2.2 – The Mass Spectrometer

2.2.1 - Describe and explain the operation of a mass spectrometer

Mass spectrometers are very complex, and are made up of a number of components, each of which performs a particular function. The principle behind it is that the movement of charged particles will be affected as they pass through the magnetic field. Their mass and their charge ($\frac{m}{z}$) ratio determines the degree to which the particles are deflected.

The operation of the mass spectrometer can be broken down into four stages:

Vaporisation - The sample is heated and vaporised, and passed through into an evacuated tube. This separates the particles

Ionisation - The atoms/molecules are then bombarded by a stream of high energy electrons, knocking electrons off the particles, resulting in ions with a 1+ charge (though in some cases 2+)

Acceleration - The positively charged ions are then accelerated along the tube by means of the attraction to negatively charged plates. The ions pass through the slits, which control the direction and velocity of their motion

Deflection - The ions are then passed into a very strong magnetic field, deflecting the ions in a curved path. In the case of a fixed size magnetic field, a lighter ion will be deflected more than a heavier one, and a 2+ ion will be deflected more than a 1+ one of the same mass.

The deflection of the ions depends on the mass/charge ratio

Modern mass spectrometers have a variable strength of magnetic field. The strength can be increased to deflect a heavier ion or one with a lower charge. This can be used when the ions are to be deflected to the same point.

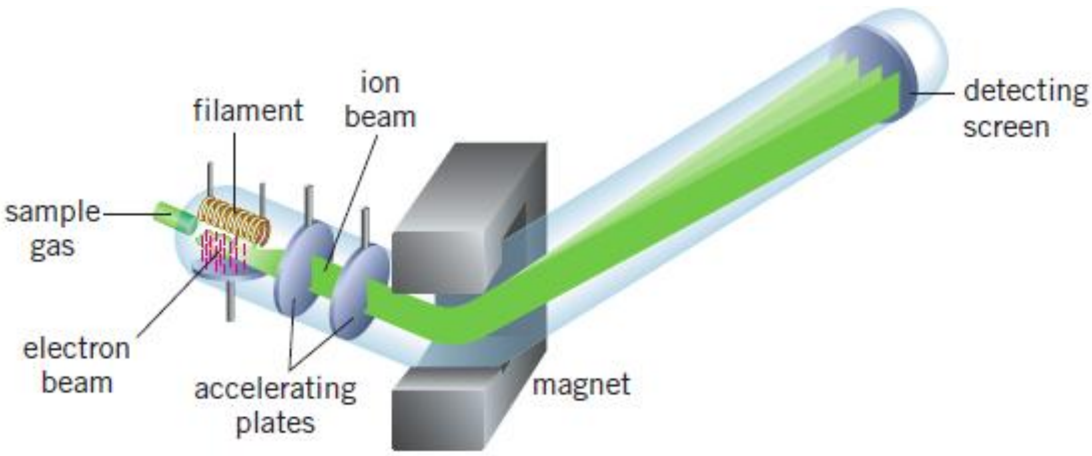
Detection - The ions are detected electronically by a device that measures both the location and the number of particles that collide with it.

Recording - The percentage abundance of the isotopes is recorded as a graph called a spectrum

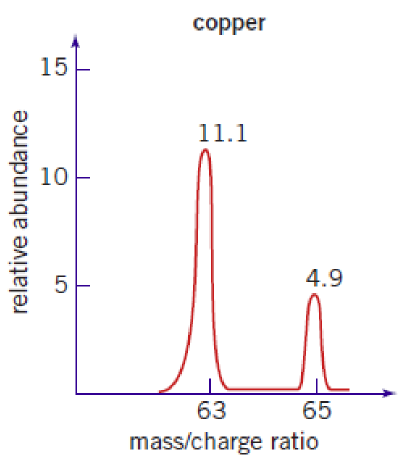
$$\frac{\textit{number of isotopes of a particular type}}{\textit{total number of particles in sample}} \times \frac{100}{1}$$

A peak is produced in the spectrum for each isotope. The peaks along the horizontal axis indicate the ratio:

$$\frac{\textit{mass of ion}}{\textit{charge on ion}}$$



The number of peaks recorded indicates the <u>number of isotopes</u> of the element present and their isotopic masses. The height of the peak indicates the abundance, a higher one meaning more. This is converted into the **percentage abundance** for the calculation of relative atomic mass. This is found by dividing the height of the particular peak by the sum of all the peaks.



$$\frac{11.1}{11.1 + 4.9} = \frac{11.1}{16.0} \times 100 = 69.4\%$$

$$\frac{4.9}{11.1 + 4.9} = \frac{4.9}{16.0} \times 100 = 30.6\%$$

2.2.2 - Describe how the mass spectrometer may be used to determine relative atomic mass using the 12C scale

To generate the relative scale of atomic masses, the carbon-12 isotope is assigned a relative mass of 12 units exactly. This is because carbon is cheap and widely available, it is easy to isolate and purify the isotope and it is in no way toxic. The mass of 12 was chosen to reflect the mass number.

So, the lightest of all elements (H) was found to have deflected 12 times further that carbon-12, while the magnesium-24 isotope deflects half as far. This is why hydrogen's relative mass is close to 1 and magnesium's is approximately 24.

These days, mass spectrometer are used in conjunction with nuclear magnetic resonance (NMR) or infrared (IR) spectrometers for the analysis of substances. The relative isotopic masses of all isotopes have been determined and are readily available

2.2.3 - Calculate non-integer relative atomic masses and abundance of isotopes from given data

The relative atomic mass of an element is the weighted mean of al its naturally occurring isotopes on the scale in which the carbon-12 isotope is 12 units exactly. Its symbol is Ar

To calculate the RAM, we multiply the relative isotopic mass (Ir) of the naturally occurring isotopes by their percentage abundance, then add these values.

$$A_r(X) = \frac{\sum(I_r \times abundance\ fraction)}{100}$$

Isotope	Relative Isotopic Mass	Percentage Abundance
^{24}Mg	23.99	78.70
^{25}Mg	24.99	10.13
^{26}Mg	25.98	11.17

$$A_r(Mg) = \frac{\Sigma(I_r \times \%\ \text{abundance})}{100}$$

$$= \frac{23.99 \times 78.70}{100} + \frac{24.99 \times 10.13}{100} + \frac{25.98 \times 11.17}{100}$$

$$= 18.88 + 2.53 + 2.90$$

$$= 24.31$$