1/2 only two direction are allowed

$$I_z = \hbar m_I \quad \text{.................... } 2$$

The total number **(multiplicity)** of possible spin states (i.e., the different value of m) is determining as follow:-

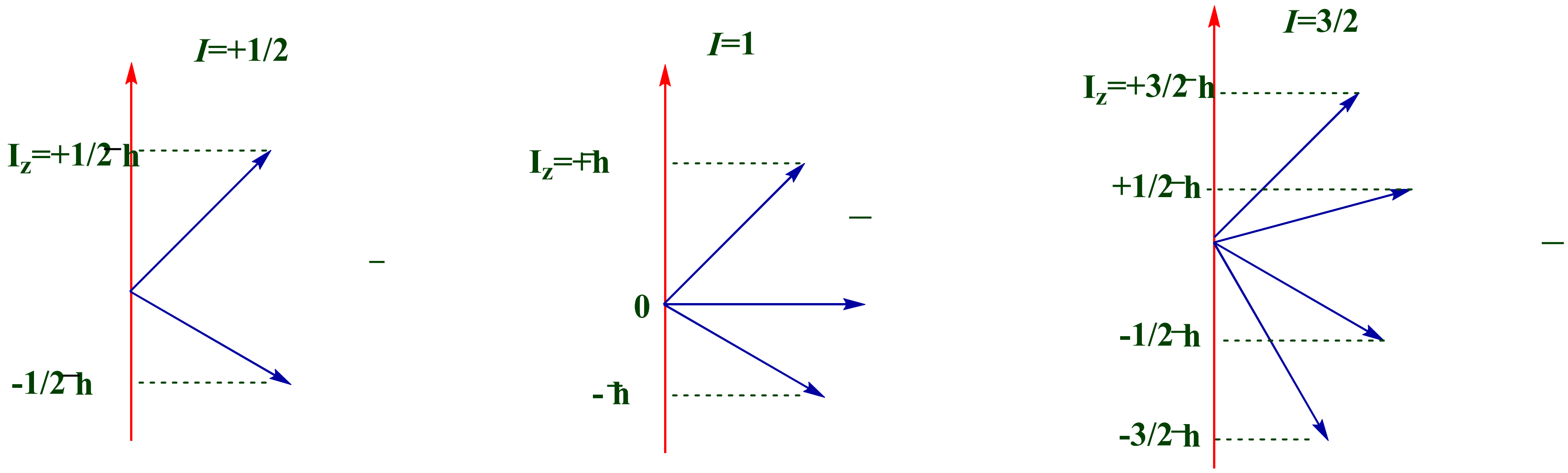
$$\textbf{Multiplicity} = 2I+1 \quad \text{........... } 3$$

Thus, the allowed values of spin, m_I are

I*, *I*-1, *I*-2,......,0,.........2-*I*, 1-*I*, -*I* .... for integer *I

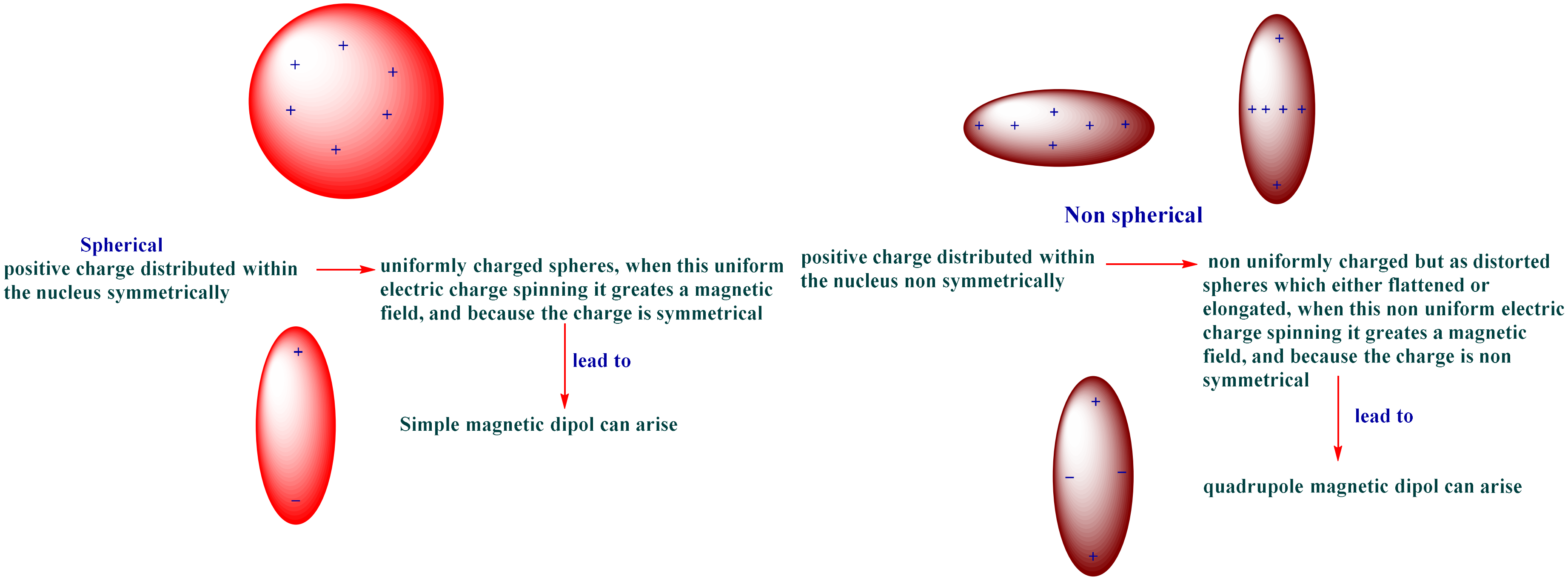
I*, *I*-1, *I*-2,......,-1/2, +1/2,......2-*I*, 1-*I*, -*I* .... for half integer *I

A combination of Eqns. 1 and 2 leads to the following spin-state diagrams for nuclei with different spins (e.g. ½, 1, ³/2 ...):-



spin-state diagrams for *I* = ½ (left), 1 (mid) and 3/2 (right).

All nuclei with I=1/2 have a spherical (symmetrical) distribution of spinning charge, so the electric and magnetic fields surrounding such nuclei are spherical, homogeneous, and isotropic in all directions. By contrast, nuclei with I> ½ have a non spherical distribution of spinning charge, resulting in nonsymmetrical electric and magnetic fields. This imparts an electric quadrupole (Q) to the nucleus, a property that can complicate their NMR behavior; As a result, the most commonly studied nuclei are those with a nuclear spin of ½ (such as ^{1}H, ^{13}C, ^{15}N, ^{31}P, ^{19}F).



Homework:- complete the following table.

Spin quantum number and derived quantities

Spin quantum number I	Examples	Angular momentum, I $\sqrt{I(I+1)}$ in units of $h/2\pi$	Number of spin state (allowed orientation) $2I+1$	Magnetic quantum number-the z-axis components of I (allowed values of spin) m_I
0	^{4}He, ^{12}C, ^{16}O			
1/2	^{1}H, ^{13}C, ^{15}N ^{19}F, ^{29}Si , ^{31}P			
1	^{2}H, ^{14}N			
3/2	^{11}Be, ^{23}Na ^{35}Cl, ^{37}Cl			
2	^{8}Li*, ^{20}F*			
5/2	^{17}O,^{27}Al			