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Mass Spectroscopy and its applications

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Abstract: The mass spectrum is a plot representation the m/e values of the various ions (i.e., parent ion as well as fragment ions) against their corresponding relative abundances. In the mass spectrum, the peak on the extreme right (i.e., particle of highest mass) corresponds to the molecular mass of the original molecule. In case of straight chain hydrocarbons, the abundance of the parent peak is fair and it is also give (M + 1) peak.

Keywords: Mass spectroscopy, molecules, Counterfeit

Introduction : Mass spectroscopy is the most accurate method for determining the molecular mass, molecular formula of the compound and its elemental composition.

Techniques: 1. Electron Impact technique (EI)
2. Chemical Ionisation technique (CI)
3. Electro Spray Ionisation technique (ESI)

Electron Impact technique (EI):

In electron Impact technique molecules of the carbon compounds in the vapour state (gas phase) are bombarded with a beam of energetic electron (nearly 70ev). The molecules are ionized and broken up into many fragments. The result of this bombardment is recorded as a spectrum of positive ions separated on the basis of m/z ratio.

A parent ion results when one electron is removed from the parent molecule of the substance.

$M + e^- \rightarrow M^{\bullet+} + 2e^-$

The molecular ions have usually the highest m/e value in this spectrum and its m/e value is equal to the molecular mass of the compound.

The molecular ion is usually not much stable and tends to fragment. The fragmentation of molecular ion produce daughter ion of definite m/e value which help in structure determination.[1]

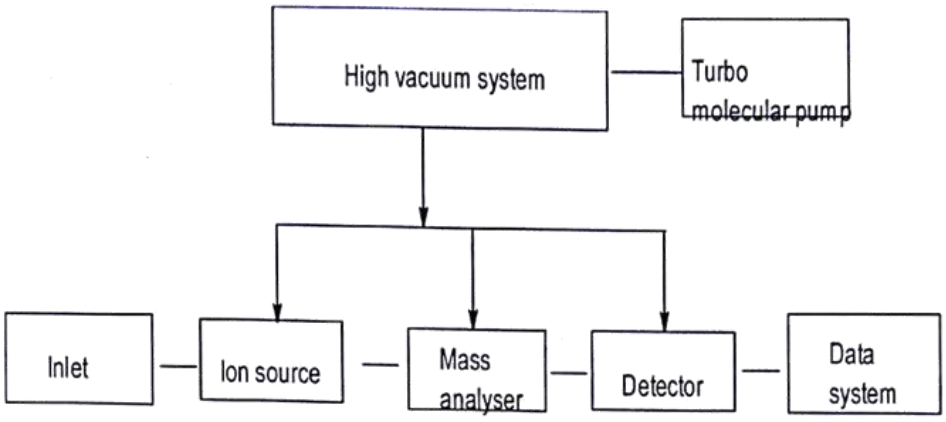
Chemical Ionisation technique (CI): It is SOFT ionization technique. In the ionization occur in this due to collisions of ionized gases with the target analyte.

Electro Spray Ionisation technique (ESI):

In this method liquid phase sample of large size (bio molecular) are ionized.

Instrumentation: Sample input system, Ionization source, Mass analyzer, Detector, Vacuum pumps, Computer based data acquisition and processing system.

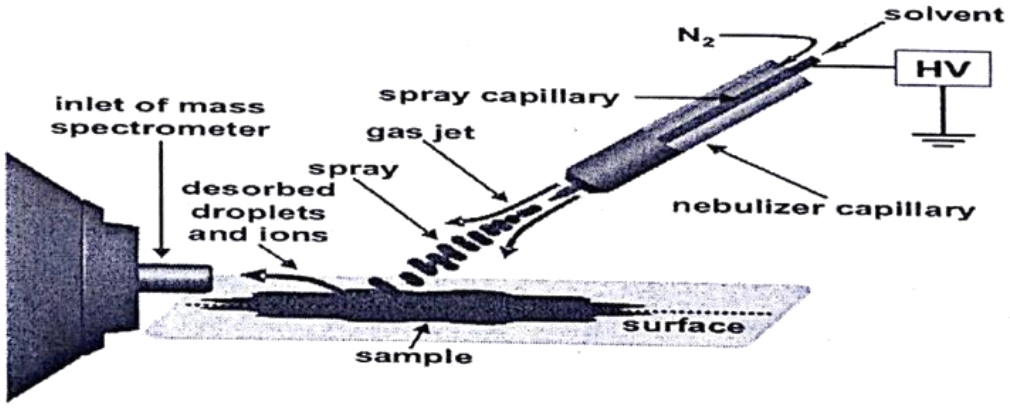
Mass Spectrometer Block Diagram



AMBIENT IONIZATION METHODS.[3]

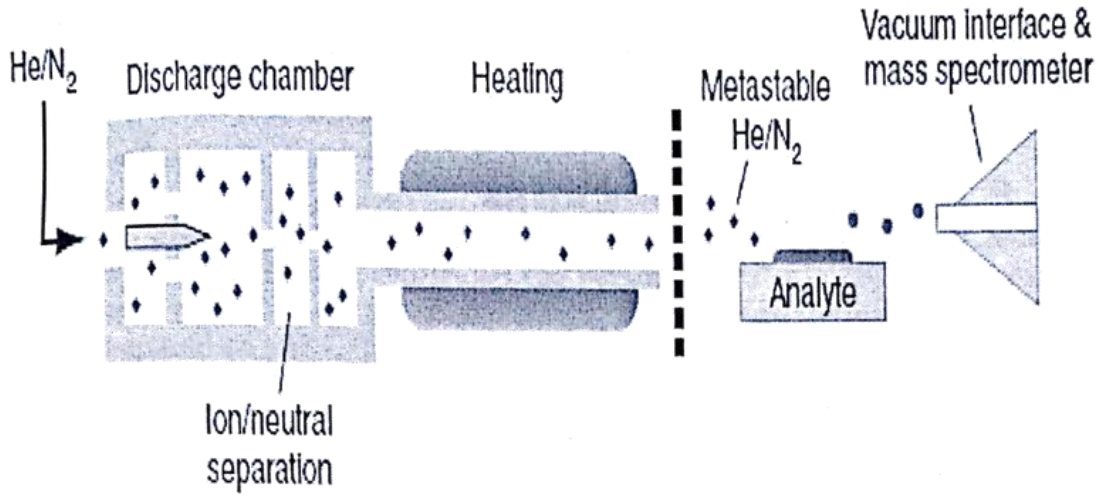
Graham Cook coined the term ambient ionization methods in 2004. The methods are DESI and DART.

Desorption Electro Spray Ionisation (DESI):



In this method analyte particals are solvated by an ionized solvent flow, the mechanism and spectra are very much similar to ESI. This can be used in Pharmaceutical testing like QC/QA, Counterfeit identification, Chemical weapons and latent fingure prints.

Direct analysis in real time (DART): Direct analysis in real time (DART) was initially developed in 2003 and reported in 2005. It is very similar to DESI (gas solvent instead of liquid). It is used Forensics, Food inspection.



Applications of Mass Spectrometry

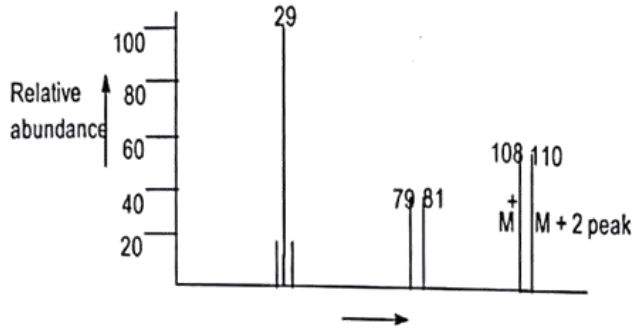
Pharmaceutical analysis, Bio availability studies, Drug metabolism studies, pharmacokinetics Characterization of potential drugs, Drug degradation product analysis, Screening of drug candidates, Identifying drug targets, Biomolecule characterization, Proteins and peptides Oligo nucleotides, Environmental analysis, Pesticides on foods, Soil and groundwater contamination etc.,

Determination of molecular formula by mass spectroscopy.[1]

The mass spectrum is a plot representating the m/e values of the various ions (i.e., parent ion as well as fragment ions) against their corresponding relative abundances. In the mass spectrum, the peak on the extreme right (i.e., particle of highest mass) corresponds to the molecular mass of the original molecule. In case of straight chain hydrocarbons, the abundance of the parent peak is fair and it is also give (M + 1) peak. In case of an organic compound gives fragment as well as parent peaks in pairs which are two units apart, then a) If the pair of peaks is in the intensity ratio of 1: 3, it must be a Chloro compound.

b) If the pair of peaks appear in the intensity ratio of 1:1 then it must be a Bromo compound.

Ex: Let us determine the molecular formula of the compound gives the following mass spectrum.



Mass spectrum of Ethyl bromide C_2H_5Br

From above spectrum, the pair on the extreme right corresponds to M^+ and (M^+ +2) peaks and also the pair of peaks are of equal intensity (1:1). Hence it is a bromo compound; the isotopes of bromine are $_{79}Br$ and $_{81}Br$.

Hence the molecular formula of the compound is C_2H_5Br (molecular mass =108)

References:

1. Y. R. Sharma, *"Elementary Organic Spectroscopy"* (2010) Page No.280 & 286
2. Jagmohan, " Text book of Organic Spectroscopy" (2007)
3. Ryan Sargeant *"Mass Spectrometry Ionization Techniques"* Mass spectrometry (Google Search)