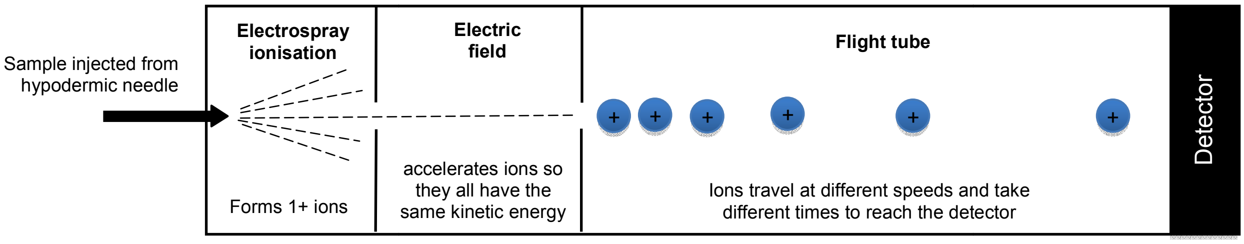
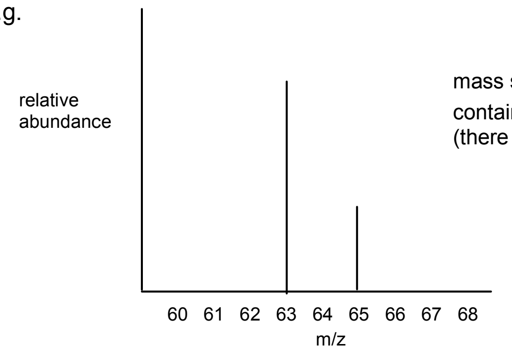
TIME OF FLIGHT MASS SPECTROMETRY 1

Mass spectroscopy is a very powerful instrumental technique used to find the relative mass of elements and compounds.



Stage	What happens
1 Ionisation	Main method in use is **electrospray ionisation**: • the sample is dissolved in a volatile solvent and injected through a fine hypodermic needle as a fine spray into a vacuum in the ionisation chamber • a very high voltage is applied to the end of the needle where the spray emerges (the needle is positively charged) – this produces tiny positively charged droplets (due to the loss of electrons to the needle) • the solvent evaporates leaving 1+ ions
2 Acceleration of ions	• the ions are accelerated using an electric field so that all the ions have the **same kinetic energy** (where kinetic energy = $\frac{1}{2}mv^2$)
3 Separation 3of charged ions	• **ion drift** - the ions then enter the flight tube • Ions with different masses have a different **time of flight** • the lighter ions travel faster and take less time to reach the detector (i.e. they have a lower time of flight)
4 Detection	• the detector is an negatively charged plate – a current is produced when the ions hit the plate – the more ions that hit the detector the bigger the current • the mass of the ions hitting the detector can be calculated from the time it takes to reach the detector • the mass spectrum shows the number of particles (abundance) of each mass that hit the detector e.g.  mass spectrum of copper contains two main isotopes: ^{63}Cu and ^{65}Cu (there are more atoms of ^{63}Cu than ^{65}Cu) • the horizontal axis is actually the mass to charge ratio (m/z) of the particles that hit the detector, but as the charge is usually +1, the m/z ratio is effectively the mass.

Finding relative atomic mass (A_r)

The mass spectrum of an element shows the mass and abundance of each isotope and can be used to work out the relative atomic mass of the element (relative atomic mass, A_r = average mass of atoms relative to 1/12th mass of ^{12}C atom).

Imagine you are working out the average mass of the following balls:

- 2 balls with mass 100 g
- 3 balls with mass 200 g
- 10 balls with mass 400 g

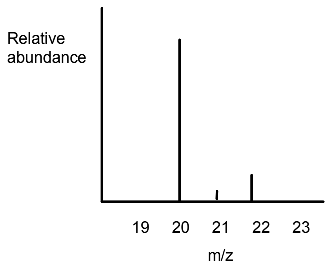
$$\text{the average mass of balls} = \frac{\text{total mass of all the balls}}{\text{total number of balls}} = \frac{(2 \times 100) + (3 \times 200) + (10 \times 400)}{2 + 3 + 10} = \frac{4800}{15} = 320\text{ g}$$

Note that the average mass of the balls must be somewhere between the mass of the heaviest and the lightest, i.e. between 200 g and 400 g.

This principle is used to find the average mass of atoms:

$$\text{the average mass of atoms} = \frac{\text{total mass of all the atoms}}{\text{total number of atoms}}$$

For example, here is the mass spectrum of neon.



^{20}Ne 90.9 %
^{21}Ne 0.26 %
^{22}Ne 8.8 %

$$A_r = \frac{[(90.9 \times 20) + (0.26 \times 21) + (8.8 \times 22)]}{(90.9 + 0.26 + 8.8)} = 20.17$$

Find the relative atomic mass of the following elements using the data from mass spectrometry.

a) lithium ^{6}Li (7.4%) ^{7}Li (92.6%)

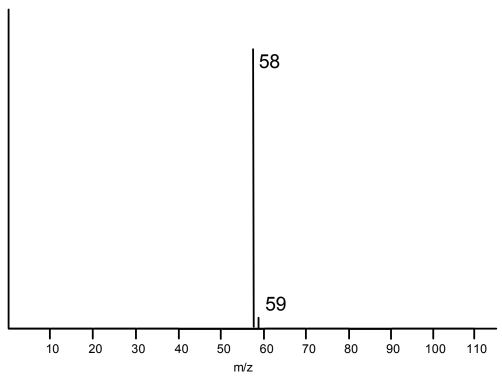
b) gallium ^{69}Ga (1.00) ^{71}Ga (0.66)

c) iron ^{54}Fe (5.8%) ^{56}Fe (91.6%) ^{57}Fe (2.2%) ^{58}Fe (0.3%)

Finding relative molecular mass (M_r)

Mass spectra can also be used to find the M_r of molecules. The main peak corresponds to the M_r. In organic molecules, there is often a small peak at the M_r+1 due to a small number of molecules containing ^{13}C or ^{2}H atoms.

e.g. this spectrum is of butane with M_r 58, with a small peak at 59 (58+1) as well due to isotopes.



In molecules containing atoms with significant amounts of isotopes, the peaks are more significant.

e.g. Cl_2 (with isotopes ^{35}Cl and ^{37}Cl in ratio 3:1).