

S.O.S. IN ENVIRONMENTAL CHEMISTRY  
JIWAJI UNIVERSITY, GWALIOR

*PRESENTATION ON:-*

*Mass Spectrometry*

*(part-I)*

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## Brief History of mass spectrometry

**1913:-** Thomson separates the  $^{20}\text{Ne}$  and the  $^{22}\text{Ne}$  isotopes, and he correctly identifies the  $m/z = 11$  signal as a doubly charged  $^{22}\text{Ne}$  particle.

**1919:-**Francis Aston constructs the first velocity focusing mass spectrograph.

**1934:-**Josef Mattauch and Richard Herzog develop the double-focusing mass spectrograph.

**1946:-**William Stephens presents the concept of a time-of-flight mass spectrometer.

**1968:-**Malcolm Dole develops electrospray ionization.

**2002:-** John Bennett Fenn and Koichi Tanaka are awarded the Nobel Prize in chemistry "for the development of soft desorption ionisation methods for mass spectrometric analyses of biological macromolecules."

## Introduction:-

- Mass spectrometry is a powerful analytical technique used to identify unknown compounds within a sample, and to elucidate the structure and chemical properties of different molecules.
- The complete process involves the conversion of the sample into gaseous ions, with or without fragmentation, which are then characterized by their mass to charge ratios ( $m/z$ ) and relative abundances.

**Basic Principle:-** A mass spectrometer generates multiple ions from the sample under investigation, it then separates them according to their specific mass-to-charge ratio ( $m/z$ ), and then records the relative abundance of each ion type.

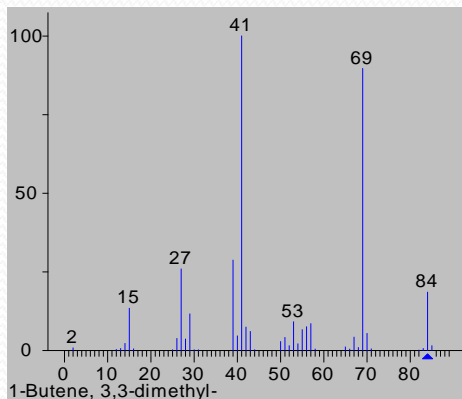
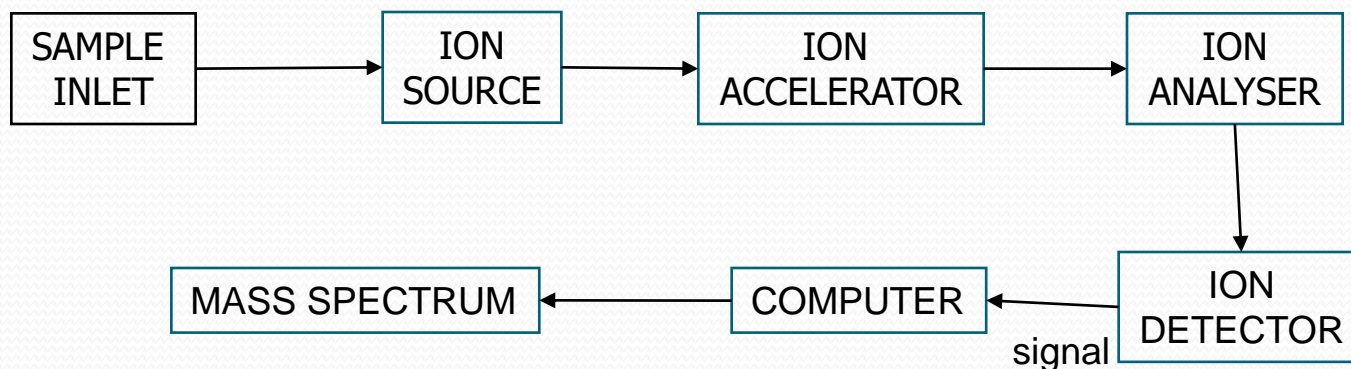
A mass spectrometer needs to perform three functions:-

- Creation of ions – the sample molecules are subjected to a high energy beam of electrons, converting some of them to ions.
- Separation of ions – as they are accelerated in an electric field, the ions are separated according to mass-to-charge ratio ( $m/z$ ).
- Detection of ions – as each separated population of ions is generated, the spectrometer needs to qualify and quantify them.

# Instrumentation:-

An instrument that generates ions from molecules and measure their masses.

The essential components of mass spectrometers:-



## Sample Inlet System:-

The purpose of the inlet system is permit introduction of a representative sample into the ion source with minimal loss of vacuum.

Most modern mass spectrometers are equipped with several types of inlets to accommodate various kinds of sample ,these include:

- 1- Batch Inlet System ( Gas+ some liquid)
- 2- The Direct Probe Inlet ( Solid+ Liquid)
- 3- Chromatography and Capillary Electrophoretic Inlet System.

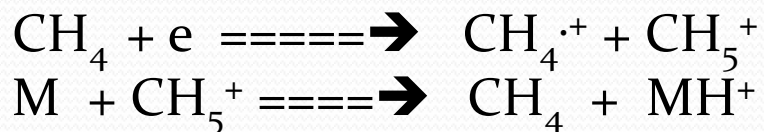
Ion Source:- For producing gaseous ions from the substance being studied.

Ways to produce ions:-

1) Electron impact (EI) - vapor of sample is bombarded with electrons.



2) Chemical ionization (CI) - sample M collides with reagent ions present in excess e.g.

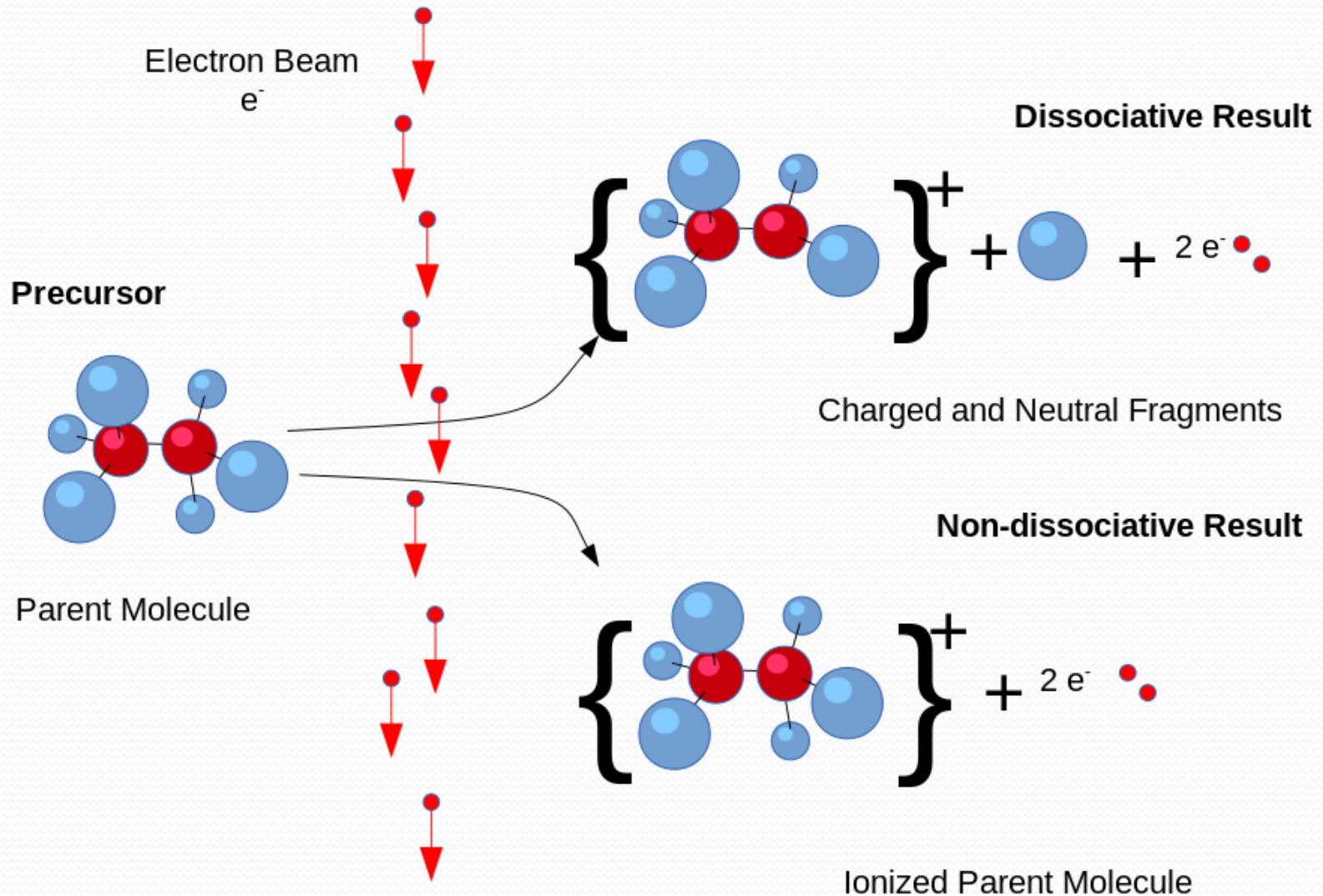


3) Fast Atom/Ion Bombardment (FAB):- Ionisation is brought by fast moving atoms.

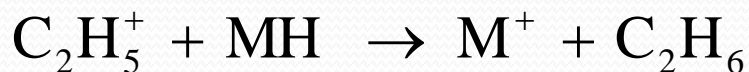
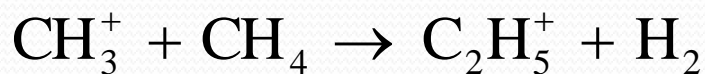
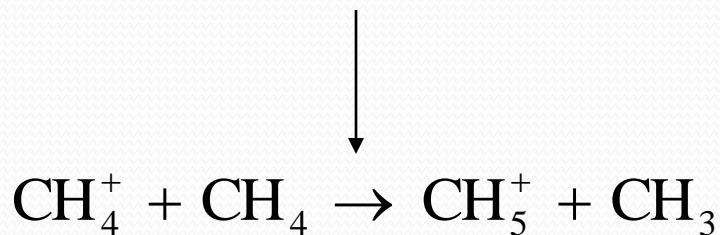
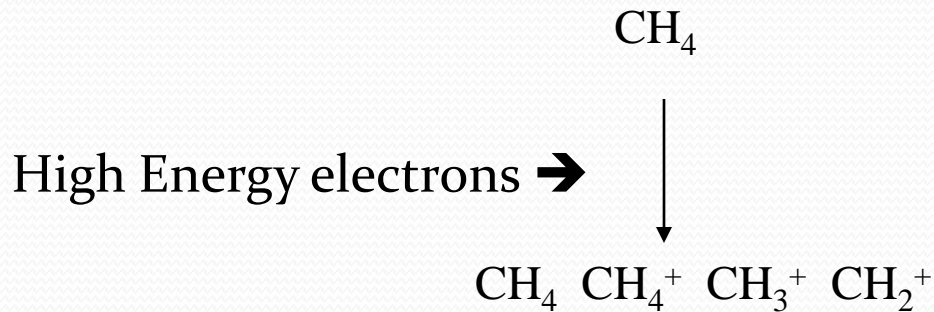
4) Electrospray Ionization (ESI) - a stream of solution passes through a strong electric field ( $10^6$  V/m).



# The Electron-Impact Source:-



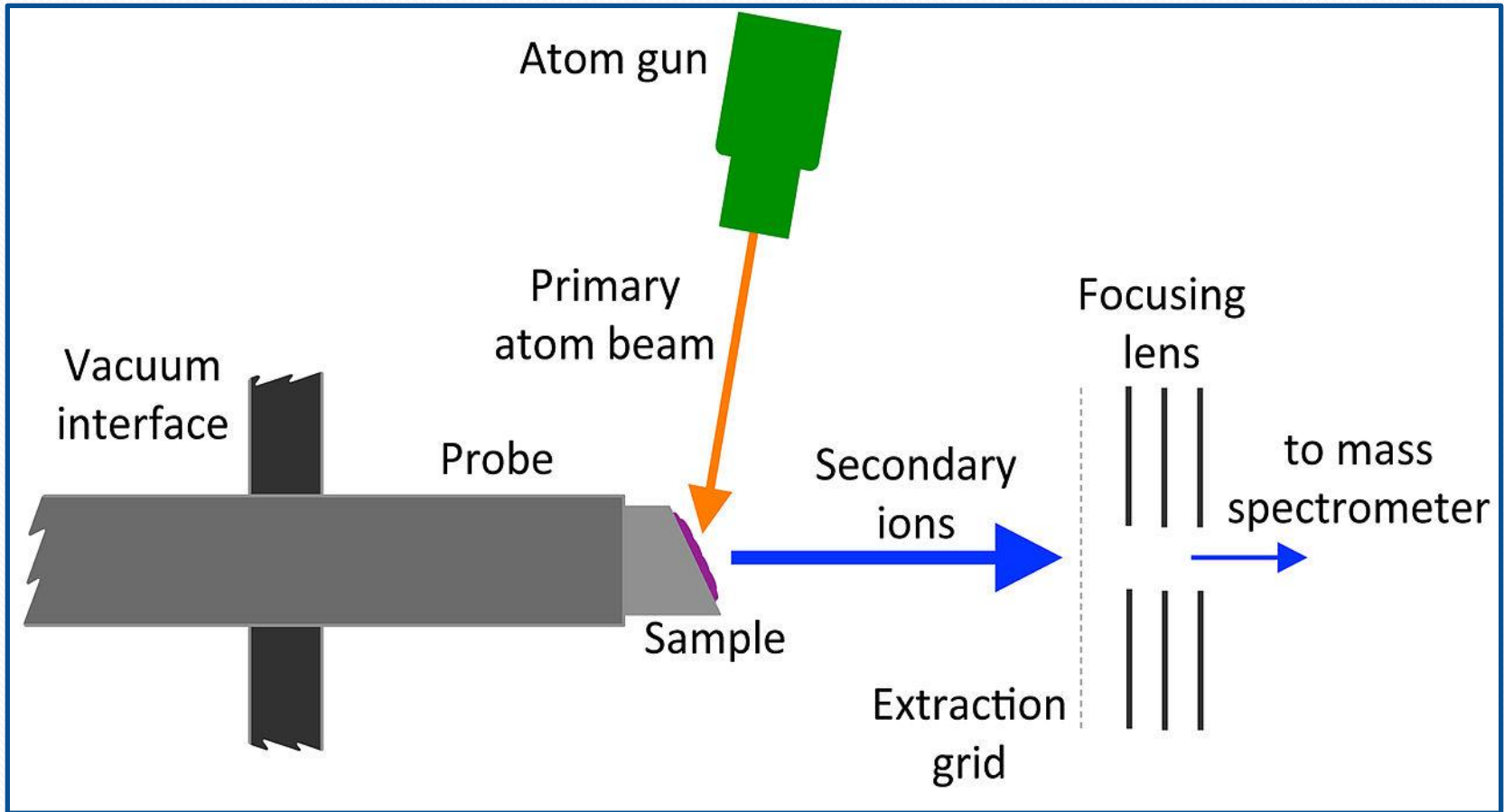
# Chemical ionisation :-



Sample Molecule MH  $\rightarrow$

Molecule Ions  $\rightarrow$

# Fast atom bombardment



# Electrospray Ionisation

