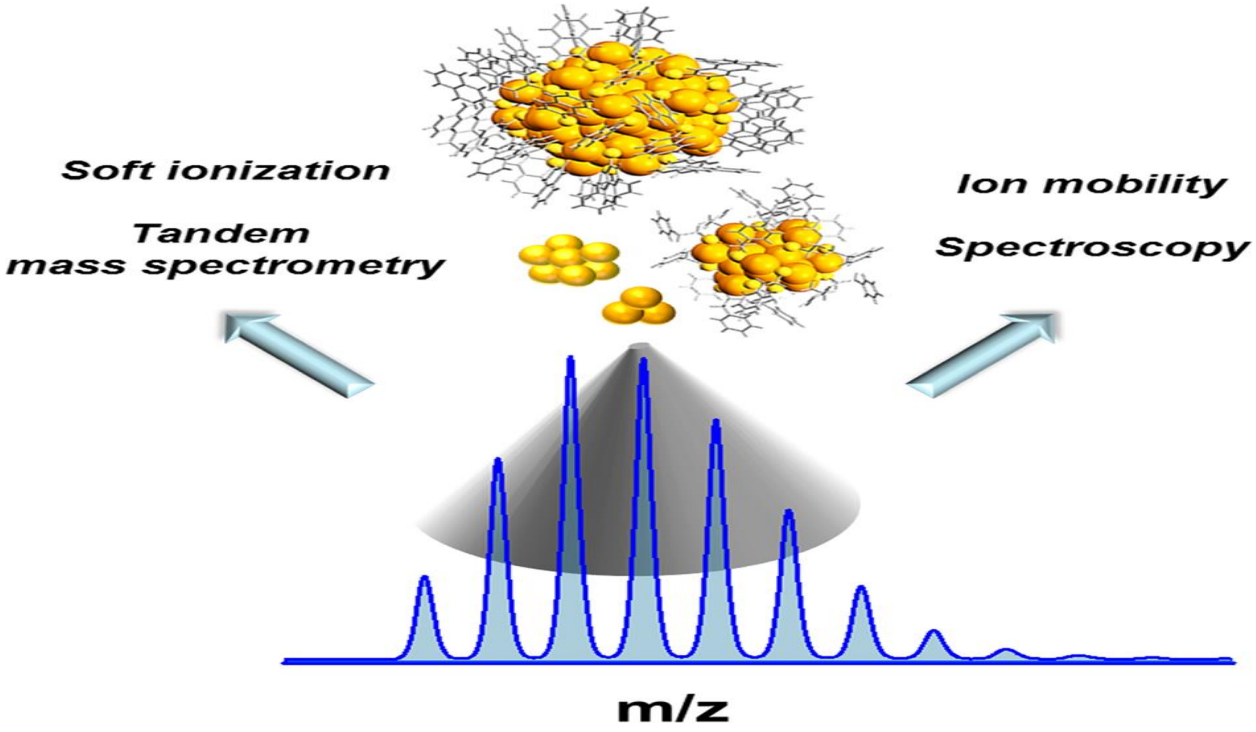
MASS SPECTROSCOPY



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INTRODUCTION

Mass spectrometry is a powerful analytical technique used to quantify known materials, to identify unknown compounds within a sample, and to elucidate the structure and chemical properties of different molecules.

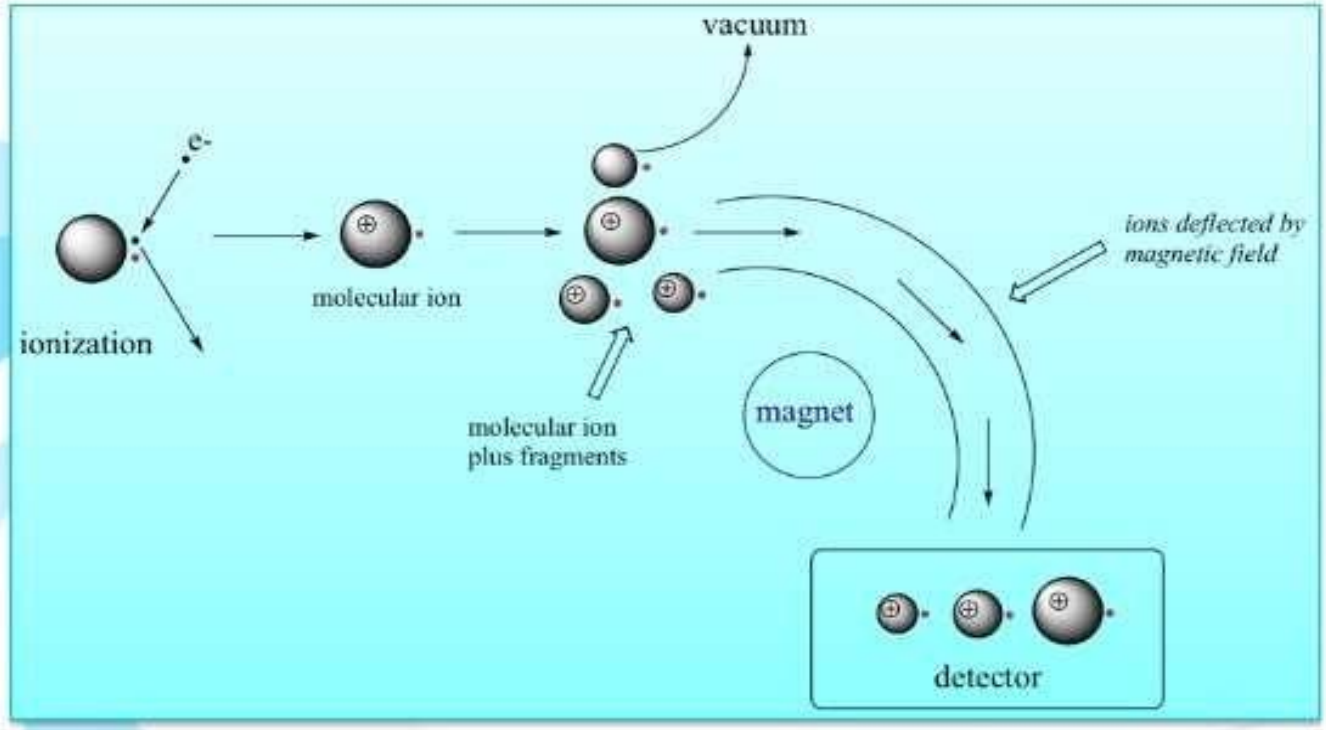
MS is the measurement of atomic mass(total number of protons and neutrons in atom) of molecules and atoms and detection of then on the **basis of mass** to **charge ratio.**

It is a micro-analytical technique requiring only a few nanomoles of the sample to obtain characteristic information pertaining to the structure and molecular weight of analyte.

It is not concerned with non- destructive interaction between molecules and electromagnetic radiation.

It is instrumental technique in which sample is converted to positive charged ions by electron bombardment and the particles are separated according to their mass, finally they are detected by detector.

Simple mass spectrometry



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.

The first step in the mass spectrometric analysis of compounds is the production of gas phase ions of the compound, basically by electron ionization. This molecular ion undergoes fragmentation. Each primary product ion derived from the molecular ion, in turn, undergoes fragmentation, and so on.

The ions are separated in the mass spectrometer according to their mass-to-charge ratio, and are detected in proportion to their abundance. A mass spectrum of the molecule is thus produced. It displays the result in the form of a plot of ion abundance versus mass-to-charge ratio. Ions provide information concerning the nature and the structure of their precursor molecule.

In the spectrum of a pure compound, the molecular ion, if present, appears at the highest value of m/z (followed by ions containing heavier isotopes) and gives the molecular mass of the compound.

Instrument

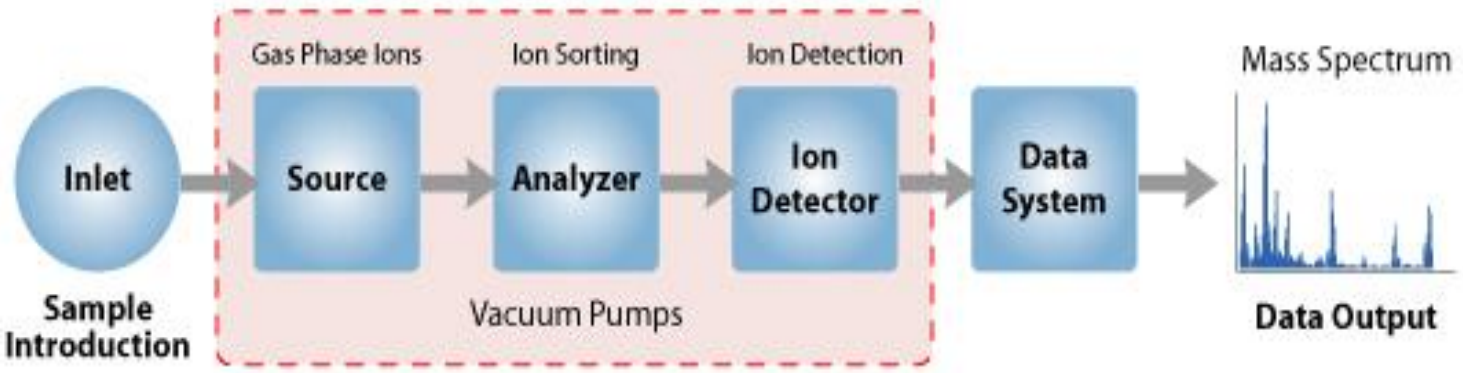
The instrument consists of three major components:

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

2. Analyzer: For resolving the ions into their characteristics mass components according to their mass-to-charge ratio.

3. Detector System: For detecting the ions and recording the relative abundance of each of the resolved ionic species.

In addition, a sample introduction system is necessary to admit the samples to be studied to the ion source while maintaining the high vacuum requirements (~10-6 to 10-8 mm of mercury) of the technique; and a computer is required to control the instrument, acquire and manipulate data, and compare spectra to reference libraries.



Applications

✓Mass Spectrometry as a technique can be coupled with other techniques such as HPLC and GC.

✓As it is used in the identification of compounds it is used in all areas of science.

✓Some of its uses are : Trace Gas Analysis, Pharmaceutical Industry, Space Exploration, Forensic Toxicology, Archaeological Dating.

✓Mass spectrometry is fast becoming an indispensable field for analyzing biomolecules. Till the1970s, the only analytical techniques which provided similar information were electrophoretic, chromatographic or ultracentrifugation methods. The results were not absolute as they were based on characteristics other than the molecular weight. Thus the only possibility of knowing the exact molecular weight of a macromolecule remained its calculation based on its chemical structure.