



Uses of mass spectrometry



One of our SciBar participants prepared this glossary, independently of Tony Bristow.

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Deflection The ions in a mass spectrometer are deflected by a magnetic field according to their mass and charge. The lighter the ion, the more it is deflected. The greater the charge, the more the ion is deflected.

Electron Negative subatomic particles.

Fragmentation The bombarding electrons in a mass spectrometer ionize the organic molecules, which may then break up into smaller pieces.

Gas chromatography A separation technique used to separate the chemicals in an unknown substance. Separation is necessary before mass spectrometry because a mixture will generate many overlapping peaks in the mass spectrum.

Ionization The removal (positive ions) or addition (negative ions) of one or more electrons from an atom or molecule. In a mass spectrometer ionization occurs when a stream of electrons from a heated metal filament bombards a vaporized sample of the substance being tested. In such collisions, the electrons have a high enough energy to knock an electron off the atom or molecule.

Ionization energy The minimum energy required to remove an electron from an atom or molecule in order to produce a positive ion.

Isotope Two or more forms of the same element with differing numbers of neutrons, giving different masses. Not all isotopes are radioactive.

Mass spectrometry A technique used to identify substances in a sample, by separating components according to their mass and counting the relative amounts of the different mass fragments.

Mass spectrum The output chart from the mass spectrometer – a pattern of lines showing the number of ions arriving at the detector for each value of mass/charge. For elements, each line represents a different isotope, and the output shows the ratio of various isotopes. For organic compounds, each line represents a different fragment produced when the molecular ion breaks up. Each organic substance has a unique ‘fingerprint’ and can be identified by computer matching against a database of the known spectra of organic compounds.

Molecular ion (also called parent ion) The ion with the highest measured mass: the molecule has been ionized, but not broken into smaller fragments.

Neutrons Neutral particles found in atomic nuclei.

Specific test A test that positively identifies the presence of a particular substance. Unlikely to give a false positive result.

Vaporization The sample to be tested must be in gas form so it is either heated to vaporize it (turn it into a gas), or passed through a gas chromatography machine.

Useful weblinks:

The SAM (Sample Analysis at Mars) suite of instruments on the Curiosity rover <http://ssed.gsfc.nasa.gov/sam/>
Chemistry and the Olympics <http://www.rsc.org/chemistryworld/2012/06/chemistry-olympics>

Next SciBar: 12 November 2012. Personalised medicine, by Ian Watson of AstraZeneca. Time: 6.30pm as usual.