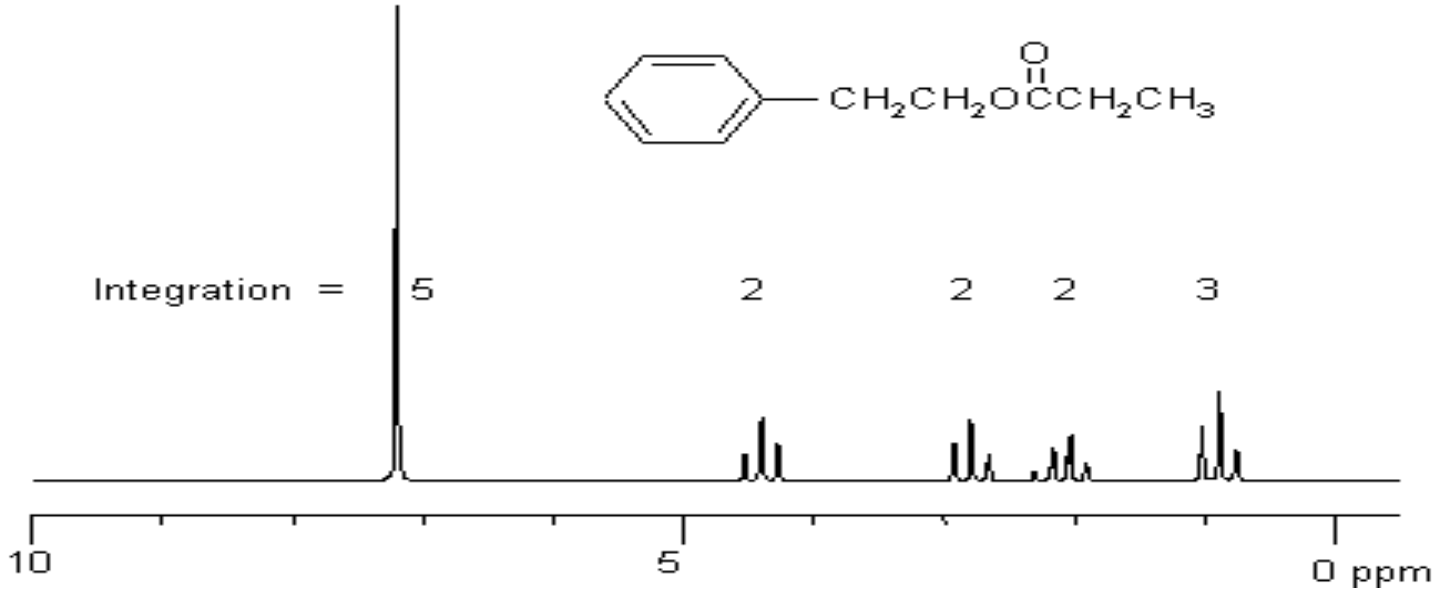
Nuclear Magnetic Resonance SPECTROSCOPY



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INTRODUCTION

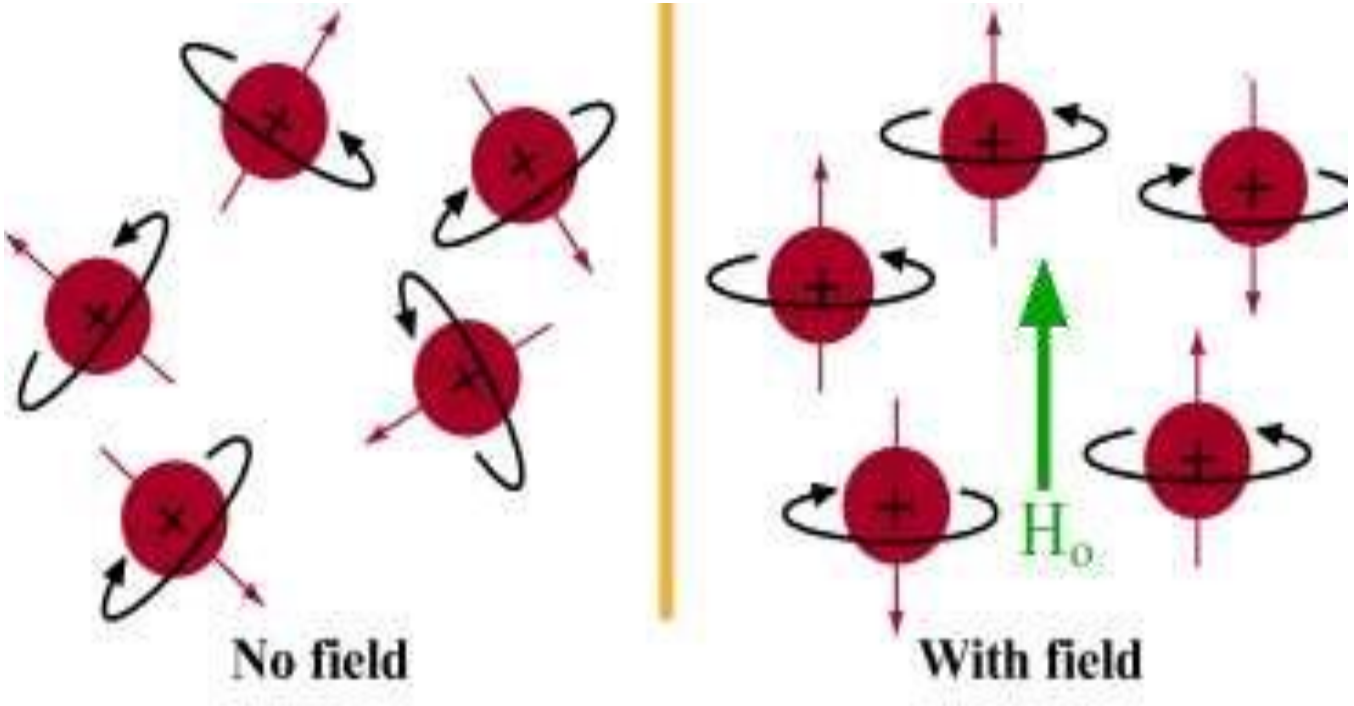
- Nuclear magnetic resonance spectroscopy(NMR) is a powerful analytical technique used to characterize organic molecules by identifying carbon-hydrogen frameworks within molecules.
- It is a research technique that exploits the magnetic properties of certain atomic nuclei. It is a spectroscopy technique which is based on the absorption of electromagnetic radiation in the radio frequency region 4 to 900 MHz by nuclei of the atoms. When low-energy radio waves interact with a molecule, they can change the nuclear spins of some elements, including ^{1}H and ^{13}C..
- It determines the physical and chemical properties of atoms or the molecules in which they are contained.

Types -

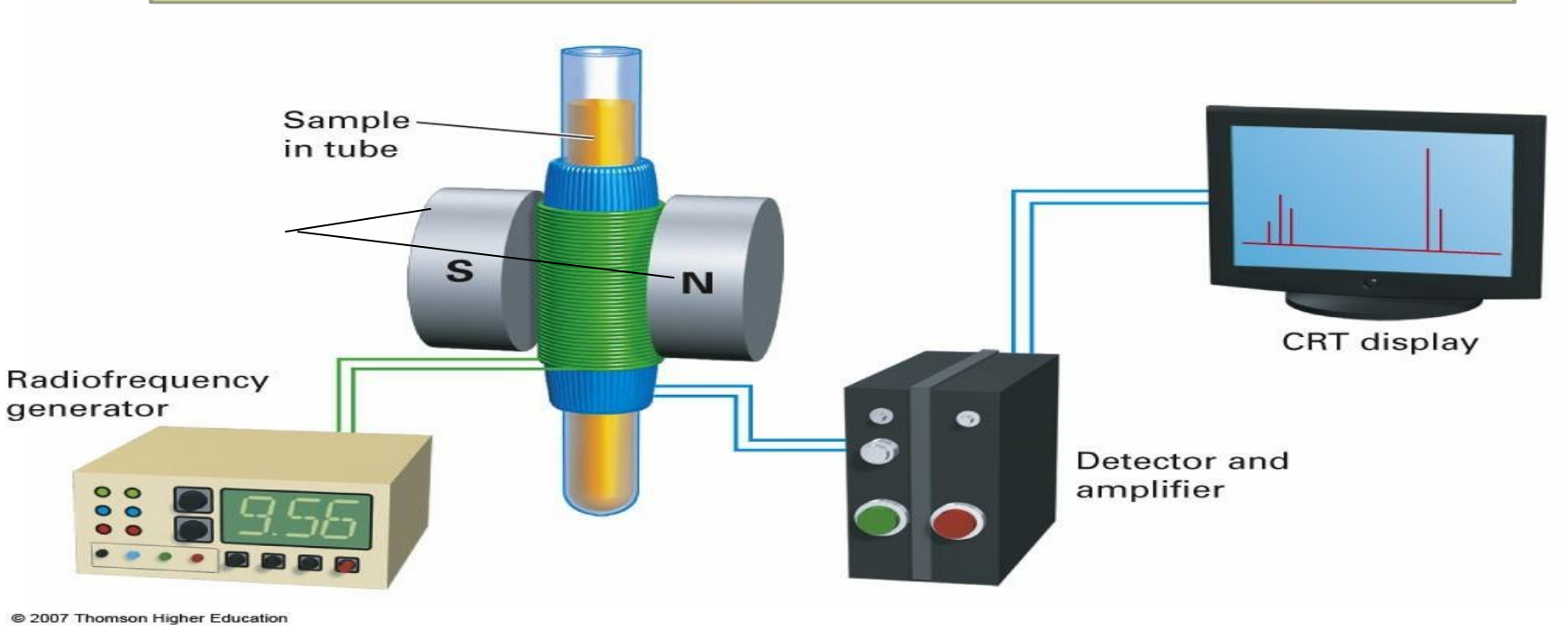
- Two common types of NMR spectroscopy are used to characterize organic structure:
- ^{1}H NMR:- Used to determine the type and number of H atoms in a molecule
- ^{13}C NMR:- Used to determine the type of carbon atoms in the molecule

Theories 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. In a magnetic field, there are now two energy states for a proton: a lower energy state with the nucleus aligned in the same direction as B_o, and a higher energy state in which the nucleus aligned against B_o.



Schematic diagram of NMR set-up



- The sample is dissolved in a solvent, usually $CDCl_3$(deutero-chloroform), and placed in a magnetic field. A radiofrequency generator then irradiates the sample with a short pulse of radiation, causing resonance. When the nuclei fall back to their lower energy state, the detector measures the energy released and a spectrum is recorded.
- Modern NMR spectrometers use a constant magnetic field strength B_0, and then a narrow range of frequencies is applied to achieve the resonance of all protons.

- Only nuclei that contain odd mass numbers (such as ^{1}H, ^{13}C, ^{19}F and ^{31}P) or odd atomic numbers (such as ^{2}H and ^{14}N) give rise to NMR signals.

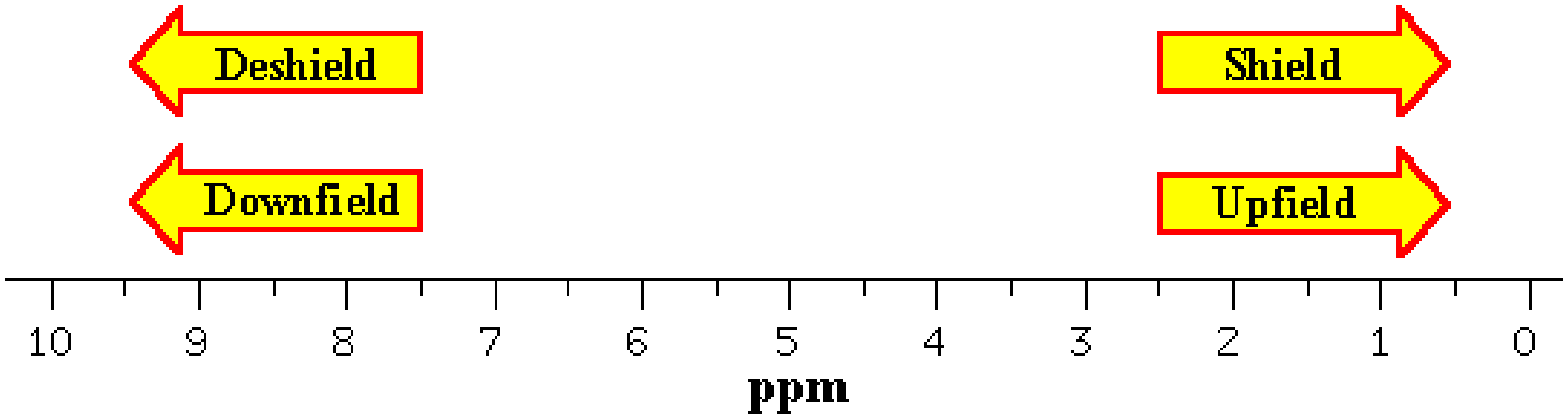
CHEMICAL SHIFT

The relative energy of resonance of a particular nucleus resulting from its local environment is called chemical shift. NMR spectra show applied field strength increasing from left to right. Left part is downfield, the right is upfield.

Nuclei that absorb on up field side are strongly shielded where nuclei that absorb on downfield side is weakly shielded. Chart is calibrated versus a reference point, set as 0, tetramethylsilane [TMS].

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



APPLICATIONS

- Nuclear magnetic resonance spectroscopy basically provides the detailed information about the structure, dynamics, reaction state, and chemical environment of molecules.
- It has various applications in food industries, food science, chemical analysis of different products, pharmaceutical approach etc.
- To analyse the carbon-hydrogen framework in the molecule is the basic work of NMR technique.

- **Application in medicine**
  - Anatomical imaging
  - Measuring physiological function
  - Flow measurement and angiography
  - Tissue perfusion studies
  - Tumors
  - MRI