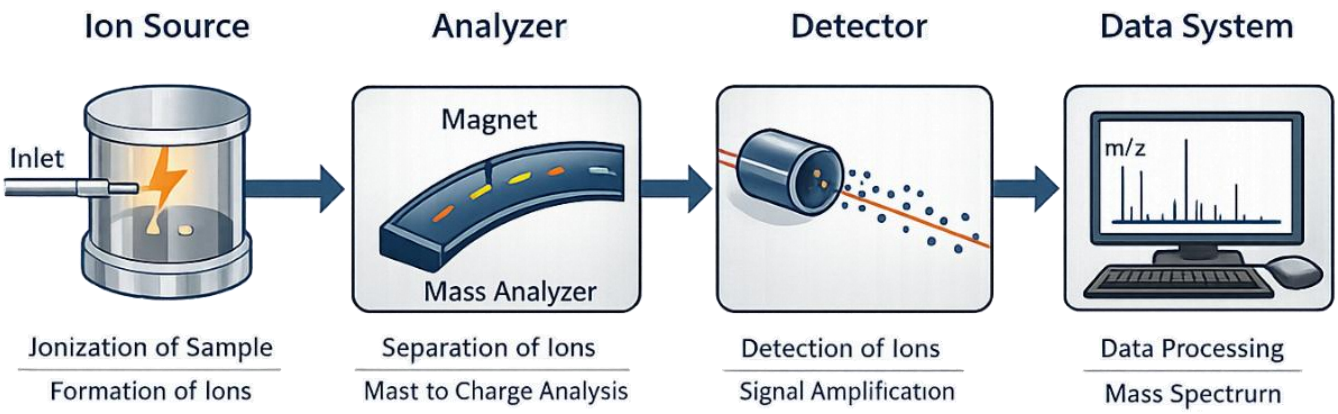
Mass Spectroscopy

Mass Spectroscopy – Principle

- Mass spectrometry is a technique used to identify and study molecules by measuring their **mass-to-charge ratio (m/z)**.

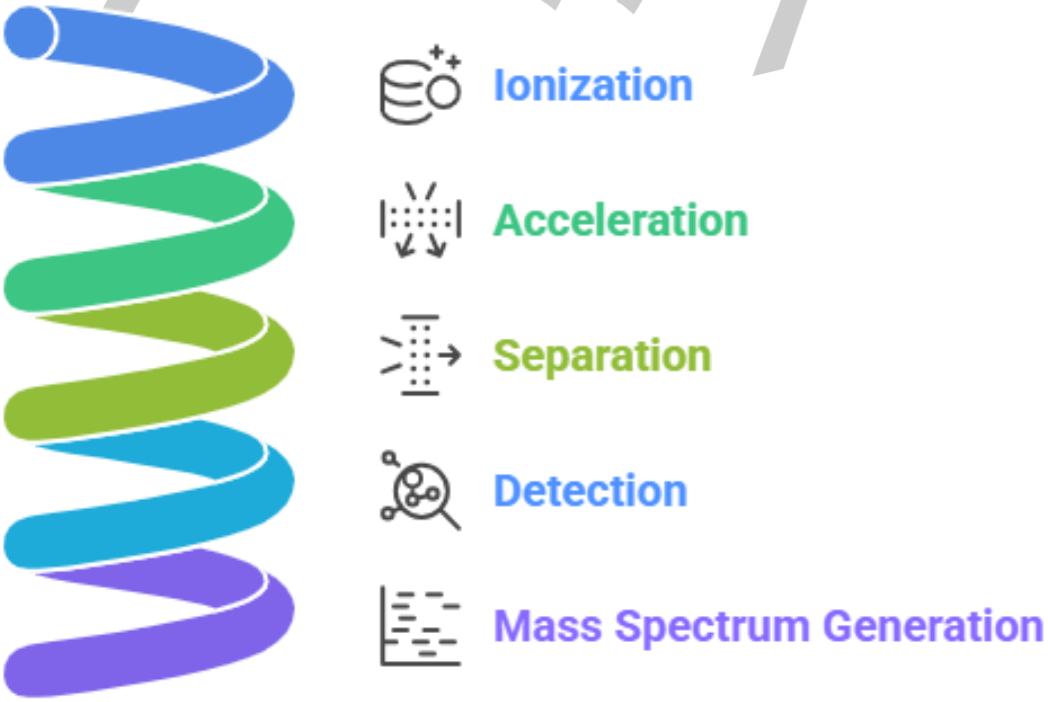


Basic idea:

- A sample is converted into charged particles (ions).
- These ions are separated based on their mass and charge.
- A detector measures how many ions of each type are present.

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Step-by-step principle:



1. Ionization

- Neutral molecules are converted into ions.
- This is necessary because only charged particles can be manipulated by electric/magnetic fields.

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2. Acceleration

- Irons are accelerated using an electric field.
- All ions are given similar kinetic energy.

3. Separation

- Ions are separated depending on their mass-to-charge ratio (m/z).
- Lighter ions or ions with higher charge move differently than heavier ones.

4. Detection

- Ions hit a detector.
- The signal produced is proportional to the number of ions.

5. Mass Spectrum

- **Output is a graph:**
  - X-axis: m/z ratio
  - Y-axis: intensity (abundance of ions)

Key concept:

- Each compound produces a **unique pattern**, like a fingerprint.

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Mass Spectroscopy – Theory

- The theory explains how ions behave under electric and magnetic fields.

Mass-to-charge ratio (m/z):

- **Defined as:**

$$m/z = \frac{\text{mass of ion}}{\text{charge of ion}}$$

- Most ions have charge = +1, so m/z ≈ mass.

Ion motion:

- **When ions are accelerated:**

$$KE = \frac{1}{2}mv^2 = zV$$

- **where:**
  - m = mass
  - v = velocity
  - z = charge

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- V = applied voltage

Important consequences:

- Lighter ions → move faster
- Heavier ions → move slower
- Higher charge → behaves like lighter ion

Separation principle:

- **Instruments separate ions based on:**
  - Speed
  - Path curvature
  - Time taken to reach detector

Fragmentation theory:

- Molecules often break into smaller pieces (fragments).
- These fragments help determine structure.

Types of peaks:

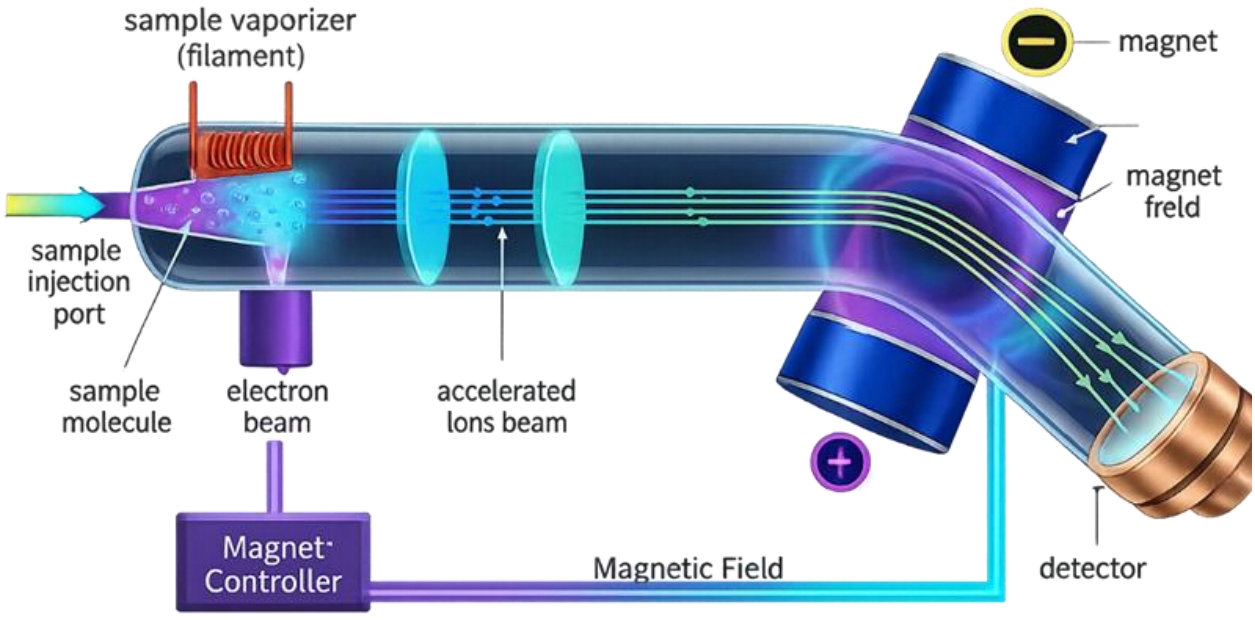
- **Molecular ion peak (M^+)** → original molecule
- **Fragment peaks** → broken parts
- **Base peak** → most intense peak (set as 100%)

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Instrumentation of Mass Spectroscopy

- A mass spectrometer has several important parts working together.

Main components:



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1. Sample Inlet System

- Introduces the sample into the instrument.
- Must convert sample into **gas phase**.
- **Types:**
  - Direct insertion
  - Gas chromatography coupling (GC-MS)
  - Liquid chromatography coupling (LC-MS)

2. Ion Source

- Converts molecules into ions.
- Different techniques used depending on sample type.
- **Examples:**
  - Electron impact (EI)
  - Electrospray ionization (ESI)
  - MALDI

3. Mass Analyzer

- Separates ions based on m/z.
- **Different analyzers:**
  - Quadrupole
  - Time-of-flight (TOF)
  - Magnetic sector

4. Detector

- Detects ions and converts them into electrical signals.
- **Common detectors:**
  - Electron multiplier
  - Faraday cup

5. Vacuum System

- Maintains **low pressure**
- Prevents ions from colliding with air molecules

6. Data System

- Converts signals into a **mass spectrum**.
- **Displays:**
  - m/z values

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- Peak intensities

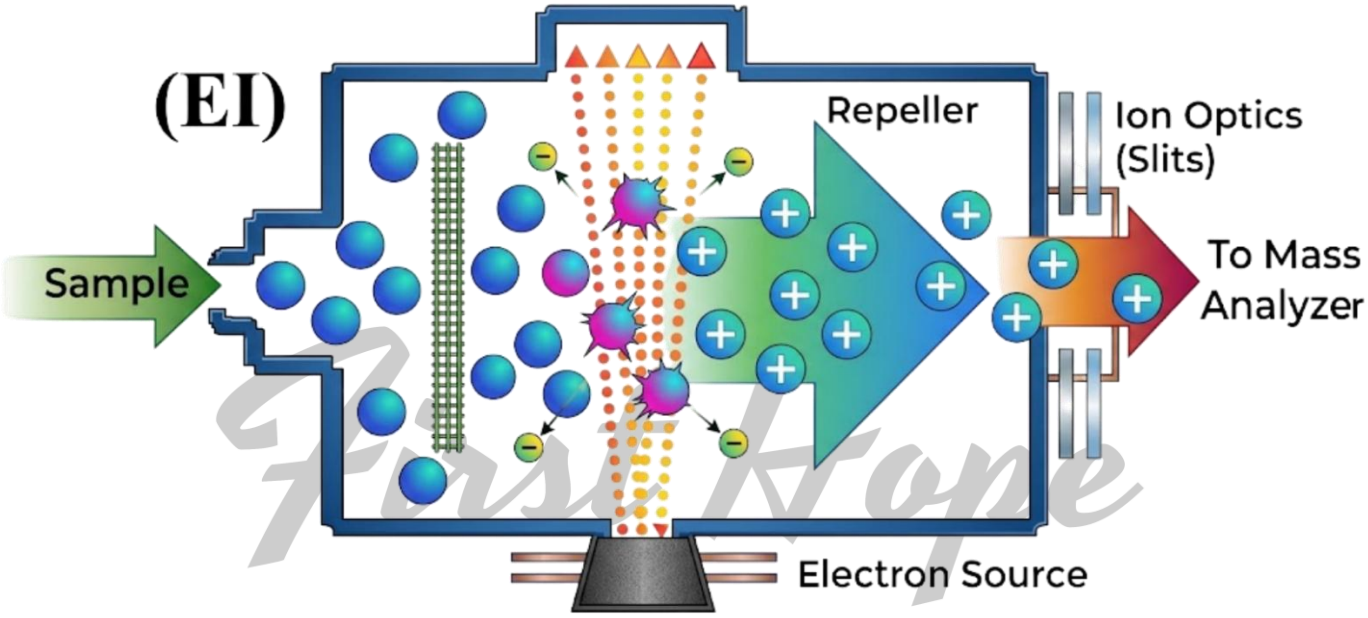
7. Flow of process

➢ Sample → Ionization → Separation → Detection → Spectrum

Electron Impact Ionization (EI)

Definition:

- A hard ionization technique where high-energy electrons collide with molecules to produce ions.



Process:

1. Sample is vaporized.
2. A beam of high-energy electrons (~70 eV) is passed through it.
3. Electron knocks out an electron from molecule:

$$M + e^- \rightarrow M^+ + 2e^-$$

Result:

- Formation of **positive ions (M^+)**.
- Excess energy causes **fragmentation**.

Characteristics:

- Produces many fragment ions.
- Gives detailed structural information.
- Molecular ion may be weak or absent.

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