NMR Spectroscopy

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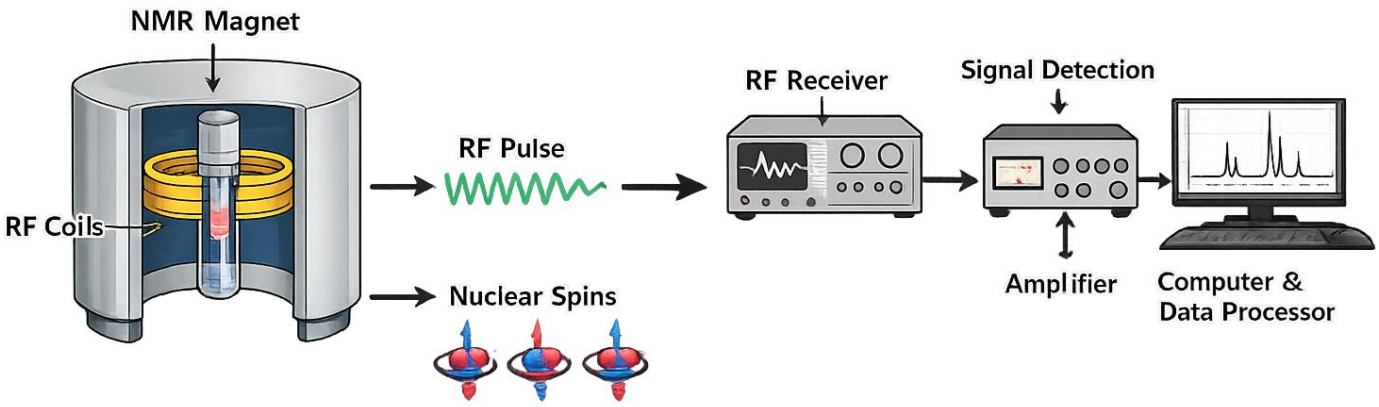
- **Nuclear Magnetic Resonance (NMR)** spectroscopy is an analytical technique used to study the structure of molecules, especially organic compounds.



- 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 ≠ 0)** are active.
- **Examples:**
  - ^{1}H (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

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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 ≠ 0** → NMR active

Examples

- ^{1}H → I = 1/2 → NMR active
- ^{13}C → I = 1/2 → NMR active
- ^{12}C → I = 0 → NMR inactive

Importance

- Only nuclei with **I ≠ 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)

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Definition

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

Possible Values

- For a given spin (I): **m = +I, +I−1, … , −I**

Example (I = 1/2)

- m = +1/2 → aligned with field
- m = −1/2 → opposed to field

Number of Orientations

- **Formula:** Number of orientations = 2I + 1
- **Example:**
  - For I = 1/2 → 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 I = 1/2)

- Lower energy → aligned with field
- Higher energy → opposed to field

Energy Difference

- **Given by:** ΔE = hv
- **Where:**
  - ΔE = Energy difference
  - h = Planck's constant
  - v = Frequency

Resonance Condition

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

Importance in NMR

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- 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

First Hope

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

Larmor Frequency

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- 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

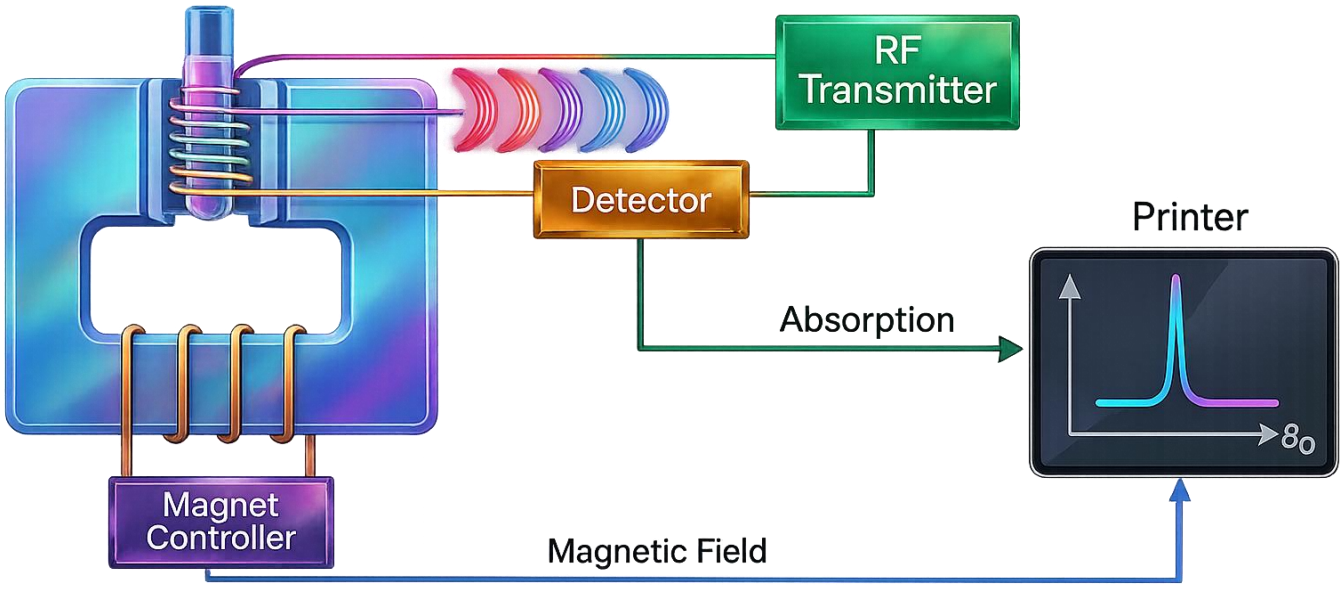
Key Concept (Chemical Shift)

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

First Hope

Instrumentation of NMR Spectroscopy

- An NMR spectrometer consists of several important components.



1. Magnet

- Provides strong and uniform magnetic field

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