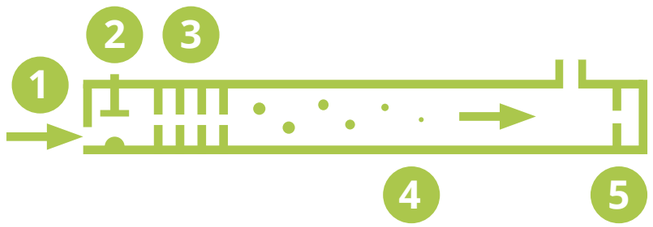
A GUIDE TO INTERPRETING MASS SPECTRA

Mass spectrometry is an analytical technique that allows us to measure the masses of atoms and molecules. The most important peak in a mass spectrum is the molecular ion peak, which can be used to determine the mass of the molecule, but fragment ions can also provide information on chemical structure.



HOW MASS SPECTROMETRY WORKS

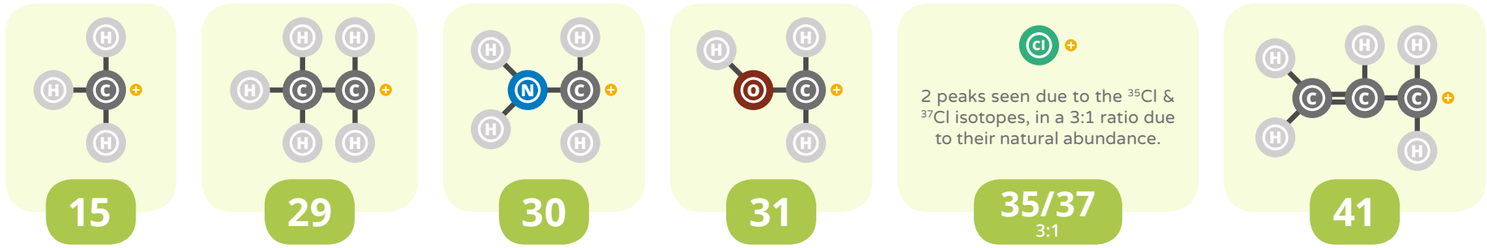
1 The sample is introduced to the mass spectrometer. Only very small samples are required. A heater is often present to vapourise the sample.

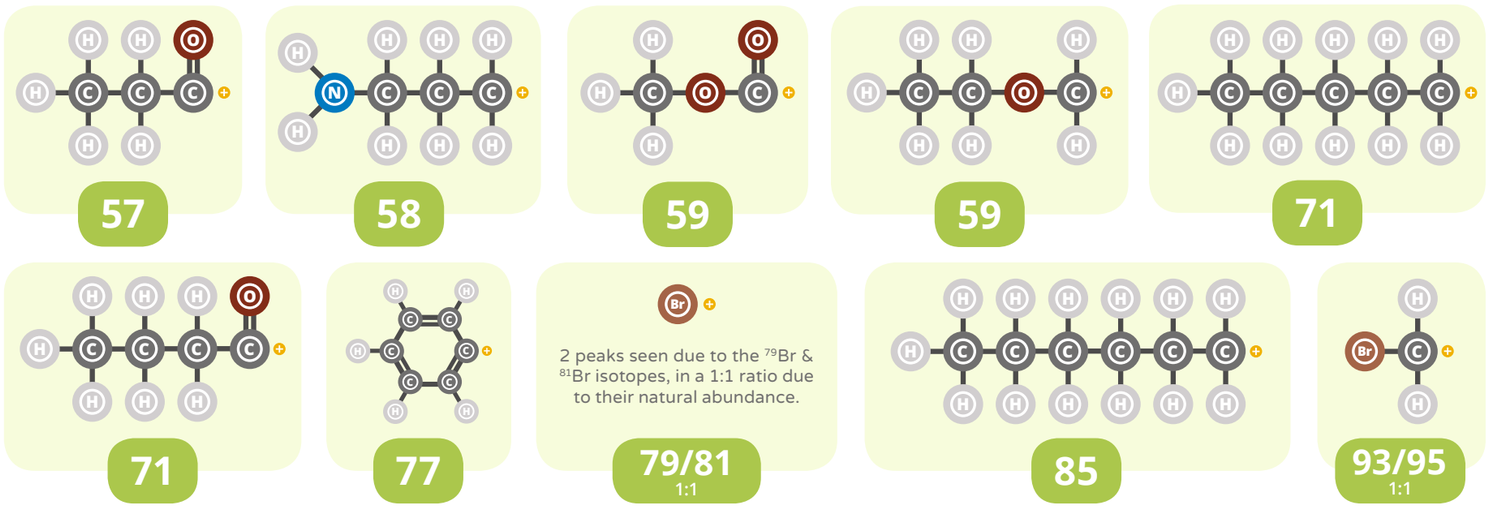
2 Molecules in the sample are ionised by an electron gun, which knocks out electrons to produce positive ions. Some molecules break into smaller ions & fragments. Some other methods of ionisation which can be used include electrospray ionisation, or matrix assisted laser desorption ionisation (MALDI) which uses a laser to ionise the sample.

3 The positive ions generated are passed through an electric field which accelerates them. All of the ions are given the same kinetic energy.

4 In time of flight mass spectrometry, lighter ions move at a higher velocity and reach the detector first. Older spectrometers used a magnetic field to deflect ions.

5 The positive ions hit a charged plate & accept electrons, creating a signal. The more ions that hit, the greater the signal. The output is a complex stick diagram.





Above are shown a selection of common fragment ions seen in mass spectra, along with their masses. Note that the structures shown are general representations, and it can also be possible for isomeric structures (those with the same constituent atoms, but a different structure) to cause the peaks in spectra. There are also many more fragments possible than those shown, but knowledge of these should suffice to interpret spectra of most simple molecules.