Chapter 13: Spectroscopy

Methods of structure determination

- Nuclear Magnetic Resonances (NMR) Spectroscopy (Sections 13.3-13.19)
- Infrared (IR) Spectroscopy (Sections 13.20-13.22)
- Ultraviolet-visible (UV-Vis) Spectroscopy (Section 13.23)
- Mass (MS) spectrometry (not really spectroscopy) (Section 13.24)

Molecular Spectroscopy: the interaction of electromagnetic radiation (light) with matter (organic compounds). This interaction gives specific structural information.

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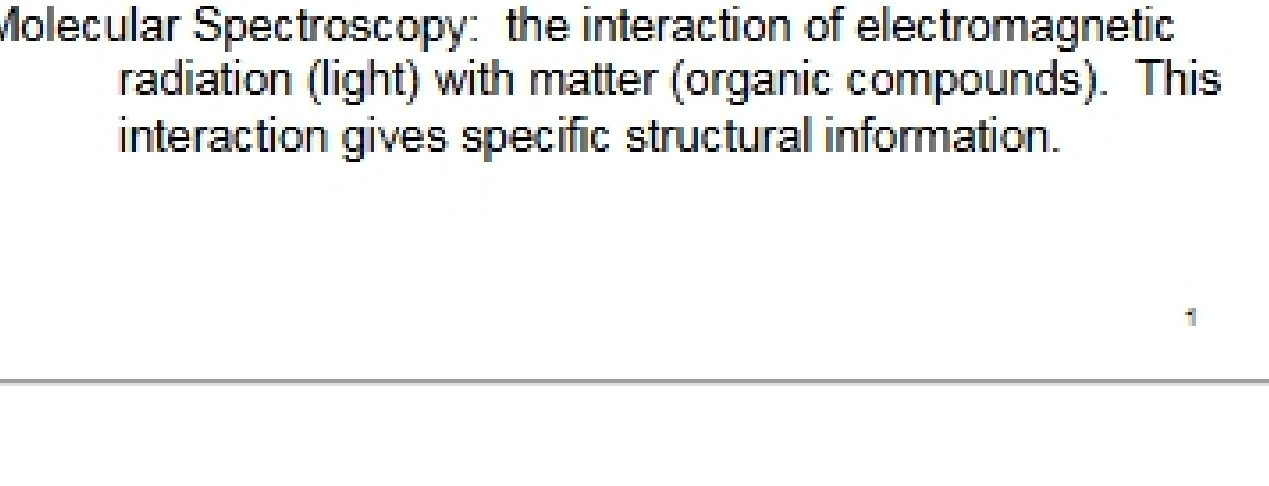
13.24: Mass Spectrometry:
molecular weight of the sample ⟶ formula

The mass spectrometer gives the mass to charge ratio *(m/z)*, therefore the sample (analyte) must be an ion.
Mass spectrometry is a gas phase technique- the sample must be "vaporized."



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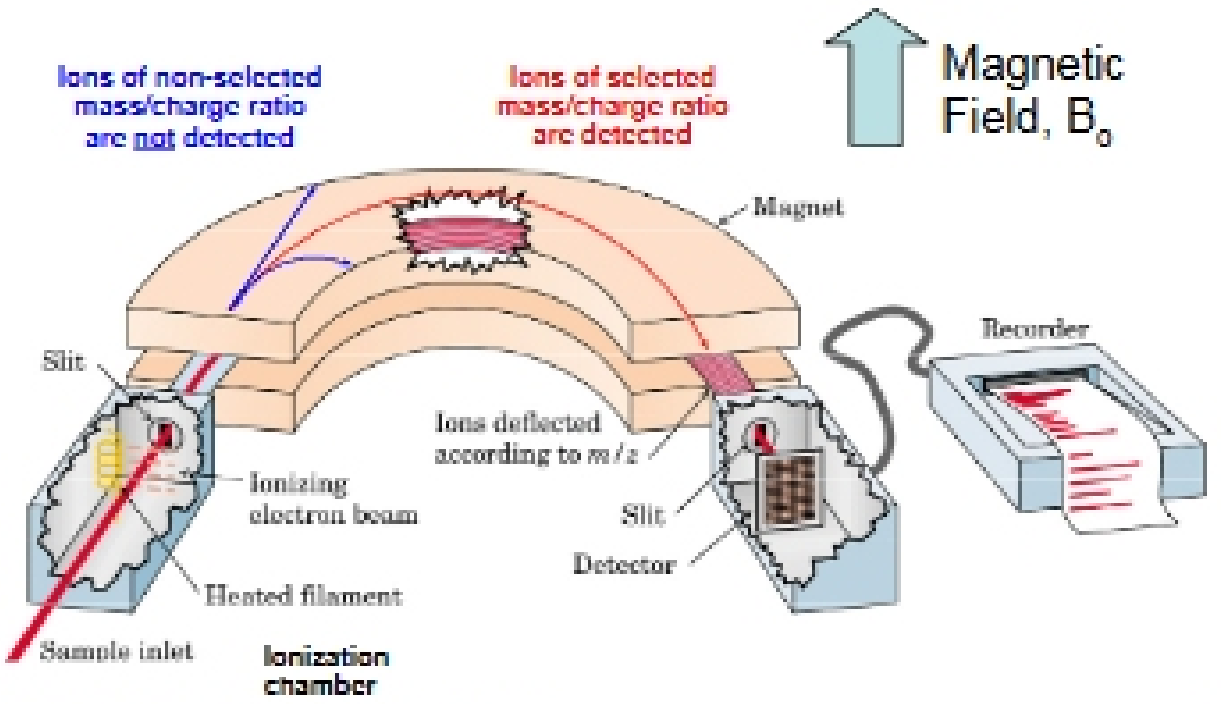
$$\frac{\text{mass}}{\text{charge}} = \frac{m}{z} = \frac{B^2 r^2}{2V}$$

B= magnetic field strength
r = radius of the analyzer tube
V= voltage (accelerator plate)



The Mass Spectrometer

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Exact Masses of Common Natural Isotopes

Isotope	mass	natural abundance
^{1}H	1.00782	99.985
^{2}H	2.01410	0.015
^{12}C	12.0000	98.892
^{13}C	13.0033	1.108 (1.11%)
^{14}N	14.00307	99.634
^{15}N	15.00010	0.366 (0.38%)
^{16}O	15.99491	99.763
^{17}O	16.99913	0.037 (0.04%)
^{18}O	17.99916	0.200 (0.20%)

Isotope	mass	natural abundance
^{19}F	18.99840	100.00
^{35}Cl	34.96885	75.77
^{37}Cl	36.96590	24.23 (32.5%)
^{79}Br	78.91839	50.69
^{81}Br	80.91642	49.31 (98%)
^{127}I	126.90447	100.00

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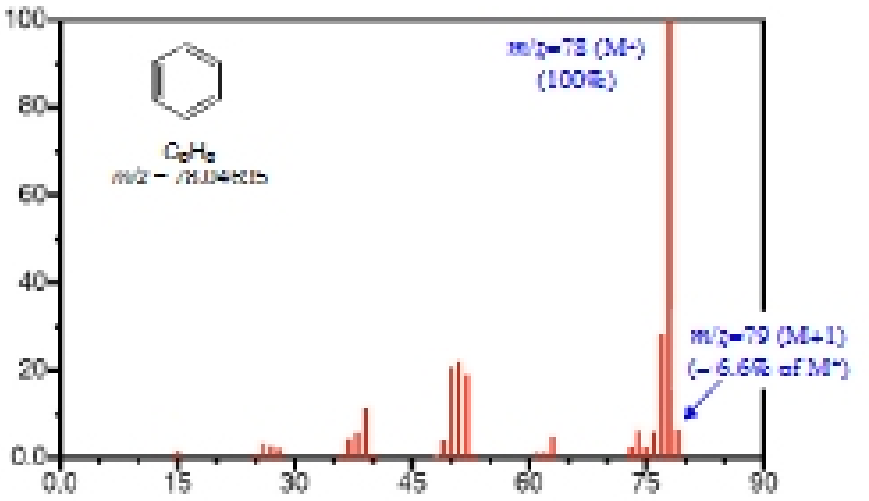
Molecular Ion (parent ion, M) = molecular mass of the analyte; sample minus an electron

Base peak- largest (most abundant) peak in a mass spectra; arbitrarily assigned a relative abundance of 100%.



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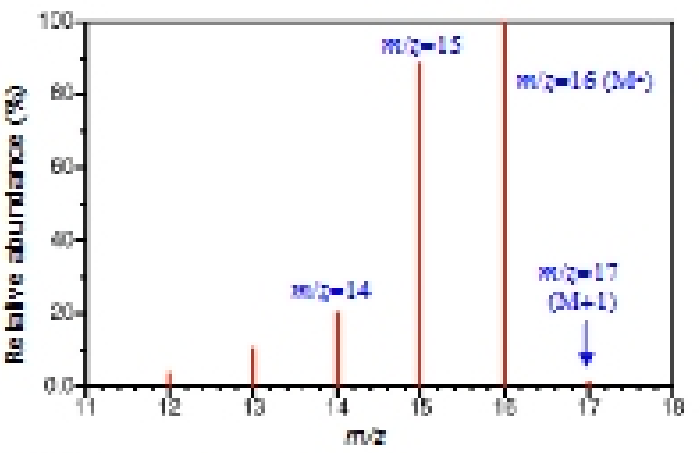
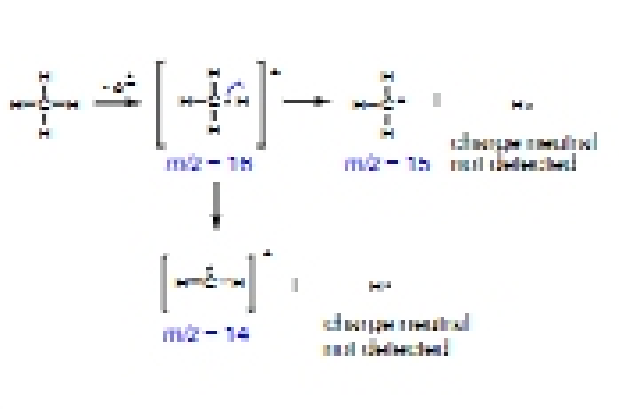
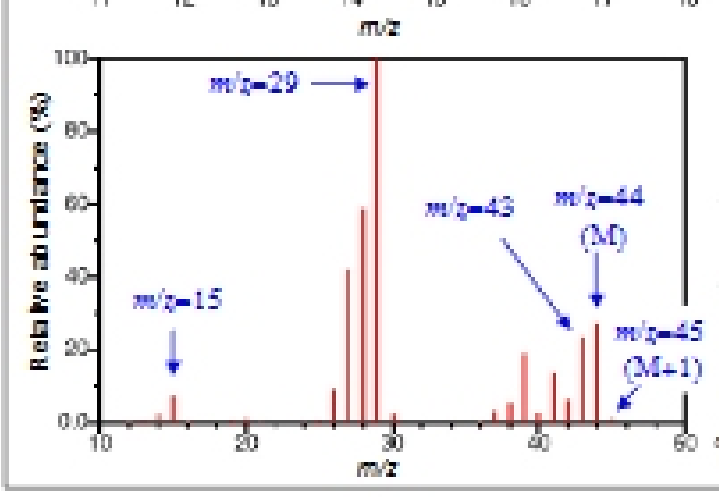
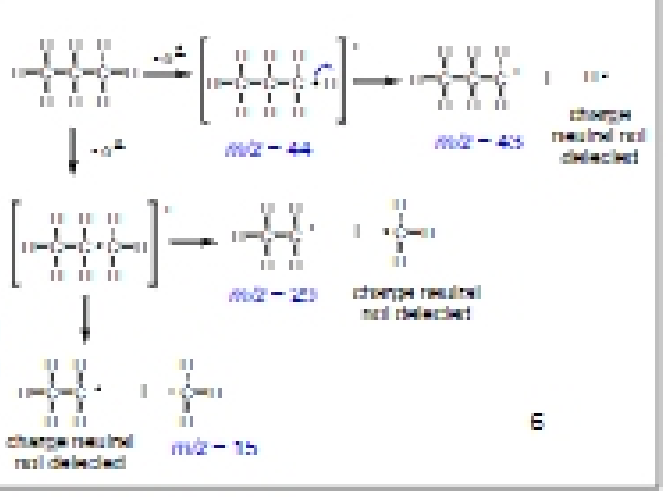
The radical cation ($M^{+\cdot}$) is unstable and will fragment into smaller ions









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