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Applications on Mass Spectroscopy

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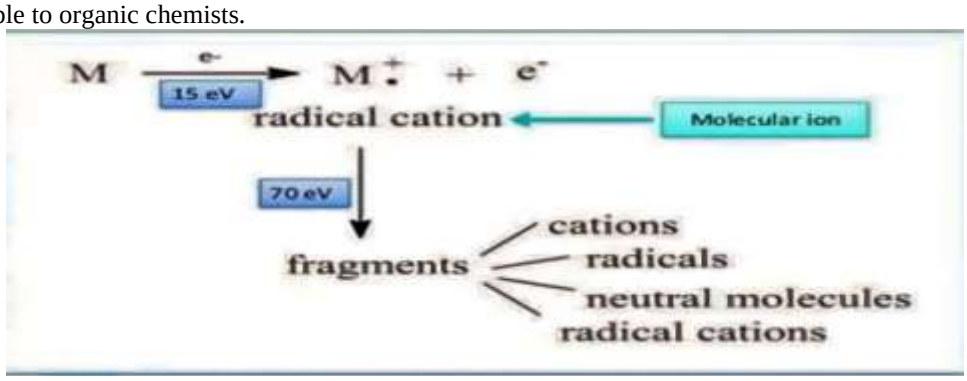
ABSTRACT:
Mass spectrometry is a highly sensitive high-throughput instrumental analytical technique. It is used to determine the molecular mass, but also gives information on molecular structure and is used for quantitation as well. Although it was developed over 100 years ago, it continues to evolve, both with respect to figures of merit (like sensitivity) and with respect to applications in various novel fields of science and technology. Mass spectrometry is capable of studying macromolecules (like proteins and protein complexes), and has very high sensitivity, now compounds at the atto- or zeptomole level can also be studied. Mass spectrometry can be coupled to separation techniques, and can be used to analyze complex mixtures, trace level compounds in biological matrices like active pharmaceutical ingredients or metabolites. In recent years, proteomics research has become a major new direction. In the present review we briefly introduce basic mass spectrometry techniques and tandem mass spectrometry.

I. INTRODUCTION :

- Mass spectroscopy is one of the primary spectroscopic methods for molecular analysis available to organic chemists.
- It is a micro analytical technique requiring only a few nano moles of the sample to obtain characteristic information relating to the structure and molecular weight of the analyte.
- It is not concerned with non-destructive interaction between molecules and electromagnetic radiation.
- In most cases , the nascent molecular ion of the analyte produces fragment ions by cleavage of the bond and the resulting fragmentation pattern constitutes the mass spectrum.
- It involves the production and separation of ionized molecules and their ionic decomposition product and finally the measurement of the relative abundance of different ions produced. It is a destructive technique in that the sample is consumed during analysis.

PRINCIPLE:

- In mass spectrometry, organic molecules are bombarded with a beam of energetic electrons (70 eV) in gaseous state under pressure between 10^{-7} to 10^{-5} mm of Hg, using tungsten or rhenium filament. Molecules are broken up into cations and many other fragments.



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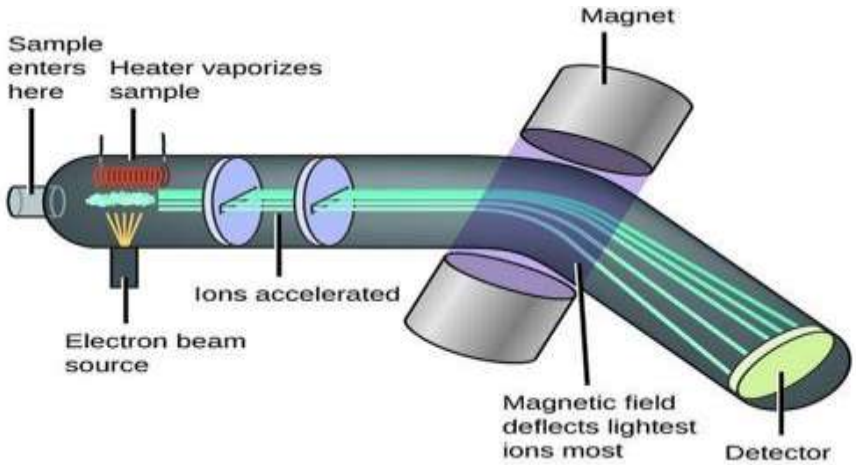
- These cations (molecular or parent ion) are formed due to loss of an electron, usually from n or π orbital from a molecule, which can further breakup into smaller ions (fragment ions or daughter ions).
- All these ions are accelerated by an electric field, sorted out according to their mass to charge ratio by deflection in a variable magnetic field and recorded. The output is known as mass spectrum.
- Each line upon the mass spectrum indicates the presence of atoms or molecules of a particular mass.
- The most intense peak in the spectrum is taken as the base peak. Its intensity is taken as 100 and other peaks are compared with it.

INSTRUMENTATION :



- Instrumentation of Mass SpectrometryWorking of Mass Spectrometry in the ion source, the sample molecules are mostly bombarded by electrons from a heated filament. The volatile liquid samples and gasses come into the ion source from the reservoir, and the non-volatile solids and liquids are added directly.
- The cations are pushed away by the charged repeller plate and moved towards other electrodes, and anions are attracted to the plate. The plate has a slit from where the ions pass as a beam. The perpendicular magnetic field deflects the ion beam into an arc. The lighter ions are deflected higher than the heavier ions.
- By analyzing the strength of the magnetic field, the ions having different masses are detected by the detector. According to the mass spectrum formed by the charged ions, one can determine the molecule or atom compared with the known molecular masses.
- The instrument used in mass spectroscopy is called "Mass spectrometer".
- It produces a mass spectrum that plots the mass - to - charge (m/z) ratio of compounds in a mixture.
- Mass spectroscopy is used in different fields and is applied to pure samples as well as complex mixtures.
- Mass spectroscopy is used for both Qualitative & Quantitative analysis of compounds.

Instrumentation of Mass SpectrometryThere are three major components present in mass spectrometry which are discussed below.

1. Ion Source: It produces gaseous ions from the given sample.
2. Analyzer: It is used to analyze and separate the ions into their characteristic mass according to their mass-to-charge ratio.
3. Detector System: Detectors in mass spectrometry detect the ions and maintain their relative abundance.Apart from these, a sample introduction system is required to add the sample to the ion source. A high vacuum is maintained (10-5-10-8 torr), and a computer system is needed to control the instrument, store the data and compare the spectrum with the references.

COMPONENTS OF MASS SPECTROSCOPY:

1) **INLET**: Samples can be introduced into the mass spectrum directly via solid probe, or in the case of mixtures by intermediary of chromatography device.
Eg: Gas chromatography

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2**) ION SOURCE :** Once in the source, sample molecules are subjected to ionization. Ions formed in the source acquire some kinetic energy & leave the source.

3) **ION ANALYZER**: Calibrated analyzer that analyzes the passing of ions as a function of their mass to change ratios. Different kinds of analyzers can be used ;

- Quadrupole mass spectrometer
- Time of flight mass spectrometer
- Double focusing analyzer
- Magnetic sector -MS
- Ion trap.

4) **DETECTOR** : The ion beam exciting the analyzer assembly is then detected & the signal is registered.

II. APPLICATIONS :

1. Environmental Analysis: It is used in water testing, soil contamination, analysis of trace elements, carbon content and pollution analysis.
2. Pharmaceutical Analysis: It is used in producing new drugs, preclinical development, etc.
3. Clinical Application: It is used in identifying infectious agents, drug therapy monitoring, clinical tests, screening of diseases, etc.
4. Forensic Analysis: It helps in confirming drug abuse, identifying explosives, arson investigation, etc.

Advantages :

1. Provides molecular weights of peptides & proteins with high accuracy (0.1 - 0.01%)
2. Highly sensitive
3. Sample purity not important
4. Can be coupled with on- line separation methods such as HPLC & capillary electrophoresis for the analysis of mixtures.

III. CONCLUSION:

MS is a powerful quantitative technique that can be used for TDM. MS offers clinical laboratories several advantages including its specificity, sensitivity, throughput, and cost-effective testing. However, MS is not without its challenges especially with the lack of standardization for TDM assays and the fear of additional regulations by the FDA on LDTs. However, many clinical laboratories are successfully using MS to perform TDM testing for the analytes discussed in this chapter. In the end, the MS applications are endless and offer clinical laboratories a way to meet the TDM needs of physicians and patients.

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