WJEC Chemistry AS-level

1.3: Chemical Calculations

Detailed Notes

English Specification

Relative Masses

Relative Atomic Mass

Relative atomic mass (Ar) is defined as:

The mean mass of an atom of an element, divided by one twelfth of the mean mass of an atom of the carbon-12 isotope.

Relative Molecular Mass

Relative molecular mass (Mr) is defined as:

The mean mass of a molecule of a compound, divided by one twelfth of the mean mass of an atom of the carbon-12 isotope.

For ionic compounds, it is known as relative formula mass.

Relative Isotopic Mass

Relative isotopic mass is defined as:

The mean mass of an atom of an isotope, divided by one twelfth of the mean mass of an atom of the carbon-12 isotope.

Mass Spectrometry

This is an **analytical technique** used to identify different **isotopes** and find the **overall relative atomic mass** of an element.

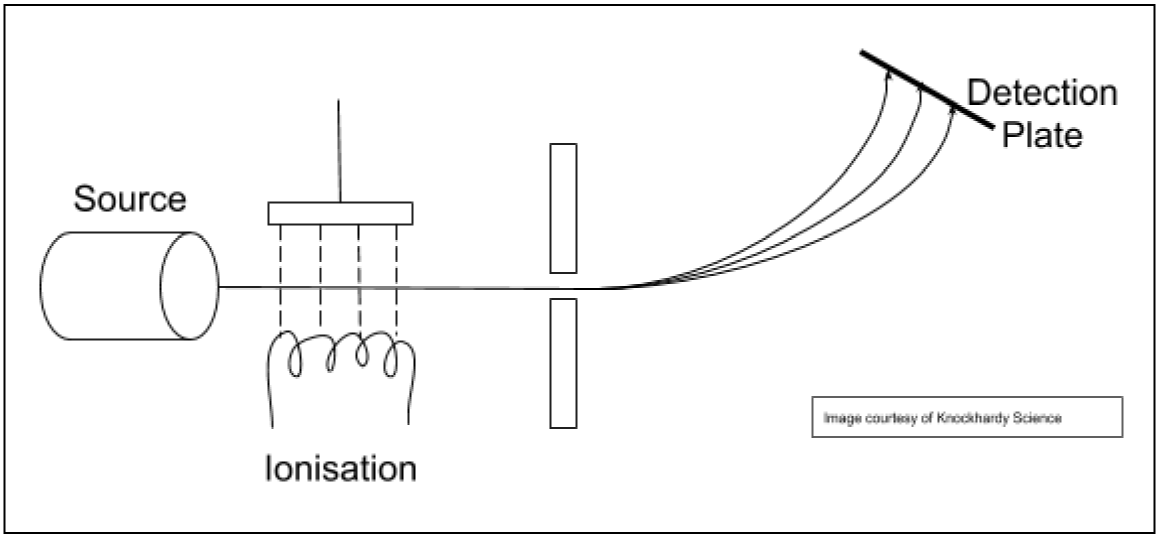
Time of Flight (TOF) Mass Spectrometry

This form of mass spectrometry records the time it takes for ions of each isotope to reach a detector. Using this, spectra can be produced showing each isotope present.

1. **Ionisation** - A sample of an element is **vapourised and injected** into the mass spectrometer where a **high voltage** is passed over the chamber. This causes electrons to be removed from the atoms (it is **ionised**) leaving +1 charged ions in the chamber.

2. **Acceleration** - These positively charged ions are then **accelerated** towards a negatively charged **detection plate**.

3. **Ion Drift** - The ions are then **deflected** by a magnetic field into a **curved path**. The **radius** of their path is dependent on the charge and mass of the ion.

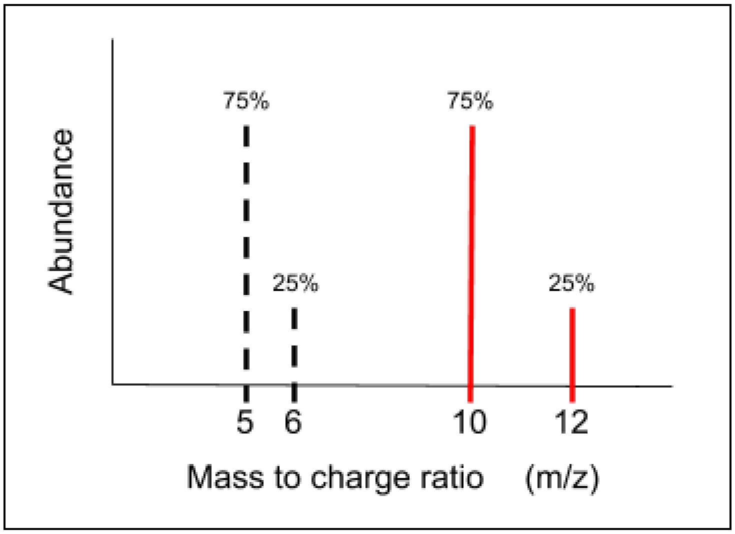


4. **Detection** - When the positive ions hit the **negatively charged detection plate**, they gain an electron producing a **flow of charge**. The greater the abundance, the greater the current produced.

5. **Analysis** - These current values are then used in combination with the **flight times** to produce a **spectra print-out** with the relative abundance of each isotope displayed.

During the ionisation process, a **2+ charged ion** may be produced. This means it will be affected more by the magnetic field producing a curved path of **smaller radius**. As a result, its **mass to charge ratio (m/z) is halved** and this can be seen on spectra as a trace at half the expected m/z value.

Example:



Determining Ar from Spectra

Using spectra like the one above, the *Ar* of the substance being analysed can be calculated:

$$\boxed{Ar = \frac{m/z \times \text{abundance}}{\text{Total abundance}}}$$

Example:

$$\mathbf{Ar = \frac{(10\times 75) + (12\times 25)}{(75 + 25)} = 10.5}$$

Chlorine Spectra

Spectra produced by the mass spectrometry of chlorine display a **characteristic pattern** in a **3:1 ratio** for Cl^+ ions and a **3:6:9 ratio** for Cl_2^+ ions. This is because one isotope is more common than the other and the chlorine molecule can form in **different combinations**.

Example:

$^{70}Cl_2^+ = 35 + 35$

$^{72}Cl_2^+ = 35 + 37$ OR $= 37 + 35$

$^{74}Cl_2^+ = 37 + 37$

Empirical and Molecular Formula

Empirical Formula

Empirical formula is the **simplest whole number ratio** of atoms of each element in a compound. It is found using **molar ratios** of each element.

Molecular Formula

Molecular formula is the **true number of each atom** in the molecule. It can be determined using the Mr of the **empirical formula** and the true **Mr of the molecule**. This gives a multiplier value which can be used to scale up the empirical formula.

Example:

$$\boxed{\frac{\text{Mr of molecule}}{\text{empirical Mr}} = \text{multiplier}}$$

Moles and the Avogadro Constant

The mole is a **standard unit of measurement** for substances. It always contains the **same number** of particles.

$$\boxed{L = 6.022\text{x}10^{23} \text{ particles}}$$

This number is the **Avogadro Constant (L)** and allows the number of particles present in a sample of a substance with known mass to be found:

$$\boxed{\text{Number of particles} = nL}$$

(n = moles) (L = Avogadro constant)

Concentration and Moles

The mole is a very important unit of measurement in many calculations:

$$\boxed{\text{Moles} = \frac{\text{mass}}{\text{Mr}} = \frac{\text{concentration x volume}}{1000}}$$

(where mass is in grams, concentration is in mol dm^{-3} and volume is in dm^3)

Molar Volume

A mole of atoms will always occupy the **same volume** when under **standard conditions**. This volume has a value of **24 dm^3**. If the pressure or temperature conditions change, the molar volume will also change.

Ideal Gas Equation

When under standard conditions, **gases and volatile liquids** follow certain trends:

Pressure is proportional to temperature.
Volume is proportional to temperature.
Pressure and volume are inversely proportional.

These relationships can be combined to give the **ideal gas equation**:

$$\boxed{pV = nRT = \frac{mRT}{Mr}}$$

p = pressure in Pascals, V = volume in m^3, T = temperature in Kelvin
n = moles, m = mass in grams

R is the **ideal gas constant**, equal to 8.31 $JK^{-1}mol^{-1}$.

Stoichiometry

Stoichiometry is the use of balanced chemical equations to calculate the **amount of products and reactants** used in the reaction. This mainly uses **ratios** between the species of the reaction to calculate quantities, such as reacting **masses**.

The Mole Ratio

When carrying out stoichiometric analysis, it is always important to consider the **molar ratios** within the reaction.

Example:

$$\boxed{Fe_2O_3 + 2Al \longrightarrow 2Fe + Al_2O_3}$$

This shows how 1 mole of Iron Oxide will react with 2 moles of Aluminium to give 2 moles of Iron and 1 mole of Aluminium Oxide.

This ratio can be **scaled up or down** as well as being used to calculate the mass of Aluminium required to react with a known mass of Iron Oxide.

Example:

What mass of Aluminium is required to react with 80g of Iron Oxide?

Firstly, find the number of moles of Iron Oxide using the Mr (Moles = Mass / Mr):

Reactant	Fe_2O_3	Al
Mass (g)	80.0	?
Mr	160	27.0
Moles	0.50	?

Then consider the molar ratio:

Reactant	Fe_2O_3	Al
Mass (g)	80.0	?
Mr	160	27.0
Moles	0.50	?
Mole Ratio	1	2

Use this to calculate the number of moles of Aluminium required (Mole ratio x Moles of Fe_2O_3):

Reactant	Fe_2O_3	Al
Mass (g)	80.0	?
Mr	160	27.0
Moles	0.50	1.00
Mole Ratio	1	2

Finally, find the mass of aluminium required (Mass = Moles x Mr):

Reactant	Fe_2O_3	Al
Mass (g)	80.0	27.0
Mr	160	27.0
Moles	0.50	1.00
Mole Ratio	1	2

This same method is very useful for **titration calculations**, but instead uses the mole formula with concentration and volume.

Atom Economy

In industrial chemical processes it is desirable to have a **high atom economy** for a reaction. This means there is **little or no waste product**, only the desired product. Therefore, it means the process is more economically viable for industrial scale manufacture. It is calculated using the following equation:

$$\boxed{\%\text{ atom economy} = \frac{\text{Mr of desired product}}{\text{Mr of reactants}} \times 100}$$

Percentage Yield

This helps to see if the reaction has been carried out correctly and if any product has been **lost** during the process. Again, it is useful in industry as it could help to highlight where product is being lost which could reduce **efficiency** of the industrial process.

$$\boxed{\%\text{ yield} = \frac{\text{Experimental mass}}{\text{Theoretical mass}} \times 100}$$