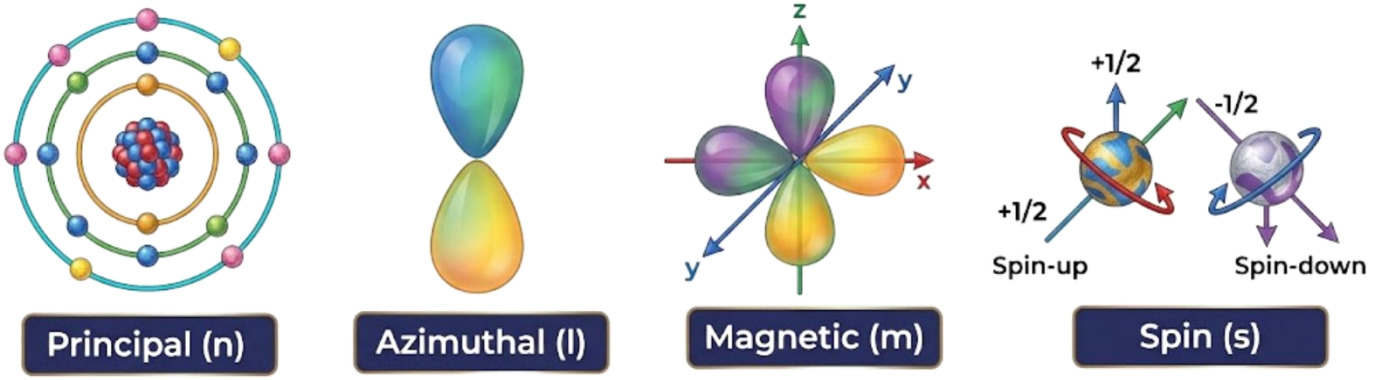
NMR Spectroscopy

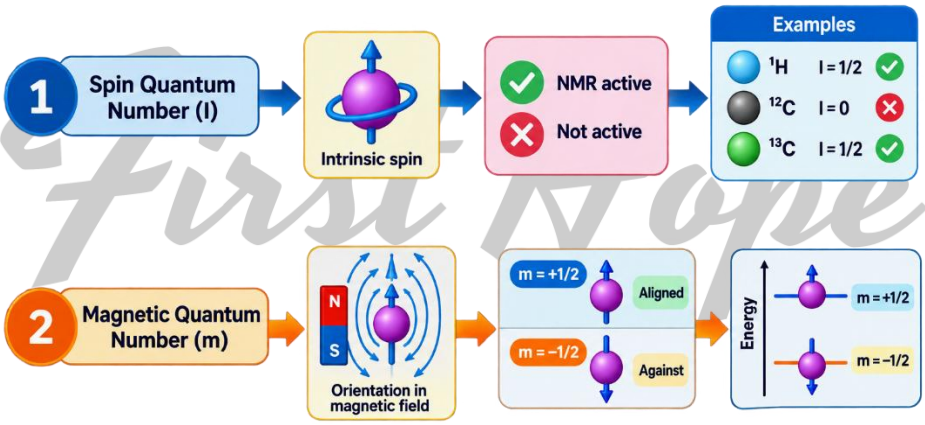
Quantum Numbers and Their Role in NMR

Definition

- Quantum numbers describe the **energy states and orientation of nuclei** in a magnetic field.



Types of Quantum Numbers in NMR



1. Spin Quantum Number (I)

- Describes intrinsic spin of nucleus
- Determines whether nucleus is NMR active
- **Example:**
  - $^{1}H \rightarrow I = 1/2$
  - $^{12}C \rightarrow I = 0$ (inactive)
  - $^{13}C \rightarrow I = 1/2$ (active)

2. Magnetic Quantum Number (m)

- Describes orientation of nucleus in magnetic field
- **Values:**
  - m = +1/2 (aligned with field)
  - m = −1/2 (against field)

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Role in NMR

- In absence of magnetic field → energy levels are equal
- In presence of magnetic field:
  - Energy levels split (Zeeman splitting)
- Transition between these levels gives **NMR signal**

Energy Difference

- **Depends on:**
  - Strength of magnetic field
  - Type of nucleus

Importance

- Only nuclei with non-zero spin show NMR
- Determines number of signals and transitions

Principle of NMR Spectroscopy

Basic Principle

- NMR (Nuclear Magnetic Resonance) is based on the **absorption of radiofrequency (RF) radiation by nuclei** when placed in a **strong magnetic field**.

Working Mechanism

- Nuclei (like ^{1}H, ^{13}C) behave like tiny magnets
- **When placed in an external magnetic field:**
  - They align either:
    - **With the field** (low energy state)
    - **Against the field** (high energy state)
- When **radiofrequency (RF) radiation** is applied:
  - Nuclei absorb energy
  - Transition from low energy → high energy state

Resonance Condition

- **Occurs when:**
  - Frequency of RF radiation = energy difference between two energy levels
- This matching condition is called **resonance**

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Signal Detection

- Absorbed energy is detected by the instrument
- Converted into an NMR spectrum

Effect of Chemical Environment

- Different nuclei absorb at different frequencies
- Depends on electron density around the nucleus

Shielding and Deshielding

A. Shielded nuclei

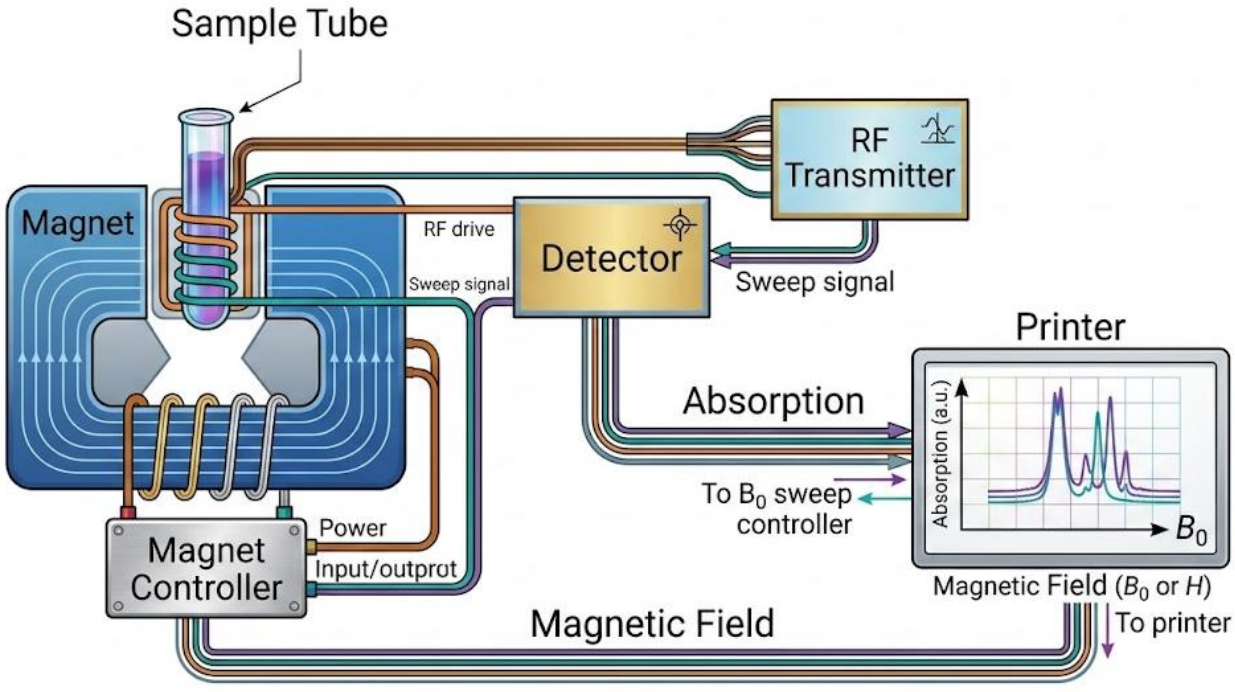
- More electron density
- Absorb at **higher field (upfield)**

B. Deshielded nuclei

- Less electron density
- Absorb at **lower field (downfield)**

Instrumentation of NMR Spectroscopy

Components



1. Magnet

- Produces a strong and uniform magnetic field

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- **Types:**
  - Permanent magnet
  - Superconducting magnet (most commonly used)

2. Radiofrequency (RF) Transmitter

- Generates radiofrequency radiation
- Causes excitation of nuclei

3. Sample Holder

- Thin glass tube containing sample
- Rotates to ensure uniform exposure to magnetic field

4. Probe

- Contains RF **coils**
- **Functions:**
  - Transmits RF radiation
  - Detects signals from nuclei

5. Detector / Receiver

- Detects emitted signals from excited nuclei
- Converts them into electrical signals

6. Computer / Data System

- Processes signals to produce NMR spectrum
- Performs Fourier Transform (FT-NMR) for signal analysis

7. Solvent System

- Uses deuterated solvents (e.g., $CDCl_3$, D_2O)
- Prevents interference from solvent signals

Working Summary

1. Sample is placed in a strong magnetic field
2. RF radiation is applied → nuclei get excited
3. Nuclei emit signals when returning to ground state
4. Signals are detected and processed
5. Final output is an NMR spectrum

Key Point

- Modern NMR uses **FT-NMR (Fourier Transform)** for **fast and accurate signal processing**

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Solvent Requirement in NMR

Need for Solvent

- Sample must be in **liquid form** for NMR analysis
- **Solvent help:**
  - Dissolve the sample
  - Provide a uniform environment

Requirements of an Ideal Solvent

- Chemical inert (does not react with sample)
- Should completely dissolve analyte
- Should not produce interfering signals

Deuterated Solvents

- Hydrogen (^{1}H) is replaced by **deuterium (^{2}H)**
- **Examples**
  - **$CDCl_3$** (deuterated chloroform)
  - **D_2O** (deuterated water)
  - **DMSO-d_6**

First Hope

Why Deuterated Solvents Are Used

- Deuterium does not interfere in ^{1}H NMR
- Provides field frequency lock
- Reduces background signals

Residual Peaks

- Small peaks may appear due to **incomplete deuteration**

Importance

- Ensures **clear and accurate spectrum**
- Prevents **overlapping of signals**

Relaxation Process in NMR

Definition

- Relaxation is the process by which **excited nuclei return to their ground state** after absorbing RF energy.

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