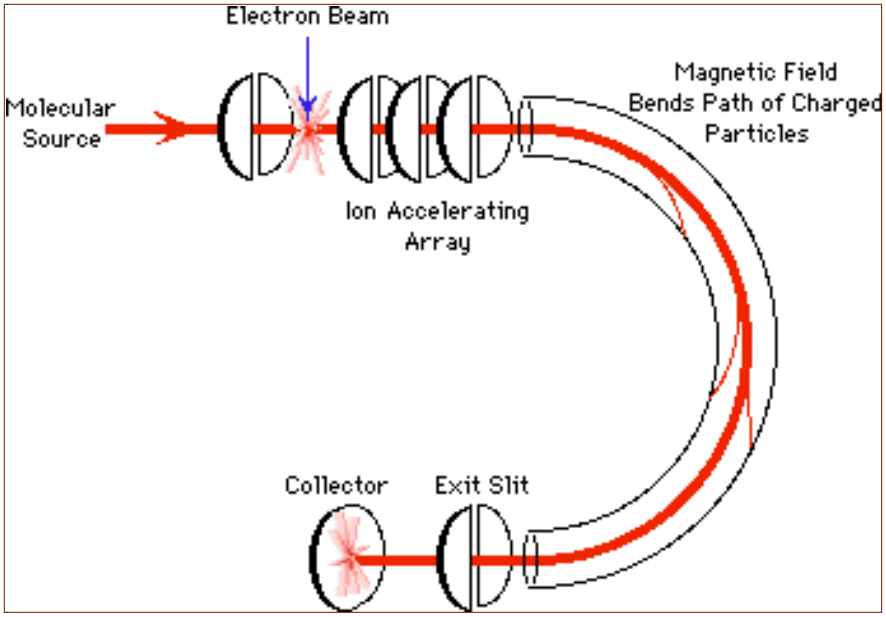
These notes can be obtained at: http://www.ndsu.nodak.edu/instruct/grcook/chem342/notes.shtml

Chapter 12: Mass Spectrometry and Infrared Spectroscopy

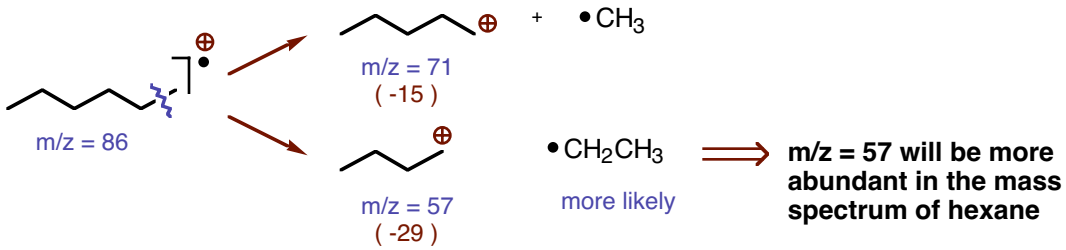
Mass Spectrometry

the mass of a molecule is determined using a mass spectrometer. Molecules are bombarded by a beam of electrons that knocks an electron out of a molecule to form a radical cation. This charged molecule is allowed to pass through a curved tube surrounded by magnets. Particles with a specific mass can be selected and only those particles strike the detector. Other particles do not make it to the detector. The magnets can be adjusted to scan for a range of masses.



Ionized Molecules will Fragment

Since the ionized molecules are highly energized, they will fragment in the mass spectrometer. The most stable cations (or radicals) are formed in higher amounts than less stable cations (or radicals).



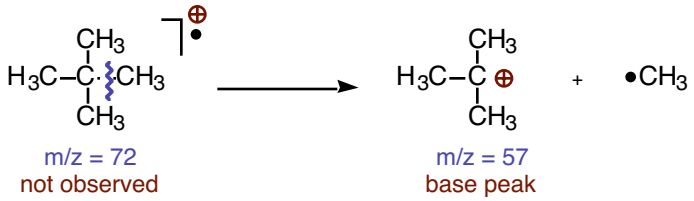
Base Peak

The most abundant (tallest) peak on the mass spectrum.

The Molecular Ion Peak

The highest peak in the mass spectrometer usually corresponds to the intact molecule.

The relative abundance of the M^+ peak in the mass spectrum is dependent on the stability of the molecule. Molecules which can very easily form very stable carbocations (tertiary or conjugated with a pi-bond) will give very small M^+ peaks which may not be seen. 2,2-dimethylpropane is one example of a molecule that fragments too readily to be seen intact in the mass spectrum.



Isotopes are seen in the mass spectrum

Carbon 13 is present in nature and makes up about 1.1 percent of all carbon. So, it is possible to detect a $M^+ + 1$ ion in the mass spectrometer. The ratio of the M^+ to the $M^+ + 1$ peaks would be 99:1.

The isotopes of chlorine and bromine are very easy to detect in a mass spectrometer. About 75% of chlorine in nature is chlorine 35 and 25% is chlorine 37 - an isotope which has 2 mass units more. Molecules which contain chlorine will show a M^+ peak and a $M^+ + 2$ peak in a ratio of about 3:1. Bromine 79 and bromine 81, also 2 mass units different, are equally abundant in nature and would give rise to equal size M^+ and $M^+ + 2$ peaks in the mass spectrum.