Mass Spectrometry

In mass Spectrometry, molecules are bombarded with a beam of energetic electrons. The molecules are ionised and broken up into many fragments. Each kind of ion has a mass to charge ratio (m/e). For most of the ions, the charge is 1 and (m/e) ratio is simply the molecular mass of ion. The molecular ion (M^+) is called the parent ion. The fragments ions are analysed in such a way that a signal is obtained for each value of m/e. The intensity of each signal represents the relative abundance of the ion producing the signal. The largest peak in the structure is called the base peak and its intensity is taken as 100. The intensities of other peaks are represented relative to the base peak.

Mass spectrum of a compound is a plot which represents the intensities of the signal at various m/e values. No two compounds can have exactly similar mass spectra. It is used (i) to prove the identity of two identity of two compounds and (ii) to establish the structure of a new compound.

THEORY

Let us consider a gaseous molecule $M_{(g)}$. A parent ion results when one electron is removed from $M_{(g)}$.

$$M_{(g)} + e \longrightarrow M^+_{(g)} + 2e$$

$$M^+_{(g)} \longrightarrow m_1^+ + m_2$$

or $$M^+_{(g)} \longrightarrow m_1 + m_2^+$$

where m_2 & m_1 are neutral particle m_1^+, m_2^+ are fragment ion

The m/e value of the parent ion is equal to the molecular mass of the compound. In a few cases, the parent ion peak may be the base peak and can be easily recognised.

The basic functions of mass spectrometer are:

(i) To vapourise compounds of varying volatility

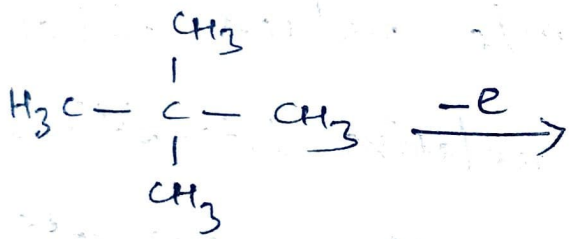
(ii) To produce ions from the neutral compounds in the vapour phase

(iii) To separate ions according to their m/e ratio and to record them.

The plot of m/e values taken along abscissa and their relative intensities along the ordinate is called the mass spectrum. Neutral particles produced in the process of fragmentation cannot be detected in the mass spectrometer.

* Mass Spectrum

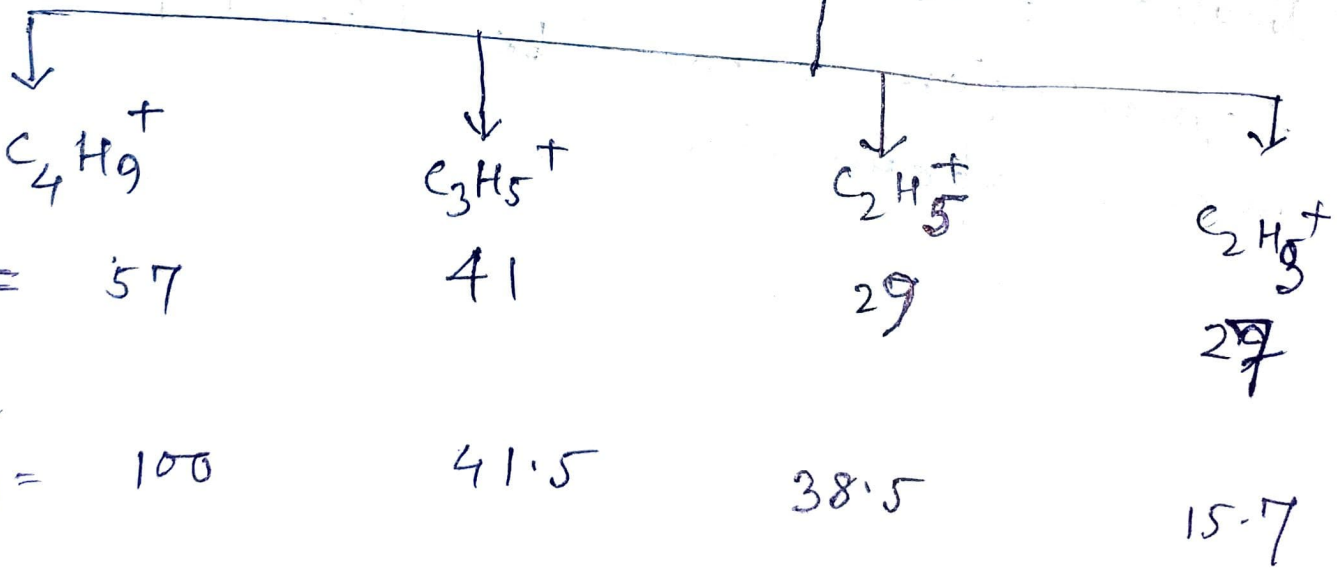
Mass spectrum is a record of the masses and the relative abundances of the molecular ion and the fragment ions. The m/e ratios are taken along the abscissa and their relative abundance along the ordinate. Base peak is the highest peak in the spectrum. eg.



neopentane

Molecular Ion

Fragmentation



m/e =	57	41	29	29
Relative Intensity =	100	41.5	38.5	15.7

The mass spectrum of neopentane is