MASS SPECTROMETRY

Mass Spectrometry:

- Molecular weight can be obtained from a very small sample.
- It does not involve the absorption or emission of light.
- A beam of high-energy electrons breaks the molecule apart.
- The masses of the fragments and their relative abundance reveal information about the structure of the molecule.

The main use of Mass spectrometry in organic chemistry is:

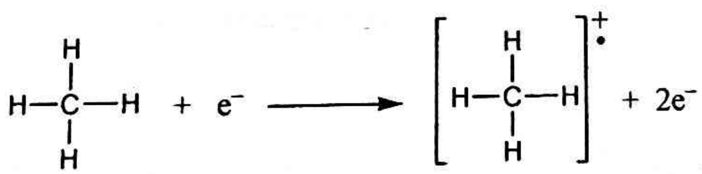
- Determine the molecular mass of organic compounds.
- Determine the molecular formula of organic compounds.

How do we achieve this?

- Persuade the molecule to enter the vapor phase (can be difficult)
- Produce ions from the molecules that enter the gas phase
- Separate the ions according to their mass-to-charge ratios (m/z))
- Measure and record these ions
- Isotopes: present in their usual abundance.
- Hydrocarbons contain 1.1% C-13, so there will be a small M^{+1} peak.
- If Br is present, M^{+2} is equal to M^{+}.
- If Cl is present, M^{+2} is one-third of M^{+}.
- If iodine is present, peak at 127, large gap.
- If N is present, M^{+} will be an odd number.
- If S is present, M^{+2} will be 4% of M^{+}.

A Mass Spectrometer: A mass spectrometer is designed to do three things

- Convert neutral atoms or molecules into a beam of positive (or negative) ions
- Separate the ions on the basis of their mass-to-charge ratio (m/z)
- Measure the relative abundance of each ion.
- Electron Ionization MS in the ionization chamber, the sample is bombarded with a beam of high-energy electrons collisions between these electrons and the sample result loss of electrons from sample molecules and formation of positive ions

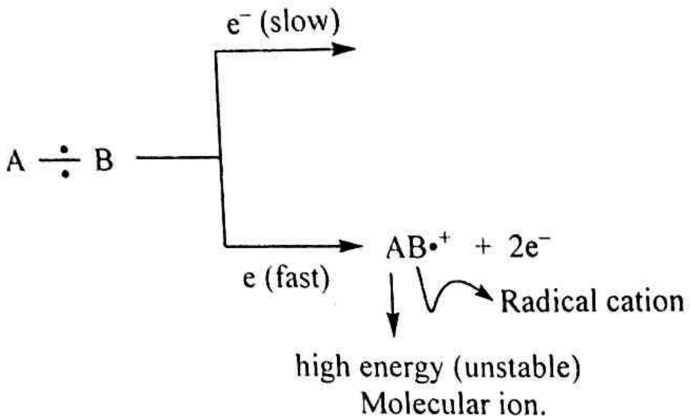


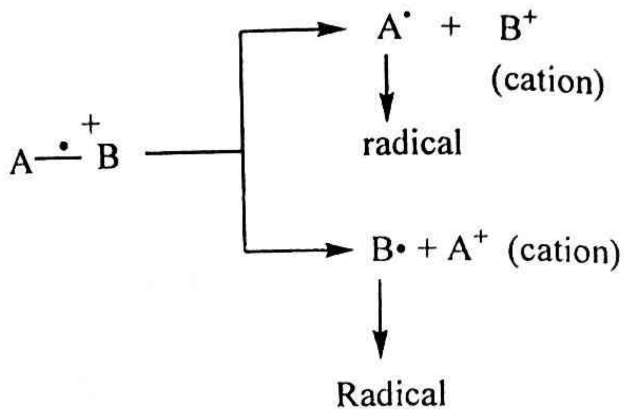
Molecular ion
A radical cations

- **Mass spectrum:** a plot of the relative abundance of each ion versus mass-to-charge ratio
- **Base peak:** the most abundant peak; assigned an arbitrary intensity of 100 .
- The relative abundance of all other ions is reported as a % of abundance of the base peak

Fragmentation by electron impact:

$$A \div B \xrightarrow[\text{gas phase}]{70\ eV}$$





Overall process is:

$$A - B \xrightarrow{e^-} AB^{+}_{\cdot} + A^{+} + B^{+} + A^{\cdot} + B^{\cdot} + AB$$