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Study Notes on Nuclear Magnetic Resonance

Nuclear Magnetic Resonance

Introduction:

Nuclear Magnetic Resonance (NMR) is part of the discipline of Magnetic Resonance, and includes NMR, Electron Paramagnetic Resonance (EPR or ESR) and Nuclear Quadrupole Resonance (NQR). Nuclear Magnetic Resonance (NMR) spectroscopy takes advantage of the magnetic properties of certain nuclei and records the absorption of energy between quantized nuclear energy levels. In an NMR experiment, the spectrometer is tuned to the frequency of a particular nucleus and the spectrum reveals all such nuclei in the molecule being investigated.

Nuclei may have spins of zero or greater than zero in units of ½, because of how the protons and neutrons are arranged relative to one another. There are three possible conditions:

No of protons	**No of neutrons**	**Spin**
Even	Even	0 → No MNR
Odd	Odd	Integral
Odd	Even	Half-Integral Spin

1. For I = 0: Nuclei that have both an even number of protons and an even number of neutrons will have zero net nuclear spin.
2. I = ½: The spin -1/2 nuclei are the most important class for NMR spectroscopy.
3. I > ½: These are known as the quadrupole nuclei, because such spins induce a so-called quadrupole magnetic moment.

For a substance to be NMR active, the I (Nuclear spin) should not be equal to 0, because these types of nuclei are unable to act like a small magnet. Those are preferred species for NMR for which spin of I = ½. These nuclei all give NMR signals that obey the same rules as do the familiar ^{1}H spectra. The highly abundant nuclei ^{1}H, ^{19}F and ^{31}P are the most important NMR nuclei to give good spectra. Some of the more common spin ½ nuclei are listed in the shorter table shown below.

Nucleus	**Natural abundance (%)**	**I**
^{1}H	99.985	½
^{19}F	100	½
^{31}P	100	½
^{13}C	1.11	½
^{15}N	0.3	½
^{77}Se	7.5	½
^{117}Sn	7.67	½
^{129}Xe	26.4	½
^{183}W	14.4	½

^{195}Pt	33.8	½

Working Principle:

Any spinning charge body generates a magnetic field. Therefore, a nucleus of an atom which possesses both electric charge and mechanical spin behaves as a tiny spinning bar magnet, and this forms the basis of Nuclear Magnetic Resonance.

The spin of nucleus can be represented by $\vec{I}$

$$\vec{I} = \left[I(I+1)\right]^{1/2} h/2\pi$$

No. of orientation = 2I + 1

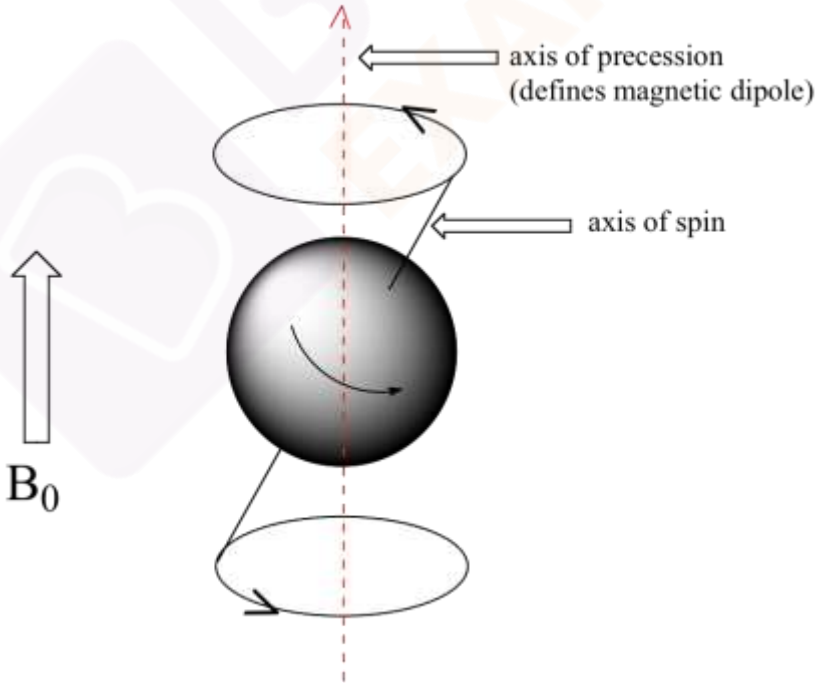
Nuclear magnetic moment is $\mu = gnB_N\left(I(I+1)\right)^{1/2}$

The spin angular momentum = $=\left(I(I+1)\right)^{1/2} h/2$

LARMOR PRECESSION:

Dipole moment of a spin nucleus is given by $\mu = gnB_N\left(I(I+1)\right)^{1/2}$

μ can be oriented so that its component is integral or half integral in the reference direction. The external magnetic field tries to align the nucleus in its direction by applying a torque on the nucleus. The spinning nucleus instead of aligning in the field direction makes a processional motion about the field direction. i.e the axis of spin describes a cone about the field direction. Such precession which is shown by the spinning nucleus is known as Larmor Precession.



The precession frequency or Larmor Frequency is given by:

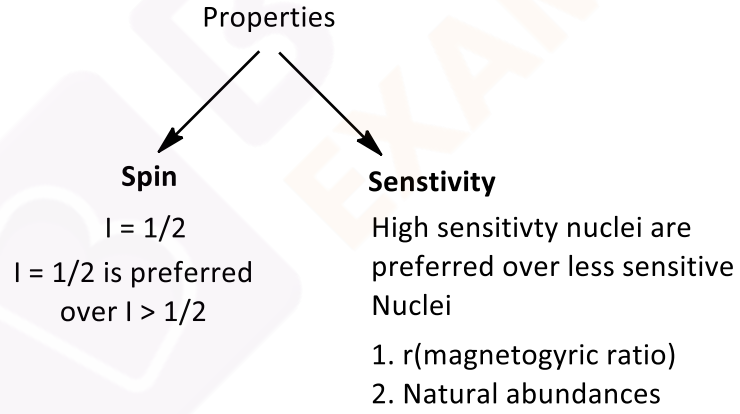
$\omega =$ (Magnetic moment/spin angular momentum) $\times B_z$

$\omega = gB_N B_z / h$

Concluding theory of NMR:
Nucleus is exposed to electromagnetic radiation of suitable frequency and subjected to an external magnetic field which is adjusted to make the processional frequency of the nucleus equal to the frequency of the radiation. Nucleus absorbs the right amount of energy and makes a transition from energy level to the next and generates a current which is further detected by the detector. The NMR signal of the nucleus is highly specific to the nucleus under study. The widest distributed magnetically active nucleus in organic compounds is H- atom and the corresponding NMR is referred to an PMR of proton Magnetic Resonance.
The points of interest in the study of NMR are: -

1. No. of signals
2. Position of signals and chemical shift.
3. Intensity of signals.
4. Splitting of signals or Spin – coupled.

Multinuclear NMR:
If an element has more than one NMR active nuclei, then most appropriate Nuclei be based on following Nuclear Properties.



Nuclei under Consideration
(a). I = ½ High abundance(^{1}H)
(b). I = ½ Low abundance(^{13}C)
(c). I > ½ Low abundance (^{15}N)

Splitting of lines by the presence of another nuclei is given by:
2nI+1
Here, n= no. of equivalent proton
I= nuclear spin

There is total 7 cases are formed while any nucleus is considered for NMR spectroscopy and these are:

1. **Molecule with one type of spin I = ½ & conc. Nuclei**
   H_2, F_2, P_4, $P4S_3$, BrF_3, BrF_5, SF_4, S_F6, H_2S, H_2O

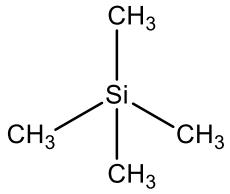
2. **Two I = ½, conc. Nuclei.**
   HF, PH_3, PF_3, PF_5, PCl_2F_3

3. **Three = I = ½, conc. Nuclei**
   PHF_2

4. **One I = ½, conc. Nuclei + I = ½ dilute Nuclei**
   2 NMR Active Nuclei
   CH_4, Hydrocarbons, SiH_4

5. **Two, I = ½ conc. Nuclei + one, I = ½ dilute Nuclei**
   3 NMR Active Nuclei
   CH_2F_2, $CH_2{=}CF_2$

6. **Two types of I = ½ spin dilute and one type of ½ spin conc.**
   The NMR Active Nuclei



7. **Molecule with Quadrupole Nuclei.**
   $CDCl_3$, NH_3, NH_4^+

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