1. Formulae, equations and amounts of substance

The mole is the key concept for chemical calculations

DEFINITION: **The mole** is the amount of substance in grams that has the same number of particles as there are atoms in 12 grams of carbon-12.

DEFINITION: **Relative atomic mass** is the weighted mean **mass** of one atom compared to one twelfth of the mass of one atom of carbon-12

DEFINITION: **Molar mass** is the mass in grams of 1 mole of a substance and is given the unit of g mol^{-1}

Molar mass for a compound can be calculated by adding up the mass numbers(from the periodic table) of each element in the compound
eg $CaCO_3$ = 40.1 + 12.0 +16.0 x3 = 100.1

For most calculations we will do at A- level we will use the following 3 equations

Learn these equations carefully and what units to use in them.

1. For pure solids, liquids and gases

$$\textbf{Amount} = \frac{\textbf{mass}}{\textbf{molar mass}}$$

Unit of Mass: grams
Unit of amount : mol

2. For Gases

Gas volume (dm^3)= amount x 24

This equation give the volume of a gas at room pressure (1atm) and room temperature 25^oC.

It is usually best to give your answers to 3sf

3. For solutions

$$\textbf{Concentration} = \frac{\textbf{amount}}{\textbf{volume}}$$

Unit of concentration: mol dm^{-3} or M
Unit of volume: **dm^3**

Converting volumes

$cm^3 \rightarrow dm^3 \div 1000$
$cm^3 \rightarrow m^3 \div 1000\ 000$
$dm^3 \rightarrow m^3 \div 1000$

For pure solids, liquids and gases

$$\textbf{amount} = \frac{\textbf{mass}}{\textbf{\textit{M}r}}$$

Unit of mass: grams
Unit of amount : mol

Example 1: Calculate the amount, in mol, in 35.0g of $CuSO_4$

amount = mass/*M*r

= 35/ (63.5 + 32 +16 x4)

= 0.219 mol

Many questions will involve changes of units
1000 mg =1g
1000 g =1kg
1000kg = 1 tonne

Example 2: Calculate the amount, in mol, in 75.0mg of $CaSO_4.2H_2O$

amount = mass/*M*r

= 0.075/ (40 + 32.0 +16.0 x4 + 18.0x2)

= 4.36×10^{-4} mol

Significant Figures
Give your answers to the same number of significant figures as the number of significant figures for the data you given in a question. If you are given a mixture of different significant figures, use the smallest

Hydrated salt

A hydrated salt contains water of crystallisation

$Cu(NO_3)_2 . 6H_2O$

hydrated copper (II) nitrate(V).

$Cu(NO_3)_2$

Anhydrous copper (II) nitrate(V).

Example 3

$Na_2SO_4 . xH_2O$ has a molar mass of 322.1

Calculate the value of x

Molar mass xH_2O = 322.1 – (23x2 + 32.1 + 16x4)

= 180

x = 180/18

=10

Heating in a crucible

This method could be used for measuring mass loss in various thermal decomposition reactions and also for mass gain when reacting magnesium in oxygen.

The water of crystallisation in calcium sulfate crystals can be removed as water vapour by heating as shown in the following equation.

$CaSO_4.xH_2O(s) \rightarrow CaSO_4(s) + xH_2O(g)$

Method.

•Weigh an empty clean dry crucible and lid .

•Add 2g of hydrated calcium sulfate to the crucible and weigh again

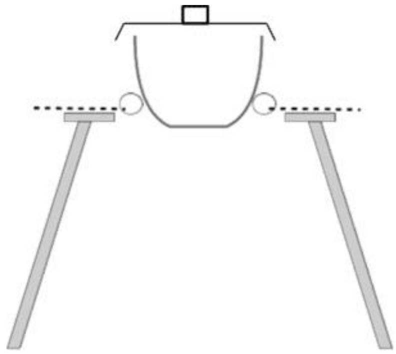
•Heat strongly with a Bunsen for a couple of minutes

•Allow to cool

•Weigh the crucible and contents again

•Heat crucible again and reweigh until you reach a constant mass (do this to ensure reaction is complete).

The lid improves the accuracy of the experiment as it prevents loss of solid from the crucible but should be loose fitting to allow gas to escape.



Large amounts of hydrated calcium sulfate, such as 50g, should not be used in this experiment as the decomposition is like to be incomplete.

The crucible needs to be dry otherwise a wet crucible would give an inaccurate result. It would cause mass loss to be too large as water would be lost when heating.

Small amounts the solid , such as 0.100 g, should **not** be used in this experiment as errors in weighing are too high.

Example 4. 3.51 g of hydrated zinc sulfate were heated and 1.97 g of anhydrous zinc sulfate were obtained.

Calculate the value of the integer x in $ZnSO_4.xH_2O$

Calculate the mass of H_2O = 3.51 – 1.97 = 1.54g

Calculate moles of $ZnSO_4$ $= \frac{1.97}{161.5}$ = 0.0122

Calculate moles of H_2O $= \frac{1.54}{18}$ =0.085

Calculate ratio of mole of $ZnSO_4$ to H_2O $= \frac{0.0122}{0.0122}$ =1 $= \frac{0.085}{0.0122}$ =7

X = 7

Avogadro's Constant

The mole is the amount of substance in grams that has the same number of particles as there are atoms in 12 grams of carbon-12.

Avogadro's constant
There are 6.02×10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.02×10^{23} of that entity':

Avogadro's constant can be used for atoms, molecules and ions

1 mole of copper atoms will contain 6.02×10^{23} atoms
1 mole of carbon dioxide molecules will contain 6.02×10^{23} molecules
1 mole of sodium ions will contain 6.02×10^{23} ions

No of particles = amount of substance (in mol) X Avogadro's constant

Example 5: How many atoms of tin are there in a 6.00 g sample of tin metal?

amount = mass/*A*r
= 6/ 118.7
= 0.05055 mol

Number atoms = amount x 6.02×10^{23}
= 0.05055 x 6.02×10^{23}
= 3.04×10^{22}

Example 6 : Calculate the number of chloride ions in a 25.0 cm^3 of a solution of magnesium chloride of concentration 0.400 mol dm^{-3}

amount= concentration x volume
$MgCl_2$ = 0.400 x **0.025**
= 0.0100 mol

Amount of chloride ions = 0.0100 x2
= 0.0200

There are two moles of chloride ions for every one mole of $MgCl_2$

Number ions of Cl^- = amount x 6.02×10^{23}
= 0.0200 x 6.02×10^{23}
= 1.204×10^{22}

Density

Density calculations are usually used with pure liquids but to work out the mass from a measured volume. It can also be used with solids and gases.

$$\textbf{Density} = \frac{\textbf{mass}}{\textbf{volume}}$$

Density is usually given in g cm^{-3}
Care needs to be taken if different units are used.

Example 7 : Calculate the number of molecules of ethanol in 0.500 dm^3 of ethanol (CH_3CH_2OH) liquid.
The density of ethanol is 0.789 g cm^{-3}

Mass ethanol = density x volume
= 0.789 x 500
= 394.5g

amount = mass/*M*r
= 394.5/ 46.0
= 8.576 mol

Number of molecules= amount x 6.022×10^{23}
= 8.576 x 6.022×10^{23}
= 5.16×10^{24}(to 3 sig fig)

Example 8: There are 980 mol of pure gold in a bar measuring 10 cm by 20 cm by 50 cm. Calculate the density of gold in kg dm^{-3}

Mass = amount x *M*r
= 980 x 197
= 193060 g
= 193.06kg

volume = 10x20x50
= 10 000cm^3
= 10dm^3

density = mass/volume
= 193/10
= 19.3 kg dm^{-3}

Parts per million (ppm)

Concentrations can be given also in parts per million. This is often used for gases in the atmosphere or in exhausts, and pollutants in water.

$$\text{parts per million (ppm) of substance, by mass} = \frac{\text{mass of substance in mixture}}{\text{total mass of mixture}} \times 1000\,000$$

Example 9 : Blood plasma typically contains 20 parts per million (ppm) of magnesium, by mass.
Calculate the mass of magnesium, in grams, present in 100 g of plasma.

$$\text{parts per million (ppm) of substance, by mass} = \frac{\text{mass of substance in mixture}}{\text{total mass of mixture}} \times 1000\,000$$

$$20 = \frac{\text{mass of substance in mixture}}{100} \times 1000\,000$$

mass of substance in mixture = 20 x100/1000 000
= 2×10^{-3} g

Empirical Formula

Definition: An empirical formula is the **simplest** ratio of atoms of each **element** in the compound.

General method

Step 1 : Divide each mass (or % mass) by the atomic mass of the element

Step 2 : For each of the answers from step 1 divide by the smallest one of those numbers.

Step 3: sometimes the numbers calculated in step 2 will need to be multiplied up to give whole numbers.

These whole numbers will be the empirical formula.

The same method can be used for the following types of data:

1. masses of each element in the compound
2. percentage mass of each element in the compound

Example 10 : Calculate the empirical formula for a compound that contains 1.82g of K, 5.93g of I and 2.24g of O

Step1: Divide each mass by the atomic mass of the element

K = 1.82 / 39.1 I = 5.93/126.9 O = 2.24/16

= 0.0465 mol = 0.0467mol = 0.14 mol

Step 2 For each of the answers from step 1 divide by the smallest one of those numbers.

K = 0.0465/0.0465 I = 0.0467/0.0465 O = 0.14 / 0.0465

=1 = 1 = 3

Empirical formula = KIO_3

Molecular formula from empirical formula

Definition: A molecular formula is the **actual** number of atoms of each element in the compound.

From the relative molecular mass (*M*r) work out how many times the mass of the empirical formula fits into the *M*r.

Example 11 : Determine the molecular formula for the compound with an empirical formula of C_3H_6O and a M_r of 116

C_3H_6O has a mass of 58

The empirical formula fits twice into M_r of 116

So the molecular formula is $C_6H_{12}O_2$

The *M*r does not need to be exact to turn an empirical formula into the molecular formula because the molecular formula will be a whole number multiple of the empirical formula.

Concentration of Solutions

A solution is a mixture formed when a solute dissolves in a solvent. In chemistry we most commonly use water as the solvent to form aqueous solutions. The solute can be a solid, liquid or a gas.

Molar concentration can be measured for solutions. This is calculated by dividing the amount in moles of the solute by the volume of the solution. The volume is measure is dm^3. The unit of molar concentration is mol dm^{-3} ; it can also be called molar using symbol M

Concentration = $\frac{\text{amount}}{\text{volume}}$

Unit of concentration: mol dm^{-3} or M
Unit of Volume: **dm^3**

Converting volumes

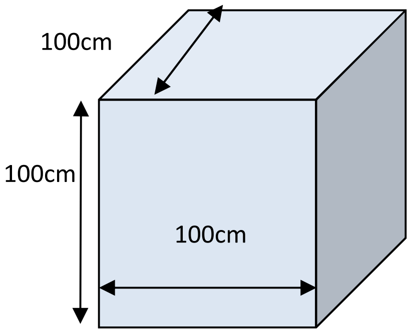
A m^3 is equivalent to a cube 100cmx100cmx100cm= 1000000 cm^3

A dm^3 is equivalent to a cube 10cmx10cmx10cm= 1000 cm^3

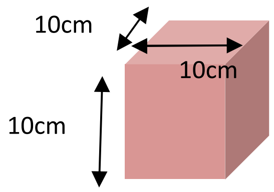
1 dm^3 = 1 litre

A cm^3 is equivalent to a cube 1cmx1cmx1cm

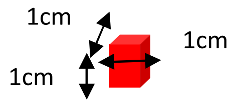
1 cm^3 = 1 ml



$1m^3$



1 dm^3 or 1 litre



$1cm^3$

1 m^3 = 1000 dm^3 or 1000L
To convert m^3 into dm^3 multiply by 1000

1 dm^3 = 1000 cm^3 or 1000 mL
To convert cm^3 into dm^3 divide by 1000

$cm^3 \rightarrow dm^3 \div 1000$
$cm^3 \rightarrow m^3 \div 1000\ 000$
$dm^3 \rightarrow m^3 \div 1000$

Example 12 Calculate the concentration of solution made by dissolving 5.00 g of Na_2CO_3 in 250 cm^3 water.

amount = mass/*Mr*

= 5 / (23.0 x2 + 12 +16 x3)

= 0.0472 mol

conc= amount/volume

= 0.0472 / **0.25**

= 0.189 mol dm^{-3}

Example 13 Calculate the concentration of solution made by dissolving 10 kg of Na_2CO_3 in 0.50 m^3 water.

amount = mass/*Mr*

= 10 000 / (23.0 x2 + 12 +16 x3)

= 94.2 mol

conc= amount/volume

= 94.2 / **500**

= 0.19 mol dm^{-3}

Mass Concentration

The concentration of a solution can also be measured in terms of mass of solute per volume of solution

Mass concentration = $\frac{\text{mass}}{\text{volume}}$

Unit of mass concentration: g dm^{-3}
Unit of mass **g**
Unit of volume: **dm^3**

To turn concentration measured in mol dm^{-3} into concentration measured in g dm^{-3} multiply by *M*r of the substance
conc in g dm^{-3} = conc in mol dm^{-3} x *M*r
The concentration in g dm^{-3} is the same as the mass of solute dissolved in $1dm^3$

Ions dissociating

When soluble ionic solids dissolve in water they will dissociate into separate ions. This can lead to the concentration of ions differing from the concentration of the solute.

Example 14

If 5.86g (0.1 mol) of sodium chloride (NaCl) is dissolved in 1 dm^3 of water then the concentration of sodium chloride solution would be $0.1moldm^{-3}$.
However the 0.1mol sodium chloride would split up to form 0.1 mol of sodium ions and 0.1 mol of chloride ions. The concentration of sodium ions is therefore 0.1 mol dm^{-3} and the concentration of chloride ions is also 0.1 mol dm^{-3}

$NaCl(s) + aq \rightarrow Na^{+}(aq) + Cl^{-}(aq)$

0.1mol 0.1mol 0.1mol

Example 15

If 9.53g (0.1 mol) of magnesium chloride ($MgCl_2$) is dissolved in 1 dm^3 of water then the concentration of magnesium chloride solution ($MgCl_2$ aq) would be $0.1moldm^{-3}$.
However the 0.1mol magnesium chloride would split up to form 0.1 mol of magnesium ions and 0.2 mol of chloride ions. The concentration of magnesium ions is therefore 0.1 mol dm^{-3} and the concentration of chloride ions is now 0.2 mol dm^{-3}

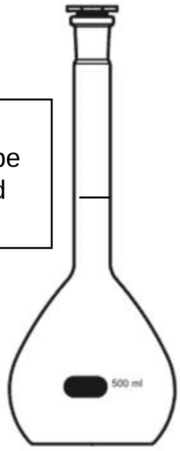
$MgCl_2(s) + aq \rightarrow Mg^{2+}(aq) + 2Cl^{-}(aq)$

0.1mol 0.1mol 0.2mol

Making a solution

- Weigh the sample bottle containing the required mass of solid on a 2 d.p. balance
- Transfer to beaker and reweigh sample bottle
- Record the difference in mass

Alternatively the known mass of solid in the weighing bottle could be transferred to beaker, washed and washings added to the beaker.



• Add 100 cm^3 of distilled water to the beaker. Use a glass rod to stir to help dissolve the solid.

•Sometimes the substance may not dissolve well in cold water so the beaker and its contents could be heated gently until all the solid had dissolved.

- Pour solution into a 250 cm^3 graduated flask via a funnel.
- Rinse beaker and funnel and add washings from the beaker and glass rod to the volumetric flask.
- make up to the mark with distilled water using a dropping pipette for last few drops.
- Invert flask several times to ensure uniform solution.

Remember to fill so the bottom of the meniscus sits on the line on the neck of the flask. With dark liquids like potassium manganate it can be difficult to see the meniscus.

Dilutions

Diluting a solution

•Pipette 25cm^3 of original solution into a 250cm^3 volumetric flask
•make up to the mark with distilled water using a dropping pipette for last few drops.
• Invert flask several times to ensure uniform solution.

Using a volumetric pipette is more accurate than a measuring cylinder because it has a smaller uncertainty

Use a teat pipette to make up to the mark in volumetric flask to ensure volume of solution accurately measured and one doesn't go over the line

Calculating Dilutions

Diluting a solution will not change the amount of moles of solute present but increase the volume of solution and hence the concentration will lower

amount= volume x concentration

If amount of moles does not change then
Original volume x original concentration = new diluted volume x new diluted concentration

so

$$\text{new diluted concentration} = \text{original concentration} \times \frac{\text{original volume}}{\text{new diluted volume}}$$

The new diluted volume will be equal to the original volume of solution added + the volume of water added.

Example 16
50 cm^3 of water are added to 150 cm^3 of a 0.20 mol dm^{-3} NaOH solution. Calculate the concentration of the diluted solution.

$$\text{new diluted concentration} = \text{original concentration} \times \frac{\text{original volume}}{\text{new diluted volume}}$$

$$\text{new diluted concentration} = 0.20 \times \frac{0.150}{0.200}$$

$$= 0.15 \text{ mol dm}^{-3}$$

Example 17
What volume of water in cm^3 must be added to dilute 5.00 cm^3 of 1.00 mol dm^{-3} hydrochloric acid so that it has a concentration of 0.050 mol dm^{-3}?

Amount in mol original solution = conc x vol
= 1.00 x 0.005
= 0.005

New volume = amount /conc
= 0.005/0.05
= 0.1dm^3 = 100cm^3

Volume of water added = 100-5 = 95cm^3

Ideal Gas Equation

The ideal gas equation applies to all gases and mixtures of gases. If a mixture of gases is used the value n will be the total moles of all gases in the mixture.

PV = nRT

Unit of Pressure (P):Pa
Unit of Volume (V): **m^3**
Unit of Temp (T): K
n= moles
R = 8.31 $JK^{-1}mol^{-1}$

The biggest problems students have with this equation is choosing and converting to the correct units, so pay close attention to the units.

Example 18: Calculate the mass of Cl_2 gas that has a pressure of 100 kPa, temperature 20 ^oC , volume 500 cm^3.   (R = 8.31)

moles = PV/RT
= 100 000 x 0.0005 / (8.31 x 293)
= 0.0205 mol

100 kPa = 100 000 Pa
20^oC = 20+273= 293K
500 cm^3 = 0.0005 m^3

Mass = amount x *M*r
= 0.0205 x (35.5 x2)
= 1.46 g

Converting temperature

$^oC \rightarrow$ K add 273

Example 19: 0.150 g of a volatile liquid was injected into a sealed gas syringe. The gas syringe was placed in an oven at 70 ^oC at a pressure of 100 kPa and a volume of 80 cm^3 was measured. Calculate the *M*r of the volatile liquid (R = 8.31)

moles = PV/RT
= 100 000 x 0.00008 / (8.31 x 343)
= 0.00281 mol

100 kPa = 100 000 Pa
80 cm^3 = 0.00008 m^3

Mr = mass/amount
= 0.15 / 0.00281
= 53.4 g mol^{-1}

Using a gas syringe

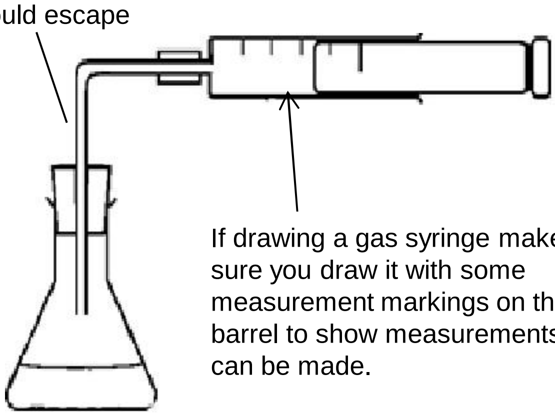
Gas syringes can be used for a variety of experiments where the volume of a gas is measured, possibly to work out moles of gas or to follow reaction rates.

The volume of a gas depends on pressure and temperature so when recording volume it is important to note down the temperature and pressure of the room.

Moles of gas can be calculated from gas volume (and temperature and pressure) using ideal gas equation PV = nRT

Potential errors in using a gas syringe
•gas escapes before bung inserted
•syringe sticks
• some gases like carbon dioxide or sulphur dioxide are soluble in water so the true amount of gas is not measured.

Make sure you don't leave gaps in your diagram where gas could escape



If drawing a gas syringe make sure you draw it with some measurement markings on the barrel to show measurements can be made.

Changing the Conditions of a gas

Questions may involve the same amount of gas under different conditions.

Example 20
40 cm^3 of oxygen and 60 cm^3 of carbon dioxide, each at 298 K and 100 kPa, were placed into an evacuated flask of volume 0.50 dm^3. Calculate the pressure of the gas mixture in the flask at 298 K

There are two approaches to solving this
1. Work out amount in mol of gas using ideal gas equation then put back into ideal gas equation with new conditions
2. Or combine the equation n= PV/RT as on right

Can do this as moles of gas do not change

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

As temperature is the same can make the above equation $P_1V_1 = P_2V_2$

$P_2 = P_1V_1 / V_2$

$= 100000 \times 1 \times 10^{-4} / 5 \times 10^{-4}$

= 20 000Pa

Reacting Volumes of Gas

Equal volumes of any gases measured under the same conditions of temperature and pressure contain equal numbers of molecules (or atoms if the gas in monatomic)

1 mole of any gas at room pressure (1atm) and room temperature 25°C will have the volume of 24dm^3

Volumes of gases reacting in a balanced equation can be calculated by simple ratio

Example 21 If one burnt 500 cm^3 of methane at 1atm and 300K what volume of Oxygen would be needed and what volume of CO_2 would be given off under the same conditions?

$CH_4(g) + \mathbf{2}\ O_2(g) \rightarrow CO_2(g) + 2\ H_2O(l)$

1 mole	**2** mole	1 mole
500cm^3	1dm^3	500cm^3

Simply multiply gas volume x2

Example 22 An important reaction which occurs in the catalytic converter of a car is
$2CO(g) + 2NO(g) \rightarrow 2CO_2(g) + N_2(g)$
In this reaction, when 500 cm^3 of CO reacts with 500 cm^3 of NO at 650 °C and at 1 atm.
Calculate the **total** volume of gases produced at the same temperature and pressure.

$2CO(g) + 2NO(g) \rightarrow 2CO_2(g) + N_2(g)$

500cm^3	500cm^3	**500cm^3**	**250cm^3**

total volume of gases produced = 750cm^3

Converting quantities between different substances using a balanced equation

$$N_2 \quad + \quad 3H_2 \rightarrow 2NH_3$$

The balancing (stoichiometric) numbers are mole ratios
e.g. 1 mol of N_2 reacts with 3 mol of H_2 to produce 2mol of NH_3

Typically we are given a quantity of one substance and are asked to work out a quantity for another substance in the reaction. Any of the above three equations can be used.

Step 1:
Use one of the above 3 equations to convert any given quantity into amount in mol
Mass → amount
Volume of gas → amount
Conc and vol of solution → amount

→

Step 2:
Use balanced equation to convert amount in mol of initial substance into amount in mol of second substance

→

Step 3
Convert amount, in mol, of second substance into quantity question asked for using relevant equation
e.g. amount ,*Mr* → mass
Amount gas → vol gas
amount, vol solution → conc

Example 23: Calculate the mass of carbon dioxide that would be produced from heating 5.50 g of sodium hydrogencarbonate.

$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$

Step 1: work out amount, in mol, of sodium hydrogencarbonate

amount = mass / *Mr*
= 5.5 /84
= 0.0655 mol

Step 2: use balanced equation to give amount in mol of CO_2

2 moles $NaHCO_3$: 1 moles CO_2
So 0.0655 HNO_3 : 0.0328mol CO_2

Step 3: work out mass of CO_2

Mass = amount x *Mr*
= 0.0328 x 44.0
=1.44g

Example 24: Calculate the mass of copper that reacts completely with 150 cm^3 of 1.60 mol dm^{-3} nitric acid.

$3Cu + 8HNO_3 \rightarrow 3Cu(NO_3)_2 + 2NO + 4H_2O$

Step 1: work out moles of nitric acid

amount = conc x vol
= 1.6 x 0.15
= 0.24 mol

Step 2: use balanced equation to give moles of Cu

8 moles HNO_3 : 3 moles Cu
So 0.24 HNO_3 : 0.09 (0.24 x $^3/_8$) mol Cu

Step 3: work out mass of Cu

Mass = amount x *Mr*
= 0.09 x 63.5
=5.71g

Example 25: What is the total volume of gas produced in dm^3 at 333K and 100kPa when 0.651 g of magnesium nitrate decomposes when heated?

$2Mg(NO_3)_{2\,(s)} \rightarrow 2MgO_{(s)} + 4NO_{2\,(g)} + O_{2\,(g)}$

Step 1: work out moles of magnesium nitrate

Moles = mass / *Mr*
= 0.651 / 148.3
= 0.00439 mol

Step 2: use balanced equation to give moles of gas produced

2 moles $Mg(NO_3)_2$: $4NO_{2\,(g)} + O_{2\,(g)}$ ie 5moles of gas
So 0.00439 $Mg(NO_3)_2$: 0.01098(0.00439 x $^5/_2$) mol gas

Step 3: work out volume of gas

Volume = nRT/P
= (0.01098 x 8.31 x 333)/ 100000
= 0.000304 m^3
= 0.303 dm^3

Example 26: 23.6cm^3 of H_2SO_4 neutralised 25.0cm^3 of 0.150 mol dm^{-3} NaOH. Calculate the concentration of the H_2SO_4

$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$

Step 1: work out moles of sodium hydroxide

amount = conc x vol
= 0.150 x 0.025
= 0. 00375 mol

Step 2: use balanced equation to give moles of H_2SO_4

2 moles NaOH : 1 moles H_2SO_4
So 0.00375 NaOH : 0.001875 mol H_2SO_4

Step 3 work out concentration of H_2SO_4

conc= amount/volume
= 0.001875 / 0.0236
= 0.0794 mol dm^{-3}

% Yield

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

% yield in a process can be lowered through incomplete reactions, side reactions, losses during transfers of substances, losses during purification stages.

Example 27: 25.0g of Fe_2O_3 was reacted and it produced 10.0g of Fe. What is the percentage yield?

$Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$

First calculate maximum mass of Fe that could be produced

Step 1: work out amount in mol of Iron oxide
amount = mass / *M*r
=25 / 159.6
= 0.1566 mol

Step 2: use balanced equation to give moles of Fe
1 moles Fe_2O_3 : 2 moles Fe
So 0.1566 Fe_2O_3 : 0.313mol Fe

Step 3: work out mass of Fe
Mass = amount x *M*r
= 0.313 x 55.8
=17.5g

% yield = (actual yield/theoretical yield) x 100
= (10/ 17.48) x 100
=57.2%

% Atom Economy

$$\text{percentage atom economy} = \frac{\text{Mass of useful products}}{\text{Mass of all reactants}} \times 100$$

Do take into account balancing numbers when working out % atom economy.

Example 28: Calculate the % atom economy for the following reaction where Fe is the desired product assuming the reaction goes to completion.

$Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$

$$\% \text{ atom economy} = \frac{(2 \times 55.8)}{(2 \times 55.8 + 3 \times 16) + 3 \times (12+16)} \times 100$$

=45.8%

Sustainable chemistry requires chemists to design processes with high atom economy that minimise production of waste products.

Reactions where there is only one product where all atoms are used making product are ideal and have 100% atom economy.
e.g. $CH_2=CH_2 + H_2 \rightarrow CH_3CH_3$

If a process does have a side, waste product the economics of the process can be improved by selling the bi-product for other uses

Displacement Reactions

Metal displacement reactions

More reactive metals will displace less reactive metals from their compounds

$Mg + CuSO_4 \rightarrow Cu + MgSO_4$

Ionically $Mg + Cu^{2+} \rightarrow Cu + Mg^{2+}$

Halogen displacement reactions

A halogen that is a strong oxidising agent will displace a halogen that has a lower oxidising power from one of its compounds

$Cl_2(aq) + 2Br^-(aq) \rightarrow 2Cl^-(aq) + Br_2(aq)$

$Cl_2(aq) + 2I^-(aq) \rightarrow 2Cl^-(aq) + I_2(aq)$

$Br_2(aq) + 2I^-(aq) \rightarrow 2Br^-(aq) + I_2(aq)$

See topic 4b Halogens for more detail

Precipitation Reactions

Insoluble salts can be made by mixing appropriate solutions of ions so that a **precipitate** is formed
Lead nitrate (aq) + sodium chloride (aq) → **lead chloride (s)** + sodium nitrate (aq)
These are called **precipitation** reactions. A **precipitate is a solid**

When making an insoluble salt, normally the salt would be removed by **filtration,** washed with distilled water to remove soluble impurities and then **dried on filter paper**

Writing ionic equations for precipitation reactions

We usually write ionic equations to show precipitation reactions. Ionic equations only show the ions that are reacting and leave out spectator ions.

Spectator ions are ions that are not
- Not changing state
- Not changing oxidation number

Take full equation

$$Pb(NO_3)_2\ (aq) + 2NaCl\ (aq) \rightarrow PbCl_2\ (s) + 2\ NaNO_3\ (aq)$$

Separate (aq) solutions into ions

$$Pb^{2+}_{(aq)} + 2NO_3^-{}_{(aq)} + 2Na^+{}_{(aq)} + 2Cl^-{}_{(aq)} \rightarrow PbCl_2\,_{(s)} + 2\ Na^+{}_{(aq)} + 2NO_3^-{}_{(aq)}$$

Cancel out spectator ions leaving ionic equation

$$Pb^{2+}_{(aq)} + 2Cl^-{}_{(aq)} \rightarrow PbCl_2\,_{(s)}$$

Reactions of Acids

A **Salt** is formed when the H^+ ion of an acid is replaced by a metal ion or an ammonium ion

The most common strong acids are :
Hydrochloric (HCl), sulfuric (H_2SO_4) and nitric (HNO_3) acid;

Neutralisation reactions form salts

Bases neutralise acids. Common bases are metal oxides, metal hydroxides and ammonia.

An alkali is a soluble base that releases OH^- ions in aqueous solution;
The most common alkalis are sodium hydroxide (NaOH), potassium hydroxide (KOH) and aqueous ammonia (NH_3)

Common Acid Reaction Equations

Acid + Base → Salt + Water

$HCl + NaOH \rightarrow NaCl + H_2O$

$2HNO_3 + Mg(OH)_2 \rightarrow Mg(NO_3)_2 + 2H_2O$

$H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$

$2HCl + CaO \rightarrow CaCl_2 + H_2O$

$HCl + NH_3 \rightarrow NH_4Cl$

Acid + Metal → Salt + Hydrogen

$2HCl + Mg \rightarrow MgCl_2 + H_2$

Observations: These reaction will effervesce because H_2 gas is evolved and the metal will dissolve

Acid + Carbonate → Salt + Water + Carbon Dioxide

$H_2SO_4 + K_2CO_3 \rightarrow K_2SO_4 + CO_2 + H_2O$

$2HCl + Na_2CO_3 \rightarrow 2NaCl + CO_2 + H_2O$

$2HCl + CaCO_3 \rightarrow CaCl_2 + CO_2 + H_2O$

Observations : In carbonate reactions there will be Effervescence due to the CO_2 gas evolved and the solid carbonate will dissolve. The temperature will also increase.

Ionic equations for reactions of acids with metals, carbonates, bases and alkalis

Ionic equations

acid + metal → salt + hydrogen

$2HCl_{(aq)} + Mg (s) \rightarrow MgCl_2 (aq) + H_2 (g)$ ⟶ $2H^+_{(aq)} + Mg_{(s)} \rightarrow Mg^{2+}_{(aq)} + H_{2\,(g)}$

acid + alkali (NaOH) → salt + water

$2HNO_2 (aq) + Ba(OH)_2 (aq) \rightarrow Ba(NO_2)_2 (aq) + 2H_2O_{(l)}$ ⟶ $H^+_{(aq)} + OH^-_{(aq)} \rightarrow H_2O_{(l)}$

acid + carbonate (Na_2CO_3) → salt + water + CO_2

$2HCl (aq) + Na_2CO_3 (aq) \rightarrow 2NaCl (aq) + H_2O (l) + CO_{2\,(g)}$ ⟶ $2H^+_{(aq)} + CO_3^{2-}{}_{(aq)} \rightarrow H_2O_{(l)} + CO_{2\,(g)}$

Example 29
The equation representing the reaction between copper(II) oxide and dilute sulfuric acid is:
$CuO(s) + H_2SO_4(aq) \rightarrow CuSO_4(aq) + H_2O(l)$
Write the ionic equation for the reaction.
Only the sulfate ion is a spectator ion in this case because it's the only ion not changing state.
$CuO(s) + 2H^+ \rightarrow Cu^{2+} (aq) + H_2O(l)$

Method for preparing a soluble salt

If using an insoluble base, metal or solid carbonate

- Add solid base to acid (gently heat to speed up reaction)
- Filter off excess solid base
- Heat filtrate solution until volume reduced by half
- Leave solution to cool and allow remaining water to evaporate slowly and crystals to form
- Filter or pick out crystals
- Leave to dry and put crystals between filter

Use excess solid base/ metal/carbonate to ensure all **acid** reacts/neutralises and that the product is neutral

The percentage yield of crystals will be less than 100% because some salt stays in solution. There will also be losses on transferring from one container to another and a loss on filtering.

If using a soluble base

An indicator can be used to show when the acid and alkali have completely reacted to produce a salt solution using the titration method. Then repeat reaction without indicator using the same volumes. Then follow above method from the reducing volume of solution stage to evaporate neutralised solution to get crystals of salt