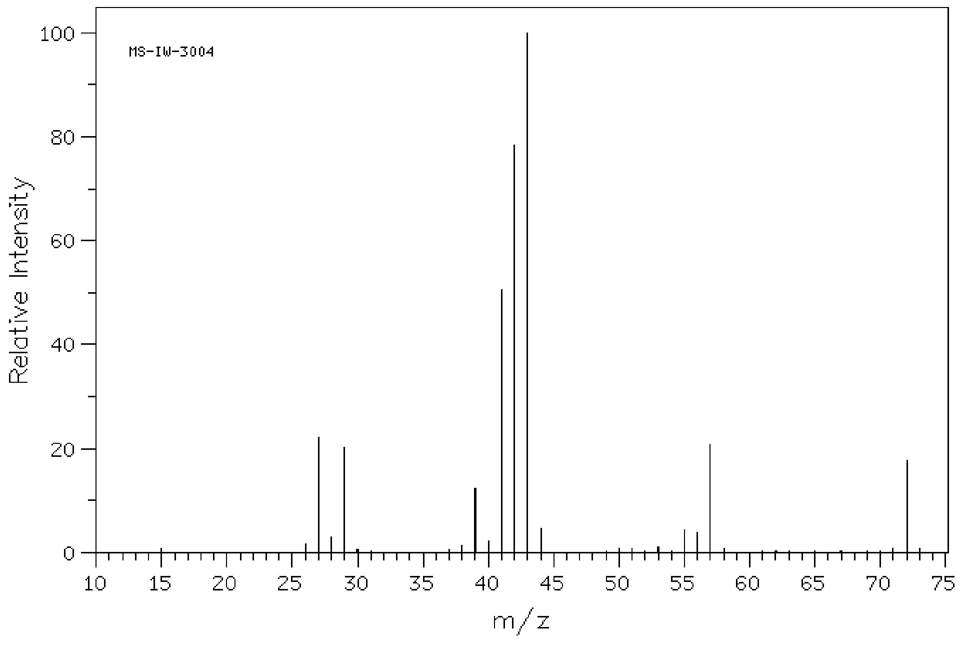
MASS SPECTROMETRY

How it works

In a mass spectrometer, molecules are bombarded with high energy particles which can remove an electron from the molecules. This leaves the molecules with a positive charge. These **molecular ions** are then accelerated through magnetic and/or electric fields which, by deflecting them relative to their mass, give information that allows their molecular mass to be calculated. Other ions, produced by fragmentation of the molecular ion are also produced. Examining the mass of these fragments provides clues about the chemical structure of the original molecule.

A typical mass spectrum is shown below, for pentane.
The x-axis is the mass/charge ratio (m/z), where z represents the charge of the ion. In most cases z = 1, therefore m/z equals the mass of the ion.
The y-axis is the intensity of the peak provided, the taller the peak is then the more common the corresponding ion.
In the diagram below the molecular ion is at 72, e.g. C_5H_{12} = (5 x 12) + (12 x 1) = 72. **The molecular ion will typically be the ion with the highest m/z ratio**.
The other peaks present are due to the fragmentation of the molecular ion, which may occur during the analysis. In simple organic compounds **fragmentation often occurs by the breaking of a carbon carbon single bond**, i.e the peak at 43 is due to the fragment $[CH_3CH_2CH_2]^+$



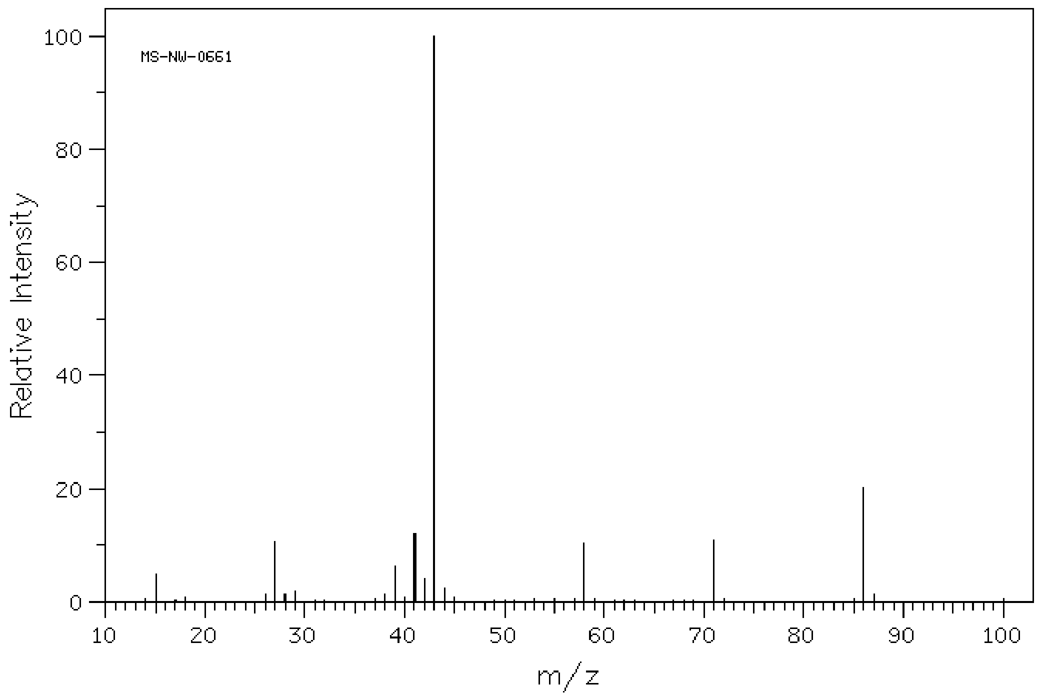
WHAT INFORMATION WE CAN GET FROM THIS DATA

a) The MOLECULAR FORMULA from the peak FURTHEREST to the RIGHT
b) The PRESENCE OF Br, from a doublet - 2 peaks of identical size, 2 m/z units apart*#
c) The PRESENCE OF Cl, from 2 peaks 2 m/z units apart, with one 3 x larger than the other*#
d) The presence of OTHER "common sections" for example, a peak @ 43 ($CH_3CH_2CH_2^+$), @ 29 ($CH_3CH_2^+$) etc – these generally come from breaks between C-C single bonds

- For Br, the isotopes ^{79}Br and ^{81}Br are found in equal abundance in nature, therefore the size of the peaks is identical, however, ^{35}Cl is 3 x more common than ^{37}Cl which gives the difference in peak size

\# For compounds containing a halogen, there is usually a peak corresponding to the chain without the halogen attached

AN EXAMPLE: MASS SPECTRUM FOR 2-PENTANONE



2-pentanone ($C_5H_{10}O$) $(5 \times 12) + (10 \times 1) + 16 = 86$