

3.1 NUCLEAR MAGNETIC RESONANCE SPECTROMETER

- It is the study of absorption of radio frequency radiation by nuclei in a magnetic field.
- For a particular nucleus an NMR absorption spectrum may consist of one to several groups of absorption lines in the radio frequency regions of the electromagnetic spectrum.
- They indicate the chemical nature of the nucleus and spatial positions of neighbouring nuclei nuclear magnetic resonance spectrometry.
- It is recognized as one of the most powerful techniques for chemical analysis.
- The importance of this technique is reflected in the efforts that have been made to extend its applicability to smaller & smaller sample sizes.
- NMR spectrometer provides an accurate & non-destructive
- method of determining structure of liquids & stable chemical compounds.
- In NMR spectroscopy the characteristic absorption of energy by certain spinning nuclei in a strong magnetic field, when irradiated by a second and weaker field perpendicular to it permits the identification of atomic configurations of molecules.
- Absorption of energy occurs when these nuclei undergo transitions from one alignment in the applied field to another one.

THEORY OF NMR

- A radically different type of interaction between matter & electromagnetic forces can be observed by subjecting a substance simultaneously to two magnetic fields, one stationary & the other varying at some radio frequency.

- At a particular combinations of fields energy is absorbed by the sample & absorption can be observed as a change in signal developed by a radio frequency detector & amplifier.
- The energy absorption can be related to the magnetic dipolar nature of spinning nuclei. This technique is known as NMR.
- Radio waves are considered to be the lowest form of Electromagnetic radiation.
- This amount of energy is not sufficient to excite or vibrate or rotate an atom or molecule. The amount of energy available in radio frequency region is just sufficient to affect the nuclear spin of the atom in a molecule & hence constitute the most fundamental part of spectroscopy.

CHEMICAL SHIFT

- This is the phenomenon that occurs in which a specification i.e., a carbon or hydrogen atom in a given molecule resonates at a slightly different frequency based on its local chemical environment.
- In other words, the difference between the field necessary for resonance in the sample & in some arbitrarily chosen reference compound is called the chemical shift.
- For protons, it is usual to refer spectra to tetramethylsilane (TMSi) with extrapolation to infinite dilution in an inert solvent such as CCl₄. TMSi gives end of the range of observed proton shifts & therefore, it does not obscure any other proton lines arising from the sample.
- The chemical shift is expressed as

$$\delta = \frac{H_{\text{sample}} - H_{\text{TMSi}}}{H_1} \times 10^6$$

When,

- δ sample & δ HTM Si are the positions of the absorption peaks for the sample & reference material, respectively in Hz & ν is the radio frequency of the signal used.
- The chemical shift δ units is expressed in parts per million.

