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MASS SPECTROMETRY APPLICATIONS

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ABSTRACT:

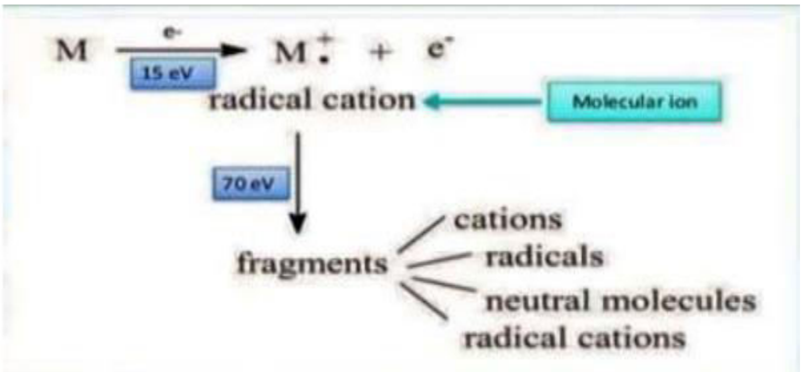
Mass spectrometry remains a highly sensitive and efficient instrumental analytical technique known for its ability to determine molecular mass, provide structural insights, and enable quantitation. Developed over a century ago, it continues to evolve in terms of sensitivity and application across diverse scientific and technological domains. Mass spectrometry's capabilities extend to studying macromolecules such as proteins and protein complexes, with sensitivity reaching levels as low as atto- or zeptomoles. Coupled with separation techniques, it can analyze complex mixtures and trace-level compounds in biological matrices like active pharmaceutical ingredients and metabolites. Recent advancements have propelled proteomics research as a significant frontier. This review briefly introduces fundamental mass spectrometry techniques and tandem mass spectrometry.

INTRODUCTION:

- Mass spectrometry stands as a cornerstone spectroscopic method for organic chemists.
- This micro-analytical technique requires only a few nanomoles of sample to provide crucial information regarding the structure and molecular weight of the analyte.
- It involves the interaction between molecules and electromagnetic radiation, providing insights through the fragmentation pattern of nascent molecular ions.
- The process entails the production, separation, and measurement of ionized molecules and their decomposition products, consuming the sample during analysis[1].

PRINCIPLE:

- In mass spectrometry, organic molecules are bombarded with a beam of energetic electrons (typically 70 eV) while in a gaseous state under pressures ranging from 10^{-7} to 10^{-5} mm of Hg, often utilizing tungsten or rhenium filaments.
- This bombardment causes molecules to fragment into cations and various other fragments, which are then analyzed to determine the molecular structure and composition[2].



Formation and Analysis of Ions

These cations (molecular or parent ions) are generated by the loss of an electron, typically from an n or π orbital of a molecule, which may further fragment into smaller ions (fragment ions or daughter ions)[3].

- All these ions are accelerated by an electric field, separated based on their mass-to-charge ratio by deflection in a variable magnetic field, and then recorded. The resulting output is known as a mass spectrum[4].
- Each peak in the mass spectrum corresponds to atoms or molecules of a specific mass.
- The most intense peak in the spectrum is identified as the base peak, with its intensity set to 100, against which other peaks are compared[5].

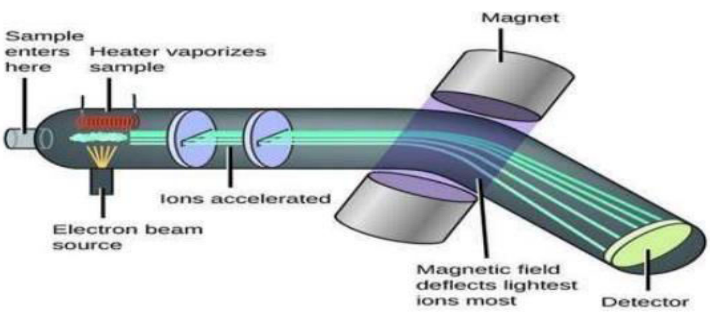
Instrumentation:

Mass spectrometry comprises three primary components:

1. **Ion Source:** This component generates gaseous ions from the sample provided.
2. **Analyzer:** It is responsible for separating and analyzing ions according to their characteristic mass-to-charge ratio[6].
3. **Detector System:** Detectors detect the ions and maintain records of their relative abundance.

Additionally, a sample introduction system is necessary to introduce the sample into the ion source. The instrument operates under high vacuum conditions (10^-5 to 10^-8 torr), and a computer system controls the instrument, stores data, and compares the obtained spectrum with reference spectra[7].

INSTRUMENTATION:



Instrumentation of Mass Spectrometry

In mass spectrometry, the ion source initiates the process by bombarding sample molecules mostly with electrons emitted from a heated filament. Volatile liquid samples and gases are introduced into the ion source from a reservoir, while non-volatile solids and liquids are directly added[8].

- Cations are repelled by a charged repeller plate and directed towards other electrodes, while anions are attracted to the plate. The plate includes a slit through which ions pass as a beam.
- A perpendicular magnetic field deflects the ion beam into an arc, with lighter ions deflecting higher than heavier ones.
- By varying the strength of the magnetic field, ions of different masses are detected by the detector. The resulting mass spectrum, depicting the mass-to-charge (m/z) ratio of compounds in the sample, allows identification of molecules or atoms based on known molecular masses.
- The instrument used for mass spectrometry is called a "mass spectrometer."
- It generates a mass spectrum that plots the m/z ratio, providing detailed information about the composition of compounds in a mixture.
- Mass spectrometry finds applications across various fields, analyzing both pure samples and complex mixtures[9].
- It serves both qualitative and quantitative purposes in compound analysis.

Components of Mass Spectrometry:

1. **Inlet:** Samples can be introduced directly into the mass spectrometer using a solid probe, or for mixtures, via an intermediary chromatography device (e.g., gas chromatography).
2. **Ion Source:** In the ion source, sample molecules undergo ionization. The ions formed acquire kinetic energy and exit the source.
3. **Ion Analyzer:** This calibrated component analyzes ions based on their mass-to-charge ratios. Various types of analyzers can be employed, including:
    - Quadrupole mass spectrometer
    - Time-of-flight mass spectrometer
    - Double focusing analyzer
    - Magnetic sector mass spectrometer
    - Ion trap
4. **Detector:** The ion beam exiting the analyzer assembly is detected, and the signal is recorded[10].

Applications:

1. **Environmental Analysis:** Used for water testing, soil contamination assessment, analysis of trace elements, carbon content, and pollution analysis.
2. **Pharmaceutical Analysis:** Applied in drug development, preclinical studies, and quality control.
3. **Clinical Applications:** Used for identifying infectious agents, monitoring drug therapy, clinical testing, and disease screening.

4. **Forensic Analysis:** Helps confirm drug abuse, identify explosives, and aid in arson investigations.

Advantages:

1. Provides molecular weights of peptides and proteins with high accuracy (0.1 - 0.01%).
2. Highly sensitive technique.
3. Sample purity is not crucial for analysis.
4. Can be coupled with online separation methods such as HPLC and capillary electrophoresis for analyzing mixtures.

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