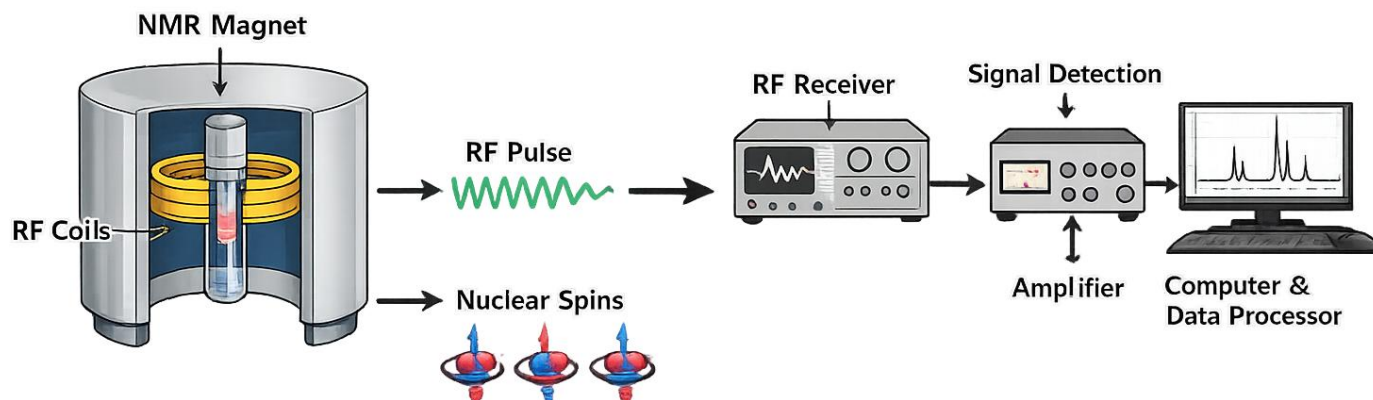


NMR Spectroscopy

NMR Spectroscopy

- **Nuclear Magnetic Resonance (NMR)** spectroscopy is an analytical technique used to study the structure of molecules, especially organic compounds.



- It gives detailed information about how atoms (mainly hydrogen and carbon) are arranged in a molecule.

Basic Idea

- Certain atomic nuclei behave like tiny magnets.
- When these nuclei are placed in a strong external magnetic field, they align in specific ways.
- When radiofrequency (RF) radiation is applied, these nuclei absorb energy and change their orientation.
- This absorption is detected and converted into a spectrum.

Nuclei That Show NMR

- Not all Nuclei give NMR signals. Only those with **spin ($I \neq 0$)** are active.
- **Examples:**
 - ^1H (proton)
 - ^{13}C
 - ^{19}F
 - ^{31}P
- **Do not show NMR:**
 - ^{12}C (spin = 0)

Why NMR is Important

- Determines structure of compounds
- Identifies number of different types of hydrogen or carbon atoms
- Gives information about neighboring atoms

Quantum Numbers and Their Role in NMR

Introduction to NMR

- Nuclear Magnetic Resonance (NMR) spectroscopy studies the behavior of atomic nuclei in a magnetic field.
- It is widely used to determine molecular structure.

What are Quantum Numbers?

- Quantum numbers describe the properties and behavior of particles such as atomic nuclei.
- In NMR, the most important quantum numbers are:
 - Spin Quantum Number (I)
 - Magnetic Quantum Number (m)

Spin Quantum Number (I)

Definition

- Represents the intrinsic angular momentum (**spin**) of a nucleus.
- Possible values: **0, 1/2, 1, 3/2, etc.**

Rules for Spin Values

- If mass number and atomic number are both **even** → $I = 0$ → NMR inactive
- If mass number is **odd** → $I \neq 0$ → NMR active

Examples

- $^1\text{H} \rightarrow I = 1/2 \rightarrow$ NMR active
- $^{13}\text{C} \rightarrow I = 1/2 \rightarrow$ NMR active
- $^{12}\text{C} \rightarrow I = 0 \rightarrow$ NMR inactive

Importance

- Only nuclei with $I \neq 0$ can be detected in NMR.
- These nuclei behave like **tiny magnets**.

Magnetic Behavior of Nuclei

- Nuclei with spin acts like small magnetic dipoles.
- In an external magnetic field:
 - Aligned with field → Low energy state
 - Opposed to field → High energy state

Magnetic Quantum Number (m)

Definition

- Describes the orientation of a nucleus in a magnetic field.

Possible Values

- For a given spin (l): $m = +l, +l-1, \dots, -l$

Example ($l = 1/2$)

- $m = +1/2 \rightarrow$ aligned with field
- $m = -1/2 \rightarrow$ opposed to field

Number of Orientations

- **Formula:** Number of orientations = $2l + 1$
- **Example:**
 - For $l = 1/2 \rightarrow 2$ orientations

Energy Levels in Magnetic Field

- **Without Magnetic Field**
 - Energy levels are equal (degenerate)
- **With Magnetic Field**
 - Energy levels split into different states
 - This phenomenon is called: Zeeman Splitting

Two Energy States (for $l = 1/2$)

- Lower energy $\rightarrow$ aligned with field
- Higher energy $\rightarrow$ opposed to field

Energy Difference

- **Given by:** $\Delta E = h\nu$
- **Where:**
 - ΔE = Energy difference
 - h = Planck's constant
 - ν = Frequency

Resonance Condition

- When **radiofrequency (RF) radiation** = ΔE :
 - Nucleus absorbs energy
 - **Transition occurs from:** lower $\rightarrow$ higher energy state

Importance in NMR

- NMR measures these energy transitions.
- **This allows scientists to:**
 - Identify atoms
 - Determine molecular structure

Principle of NMR Spectroscopy

- NMR spectroscopy is based on the absorption of radiofrequency radiation by nuclei in a magnetic field.

Basic Concept

- A sample is placed in a strong magnetic field
- **Nuclei align in two orientations:**
 - With the field → Low energy
 - Against the field → High energy
- Radiofrequency (RF) radiation is applied
- Nuclei absorb energy and change orientation
- This absorption is detected and recorded

Step-by-Step Explanation

- Sample is placed in magnetic field
- Nuclei align in different energy states
- RF radiation is applied
- **When frequency matches energy difference:**
 - Absorption occurs (resonance)
- Nuclei move from lower → higher energy state
- Signal is recorded to produce spectrum

Resonance Condition

$$\nu = \frac{\gamma B_0}{2\pi}$$

- **Where:**
 - ν = Frequency (Larmor frequency)
 - γ = Gyromagnetic ratio
 - B_0 = Magnetic field strength

Larmor Frequency

- Frequency at which nuclei absorb radiation
- **Depends on:**
 - Type of nucleus
 - Strength of magnetic field

Important Points

- Different nuclei absorb at different frequencies
- Chemical environment affects absorption frequency
- Leads to chemical shift

Result

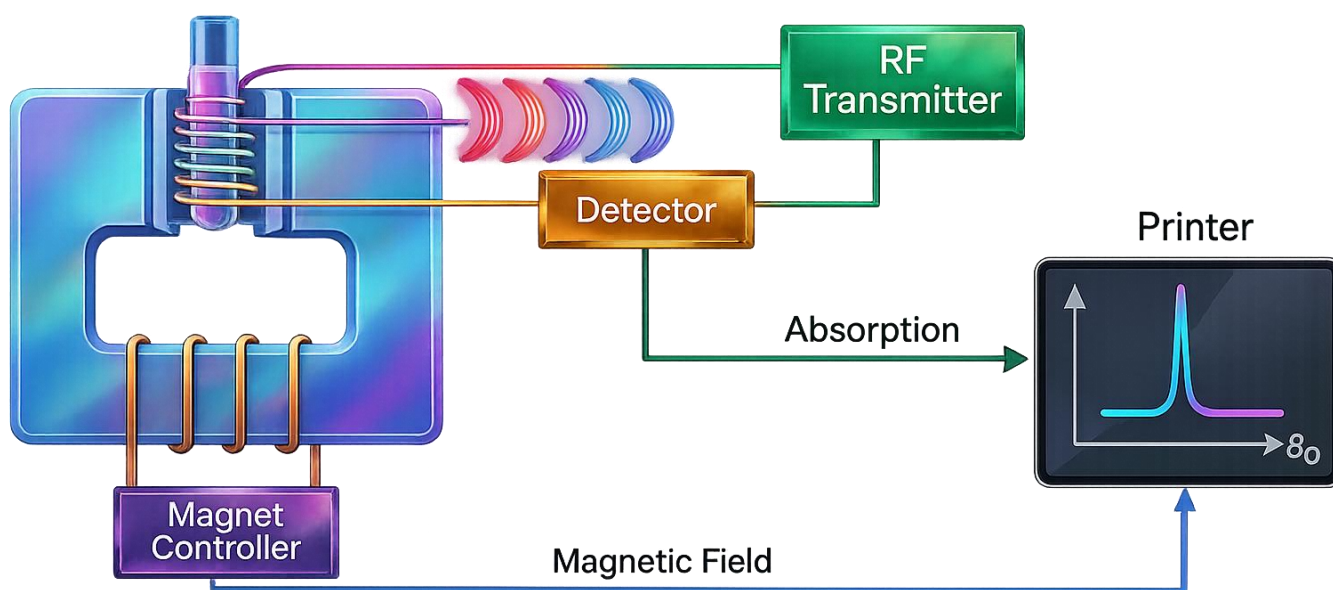
- NMR spectrum is obtained
- Shows signals corresponding to different nuclei
- Helps in structure determination

Key Concept (Chemical Shift)

- Nuclei in different chemical environments absorb at slightly different frequencies
- This difference is called **chemical shift**
- Used to identify molecular structure

Instrumentation of NMR Spectroscopy

- An NMR spectrometer consists of several important components.



1. Magnet

- Provides strong and uniform magnetic field



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