Introduction to NMR- Spectra
(Lecture – 24)

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- **Spectroscpy** is the study of interaction of EMR with matter, which may result in absorption, transmission, emission,reflection , rotation of EMR
- **Nuclear magnetic resonance spectroscopy**, most commonly known as **NMR spectroscopy.**

Nuclear Magnetic Resonance (NMR) is a spectroscopy technique which is based on the absorption of electromagnetic radiation in the radio frequency region 4 to 900 MHz by nuclei of the atoms.

- Proton Nuclear magnetic resonance spectroscopy is one of the most powerful tools for elucidating the number of hydrogen or proton in the compound.
- **Spectroscopy** determines the physical and chemical properties of atoms or the molecules in which they are contained and provide detailed information about the structure, dynamics, reaction state, and chemical environment of molecules.
- It is used to study a wide variety of nuclei:
  - 1H
  - 15N
  - 19F
  - 13C
  - 31P

Theory of NMR

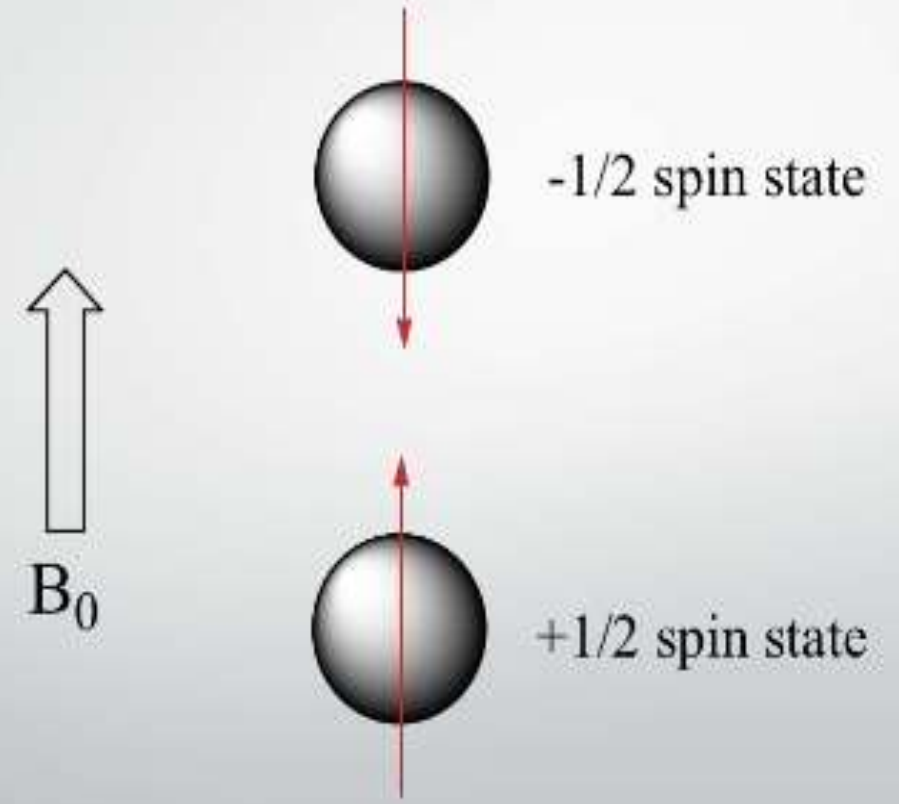
Spin quantum number (I) is related to the atomic and mass number of the nucleus

I	Z	A	Eg;
Half integer	Odd	Odd	1H (1/2)
Half integer	Odd	Even	13C (1/2)
Integer	Even	Odd	2H(1)
Zero	Even	Even	12C (0)

Elements with either odd mass or odd atomic number have the property of nuclear "spin"

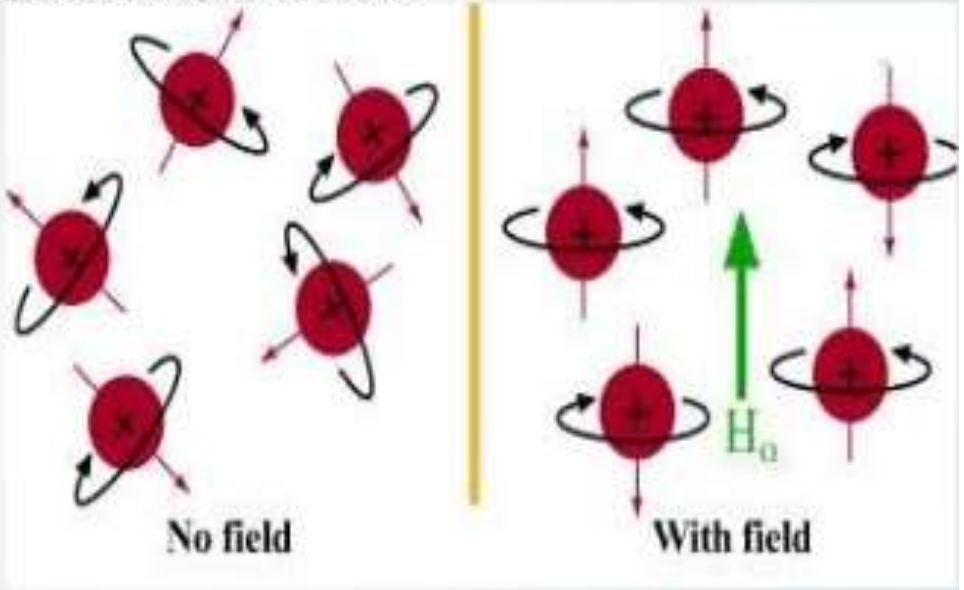
- If an external magnetic field is applied,the number of possible orientations calculated by **(2I+1).**

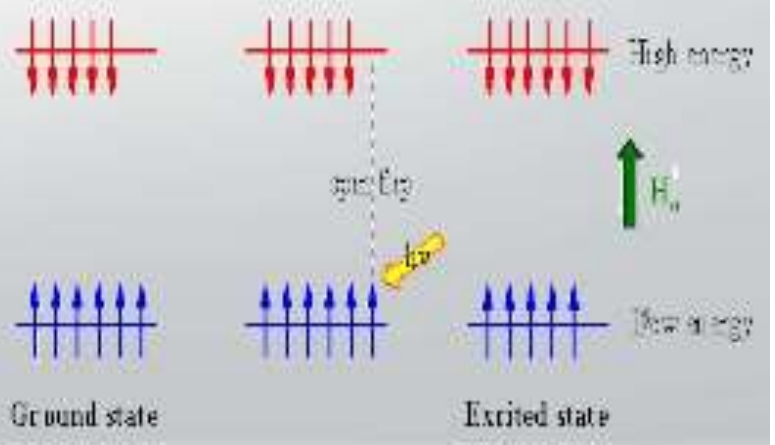
Eg.:-Hydrogen has spin quantum number I=1/2 and possible orientation is (2*1/2+1=2) two , ie,+1/2 and -1/2.



PRINCIPLE OF NMR

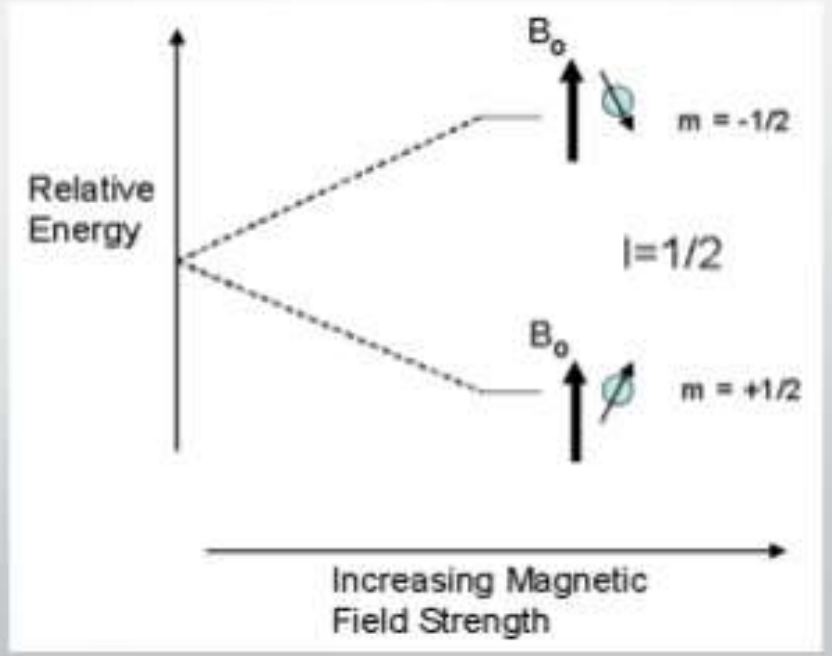
- The principle is based on the-spinning of nucleus and generating a magnetic field.
- Without external magnetic(Bo) – field nuclear spin are random in direction.
- With Bo ,nuclei align themselves either with or against field of external magnetic field





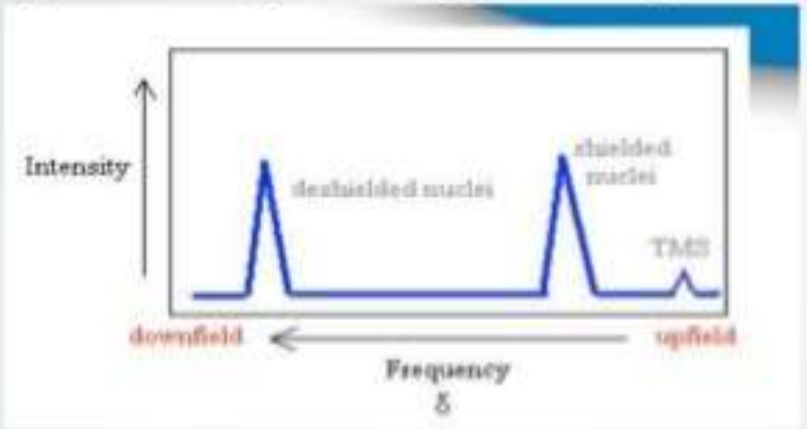
Eg, Liq.N2 Vs Liq. O2

- If an external magnetic field is applied, an energy transfer (ΔE) is possible between ground state to excited state.
- When the spin returns to its ground state level, the absorbed radiofrequency energy is emitted at the same frequency level.
- The emitted radiofrequency signal that give the NMR spectrum of the concerned nucleus.and is directly proportional to the strength of the applied field



NMR SPECTRUM

NMR spectrum is a plot of intensity of NMR signals VS magnetic field (frequency) in reference to TMS



Reasons for taking TMS as reference Standard

1. Chemically inert, magnetically isotopic, volatile & soluble in most organic solvents.
2. TMS gives an intense signal.
3. TMS can be easily removed.
4. Electro negativity is low.
5. It doesn't make any intermolecular association with sample

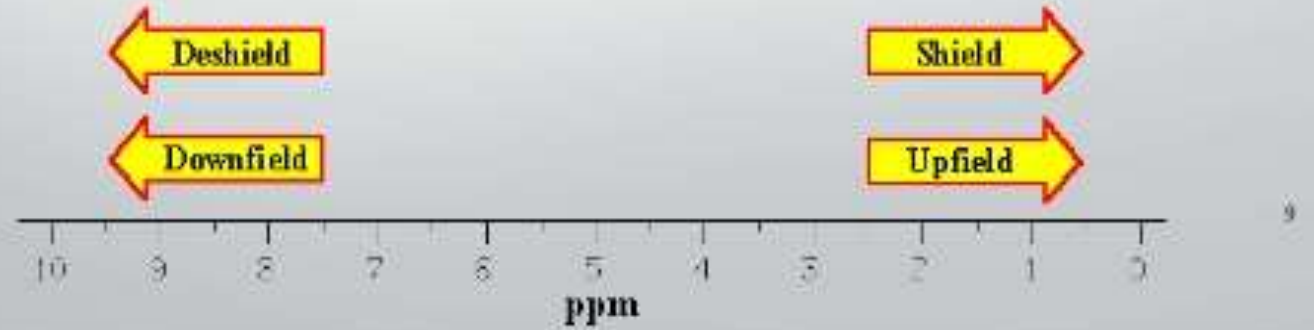
Chemical shift

- Is the resonance frequency of a nucleus relative to a standard in a magnetic field.
- TMS is the most common reference compound in NMR, it is set at $\delta = 0ppm$

$$\delta = \frac{\nu sample - \nu ref}{\nu ref}$$

Shielding of protons:- High electron density around a nucleus shields the nucleus from the external magnetic field and the signals are upfield in the NMR spectrum

Deshielding of protons:- Lower electron density around a nucleus deshields the nucleus from the external magnetic field and the signals are downfield in the NMR spectrum



Factors affecting chemical shift

- Electronegative groups/ Inductive effect
- Magnetic anisotropy of π-systems / diamagnetic effect of pi bond
- Hydrogen bonding
- Vander Waal's deshielding
- Effect of temperature &Effect of solvent

Electronegative groups:- Electronegative groups attached to the C-H system decrease the electron density around the protons, and there is less shielding (i.e.deshielding) and chemical shift increases

Compound	Chemical shift
CH3I	2.16
CH3Br	2.65
CH3Cl	3.10
CH3F	4.26

Thank You