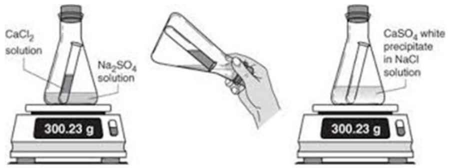
C3 Quantitative Chemistry

1. Conservations of mass.

The law of conversation of mass states that no atoms are lost or gained during a chemical reaction so the mass of the products equals the mass of the reactants.

Proving the conversion of mass:



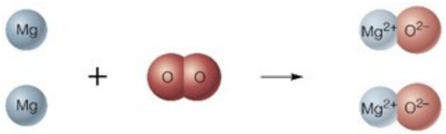
Calcium chloride + sodium sulfate —> calcium sulfate + sodium chloride

$CaCl_{2(aq)}$ + $Na_2SO_{4\,(aq)}$ —> $CaSO_{4\,(s)}$ + **2**$NaCl_{\,(aq)}$

To check conservation of atoms:

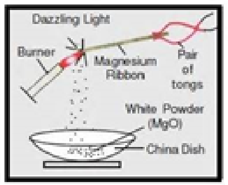
Reactants use: 1 x Ca, 2 x Cl, 2 x Na, 1 x SO_4
Products makes: 1 x Ca, 2 x Cl, 2 x Na, 1 x SO_4

Some reactions may appear to involve a change in mass but this is explained because a reactant or product is a gas and its mass has not been taken into account.
The conservation of mass is explained using the balanced symbol equations:
When a metal reacts with oxygen the mass of the oxide produced is greater than the mass of the metal



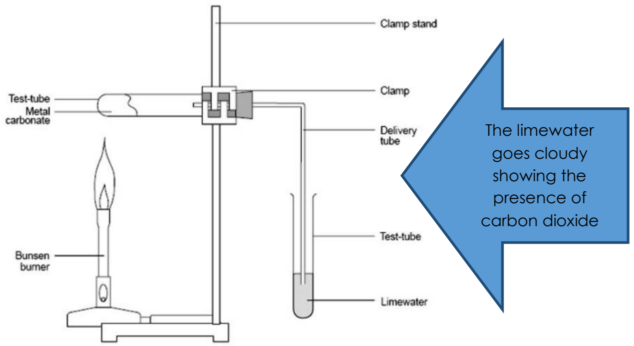
2 Mg + O_2 —-> 2MgO

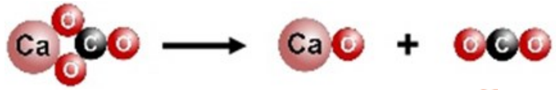
48.6g + 32.0g —-> 80.6g



Chemical Reaction - Burning of Mg ribbon in the air.

2. In **thermal decomposition** of metal carbonates carbon dioxide is produced and escapes into the atmosphere leaving the metal oxide as the only solid product.





$CaCO_3$ —> CaO + CO_2

100g —-> 56g + 44g

3. Relative Atomic Mass

The **Relative Atomic Mass (RAM or Ar)** is calculated in comparison to CARBON 12. It is the sum of the protons and neutrons in the nucleus.
Isotope – This is an element with the same number of protons – but a different number of neutrons in its nucleus.
If you look at chlorine on the periodic table its RAM is **35.5** this is because it exists as the two isotopes of:

$^{35}_{17}Cl$ $^{37}_{17}Cl$

4. To calculate the RAM you need to know:
The abundance (amount) of each isotope;
The RAM of each isotope.
If the relative abundances are 75% of Cl_{35} and 25% of Cl_{37}.
The equation can then be used:

$$\frac{(\% \text{ of } Cl_{35} \times \text{RAM of } Cl_{35}) + (\% \text{ of } Cl_{37} \times \text{RAM of } Cl_{37})}{100}$$

$$\frac{(75 \times 35) + (25 \times 37) = 2625 + 925 = 3550}{100} = \mathbf{35.5}$$

The **Relative Molecular Mass (RMM or Mr)** is calculated using the RAM/Ar of the atoms making up the molecule.

Mr of $CaCO_3$ = Ar of Ca + Ar of C + 3xAr of O
= 40 + 12 + 3x16 = 48
= 100

Remember – in a balanced equation, the sum of the Mr of the reactants equals the sum of the Mr of the products – this shows conservation of mass.

5. Moles and reacting mass (HT ONLY)

Avogadro's number 6.02×10^{23} atoms is the number of atoms in the relative atomic mass of an atom.
So, a 24 g piece of magnesium contains 6.02×10^{23} atoms.
This also refers to one mole of a substance.
The relative molecular mass of a compound also refers to Avogadro's number.

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6. <u>Calculating molar mass</u>

Unit is g/mol or $gmol^{-1}$.

The mass of one mole of a substance is calculated by adding up the relative atomic masses of the atoms in the formula.

Eg for H_2O

$H + H + O = H_2O$

1 + 1 + 16 = 18g

One mole of water = 18g/mol

Eg for formula containing brackets, these must be considered in the calculation:

$Mg(NO_3)_2$ atoms in the brackets must be multiplied by 2

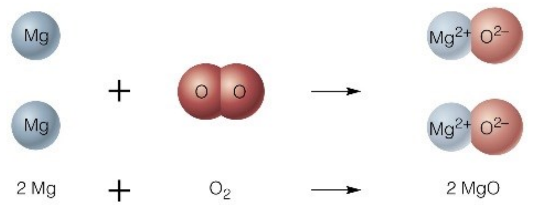
Mg = 24, N = 14, O = 16

So —> 24 + (2x14) + (2x(3x16) = 148 g/mol.

7. <u>Amounts of substances in equations (HT ONLY)</u>

Using balanced symbol equations the masses of reactants and products can be calculated.

For the reaction:



The equation also shows us that 2 moles of magnesium will react with 1 mole of oxygen to produce 2 moles of magnesium oxide.

Mg = 24 O =16

So —>

48g + 32g —> 80g

To calculate different masses the equation is needed:

$$\frac{\text{molar mass of substance A}}{\text{mass of A}} = \frac{\text{molar mass of substance B}}{\text{mass of B}}$$

Worked example – calculate the mass of MgO made from 6.0g of Mg.

Rearrange the equation to become:

$$\text{Mass of B} = \text{mass A} \times \frac{\text{molar mass of B}}{\text{Molar mass of A}}$$

Substitute in numbers

$$\text{Mass of MgO} = 6.0 \times \frac{80}{48}$$

Calculate = **10g Don't forget the units**

8. <u>Using moles to balance equations</u>

$$\textbf{Number or moles} = \frac{\textbf{mass of the chemical}}{\textbf{Molar mass}}$$

Worked example – Aluminium oxide Al_2O_3 produces aluminium, Al and oxygen O_2.

If 204g of Al_2O_3 produces 108g of Al work out the number of moles of Al_2O_3, Al and O_2 involved hence write out the full balanced equation.

Use the equation:

$$\textbf{Number or moles} = \frac{\textbf{mass of the chemical}}{\textbf{Molar mass}}$$

Al_2O_3 —> Al + O_2

204g —> 108g + ??g (204 – 108 = 96g)

$$\text{Number of moles of aluminium oxide} = \frac{204}{102} = 2$$

$$\text{Number of moles of aluminium} = \frac{108}{27} = 4$$

$$\text{Number of moles of oxygen} = \frac{96}{32} = 3$$

Balanced equation:

<u>2</u>Al_2O_3 —> **<u>4</u>**Al + **<u>3</u>**O_2

9. <u>Concentration of solutions</u>

CONCENTRATION – the amount of a chemical dissolved in a certain volume of a solution. It is calculated using:

$$\textbf{Concentration} = \frac{\textbf{mass of solute}}{\textbf{volume}}$$

The units for volume is **dm^3** this is equal to $1000cm^3$ to convert cm^3 to dm^3 **divide by 1000.**

Worked example:

A solution has a concentration of $4.2g/dm^3$. Calculate the mass of solute dissolved in 250 cm^3 of solution.

1. Use the equation. Substitute in known values.

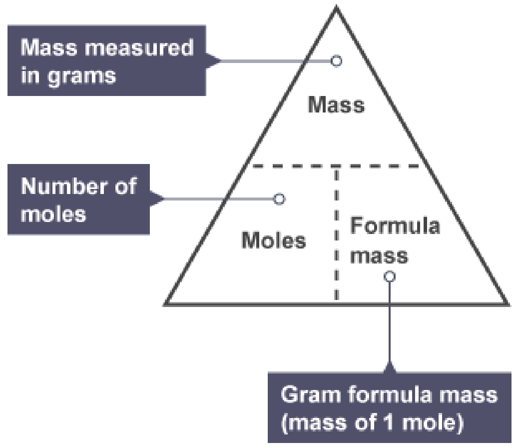
$$\text{Concentration} = \frac{\text{mass of solute}}{\text{Volume}}$$

$$4.2\ g/dm^3 = \frac{??}{(250/1000)}$$

2. Rearrange

Mass of solute = 4.2 x (250/1000)

= 1.05 **g Don't forget the units**



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10. Using moles to calculate concentration of solutions

You can work out the concentration of a solution using this equation:

$$\text{concentration in mol dm}^{-3} = \frac{\text{number of moles of solute}}{\text{volume of solution in dm}^3}$$

Worked example:

25.00cm³ of sodium hydroxide solution was titrated against 0.10mol dm⁻³ hydrochloric acid. An average of 20.00cm³ of the acid was needed to react completely. What is the concentration of the sodium hydroxide solution?

Step 1:

Number of moles of hydrochloric acid = Concentration of hydrochloric acid (mol dm⁻³) X Volume used (dm⁻³)

So, number of moles of hydrochloric acid $= 0.1 \times \frac{20.0}{1000} = 0.002$ mol

Step 2: Write the balanced equation for the reaction and use this to work out how many moles of sodium hydroxide reacted with this number of moles of acid:

The equation shows that 1mol of hydrochloric acid reacts

Sodium Hydroxide	+	Hydrochloric Acid	→	Sodium chloride	+	Water
NaOH		**HCl**		**NaCl**		H_2O

with 1mol of sodium hydroxide. So, 0.002mol of hydrochloric acid reacts with 0.002mol of sodium hydroxide

Step 3:

Concentration of sodium hydroxide = Moles of sodium hydroxide / Volume of sodium hydroxide solution (dm⁻³)

$= \frac{0.002}{0.025} = 0.08$ mol dm⁻³

11. Amounts of substances in volumes of gases

We find that is the **formula mass** of a gas is measured in grams and the **volume** it occupies is measured (at **room temperature and pressure**) then a gas occupies **24dm³.**

Number of moles of gas = volume of gas in dm³ / 24

Volumes from balanced equations

If propane reacts with oxygen the equation is:

$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$

If 24dm³ of C_3H_8 is used then 5 x 24dm³ of O_2 is needed (120 dm³)

If 2.4dm³ of C_3H_8 is used then 3 x 2.4dm³ of CO_2 is made (7.2 dm³)

This is calculated using the equation:

$$\frac{\text{Volume 1 (v1)}}{\text{Moles 1 (n1)}} = \frac{\text{volume 2 (v2)}}{\text{Moles 2 (n2)}}$$

Rearranged to become:

$$\frac{v1 \times n2}{n1} = v2$$

worked example:

Calculate the volume of water vapour made at rtp when 1.5 dm³ of C_3H_8 reacts with oxygen in the equation above.

1.5 dm³ C_3H_8 is used to produce 4x1.5dm³ of water = 6dm³

12. Percentage yield

The more reactant used the more product is made.

There may not be 100% of the product because:

Loss of filtration – small amounts stay on the filters

Loss in evaporation – some chemicals evaporate

Loss in transferring liquids – it sticks to the glass vessels

The **percentage yield** of a reaction is a way of comparing the mass of product made (the **actual yield)** to the mass we expect to make (the **theoretical** mass).

Percentage yield = actual yield / theoretical yield x 100

Worked example:

For example, in the reaction between hydrogen and oxygen the theoretical maximum yield of water which could be produced from reacting 32 g of oxygen is 36 g. The actual yield obtained was 28 g. So:

Actual yield (in grams)	28
Theoretical maximum yield (in grams)	36
Percentage yield = actual yield / theoretical yield x100	$\frac{28}{36} \times 100 = 78.8\%$

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13. Atom economy:

Atom economy is a way of measuring how many of the starting materials end up as **useful products** in a chemical reaction. It is measured in terms of the atoms taking part in the reaction.

It is calculated using:

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

A company makes magnesium sulfate $MgSO_4$ for use as bath salts. They need to find the best method.
A_r: Mg = 24, O = 16, H = 1, S = 32
M_r of $MgSO_4$ (desired) = 24 + 32 + (16 × 4) = 24 + 32 + 64 = **120**

Method 1:	**Method 2:**
$MgO + H_2SO_4 \rightarrow MgSO_4 + H_2O$	$MgCO_3 + H_2SO_4 \rightarrow MgSO_4 + H_2O + CO_2$
M_r reactants:	M_r reactants:
24 + 16 + 2 + 32 + 64 = 138	24 + 12 + 48 + 2 + 32 + 64 = 182
% atom economy =	% atom economy =

Which method is best? The higher the atom economy, the fewer atoms are in the wasted product, so the first method is a less wasteful process.

Calculating theoretical yields

The reactant used to calculate the theoretical maximum should be the limiting factor of the reaction

14. Choosing reactions pathways

All chemicals are produced following an extensive period of research and development. Chemicals made in the laboratory need to be "scaled up" to be manufactured on the plant.

To make a process viable industry tries:
to find suitable conditions – compromise between rate and equilibrium
to find a suitable catalyst – increases rate and cost effective as not used up in the process.

The hydrogen fuel cell car:
Looking at by-products, some reactions can give a low atom economy, e.g., hydrogen for vehicles made from water is:

$$2H_2O \rightarrow O_2 + 2H_2$$

Using the atom economy formula we find this atom economy is 12.5%. However, if oxygen were the desired product, this reaction would have an atom economy of 87.5%.

15. Considerations for reaction pathways – extension