

## 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  $6.022 \times 10^{23}$  atoms in 12 grams of carbon-12.

Therefore explained in simpler terms 'One mole of any specified entity contains  $6.022 \times 10^{23}$  of that entity':

For most calculations we will do at AS we will use the following 3 equations

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

### 1. For pure solids and gases

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

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):  $\text{m}^3$   
Unit of Temp (T): K  
n= moles  
R = 8.31

### Converting temperature

$$^{\circ}\text{C} \rightarrow \text{K add } 273$$

### 3. For solutions

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

Unit of concentration:  $\text{mol dm}^{-3}$  or M  
Unit of Volume:  $\text{dm}^3$

### Converting volumes

$$\begin{aligned} \text{cm}^3 &\rightarrow \text{dm}^3 \div 1000 \\ \text{cm}^3 &\rightarrow \text{m}^3 \div 1000\ 000 \\ \text{dm}^3 &\rightarrow \text{m}^3 \div 1000 \end{aligned}$$

Note the different unit for volume

### Typical mole calculations

Some Simple calculations using above equations

**Example 1:** What is the number of moles in 35.0g of  $\text{CuSO}_4$ ?

$$\begin{aligned} \text{moles} &= \text{mass}/\text{Mr} \\ &= 35.0 / (63.5 + 32.0 + 16.0 \times 4) \\ &= 0.219 \text{ mol} \end{aligned}$$

**Example 2:** What is the concentration of solution made by dissolving 5.00g of  $\text{Na}_2\text{CO}_3$  in  $250 \text{ cm}^3$  water?

$$\begin{aligned} \text{moles} &= \text{mass}/\text{Mr} \\ &= 5.00 / (23 \times 2 + 12 + 16 \times 3) \\ &= 0.0472 \text{ mol} \\ \text{conc} &= \text{moles}/\text{Volume} \\ &= 0.0472 / 0.25 \\ &= 0.189 \text{ mol dm}^{-3} \end{aligned}$$

**Example 3:** What is the mass of  $\text{Cl}_2$  gas that has a pressure of 100kPa, temperature 293K, volume  $500 \text{ cm}^3$ . (R = 8.31)

$$\begin{aligned} \text{moles} &= PV/RT \\ &= 100\ 000 \times 0.0005 / (8.31 \times 293) \\ &= 0.0205 \text{ mol} \\ \text{Mass} &= \text{moles} \times \text{Mr} \\ &= 0.0205 \times (35.5 \times 2) \\ &= 1.46 \text{ g} \end{aligned}$$

100 kPa = 100 000 Pa  
500  $\text{cm}^3$  = 0.0005  $\text{m}^3$

### 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

## 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  $6.02 \times 10^{23}$  atoms in 12 grams of carbon-12. Therefore explained in simpler terms 'One mole of any specified entity contains  $6.02 \times 10^{23}$  of that entity':

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

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

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

**Example 4** : How many atoms of Tin are there in a 6.00 g sample of Tin metal?

$$\begin{aligned}\text{amount} &= \text{mass}/A_r \\ &= 6.00/118.7 \\ &= 0.05055 \text{ mol} \\ \text{Number atoms} &= \text{amount} \times 6.02 \times 10^{23} \\ &= 0.05055 \times 6.02 \times 10^{23} \\ &= 3.04 \times 10^{22}\end{aligned}$$

**Example 5** : How many chloride ions are there in a 25.0 cm<sup>3</sup> of a solution of magnesium chloride of concentration 0.400 mol dm<sup>-3</sup> ?

$$\begin{aligned}\text{amount} &= \text{concentration} \times \text{Volume} \\ \text{MgCl}_2 &= 0.400 \times 0.025 \\ &= 0.0100 \text{ mol} \\ \text{Amount of chloride ions} &= 0.0100 \times 2 \\ &= 0.0200 \quad \text{There are two moles of chloride ions for every one mole of MgCl}_2 \\ \text{Number ions of Cl}^- &= \text{amount} \times 6.02 \times 10^{23} \\ &= 0.0200 \times 6.02 \times 10^{23} \\ &= 1.20 \times 10^{22} \text{ (to 3 sig fig)}\end{aligned}$$

## Density

$$\text{density} = \frac{\text{mass}}{\text{Volume}}$$

Density is usually given in g cm<sup>-3</sup>  
Care needs to be taken if different units are used.

**Example 6** : How many molecules of ethanol are there in a 0.500 dm<sup>3</sup> of ethanol (CH<sub>3</sub>CH<sub>2</sub>OH) liquid ? The density of ethanol is 0.789 g cm<sup>-3</sup>

$$\begin{aligned}\text{Mass} &= \text{density} \times \text{Volume} \\ \text{ethanol} &= 0.789 \times 500 \\ &= 394.5 \text{ g} \\ \text{amount} &= \text{mass}/M_r \\ &= 394.5/46.0 \\ &= 8.576 \text{ mol} \\ \text{Number of molecules} &= \text{amount} \times 6.02 \times 10^{23} \\ &= 8.576 \times 6.02 \times 10^{23} \\ &= 5.16 \times 10^{23} \text{ (to 3 sig fig)}\end{aligned}$$

## 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

$$\begin{array}{lll} \text{K} = 1.82 / 39.1 & \text{I} = 5.93/126.9 & \text{O} = 2.24/16 \\ = 0.0465 \text{ mol} & = 0.0467\text{mol} & = 0.14\text{mol} \end{array}$$

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

$$\begin{array}{lll} \text{K} = 0.0465/0.0465 & \text{I} = 0.0467/0.0465 & \text{O} = 0.14 / 0.0465 \\ =1 & = 1 & = 3 \end{array}$$

Empirical formula =KIO<sub>3</sub>

### 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 (Mr) work out how many times the mass of the empirical formula fits into the Mr.

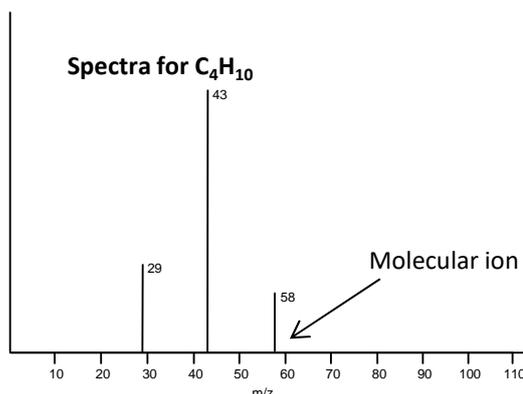
**Example 8 :** work out the molecular formula for the compound with an empirical formula of C<sub>3</sub>H<sub>6</sub>O and a Mr of 116

C<sub>3</sub>H<sub>6</sub>O has a mass of 58

The empirical formula fits twice into Mr of 116

So molecular formula is C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>

Remember the Mr 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 Mr.



The Mr 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

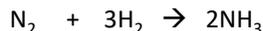
### Balancing ionic equations

Ionic equations need to be balanced both in terms of mass and charge

$\text{Fe}^{3+} + \text{Zn} \rightarrow \text{Fe}^{2+} + \text{Zn}^{2+}$  This is not balanced in terms of charge as there is a total reactant charge of +3 and product charge of +4

$2\text{Fe}^{3+} + \text{Zn} \rightarrow 2\text{Fe}^{2+} + \text{Zn}^{2+}$  This is now balanced in terms of atoms and charges

## Converting quantities between different substances using a balanced equation



The balancing (stoichiometric) numbers are mole ratios  
e.g. 1 mole of  $\text{N}_2$  reacts with 3 moles of  $\text{H}_2$  to produce 2 moles of  $\text{NH}_3$

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 moles  
Mass  $\rightarrow$  moles  
PVT of gas  $\rightarrow$  moles  
Conc and vol of solution  $\rightarrow$  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  $\rightarrow$  mass  
Mole, P, T gas  $\rightarrow$  vol gas  
Moles, vol solution  $\rightarrow$  conc

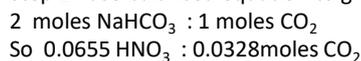
**Example 9:** What mass of Carbon dioxide would be produced from heating 5.50 g of sodium hydrogencarbonate?



Step 1: work out moles of sodium hydrogencarbonate

$$\begin{aligned}\text{Moles} &= \text{mass} / \text{Mr} \\ &= 5.50 / 84 \\ &= 0.0655 \text{ mol}\end{aligned}$$

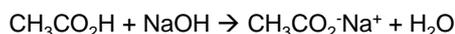
Step 2: use balanced equation to give moles of  $\text{CO}_2$



Step 3: work out mass of  $\text{CO}_2$

$$\begin{aligned}\text{Mass} &= \text{moles} \times \text{Mr} \\ &= 0.0328 \times 44.0 \\ &= 1.44 \text{ g}\end{aligned}$$

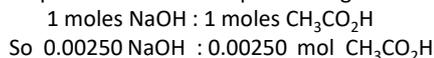
**Example 11:** A 25.0cm<sup>3</sup> sample of vinegar was diluted in a 250cm<sup>3</sup> volumetric flask. This was then put in a burette and 23.10cm<sup>3</sup> of the diluted vinegar neutralised 25.0 cm<sup>3</sup> of 0.100 M NaOH. What is the concentration of the vinegar in gdm<sup>-3</sup> ?



Step 1: work out moles of sodium hydroxide

$$\begin{aligned}\text{Moles} &= \text{conc} \times \text{vol} \\ &= 0.100 \times 0.0250 \\ &= 0.00250 \text{ mol}\end{aligned}$$

Step 2: use balanced equation to give moles of  $\text{CH}_3\text{CO}_2\text{H}$



Step 3 work out concentration of diluted  $\text{CH}_3\text{CO}_2\text{H}$  in 23.1 (and 250 cm<sup>3</sup>) in mol dm<sup>-3</sup>

$$\begin{aligned}\text{conc} &= \text{moles} / \text{Volume} \\ &= 0.00250 / 0.0231 \\ &= 0.108 \text{ mol dm}^{-3}\end{aligned}$$

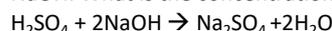
Step 4 work out concentration of original concentrated  $\text{CH}_3\text{CO}_2\text{H}$  in 25cm<sup>3</sup> in mol dm<sup>-3</sup>

$$\text{conc} = 0.108 \times 10 = 1.08 \text{ mol dm}^{-3}$$

Step 5 work out concentration of  $\text{CH}_3\text{CO}_2\text{H}$  in original concentrated 25 cm<sup>3</sup> in gdm<sup>-3</sup>

$$\begin{aligned}\text{conc in gdm}^{-3} &= \text{conc in mol dm}^{-3} \times \text{Mr} \\ &= 1.08 \times 60.0 = 64.8 \text{ g dm}^{-3}\end{aligned}$$

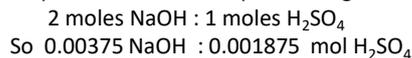
**Example 10:** 23.6cm<sup>3</sup> of  $\text{H}_2\text{SO}_4$  neutralised 25.0cm<sup>3</sup> of 0.150M NaOH. What is the concentration of the  $\text{H}_2\text{SO}_4$ ?



Step 1: work out moles of sodium hydroxide

$$\begin{aligned}\text{Moles} &= \text{conc} \times \text{vol} \\ &= 0.150 \times 0.025 \\ &= 0.00375 \text{ mol}\end{aligned}$$

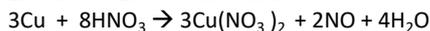
Step 2: use balanced equation to give moles of  $\text{H}_2\text{SO}_4$



Step 3 work out concentration of  $\text{H}_2\text{SO}_4$

$$\begin{aligned}\text{conc} &= \text{moles} / \text{Volume} \\ &= 0.001875 / 0.0236 \\ &= 0.0794 \text{ mol dm}^{-3}\end{aligned}$$

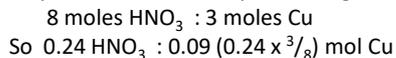
**Example 12:** What mass of Copper would react completely with 150 cm<sup>3</sup> of 1.60M nitric acid?



Step 1: work out moles of nitric acid

$$\begin{aligned}\text{Moles} &= \text{conc} \times \text{vol} \\ &= 1.6 \times 0.15 \\ &= 0.24 \text{ mol}\end{aligned}$$

Step 2: use balanced equation to give moles of Cu



Step 3: work out mass of Cu

$$\begin{aligned}\text{Mass} &= \text{moles} \times \text{Mr} \\ &= 0.09 \times 63.5 \\ &= 5.71 \text{ g}\end{aligned}$$

To turn concentration measured in mol dm<sup>-3</sup> into concentration measured in g dm<sup>-3</sup> multiply by Mr of the substance

$$\text{conc in g dm}^{-3} = \text{conc in mol dm}^{-3} \times \text{Mr}$$

The concentration in g dm<sup>-3</sup> is the same as the mass of solute dissolved in 1dm<sup>3</sup>

**Example 13:** What is the total volume of gas produced in dm<sup>3</sup> at 333K and 100kPa when 0.651 g of magnesium nitrate decomposes when heated?



Step 1: work out moles of magnesium nitrate

$$\begin{aligned} \text{Moles} &= \text{mass} / \text{Mr} \\ &= 0.651 / 148.3 \\ &= 0.00439 \text{ mol} \end{aligned}$$

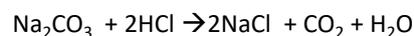
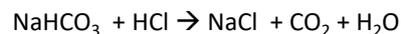
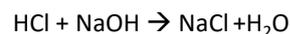
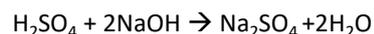
Step 2: use balanced equation to give moles of gas produced

2 moles Mg(NO<sub>3</sub>)<sub>2</sub> : 4NO<sub>2</sub>(g) + O<sub>2</sub>(g) ie 5moles of gas  
So 0.00439 Mg(NO<sub>3</sub>)<sub>2</sub> : 0.01098( 0.00439 x 5/2) moles gas

Step 3: work out volume of gas

$$\begin{aligned} \text{Volume} &= nRT/P \\ &= (0.01098 \times 8.31 \times 333) / 100000 \\ &= 0.000304\text{m}^3 \\ &= 0.303\text{dm}^3 \end{aligned}$$

### Common Reaction Equations



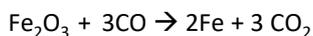
Other calculations

### % Yield and % Atom economy

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

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

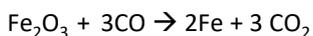
**Example 14:** What is the % atom economy for the following reaction where Fe is the desired product assuming the reaction goes to completion?



$$\begin{aligned} \% \text{ atom economy} &= \frac{(2 \times 55.8)}{(2 \times 55.8 + 3 \times 16) + 3 \times (12 + 16)} \times 100 \\ &= 45.8\% \end{aligned}$$

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

**Example 15:** 25.0g of Fe<sub>2</sub>O<sub>3</sub> was reacted and it produced 10.0g of Fe. What is the percentage yield?



First calculate maximum mass of Fe that could be produced

Step 1: work out moles of Iron oxide

$$\begin{aligned} \text{Moles} &= \text{mass} / \text{Mr} \\ &= 25.0 / 159.6 \\ &= 0.1566 \text{ mol} \end{aligned}$$

Step 2: use balanced equation to give moles of Fe

1 moles Fe<sub>2</sub>O<sub>3</sub> : 2 moles Fe  
So 0.1566 Fe<sub>2</sub>O<sub>3</sub> : 0.313 moles Fe

Step 3: work out mass of Fe

$$\begin{aligned} \text{Mass} &= \text{moles} \times \text{Mr} \\ &= 0.313 \times 55.8 \\ &= 17.5\text{g} \end{aligned}$$

$$\begin{aligned} \% \text{ yield} &= (\text{actual yield} / \text{theoretical yield}) \times 100 \\ &= (10 / 17.5) \times 100 \\ &= 57.1\% \end{aligned}$$

## 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 is monatomic)

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

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

**Example 16** If one burnt 500 cm<sup>3</sup> of methane at 1atm and 300K what volume of Oxygen would be needed and what volume of CO<sub>2</sub> would be given off under the same conditions?



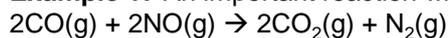
1 mole      2 mole      1 mole

500cm<sup>3</sup>    1dm<sup>3</sup>      500cm<sup>3</sup>

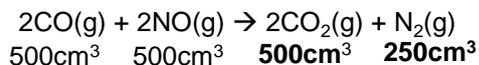


Simply multiply  
gas volume x2

**Example 17** An important reaction which occurs in the catalytic converter of a car is



In this reaction, when 500 cm<sup>3</sup> of CO reacts with 500 cm<sup>3</sup> of NO at 650 °C and at 1 atm. Calculate the **total** volume of gases produced at the same temperature and pressure ?



**total** volume of gases produced = 750cm<sup>3</sup>

# Experiments

## Safety and hazards

Irritant - dilute acid and alkalis- wear goggles  
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.

## 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 sulphate crystals can be removed as water vapour by heating as shown in the following equation.



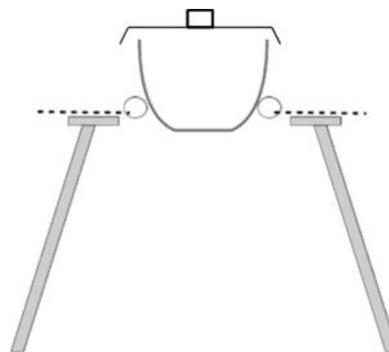
### Method.

- Weigh an empty clean dry crucible and lid .
- Add 2g of hydrated calcium sulphate 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).

Large amounts of hydrated calcium sulphate, 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 water would be lost when heating.

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.



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

**Example 18.** 3.51 g of hydrated zinc sulphate were heated and 1.97 g of anhydrous zinc sulphate were obtained.

Use these data to calculate the value of the integer  $x$  in  $\text{ZnSO}_4 \cdot x\text{H}_2\text{O}$

Calculate the mass of  $\text{H}_2\text{O} = 3.51 - 1.97 = 1.54\text{g}$

Calculate moles of $\text{ZnSO}_4$	$= \frac{1.97}{161.5}$	Calculate moles of $\text{H}_2\text{O}$	$= \frac{1.54}{18}$
	$= 0.0122$		$= 0.085$

Calculate ratio of mole of $\text{ZnSO}_4$ to $\text{H}_2\text{O}$	$= \frac{0.0122}{0.0122}$		$= \frac{0.085}{0.0122}$
	$= 1$		$= 7$

$$X = 7$$

## 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.

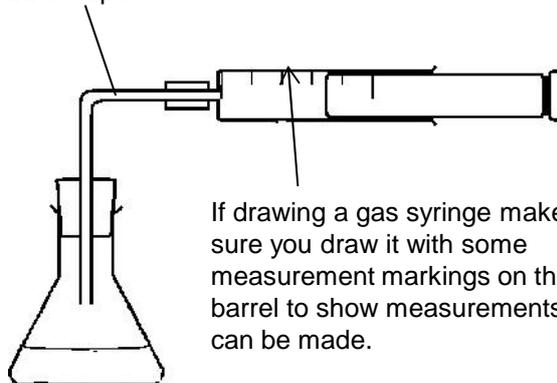
The volume of a gas depends on pressure and temperature so when recording volume it is important to note down the temperature and pressure of the room.

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



**Example 19:** 0.150g of a volatile liquid was injected into a sealed gas syringe. The gas syringe was placed in an oven at 70°C at a pressure of 100kPa and a volume of 80cm<sup>3</sup> was measured. What is the Mr of the volatile liquid ? (R = 8.31)

$$\begin{aligned} \text{moles} &= PV/RT \\ &= 100\,000 \times 0.00008 / (8.31 \times 343) \\ &= 0.00281 \text{ mol} \end{aligned}$$

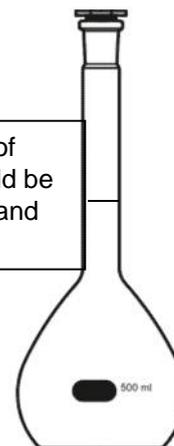
$$\begin{aligned} \text{Mr} &= \text{mass/moles} \\ &= 0.15 / 0.00281 \\ &= 53.4 \text{ g mol}^{-1} \end{aligned}$$

$$\begin{aligned} 100 \text{ kPa} &= 100\,000 \text{ Pa} \\ 80 \text{ cm}^3 &= 0.00008 \text{ m}^3 \end{aligned}$$

## 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
- Add 100cm<sup>3</sup> 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<sup>3</sup> 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.

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



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.

# Titration

The method for carrying out the titration

- rinse equipment** (burette with acid, pipette with alkali, conical flask with distilled water)
- pipette 25 cm<sup>3</sup> 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

## Working out average titre results

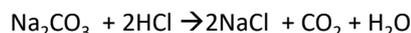
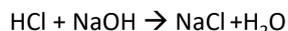
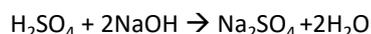
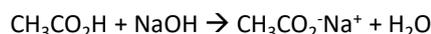
Only make an average of the concordant titre results

If **2 or 3 values** are within **0.10cm<sup>3</sup>** and therefore **concordant** or close then we can say results are accurate and **reproducible** 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<sup>3</sup>)**

## Common Titration Equations



## Titration 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<sub>3</sub>) and calcium carbonate (CaCO<sub>3</sub>) 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<sub>2</sub> 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.

## 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 we only add a few drops of them. If too much is added it will affect the titration result

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.

# 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  $\pm 0.5$  of the smallest scale reading.  
The uncertainty of a measurement (two judgements) is at least  $\pm 1$  of the smallest scale reading.

### Calculating Apparatus Uncertainties

Each type of apparatus has a sensitivity uncertainty

- balance  $\pm 0.001$  g
- volumetric flask  $\pm 0.1$  cm<sup>3</sup>
- 25 cm<sup>3</sup> pipette  $\pm 0.1$  cm<sup>3</sup>
- burette (start & end readings and end point)  $\pm 0.15$  cm<sup>3</sup>

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

$$\% \text{ uncertainty} = 0.15 / \text{average titre result} \times 100$$

To calculate the maximum 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  $\pm 0.05$  cm<sup>3</sup> then during a titration two readings would be taken so the uncertainty on the titre volume would be  $\pm 0.10$  cm<sup>3</sup>. 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 error

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 more accurate balance or 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  $214 - 203 = 11$   
 $\% = 11 / 214 \times 100$   
 $= 5.41\%$

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 errors in the results can be explained by the sensitivity of the equipment.