1.2 Calculations

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 **average mass** of one atom compared to one twelfth of the mass of one atom of carbon-12

DEFINITION: **Relative molecular mass** is the **average mass** of a molecule compared to one twelfth of the mass of one atom of carbon-12

Avogadro's Number

There are 6.022×10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.022×10^{23} of that entity':

For most calculations at A-level we use the following 3 equations to calculate moles:

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

1. For pure solids, liquids and gases

$$\textbf{moles} = \frac{\textbf{mass}}{Mr}$$

Unit of mass: grams
Unit of moles : mol

Remember the *Mr* must be calculated and quoted to 1dp

2. For gases

$$PV = nRT$$

Unit of pressure (P):Pa
Unit of volume (V): **m^3**
Unit of temp (T): K
n= moles
R = 8.31

Note the different unit for volume

Converting temperature

$^oC \rightarrow K$ add 273

3. For solutions

$$\textbf{concentration} = \frac{\textbf{moles}}{\textbf{volume}}$$

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

Converting volumes

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

Using Equation 1

1. For pure solids, liquids and gases

$$\text{moles} = \frac{\text{mass}}{Mr}$$

Unit of mass: grams
Unit of moles : mol

Molar mass (*Mr*) 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

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

Example 1: Calculate the number of moles of $CuSO_4$ in 35.0g of $CuSO_4$

$$\text{moles} = \frac{\text{mass}}{Mr}$$

= 35.0/ (63.5 + 32.0 +16.0 x4)

= 0.219 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.

Example 2: What is the number of moles in 75.0mg of $CaSO_4.2H_2O$?

$$\text{moles} = \frac{\text{mass}}{Mr}$$

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

= 4.36×10^{-4} mol

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 (L)

There are 6.022×10^{23} atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains 6.022×10^{23} of that entity':

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

1 mole of copper atoms will contain 6.022×10^{23} atoms
1 mole of carbon dioxide molecules will contain 6.022×10^{23} molecules
1 mole of sodium ions will contain 6.022×10^{23} ions

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

Example 3 : Calculate the number of atoms of tin in a 6.00 g sample of tin metal.

moles = mass/*A*r
= 6.00/ 118.7
= 0.05055 mol

number atoms = moles x 6.022×10^{23}
= 0.05055 x 6.022×10^{23}
= 3.04×10^{22}

Example 4 : 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}

moles $MgCl_2$ = concentration x volume
= 0.400 x **0.0250**
= 0.0100 mol

moles 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^- = moles x 6.022×10^{23}
= 0.0200 x 6.022×10^{23}
= 1.20×10^{22} (to 3 sig fig)

Density

Density calculations are usually used with pure liquids 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 5 : Calculate the number of molecules of ethanol in a 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
= 394.5 g

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

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

Example 6 : 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 = moles x *M*r
= 980 x 197
= 193060 g
= 193.06 kg

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

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

Empirical formulae

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 7 : 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 to give moles

K = 1.82 / 39.1	I = 5.93/126.9	O = 2.24/16
= 0.0465 mol	= 0.0467mol	= 0.14mol

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 8 : Deduce the molecular formula for the compound with an empirical formula of C_3H_6O and a M_r of 116

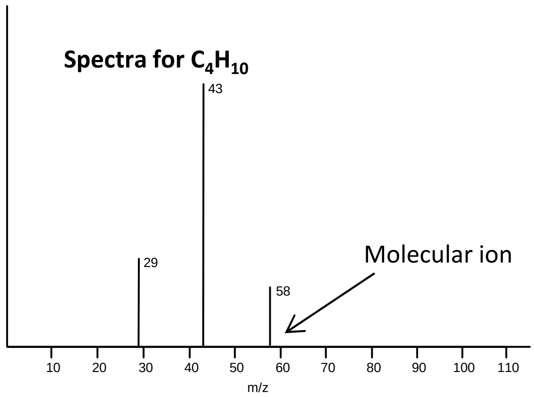
C_3H_6O has a mass of 58

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

Remember the *M*r of a substance can be found out from using a mass spectrometer. The molecular ion (the peak with highest m/z) will be equal to the *M*r.



Hydrated salt

A hydrated salt contains water of crystallisation

$Cu(NO_3)_2 \cdot 6H_2O$

hydrated copper (II) nitrate(V).

$Cu(NO_3)_2$

Anhydrous copper (II) nitrate(V).

Example 9

$Na_2SO_4 . xH_2O$ 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.

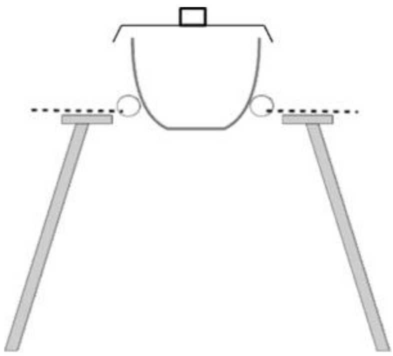
The water of crystallisation in calcium sulfate crystals can be removed as water vapour by heating as shown in the following equation.

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

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 likely 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 the water would be lost when heating.

Small amounts of the solid, such as 0.100 g, should **not** be used in this experiment as the percentage uncertainties in weighing will be too high.

Example 10. 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

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

$$\textbf{concentration} = \frac{\textbf{moles}}{\textbf{volume}}$$

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

Converting volumes

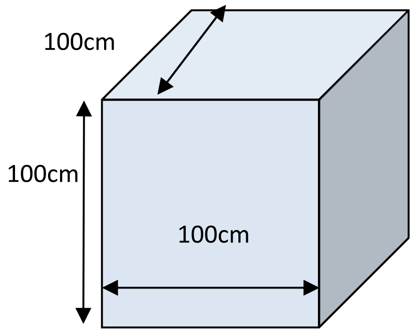
A m^3 is equivalent to a cube 100cmx100cmx100cm= 1000000 cm^3

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

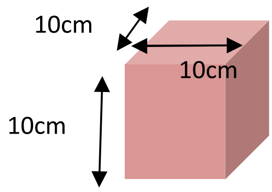
$1dm^3$ = 1litre

A cm^3 is equivalent to a cube 1cmx1cmx1cm

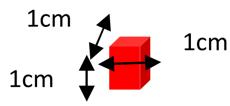
$1cm^3$ = 1 mL



1 m^3



1 dm^3 or 1 litre



1 cm^3

1 m^3 = 1000 dm^3 or 1000 L
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 11 Calculate the concentration of solution made by dissolving 5.00 g of Na_2CO_3 in 250 cm^3 water.

moles = mass/*Mr*

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

= 0.0472 mol

conc= moles/volume

= 0.0472 / **0.25**

= 0.189 mol dm^{-3}

Example 12 Calculate the concentration of solution made by dissolving 10 kg of Na_2CO_3 in 0.50 m^3 water.

moles = mass/*Mr*

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

= 94.2 mol

conc= moles/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

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

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

To convert 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 1 dm^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 13

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 0.1 mol dm^{-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}

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

0.1 mol   0.1 mol   0.1 mol

Example 14

If 9.53g (0.1 mol) of magnesium chloride ($MgCl_2$) is dissolved in 1dm^3 of water then the concentration of magnesium chloride solution ($MgCl_2$ aq) would be 0.1mol dm^{-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}

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

0.1 mol   0.1 mol   0.2 mol

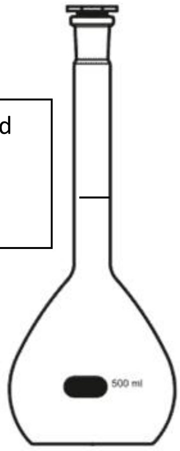
Making a solution

- Weigh the sample bottle containing the required mass of solid on a 2 dp 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 100cm^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 250cm^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.

Moles = 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 15
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 16
Calculate the volume of water in cm^3 that 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}

Moles original solution = conc x vol
= 1.00 x 0.005
= 0.005

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

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

Safety and hazards

Irritant - dilute acid and alkalis- wear googles
Corrosive- stronger acids and alkalis wear goggles
Flammable – keep away from naked flames
Toxic – wear gloves- avoid skin contact- wash hands after use
Oxidising- Keep away from flammable / easily oxidised materials

Hazardous substances in low concentrations or amounts will not pose the same risks as the pure substance.

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.

Converting temperature

$^oC \rightarrow K$ add 273

Example 17: 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 = moles x *M*r
= 0.0205 x (35.5 x2)
= 1.46 g

Example 18: 0.150g 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 100kPa and a volume of 80.0cm^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

*M*r = mass/moles
= 0.15 / 0.00281
= 53.4 g mol^{-1}

Using a gas syringe

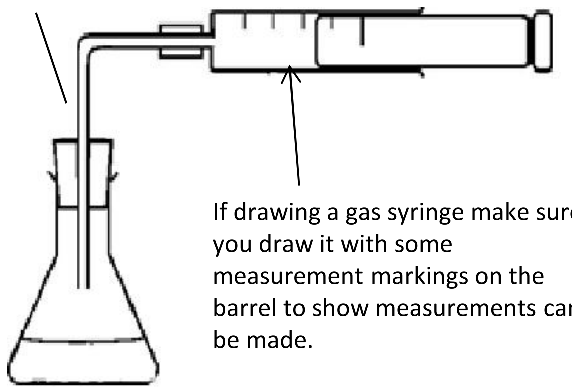
Gas syringes can be used for a variety of experiments where the volume of a gas is measured, possibly to work out moles of gas or to follow reaction rates.

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 sulfur 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 19
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 moles 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

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

We can do this as the moles of gas do not change

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

$P_2 = P_1V_1 / V_2$

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

$= 20\ 000$ Pa

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 20 500 cm^3 of methane is combusted at 1atm and 300K. Calculate the volume of oxygen needed to react and calculate the volume of CO_2 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 21 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

$N_2 + 3H_2 \rightarrow 2NH_3$

The balancing (stoichiometric) numbers are mole ratios
e.g. 1 mole of N_2 reacts with 3 moles of H_2 to produce 2 moles 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 three equations below can be used.

1. For pure solids, liquids and gases

$$\text{moles} = \frac{\text{mass}}{Mr}$$

2. For gases

$$PV = nRT$$

3. For solutions

$$\text{concentration} = \frac{\text{moles}}{\text{volume}}$$

Step 1:
Use one of the above 3 equations to convert any given quantity into moles
Mass → moles
PVT of gas → moles
Conc and vol of solution → moles

→

Step 2:
Use balanced equation to convert moles of initial substance into moles of second substance

→

Step 3
Convert moles of second substance into quantity question asked for using relevant equation
e.g. Moles ,*Mr* → mass
Mole, P, T gas → vol gas
Moles, vol solution → conc

Example 22: Calculate the mass of carbon dioxide produced from heating 5.50 g of sodium hydrogencarbonate.
$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$

Step 1: calculate moles of sodium hydrogencarbonate
Moles = mass / *Mr*
= 5.50 /84
= 0.0655 mol

Step 2: use balanced equation to give moles of CO_2
2 moles $NaHCO_3$: 1 moles CO_2
So 0.0655 HNO_3 : 0.0328moles CO_2

Step 3: calculate mass of CO_2
Mass = moles x *Mr*
= 0.0328 x 44.0
=1.44 g

Example 23: 23.6cm^3 of H_2SO_4 neutralised 25.0 cm^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: calculate moles of sodium hydroxide
Moles = 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 calculate concentration of H_2SO_4
conc= moles/volume
= 0.001875 / 0.0236
= 0.0794 mol dm^{-3}

Example 24: Calculate the total volume of gas produced in dm^3 at 333K and 100kPa when 0.651 g of magnesium nitrate is heated.
$2Mg(NO_3)_{2\,(s)} \rightarrow 2\,MgO_{(s)} + 4NO_{2\,(g)} + O_{2\,(g)}$

Step 1: calculate 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 $Mg(NO_3)_2$: $4NO_{2\,(g)} + O_{2\,(g)}$ i.e. 5moles of gas
So 0.00439 $Mg(NO_3)_2$: 0.01098(0.00439 x $^5/_2$) moles gas

Step 3: calculate volume of gas
volume = nRT/P
= (0.01098 x 8.31 x 333)/ 100000
= 0.000304m^3
= 0.303dm^3

Example 25: 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: calculate moles of nitric acid
moles = 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: calculate mass of Cu
mass = moles x *Mr*
= 0.09 x 63.5
=5.71g

Limiting and excess reactants

Example 26 Calculate the maximum mass of titanium that could be produced from reacting 100 g of $TiCl_4$ with 80.0 g of sodium.

$TiCl_4 + 4\ Na \rightarrow 4\ NaCl + Ti$

Step 1: calculate amount, in mol, $TiCl_4$
amount = mass / *Mr*
= 100 /189.9
= 0.527 mol

Step 1: calculate amount, in mol, Na
amount = mass / *Mr*
= 80/23.0
= 3.48 mol

Step 2 use balanced equation to work out which reactant is in excess
Using $1TiCl_4$:4 Na ratio we can see that 0.527mol of $TiCl_4$ should react with 2.108 mol of Na. We actually have 3.48 mol of Na which is an excess of 1.372 mol. We can complete calculation using the limiting reactant of $TiCl_4$

Step 3: use balanced equation to calculate amount in mol of Ti formed
1 mol $TiCl_4$: 1 mole Ti
So 0.527mol $TiCl_4$ produces 0.527 mole Ti

Step 4: calculate mass of Ti formed
Mass = amount x *Mr*
= 0.527 x 47.9
=25.2 g

% Yield and % Atom economy

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

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

Example 27: Calculate the % atom economy for the following reaction where Fe is the desired product assuming the reaction goes to completion.

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

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

=45.8%

Do use **balancing numbers** when calculating % atom economy.

Example 28: 25.0g of Fe_2O_3 was reacted and it produced 10.0g of Fe. Calculate the percentage yield.

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

First calculate maximum mass of Fe that could be produced.

Step 1: work out moles of iron oxide
Moles = mass / *Mr*
=25.0 / 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 : 0.313moles Fe

Step 3: work out mass of Fe
Mass = moles x *Mr*
= 0.313 x 55.8
=17.5 g

% yield = (actual yield/theoretical yield) x 100

= (10/ 17.5) x 100

=57.1%

Chemists want a high percentage yield as means there has been an efficient conversion of reactants to products.

Chemists want a high percentage atom economy so that the maximum mass of reactants ends up in the desired product (so minimising the amount of by-product).

Titrations

The method for carrying out the titration

•**rinse equipment** (burette with acid, pipette with alkali, conical flask with distilled water)
•**pipette 25 cm^3 of alkali into conical flask**
•**touch surface of alkali with pipette** (to ensure correct amount is added)
•**adds acid solution from burette**
•**make sure the jet space** in the burette **is filled** with acid
•add **a few drops of indicator** and refer to colour change at end point
•phenolphthalein [pink (alkali) to colourless (acid): end point pink colour just disappears] [use if NaOH is used]
•methyl orange [yellow (alkali) to red (acid): end point orange] [use if HCl is used]
•use a white tile underneath the flask to help observe the colour change
•add acid to alkali whilst **swirling the mixture** and **add acid dropwise at end point**
•**note burette reading** before and after addition of acid
•**repeats titration** until **at least 2 concordant results** are obtained- two readings within 0.1 of each other

Safety precautions

Acids and alkalis are corrosive
(at low concentrations acids are irritants)
Wear eye protection and gloves
If spilled immediately wash affected parts after spillage

If substance is unknown treat it as potentially toxic and wear gloves.

If the jet space is not filled properly prior to commencing the titration it will lead to errors if it then fills during the titration, leading to a larger than expected titre reading.

A conical flask is used in preference to a beaker because it is easier to swirl the mixture in a conical flask without spilling the contents.

Indicators are generally weak acids so only add a few drops of them. If too much is added it will affect the titration result.

Working out average titre results
Only make an average of the concordant titre results

If **2 or 3 values are within 0.10cm^3** and therefore **concordant** or close then we can say results are accurate and **repeatable** and **the titration technique is good/ consistent**

Recording results
•Results should be clearly recorded in a table
•Result should be recorded in full (i.e. both initial and final readings)
•**Record titre volumes to 2dp (0.05 cm^3)**

Distilled water can be added to the conical flask during a titration to wash the sides of the flask so that all the acid on the side is washed into the reaction mixture to react with the alkali.
It does not affect the titration reading as water does not react with the reagents or change the number of moles of acid added.

Common Titration Equations

$CH_3CO_2H + NaOH \rightarrow CH_3CO_2^-Na^+ + H_2O$

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

$HCl + NaOH \rightarrow NaCl + H_2O$

$NaHCO_3 + HCl \rightarrow NaCl + CO_2 + H_2O$

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

Titrating mixtures
If titrating a mixture to work out the concentration of an active ingredient it is necessary to consider if the mixture contains other substances that have acid base properties.
If they don’t have acid base properties we can titrate with confidence.

Testing batches
In quality control it will be necessary to do titrations/testing on several samples as the amount/concentration of the chemical being tested may vary between samples.

Safely dealing with excess acid
Sodium hydrogen carbonate ($NaHCO_3$) and calcium carbonate ($CaCO_3$) are good for neutralising excess acid in the stomach or acid spills because they are not corrosive and will not cause a hazard if used in excess. They also have no toxicity if used for indigestion remedies but the CO_2 produced can cause wind.
Magnesium hydroxide is also suitable for dealing with excess stomach acid as it has low solubility in water and is only weakly alkaline so not corrosive or dangerous to drink (unlike the strong alkali sodium hydroxide). It will also not produce any carbon dioxide gas.

More complicated titration calculations- taking samples

Example 29: A 25.0 cm^3 sample of vinegar was diluted in a 250 cm^3 volumetric flask. This was then put in a burette and 23.10 cm^3 of the diluted vinegar neutralised 25.0 cm^3 of 0.100 mol dm^{-3} NaOH. Calculate the concentration of the vinegar in g dm^{-3}

$CH_3CO_2H + NaOH \rightarrow CH_3CO_2^-Na^+ + H_2O$

Step 1: work out moles of sodium hydroxide
moles = conc x vol
= 0.10 x 0.025
= 0. 00250 mol

Step 2: use balanced equation to give moles of CH_3CO_2H
1 moles NaOH : 1 moles CH_3CO_2H
So 0.00250 NaOH : 0.00250 moles CH_3CO_2H

Step 3 work out concentration of diluted CH_3CO_2H in 23.1 (and 250 cm^3) in mol dm^{-3}

conc= moles/volume

= 0.00250 / 0.0231

= 0.108 mol dm^{-3}

Step 4 work out concentration of original concentrated CH_3CO_2H in 25 cm^3 in mol dm^{-3}

conc = 0.108 x 10 = 1.08 mol dm^{-3}

Step 5 work out concentration of CH_3CO_2H in original concentrated 25 cm^3 in gdm^{-3}

conc in g dm^{-3} = conc in mol dm^{-3} x *Mr*

= 1.08 x 60 = 64.8 g dm^{-3}

Example 30. An unknown metal carbonate reacts with hydrochloric acid according to the following equation.

$M_2CO_3(aq) + 2\ HCl(aq) \rightarrow 2\ MCl(aq) + CO_2(g) + H_2O(l)$

A 3.96 g sample of M_2CO_3 was dissolved in distilled water to make 250 cm^3 of solution. A 25.0 cm^3 portion of this solution required 32.8 cm^3 of 0.175 mol dm^{-3} hydrochloric acid for complete reaction. Calculate the *M*r of M_2CO_3 and identify the metal M

1. Calculate the number of moles of HCl used
moles = conc x vol
= 0.175 x 0.0328
= 0. 00574 mol

2. Work out number of moles of M_2CO_3 in 25.0 cm^3 put in conical flask
use balanced equation to give moles of M_2CO_3
2 mol HCl : 1 mol M_2CO_3
So 0. 00574 NaOH : 0.00287 mol M_2CO_3

3. Calculate the number of moles M_2CO_3 acid in original 250 cm^3 of solution
Moles in 250 cm^3 = 0.00287 x 10
= 0.0287 mol

4. work out the *Mr* of M_2CO_3
Mr= mass / moles
= 3.96/ 0.0287 = 138.0

5. Work out *Ar* of M = $\frac{138-12-16x3}{2}$

Ar of M = 39 M= potassium

Common Titration Equations

$CH_3CO_2H + NaOH \rightarrow CH_3CO_2^-Na^+ + H_2O$

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

$HCl + NaOH \rightarrow NaCl + H_2O$

$NaHCO_3 + HCl \rightarrow NaCl + CO_2 + H_2O$

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

Example 31 – back titration

950 mg of impure calcium carbonate tablet was crushed. 50.0 cm^3 of 1.00 mol dm^{-3} hydrochloric acid, an excess, was then added. After the tablet had reacted, the mixture was transferred to a volumetric flask. The volume was made up to exactly 100 cm^3 with distilled water. 10.0 cm^3 of this solution was titrated with 11.1 cm^3 of 0.300 mol dm^{-3} sodium hydroxide solution.
Calculate the percentage of $CaCO_3$ by mass in the tablet.

1. Calculate the number of moles of sodium hydroxide used
moles= conc x vol
= 0.30 x 0.0111
= 0. 00333 mol

2. Work out number of moles of hydrochloric acid left in 10.0 cm^3
use balanced equation to give moles of HCl
1 mol NaOH : 1 mol HCl
So 0.00333 NaOH : 0.00333 mol HCl

3. Calculate the number of moles of hydrochloric acid left in 100 cm^3 of solution
Moles in 100cm^3 = 0.00333 x10
=0.0333 mol

4. Calculate the number of moles of HCl that reacted with the indigestion tablet.
In original HCl 50.0 cm^3 of 1.00 mol dm^{-3} there are 0.05 mol

moles of HCl that reacted with the indigestion tablet. =0.05 -0.0333
=0.0167 mol

5 Use balanced equation to give moles of $CaCO_3$
$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + CO_2(g) + H_2O(l)$
2 mol HCl : 1 mol $CaCO_3$
So 0.0167 HCl : 0.00835 mol $CaCO_3$

6. work out the mass of $CaCO_3$ in original tablet
mass= moles x *Mr*
= 0.00835 x 100 = 0.835 g

percentage of $CaCO_3$ by mass in the tablet = 0.835/0.950 x100
= 87.9 %

Uncertainty

Readings and Measurements

Readings
the values found from a single judgement when using a piece of equipment

Measurements
the values taken as the difference between the judgements of two values (e.g. using a burette in a titration)

The uncertainty of a reading (one judgement) is at least ±0.5 of the smallest scale reading.
The uncertainty of a measurement (two judgements) is at least ±1 of the smallest scale reading.

Calculating apparatus uncertainties
Each type of apparatus has a sensitivity uncertainty

- balance ± 0.001 g (if using a 3 d.p. balance)
- volumetric flask ± 0.1 cm^3
- 25 cm^3 pipette ± 0.1 cm^3
- burette (start & end readings and end point) ± 0.15 cm^3

Calculate the percentage error for each piece of equipment used by

$$\% \text{ uncertainty} = \pm \frac{\text{uncertainty}}{\text{measurement made on apparatus}} \times 100$$

e.g. for burette
% uncertainty = 0.15/average titre result x 100

To calculate the maximum **total** percentage apparatus uncertainty in the final result add all the individual equipment uncertainties together.

To decrease the apparatus uncertainties you can either decrease the sensitivity uncertainty by using apparatus with a greater resolution (finer scale divisions) or you can increase the size of the measurement made.

Uncertainty of a measurement using a burette. If the burette used in the titration had an uncertainty for each reading of ± 0.05 cm^3 then during a titration two readings would be taken so the uncertainty on the titre volume would be ± 0.10 cm^3 . Then often another 0.05 is added on because of uncertainty identifying the end point colour change

Reducing uncertainties in a titration

Replacing measuring cylinders with pipettes or burettes which have lower apparatus uncertainty will lower the % uncertainty.

To reduce the % uncertainty in a burette reading it is necessary to make the titre a larger volume. This could be done by: increasing the volume and concentration of the substance in the conical flask or by decreasing the concentration of the substance in the burette.

If looking at a series of measurements in an investigation, the experiments with the smallest readings will have the highest experimental uncertainties.

Reducing uncertainties in measuring mass
Using a balance that measures to more decimal places or using a larger mass will reduce the % uncertainty in weighing a solid.

Weighing sample before and after addition and then calculating difference will ensure a more accurate measurement of the mass added.

Calculating the percentage difference between the actual value and the calculated value

If we calculated an *Mr* of 203 and the real value is 214, then the calculation is as follows:
Calculate difference 214-203 = 11
% = 11/214 x100
=5.41%

If the % **uncertainty** due to the apparatus **<** percentage difference between the actual value and the calculated value then there is a discrepancy in the result due to other errors.

If the % **uncertainty** due to the apparatus **>** percentage difference between the actual value and the calculated value then there is no discrepancy and all the difference between values can be explained by the sensitivity of the equipment.