Nuclear Magnetic Resonance

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ILOs

01 Define NMR

02 Discuss the principle of NMR

03 Describe the composition of NMR

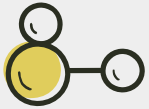
04 Discuss interpretation of NMR

05 List types of NMR

06 Compare between types of NMR

07 Outline applications of NMR

08 List advantages and disadvantages of NMR

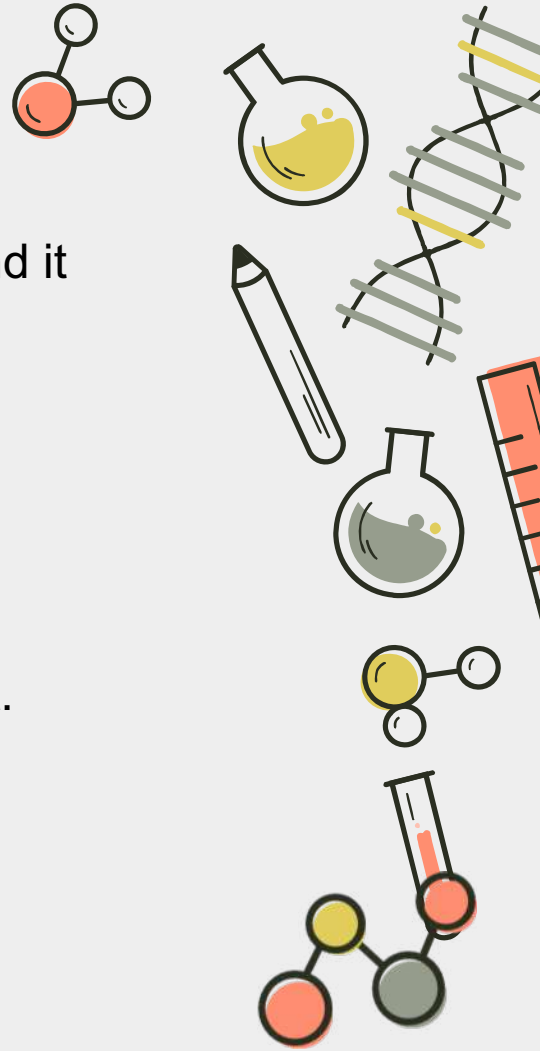


What is NMR

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.

The Principle of NMR:

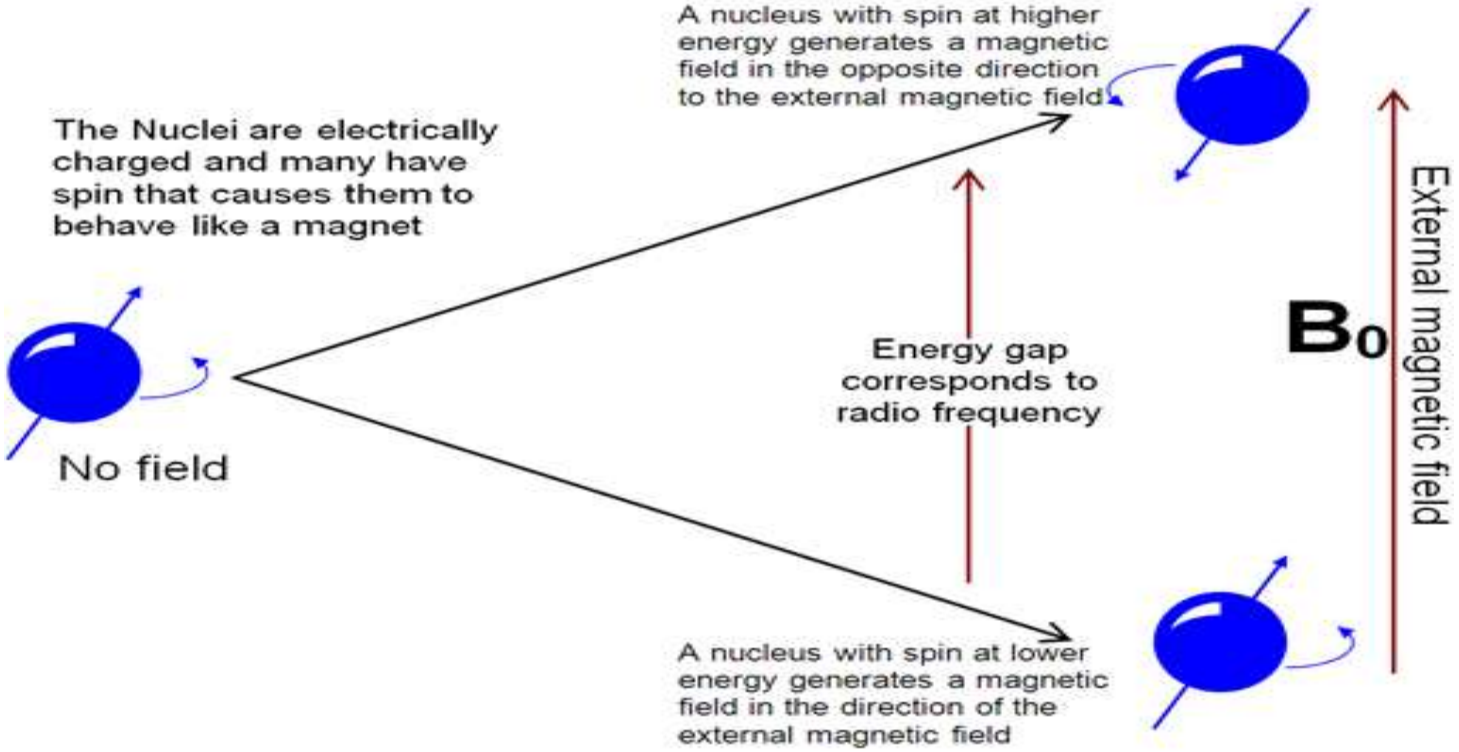
- The theory behind NMR comes from the spin of a nucleus and it generates a magnetic field.
- With out an external applied magnetic the nuclear spins are random in directions.
- When an external magnetic field, is present the nuclei align themselves either with or against the field of external magnet.



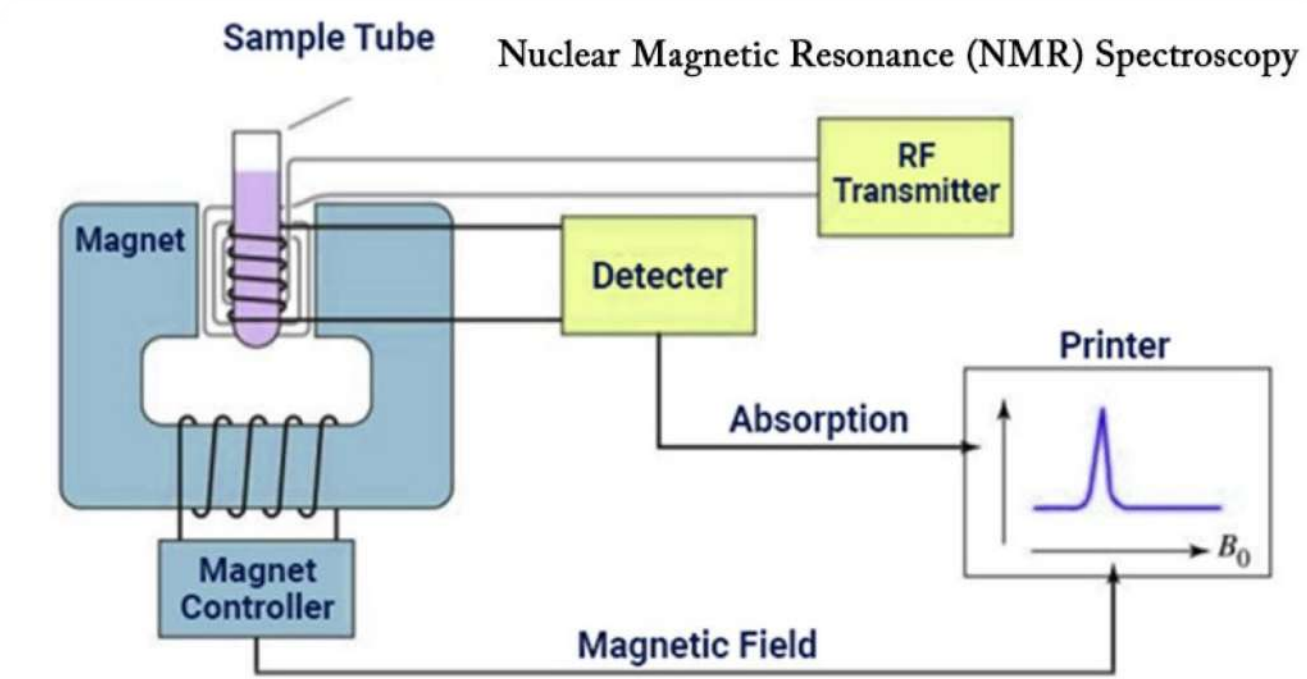
The Principle of NMR:

- The external magnetic field is applied, an energy transfer 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 concerned nucleus.

The case of the spin-½ nucleus



Composition of NMR:



Interpretation of NMR:

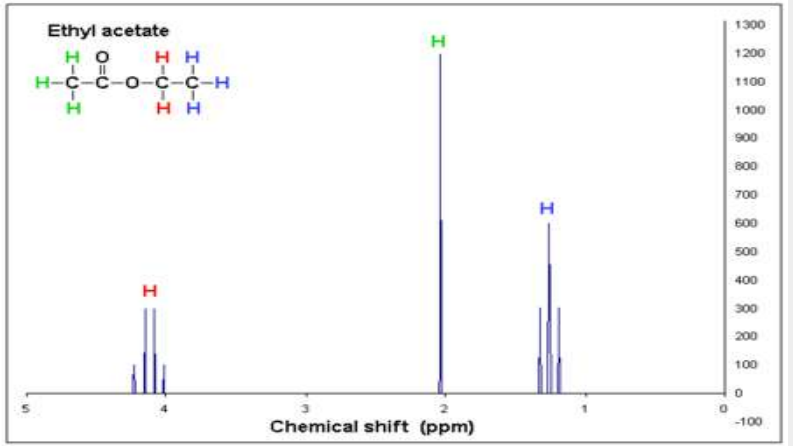
NMR interpretation plays a pivotal role in molecular identifications. As interpreting NMR spectra, the structure of an unknown compound, as well as known structures, can be assigned by several factors such as:

1. chemical shift.
2. spin multiplicity.
3. coupling constants.
4. integration.

Types of NMR

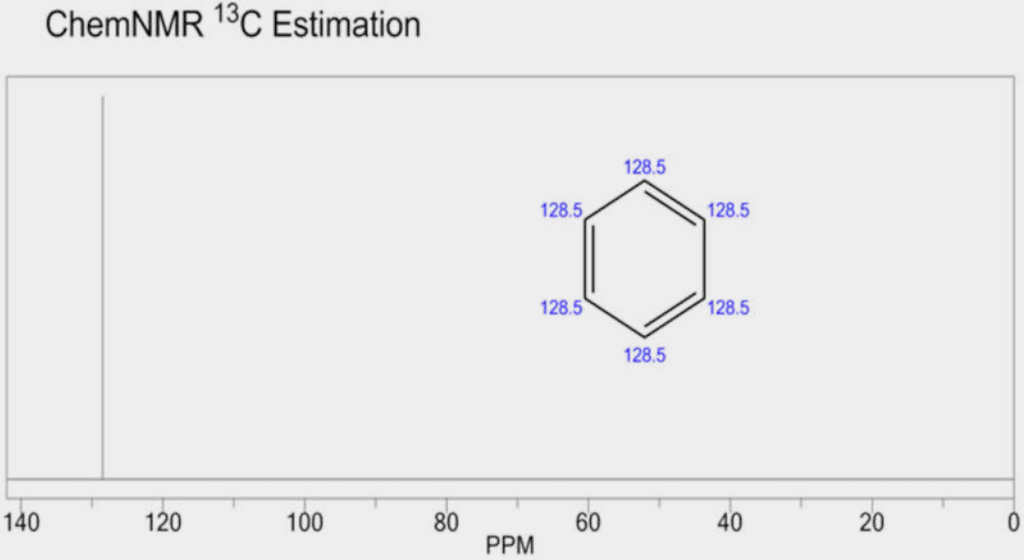
There are two types of NMR:

01 H1 NMR is a spectroscopic method used to determine the types and number of hydrogen atoms present in a molecule. In this technique, the sample (molecule/compound) is dissolved in a suitable solvent and is placed inside the NMR spectrophotometer.



Types of NMR:

02 13C NMR: is used to determine the type and number of carbon atoms in a molecule. Here also, the sample (molecule/compound) is dissolved in a suitable solvent and is placed inside the NMR spectrophotometer.



Comparison between types of NMR:

Property Used to Compare	1H NMR	13C NMR
Detection	1H NMR detect proton nuclei	13C NMR detects carbon nuclei
Method	In obtaining the NMR spectra for 1H NMR, continuous wave method is used. .	To obtain the NMR spectrum, can use Fourier transform method.
Chemical Shift Range	The chemical shift range of 1H NMR is 0-14 ppm.	The chemical shift range of 13C NMR is 0-240 ppm.

Comparison between Types of NMR:

Property Used to Compare	1H NMR	13C NMR
Progression	1H NMR process is slow	13C NMR process is fast

Applications of NMR:

- **Molecular interaction:** NMR can identify molecules, to probe molecular dynamics and study the molecular interactions.
- **Metabolic proliferation**: NMR is used to determine structure of proteins, amino acid profile
- **Drug discovery**: which the identity of an unknown compound (like a potential new drug) may be identified by the resonant properties
- **medical diagnostic:** NMR metabolomics has been used in the identification of biomarker for cardiovascular diseases and risk stratification.

List advantages and disadvantages of NMR:

Advantages	Disadvantages
Highly reproducible	Poor sensitivity
Structural Details can be obtained	Needs well trained personnel to operate it
Non Destructive analysis	Expensive instrumentation
Easy sample preparation	Use of C13 NMR requires large sample volume
Can be used to study oxidation of lipid	

Summary

- Nuclear Magnetic Resonance (NMR) is a spectroscopy technique which is based on the absorption of electromagnetic radiation in the radio.
- The Principle of NMR The theory behind NMR comes from the spin of a nucleus and it generates a magnetic field.
- Interpitation of NMR can be assigned by several factors
- There are two types of NMR: 13C NMR and H1 MNR
- Comparison between Types of NMR property used to Compare: Detection, Method, Chemical Shift Range and Progression.
- Applications of NMR: Molecular interaction ,Metabolic proliferation ,Drug discovery and medical diagnostic

References:

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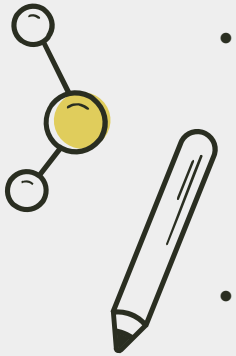

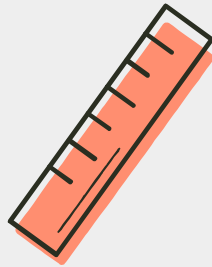

THANKS!

Do you have any questions?