Mass spectrometry

Principle of Mass Spectrometry

Definition

- Mass spectrometry (MS) is an analytical technique used to **determine molecular weight and structure** of compounds by measuring **mass-to-charge ratio (m/z)**.

Basic Principle

- A sample is converted into **charged ions**.
- These ions are separated based on their **mass-to-charge ratio (m/z)**.
- Detector records ions and produces a **mass spectrum**.

Steps Involved

- Ionization of sample
- Separation of ions
- Detection of ions

Mass Spectrum

- **Graph of:**
  - m/z (x-axis)
  - Intensity (y-axis)
- **Important peaks:**
  - **Molecular ion peak (M^+)** → gives molecular weight
  - **Base peak** → most intense peak

Working Concept

- Lighter ions → reach detector faster
- Heavier ions → reach slower

Applications

- Molecular weight determination
- Structural elucidation
- Identification of unknown compounds

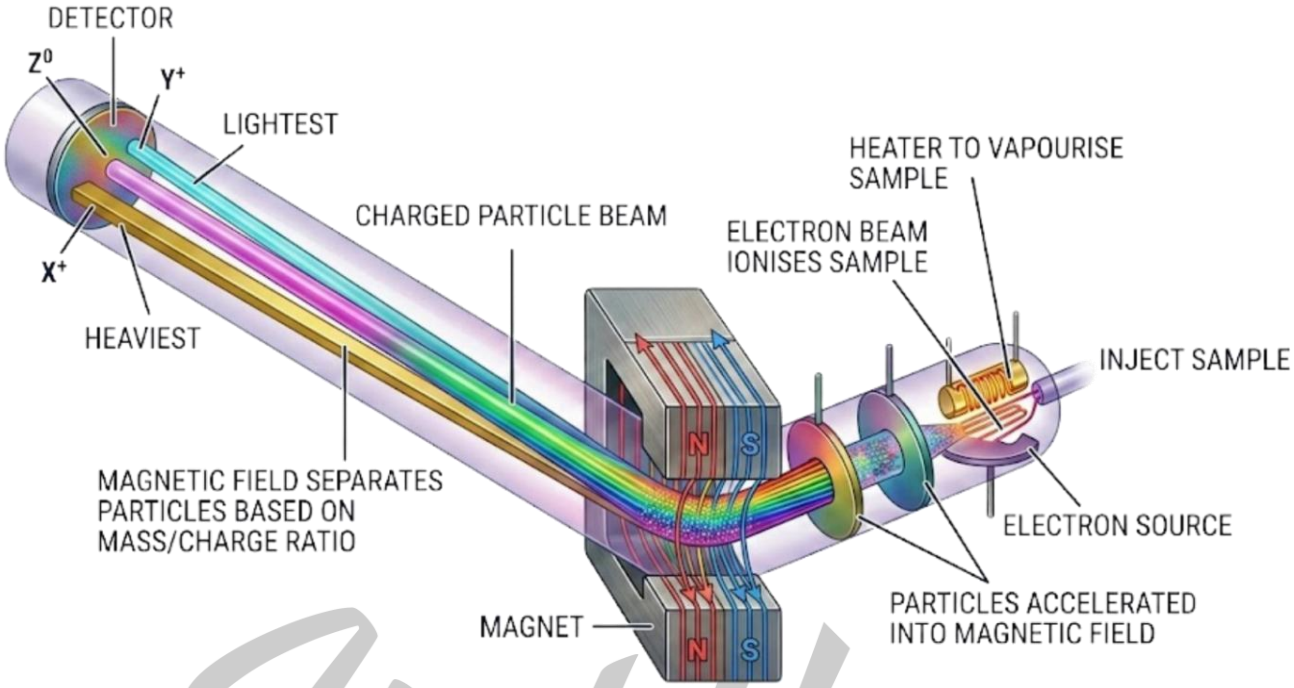
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Theory of Mass Spectrometry

Basic Concept

- **Mass** spectrometry is an analytical technique used to identify compounds based on their mass-to-charge ratio (m/z).



Ion Formation

- **Neutral** molecules are converted into **ions**:
  - **Positive ions** (most common)
  - **Negative ions**
- This process is called **ionization**

Mass-to-Charge Ratio (m/z)

- Fundamental parameter in MS
- m= mass of ion
- z= charge of ion
- Determines **position of peak in spectrum**

Molecular Ion (M^+)

- Formed by removal of one electron
- Represents the intact molecule
- Gives molecular weight of compound

Fragmentation

- Molecular ion breaks into smaller ions (fragments)

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- Produces a fragmentation pattern
- Helps in structure determination

Base Peak

- Most intense peak in spectrum
- Assigned **100% intensity**
- Represents the most stable fragment ion

Isotopic Peaks

- Arise due to natural isotopes (e.g., Cl, Br)
- Appear at higher m/z values
- Useful for element identification

Resolution

- Ability to distinguish between closely spaced m/z values
- Higher resolution → better separation of peaks

Accuracy

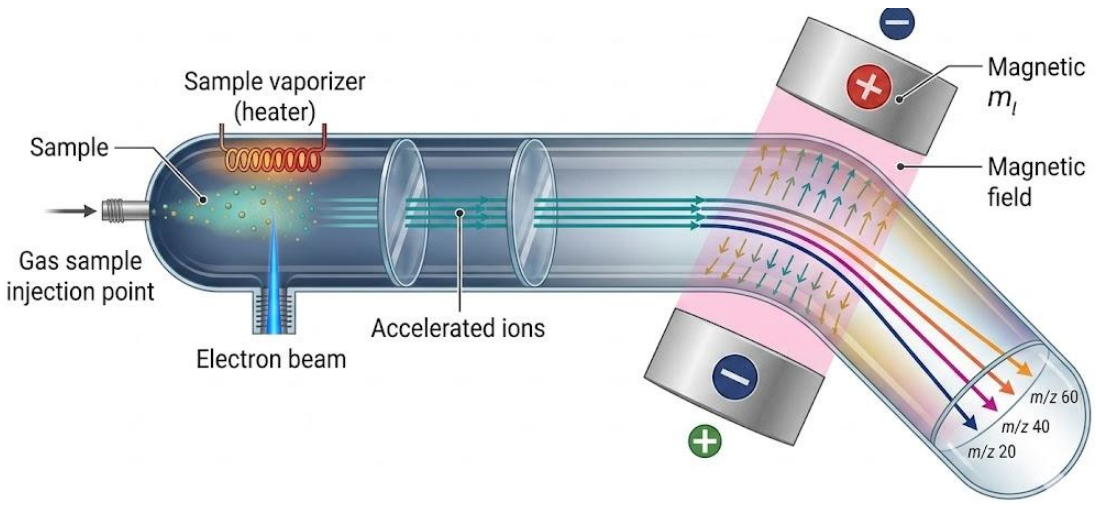
- How close the measured mass is to the true mass
- Important for exact mass determination

Importance

- Provides detailed structural information
- Helps in identifying unknown compounds
- Widely used in pharmaceutical, chemical, and biological analysis

Instrumentation of Mass Spectrometry

Components



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1. Sample Introduction System

- Introduces sample into the **ion source**
- **Can handle:**
  - Gases
  - Liquids
  - Solids

2. Ion Source

- Converts sample molecules into **ions**
- **Common Types:**
  - Electron Impact (EI)
  - Chemical Ionization (CI)
  - Electrospray Ionization (ESI)
  - MALDI (Matrix-Assisted Laser Desorption Ionization)

3. Mass Analyzer

- Separates ions based on mass-to-charge ratio (m/z)
- **Examples:**
  - Quadrupole
  - TOF
  - Ion trap

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4. Detector

- Detects ions after separation
- Converts them into electrical signals

5. Vacuum System

- Maintains high vacuum conditions
- Prevents collision of ions with air molecules
- Ensures accurate ion movement

6. Data System

- Records and processes signals
- Produces the mass spectrum
- Provides peak analysis

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Working Summary

- **Sample → Ionization → Separation → Detection → Spectrum**

Importance

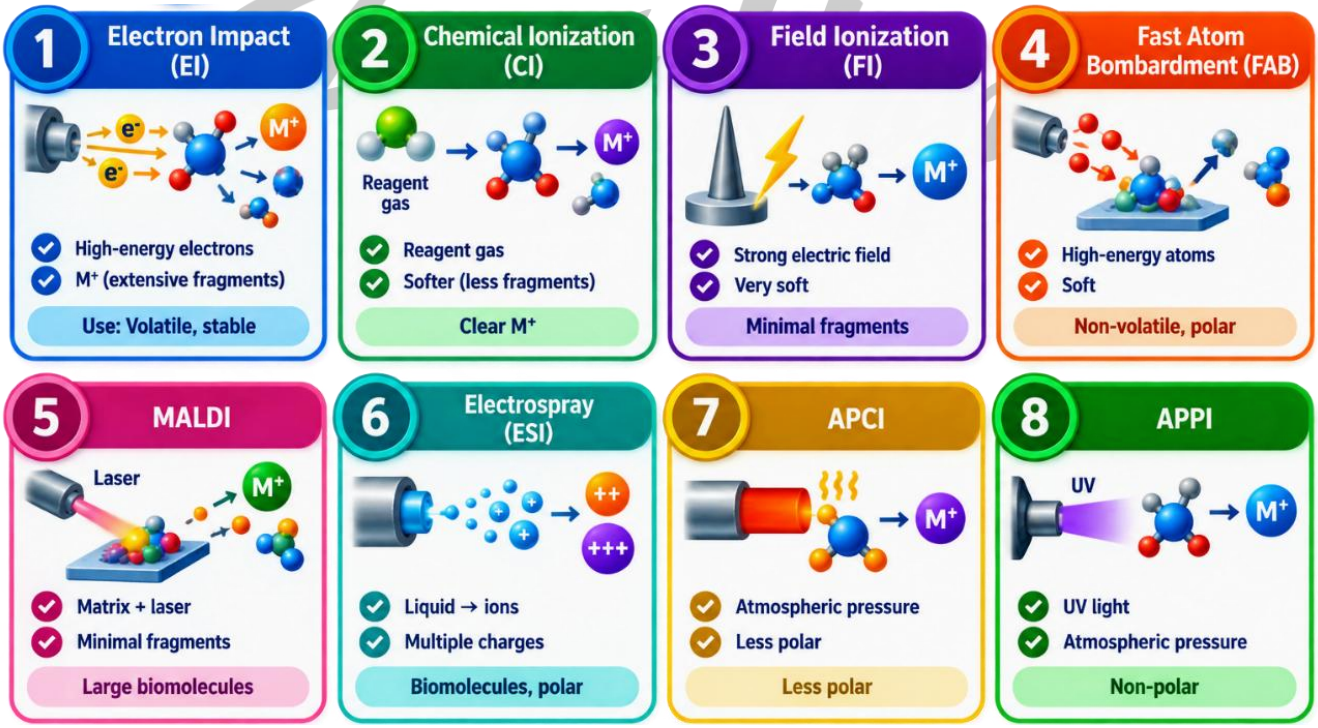
- Each component is essential for accurate analysis
- **Ensures:**
  - Proper ion formation
  - Accurate separation
  - Reliable detection and results

Ionization Methods in Mass Spectrometry

Definition

- Ionization is the process of converting **neutral molecules into charged ions** for analysis in mass spectrometry.

Types of Ionization Methods



1. Electron Impact Ionization (EI)

- Sample bombarded with high-energy electrons
- Produces positive ions (M^+)
- Causes extensive fragmentation
- **Use:**
  - Volatile and thermally stable compounds

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