1.3 – Chemical calculations I

1. Relative mass terms

Relative atomic mass (A_r) – the <u>average</u> mass of one atom of the element relative to one-twelfth the mass of an atom of carbon-12

Most elements exist as two or more different isotopes, so an average mass is used, relating to the relative abundance of all the isotopes present. It has no units as the masses are relative to another mass.

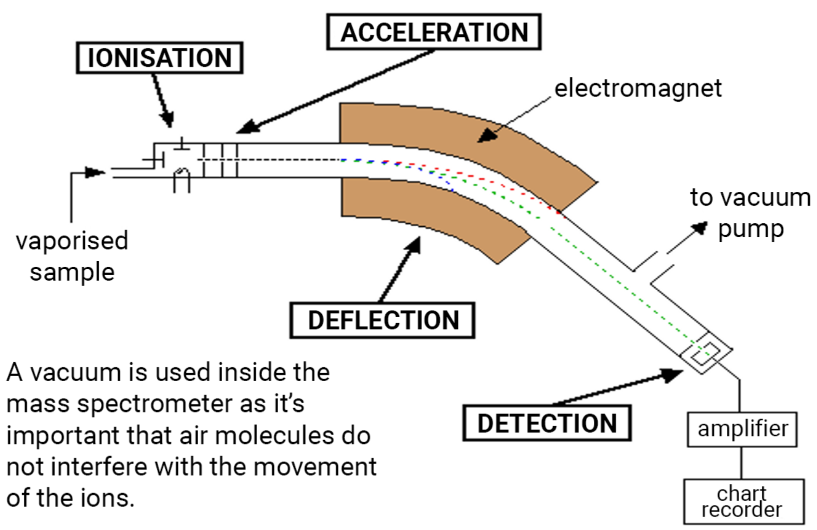
Relative isotopic mass – the mass of one atom of an isotope relative to one-twelfth the mass of one atom of carbon-12

Relative formula mass (M_r) – the total <u>average</u> mass of all the atoms in the formula relative to one-twelfth the mass of an atom of carbon-12

2. The mass spectrometer

A **mass spectrometer** can be used to find the **relative atomic mass** of an element. It measures:

- the relative mass of each different isotope of an element
- the relative abundance of each isotope of the element.



There are four main processes.

<u>Ionisation</u>

The **vaporised** sample passes into the ionisation chamber. The particles in the sample are **bombarded with a stream of electrons** and some of the collisions knock an electron out of the particles to make positive ions.

<u>Acceleration</u>

The positive ions are **accelerated** to a high speed by an **electric field**.

<u>Deflection</u>

Different ions are **deflected** by the **magnetic field** by different amounts. The amount of deflection depends on the mass of the ions and their charge:

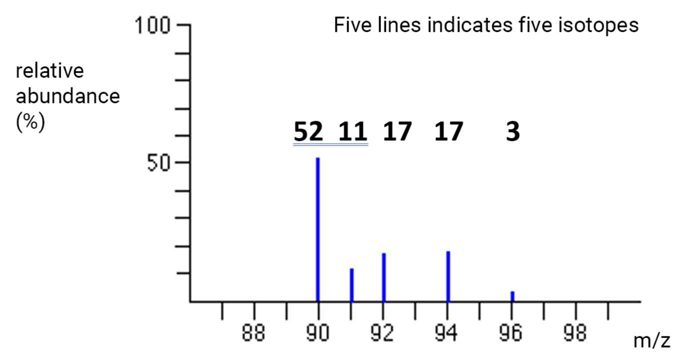
- the lighter ions are deflected more than the heavier ones
- ions with two positive charges are deflected more than ones with one positive charge.

These two factors are combined in the **mass/charge (m/z)** ratio.

<u>Detection</u>

Only ions with a given m/z ratio make it right through the machine to the ion detector. Electrons are transferred from the detector plate to the positive ion and this produces a current. The larger the current, the higher the abundance of that isotope. The signal is then amplified and recorded. When the magnetic field is varied, each ion stream can be brought in turn onto the detector to produce a current which is proportional to the number of ions arriving.

<u>Determining relative atomic mass (A_r) of an element</u>



$$A_r = \frac{(52 \times 90) + (11 \times 91) + (17 \times 92) + (17 \times 94) + (3 \times 96)}{100} = 91.3$$

Looking at the Periodic Table, the element that has the closest A_r to 91.3 is zirconium. Note that relative abundances do not have to be given as percentages, so you may have to divide by a different number.

<u>The mass spectrum of a diatomic molecule e.g. chlorine</u>

Chlorine has two isotopes – chlorine-35 (^{35}Cl) and chlorine-37 (^{37}Cl).

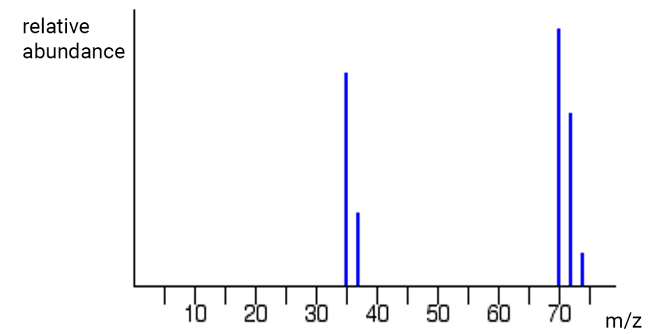
^{35}Cl is three times more common than ^{37}Cl.

The mass spectrum therefore consists of two peaks in the ratio 3:1 relating to $^{35}Cl^+$ (m/z 35) and $^{37}Cl^+$ (m/z 37) and three peaks in the ratio 9:6:1 relating to Cl_2^+ ions:

$^{35}Cl—^{35}Cl^+$ (m/z 70)

$^{35}Cl—^{37}Cl^+$ and $^{37}Cl—^{35}Cl^+$ (m/z 72)

$^{37}Cl—^{37}Cl^+$ (m/z 74)



Explaining the 9:6:1 ratio

The ^{35}Cl isotope is three times more common than the ^{37}Cl isotope.

The probability of an atom being ^{35}Cl is $\frac{3}{4}$ and being ^{37}Cl is $\frac{1}{4}$

Molecule	$^{35}Cl—^{35}Cl$	[$^{35}Cl—^{37}Cl$ and $^{37}Cl—^{35}Cl$]	$^{37}Cl—^{37}Cl$
Probability	$\frac{3}{4} \times \frac{3}{4}$	$[\frac{3}{4} \times \frac{1}{4} + \frac{1}{4} \times \frac{3}{4}]$	$\frac{1}{4} \times \frac{1}{4}$
⟶	$\frac{9}{16}$	$\frac{6}{16}$	$\frac{1}{16}$

⟶ ratio of peaks is 9:6:1

3. The avogadro constant, moles and molar mass

A mole is the amount of a substance in grams which has the same number of particles as there are atoms in 12g of carbon-12.

1 mol = 6.02×10^{23} particles

6.02×10^{23} is called the **Avogadro constant, N_A**

Molar mass is the mass of one mole of a substance.

It is the same number as A_r or M_r but has the unit g mol^{-1}.

$$\textbf{number of moles} = \frac{\textit{mass of substance (in g)}}{\textit{molar mass}}$$

4. Calculating reacting masses

Example: What mass of sodium oxide will form if 0.920g of sodium is burned in excess oxygen?

$$4Na + O_2 \longrightarrow 2Na_2O$$

Step 1 – Calculate the number of moles of sodium (the substance you have information about).

number of moles of sodium = $\frac{0.920}{23.0}$ = 0.040 mol

Step 2 – Use the balanced equation to find the mole ratio of sodium to sodium oxide and from this deduce the number of moles of sodium oxide formed in this example.

From the equation ⟶ 4 mol Na : 2 mol Na_2O

⟶ 0.040 mol : 0.020 mol

Step 3 – Rearrange the equation ⟶ mass = moles × M_r

Mass sodium oxide formed = 0.020 × 62.0 = 1.240g