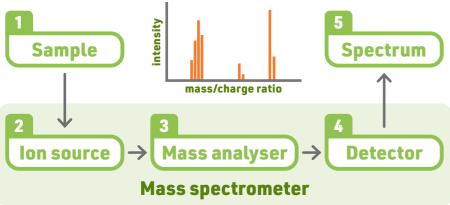
A guide to interpreting mass spectra

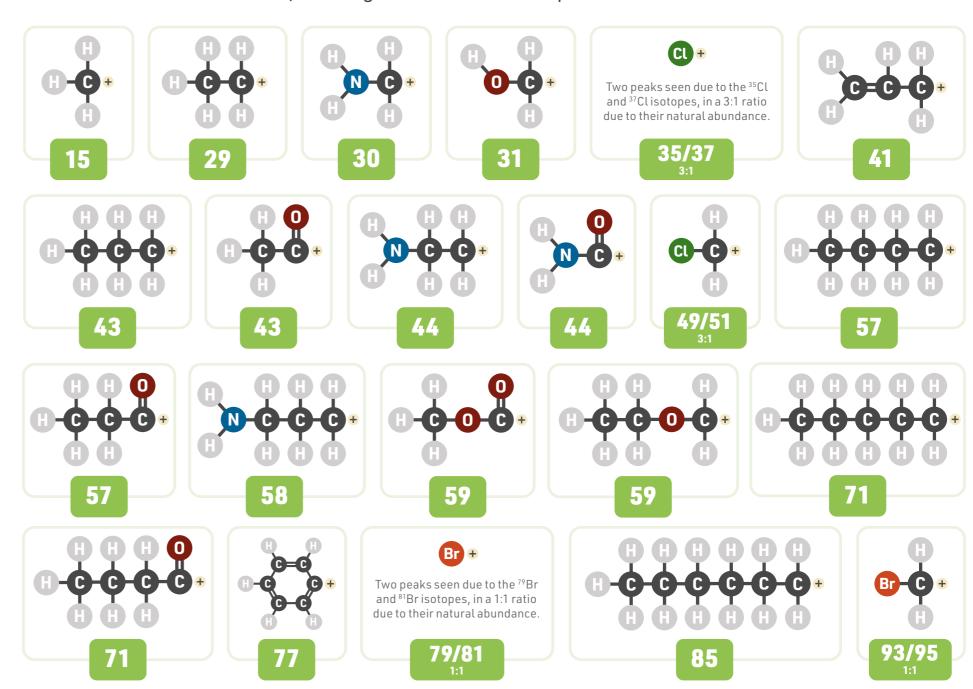


Mass spectrometry is an analytical technique that allows us to measure the masses of atoms and molecules. The most important peak in a mass spectrum is the molecular ion peak, which can be used to determine the mass of the molecule, but fragment ions can also provide information on chemical structure.

How mass spectrometry works



- A small sample of the substance to be analysed is added to the mass spectrometer.
- The mass spectrometer ionises the sample. This can be done in a number of ways, including with a laser, applying a voltage to a liquid sample spray, or firing electrons at a gaseous sample. Some molecules fragment into smaller ions.
- A mass analyser separates ions based on their mass/charge ratio. This can be done in a number of ways using an electric and/or magnetic field.
- Ions hit the detector and it converts them into a signal, amplifies it, and records it.
- The signal is output as a mass spectrum.



A selection of common fragment ions seen in mass spectra are shown above, 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 many more fragments possible than those shown, but knowledge of these fragments should suffice to interpret spectra of most simple molecules.

