



# NUCLEAR MAGNETIC RESONANCE

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# INTRODUCTION

- Nuclear Magnetic Resonance (NMR) spectroscopy is an analytical technique used in quality control and research for determining the content and purity of a sample as well as its molecular structure.
- It is a technique that exploits the magnetic properties of nuclei.
- It determines the physical and chemical properties of atoms or the molecules in which they are contained.

# PRINCIPLE

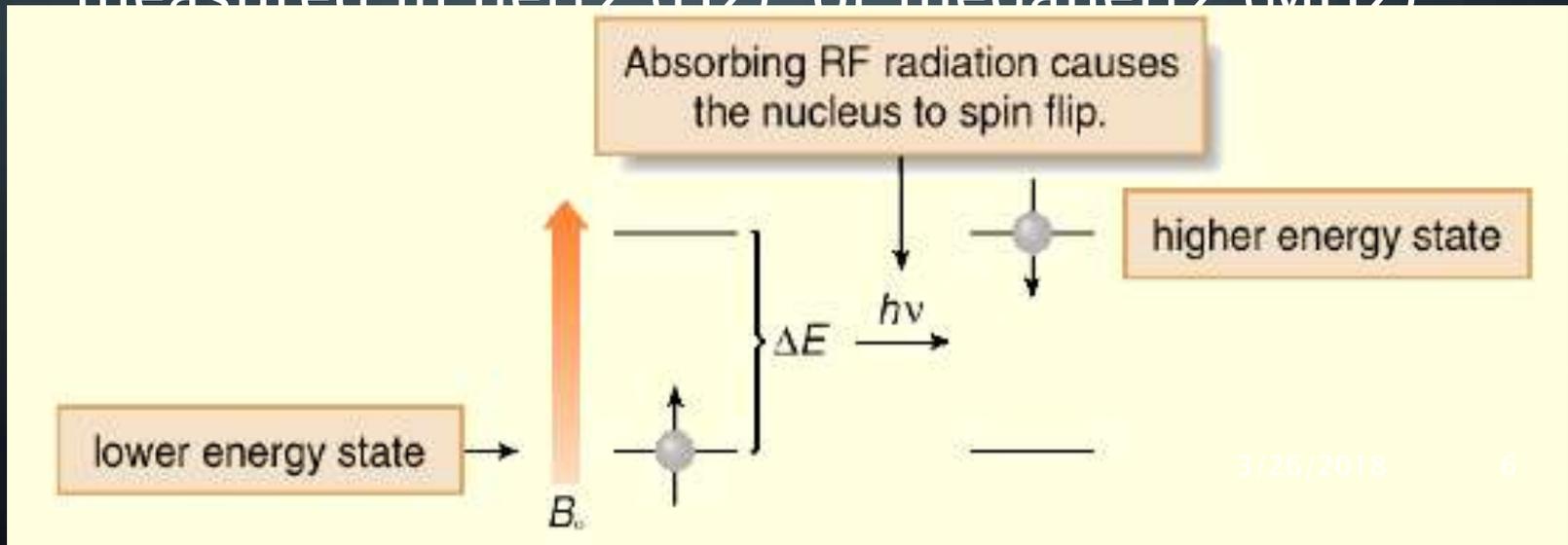
- The principle behind NMR is that many nuclei have spin and all nuclei are electrically charged. If an external magnetic field is applied, an energy transfer is possible between the base energy to a higher energy level (generally a single energy gap). The energy transfer takes place at a wavelength that corresponds to radio frequencies and when the spin returns to its base level, energy is emitted at the same frequency.
- The signal that matches this transfer is measured in many ways and processed in order to yield an NMR spectrum for the nucleus concerned.

# THEORY OF NMR

- When a charged particle such as a proton spins on its axis, it creates a magnetic field. Thus, the nucleus can be considered to be a tiny bar magnet.
- Normally, these tiny bar magnets are randomly oriented in space. However, in the presence of a magnetic field  $B_0$ , they are oriented with or against this applied field.
- In a magnetic field ( $B_0$ ), there are now two energy states for a proton: a lower energy state with the nucleus aligned in the same direction as  $B_0$ , and a higher energy state in which the nucleus aligned against  $B_0$ .

# CONTI...

- Thus, two variables characterize NMR: an applied magnetic field  $B_0$ , the strength of which is measured in tesla (T), and the frequency ( $\nu$ ) of radiation used for resonance, measured in hertz (Hz) or megahertz (MHz)



# CONTI..

- The frequency needed for resonance and the applied magnetic field strength are proportionally related:

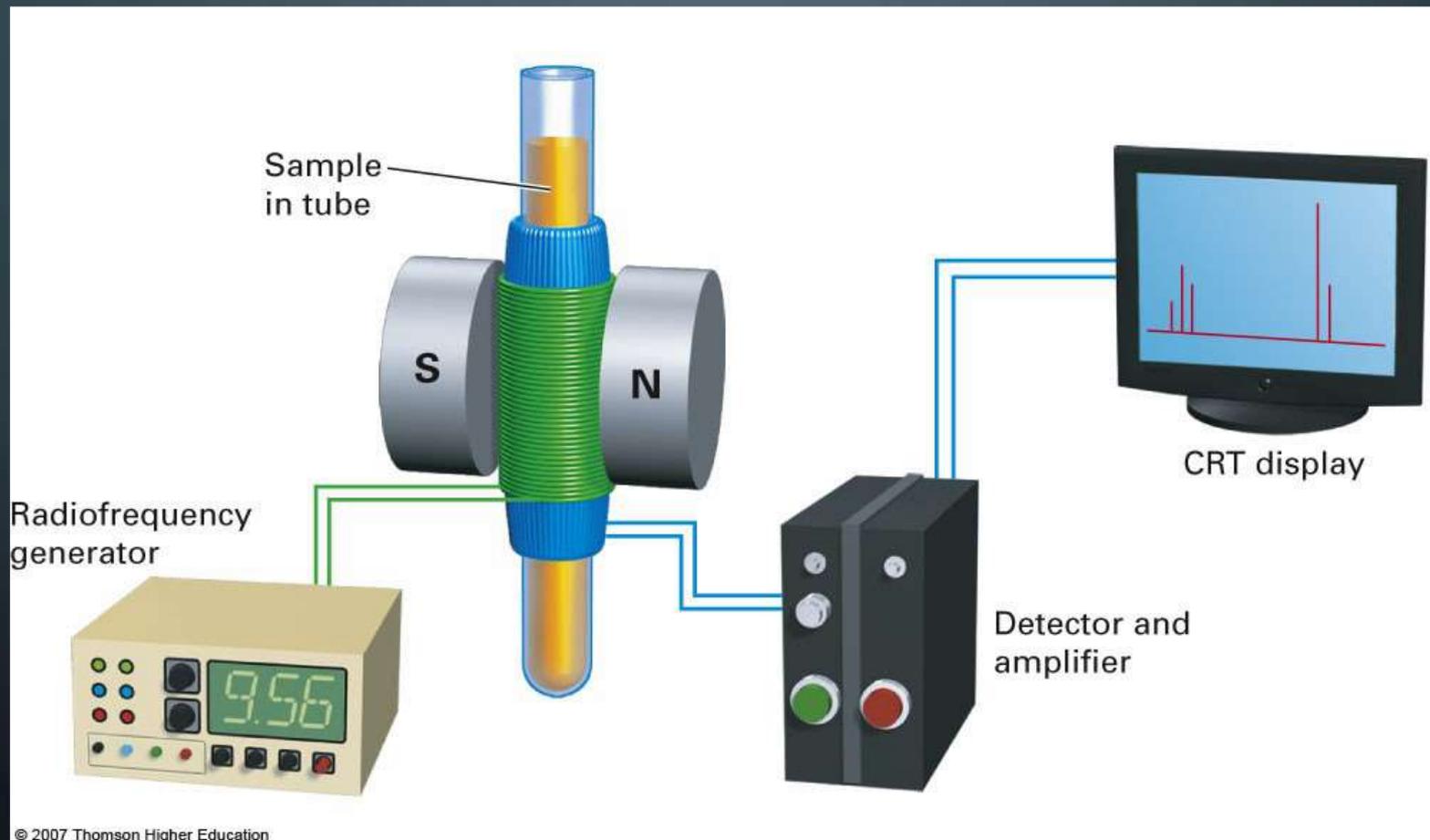
$$\nu \propto B_0$$

- The stronger the magnetic field, the larger energy difference between two nuclear spin states and higher the  $\nu$  needed for the resonance.

# TYPES OF SAMPLES

- Both liquid and solid type of samples can be used in NMR spectroscopy.
- In solid-phase media, samples like crystals, microcrystalline powders, gels, anisotropic solutions, proteins, protein fibrils or all kinds of polymers etc can be used.
- In liquid phase, different types of liquid solutions, nucleic acid, protein, carbohydrates etc. can be used.

# SCHEMATIC DIAGRAM FOR NMR SETUP



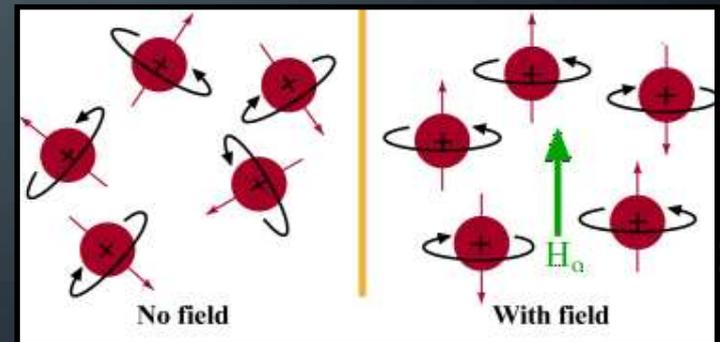
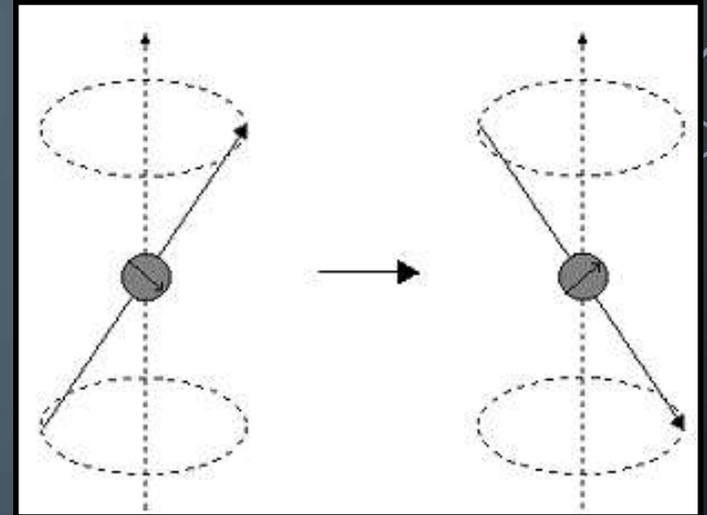
# MAGNETIC PROPERTIES OF NUCLEI

- Nuclei of certain isotopes possess a mechanical spin, or angular momentum. The total angular momentum depends on nuclear spin or spin number  $I$ , which has values of  $0, 1/2, 1, 3/2, \dots$
- The numerical value of spin number  $I$  is related to the mass number and the atomic number.

Mass no.	Atomic no.	Spin no. $I$
odd	even or odd	$1/2, 3/2, 5/2, \dots$
even	even	0
even	odd	$1, 2, 3, \dots$

- Atomic charge is associated with atomic nucleus, the spinning of nucleus gives rise to magnetic field whose axis is coincident with axis of spin.

- Each nucleus for which  $I > 0$  will have characteristic magnetic moment.
- Quantised system
- $(2I+1)$  orientation.
- The nuclear magnet is oriented exactly parallel or antiparallel with the applied magnetic field. But because the nucleus is spinning, its rotational axis draws out circle perpendicular to the applied field. This motion of nucleus is called as precession.



# NUCLEAR RESONANCE

- A proton in a static magnetic field may assume only two orientations corresponding to energies  $+/- \mu H$ . The low energy orientation and high energy orientation.
- The precessional frequency of the spinning nucleus is exactly equal to the frequency of electromagnetic radiation necessary to induce a transition from one nuclear spin state to another.
- When the frequency of rotating magnetic field and the frequency of precessing nucleus becomes equal they are said to be in resonance.
- Spontaneous transition from higher energy state to lower energy state is negligible in radio frequency region.

# CHEMICAL SHIFT

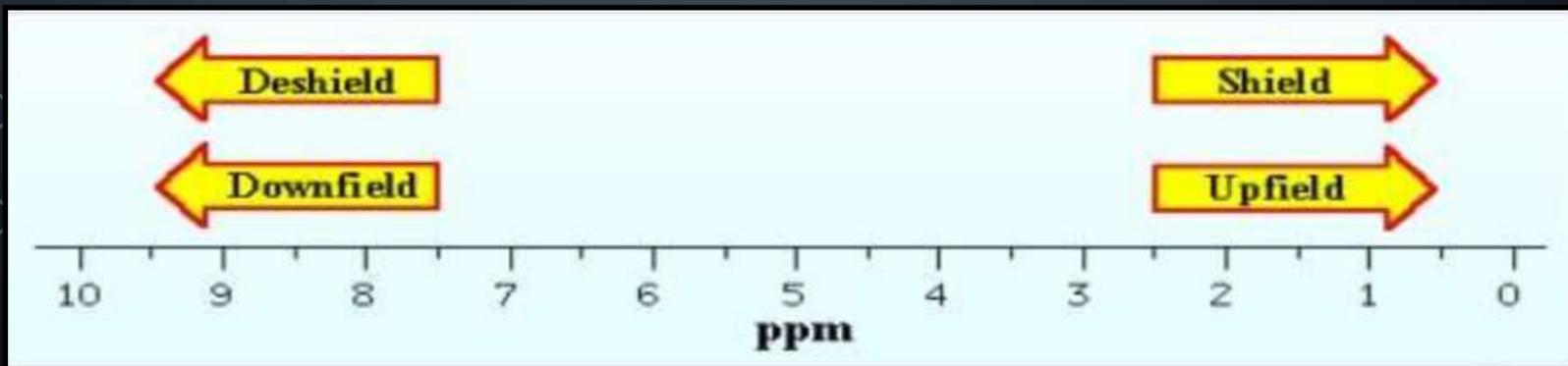
- A chemical shift is defined as the difference in parts per million (ppm) between resonance frequency of observed proton to tetraethylsilane (TMS) hydrogen.
- TMS is common reference standard used in NMR, it is set at  $\delta=0$  ppm.

- **Shielding**

High electron density around the nucleus shields the nucleus from external magnetic field and the signals are upfield in the NMR spectrum.

- **Deshielding**

Lower electron density around the nucleus deshields the nucleus from external magnetic field and the signals are downfield in the NMR spectrum



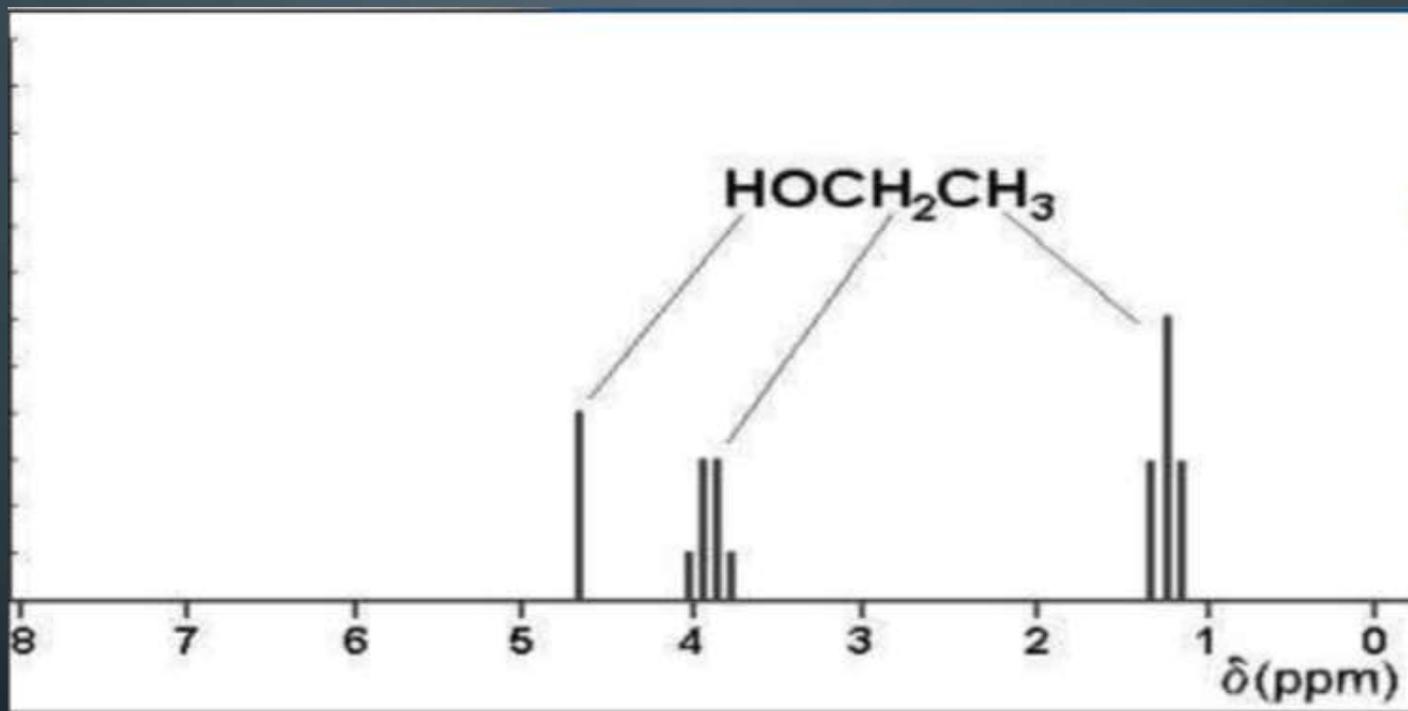
# FACTORS AFFECTING CHEMICAL SHIFT

- Electronegative group
- Electronegative group attached to C–H system decreases the electron density around the proton and there is less shielding thus chemical shift increases.
- Magnetic anisotropy
- Hydrogen bonding

# PROTON NMR

- The most common form of NMR is based on the hydrogen nucleus.
- It can give information of any molecule containing hydrogen atom.

# NMR spectra of Ethanol



# APPLICATIONS

## ❖ Chemistry

- By studying the peaks of nuclear magnetic resonance spectra, chemists can determine the structure of many compounds.
- It can be a very selective technique, distinguishing among many atoms within a molecule or collection of molecules of the same type but which differ only in terms of their local chemical environment.
- NMR spectroscopy is used to unambiguously identify known and novel compounds, and as such, is usually required by scientific journals for identity confirmation of synthesized new compounds
- The detailed investigation includes
  - Identification of structural isomers
  - Detection of hydrogen bonding
  - Detection of aromaticity
  - Detection of electronegative atom or group
- Purity determination (w/w NMR)
  - NMR is primarily used for structural determination, however it can also be used for purity determination, providing that the structure and molecular weight of the compound is known. This technique requires the use of an internal standard of a known purity

## ❖ Medicine

- useful for identifying drug leads and determining the conformations of the compounds bound to enzymes, receptors, and other proteins.
- best known application of nuclear magnetic resonance to the general public is **magnetic resonance imaging** for medical diagnosis and magnetic resonance microscopy in research settings
  - MRI scanners use strong magnetic fields, electric field gradients, and radio waves to generate images of the organs in the body
  - In most medical applications, protons (hydrogen atoms) in tissues containing water molecules create a signal that is processed to form an image of the body.
  - Each subatomic particle, such as a proton, has a certain level of spin.
  - By adjusting the magnetic field surrounding these subatomic particles, the spin rate is altered.
  - As the spin returns to normal, the MRI machine is able to determine its location.
  - By locating a plethora of these subatomic particles, an image of tissues can be developed, giving researchers a picture of the subject's particular area



## OTHER

### ❖ Data acquisition in the petroleum industry

- Another use for nuclear magnetic resonance is data acquisition in the petroleum industry for petroleum and natural gas exploration and recovery.
- A borehole is drilled into rock and sedimentary strata into which nuclear magnetic resonance logging equipment is lowered.
- Nuclear magnetic resonance analysis of these boreholes is used to measure rock porosity, estimate permeability from pore size distribution and identify pore fluids (water, oil and gas)

### ❖ To study molecular structure and interactions and for determining 3D structure of proteins and other macromolecules. Moreover, in Polymer production, cosmetics and food manufacturing

### ❖ Process control

- NMR has now entered the arena of real-time process control and process optimization
- different types of NMR analysis are utilized to provide real time analysis of feeds and products in order to control and optimize unit operation

## PROS AND CONS OF NMR SPECTROSCOPY

Advantages	Disadvantages
Provides high resolution information	Requires high concentrations of soluble protein
Does not require a protein crystal and is not affected by crystal contacts	Can not be applied to large proteins (800kD max so far)
Can be used to study flexible proteins	Can not be used with amyloid fibril
conformational structure	

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