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.

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

1. **For pure solids, liquids 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): m³
   Unit of Temp (T): K
   \( n = \text{moles} \)
   \( R = 8.31 \)
   Note the different unit for volume

3. **For solutions**
   \[
   \text{Concentration} = \frac{\text{moles}}{\text{volume}}
   \]
   Unit of concentration: mol dm⁻³ or M
   Unit of Volume: dm³

**Converting volumes**

- cm³ → dm³ ÷ 1000
- cm³ → m³ ÷ 1000 000
- dm³ → m³ ÷ 1000

**Converting temperature**

\( ^{\circ} \text{C} \rightarrow \text{K} \text{ add 273} \)

**Using Equation 1**

1. **For pure solids, liquids and gases**

   \[
   \text{moles} = \frac{\text{mass}}{\text{Mr}}
   \]
   Unit of Mass: grams
   Unit of moles: mol

   **Example 1:** What is the number of moles in 35.0g of CuSO₄?
   \[
   \text{moles} = \frac{35.0}{(63.5 + 32.0 + 16.0 \times 4)}
   \]
   \[
   = 0.219 \text{ mol}
   \]

2. **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 CaCO₃ = 40.1 + 12.0 + 16.0 x3 = 100.1

   **Example 2:** What is the number of moles in 75.0mg of CaSO₄₂H₂O?
   \[
   \text{moles} = \frac{0.075}{(40 + 32.0 + 16.0 \times 4 + 18.0 \times 2)}
   \]
   \[
   = 4.36 \times 10^{-4} \text{ mol}
   \]

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 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':
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 can be used for atoms, molecules and ions

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

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

Example 3: How many atoms of Tin are there in a 6.00 g sample of Tin metal?

moles = mass/Ar
= 6.00/ 118.7
= 0.05055 mol

Number atoms = moles x $6.022 \times 10^{23}$
= 0.05055 x $6.022 \times 10^{23}$
= 3.04 x$10^{22}$

Example 4: How many chloride ions are there in a 25.0 cm$^3$ of a solution of magnesium chloride of concentration 0.400 mol dm$^{-3}$?

moles = concentration x Volume
MgCl$_2$ = 0.400 x 0.0250
= 0.0100 mol

moles of chloride ions = 0.0100 x2
= 0.0200

Number ions of Cl$^-$ = moles x $6.022 \times 10^{23}$
= 0.0200 x $6.022 \times 10^{23}$
= 1.20 x$10^{22}$ (to 3 sig fig)

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.

density = mass/Volume

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

Example 5: How many molecules of ethanol are there in a 0.500 dm$^3$ of ethanol (CH$_3$CH$_2$OH) liquid? The density of ethanol is 0.789 g cm$^{-3}$

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

moles = mass/Mr
= 394.5/ 46.0
= 8.576 mol

Number of molecules= moles x $6.022 \times 10^{23}$
= 8.576 x $6.022 \times 10^{23}$
= 5.16 x$10^{24}$ (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. What is the density of gold in kg dm$^{-3}$?

Mass = moles x Mr
= 980 x 197
= 193060 g
= 193.06 kg

Volume = 10x20x50
= 10 000cm$^3$
= 10dm$^3$

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**

1. **Step 1:** Divide each mass (or % mass) by the atomic mass of the element
2. **Step 2:** For each of the answers from step 1 divide by the smallest one of those numbers.
3. **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.

**Example 7:** Calculate the empirical formula for a compound that contains 1.82g of K, 5.93g of I and 2.24g of O

Step 1: Divide each mass by the atomic mass of the element to give moles

\[
\begin{align*}
\text{K} &= 1.82 / 39.1 = 0.0465 \text{ mol} \\
\text{I} &= 5.93 / 126.9 = 0.0467 \text{ mol} \\
\text{O} &= 2.24 / 16 = 0.14 \text{ mol}
\end{align*}
\]

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

\[
\begin{align*}
\text{K} &= 0.0465 / 0.0465 = 1 \\
\text{I} &= 0.0467 / 0.0465 = 1 \\
\text{O} &= 0.14 / 0.0465 = 3
\end{align*}
\]

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 (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$_3$H$_6$O and a Mr of 116

C$_3$H$_6$O has a mass of 58
The empirical formula fits twice into Mr of 116

So molecular formula is C$_6$H$_{12}$O$_2$

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.

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

\[ \text{CaSO}_4 \cdot x \text{H}_2\text{O}(s) \rightarrow \text{CaSO}_4(s) + x \text{H}_2\text{O}(g) \]

**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).

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.

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 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.

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.

**Example 10.** 3.51 g of hydrated zinc sulfate were heated and 1.97 g of anhydrous zinc sulfate were obtained. Use these data to calculate the value of the integer \( x \) in ZnSO\(_4\).xH\(_2\)O

<table>
<thead>
<tr>
<th>Calculation</th>
<th>( \text{ZnSO}_4 )</th>
<th>( \text{H}_2\text{O} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass lost</td>
<td>1.97</td>
<td>1.54</td>
</tr>
<tr>
<td>Moles</td>
<td>0.0122</td>
<td>0.085</td>
</tr>
<tr>
<td>Ratio</td>
<td>1</td>
<td>7</td>
</tr>
</tbody>
</table>

\( \text{X} = 7 \)
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.

**Concentration** = \( \frac{\text{moles}}{\text{volume}} \)

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

### Converting volumes

- A m$^3$ is equivalent to a cube 100cmx100cmx100cm = 1000000cm$^3$
- A dm$^3$ is equivalent to a cube 10cmx10cmx10cm = 1000cm$^3$
- A cm$^3$ is equivalent to a cube 1cmx1cmx1cm

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

\[
\begin{align*}
\text{cm}^3 & \rightarrow \text{dm}^3 \div 1000 \\
\text{cm}^3 & \rightarrow \text{m}^3 \div 1000000 \\
\text{dm}^3 & \rightarrow \text{m}^3 \div 1000
\end{align*}
\]

Example 11 Calculate the concentration of solution made by dissolving 5.00g of Na$_2$CO$_3$ in 250 cm$^3$ water

moles = \( \frac{\text{mass}}{\text{Mr}} \)

= \( \frac{5}{(23.0 \times 2 + 12 + 16 \times 3)} \)

= 0.0472 mol

conc = \( \frac{\text{moles}}{\text{Volume}} \)

= 0.0472 / 250

= 0.189 mol dm$^{-3}$

Example 12 Calculate the concentration of solution made by dissolving 10kg of Na$_2$CO$_3$ in 0.50 m$^3$ water

moles = \( \frac{\text{mass}}{\text{Mr}} \)

= \( \frac{10000}{(23.0 \times 2 + 12 + 16 \times 3)} \)

= 94.2 mol

conc = \( \frac{\text{moles}}{\text{Volume}} \)

= 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.

\[
\text{Mass Concentration} = \frac{\text{mass}}{\text{volume}}
\]

Unit of mass concentration: g dm\(^{-3}\)
Unit of Mass g
Unit of Volume: dm\(^3\)

Ions dissolving

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 0.1mol dm\(^{-3}\).

However the 0.1mol sodium chloride would split up to form 0.1mol of sodium ions and 0.1mol of chloride ions. The concentration of sodium ions is therefore 0.1mol dm\(^{-3}\) and the concentration of chloride ions is also 0.1mol dm\(^{-3}\).

\[
\text{NaCl(s)} \rightarrow \text{Na}^{+}(aq) + \text{Cl}^{-}(aq)
\]

| 0.1mol | 0.1mol | 0.1mol |

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 0.1mol of magnesium ions and 0.2mol of chloride ions. The concentration of magnesium ions is therefore 0.1mol dm\(^{-3}\) and the concentration of chloride ions is now 0.2mol dm\(^{-3}\).

\[
\text{MgCl}_2(s) +aq \rightarrow \text{Mg}^{2+}(aq) + 2\text{Cl}^{-}(aq)
\]

| 0.1mol | 0.1mol | 0.2mol |

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\(^3\) 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.

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.
**Dilutions**

**Diluting a solution**

- Pipette 25cm³ of original solution into a 250cm³ 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.

\[
\text{moles} = \text{volume} \times \text{concentration}
\]

If amount of moles does not change then:

\[
\text{original volume} \times \text{original concentration} = \text{new diluted volume} \times \text{new diluted concentration}
\]

So:

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

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

**Example 15**

50 cm³ of water are added to 150 cm³ of a 0.20 mol dm⁻³ NaOH solution. Calculate the concentration of the diluted solution.

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

\[
\text{new diluted concentration} = \frac{0.20 \times 0.150}{0.200} = 0.15 \text{ mol dm}^{-3}
\]

**Example 16**

Calculate the volume of water in cm³ that must be added to dilute 5.00 cm³ 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

\[
= 1.00 \times 0.005
\]

\[
= 0.005
\]

New volume = moles /conc

\[
= \frac{0.005}{0.05}
\]

\[
= 0.1 \text{ dm}^3 = 100 \text{ cm}^3
\]

Volume of water added = 100-5 = 95 cm³

**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.**
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.

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

\[
PV = nRT
\]

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

Example 17: Calculate the mass of Cl\(_2\) gas that has a pressure of 100 kPa, temperature 20\(^\circ\)C, volume 500 cm\(^3\). (\( R = 8.31 \))

\[
\text{moles} = \frac{PV}{RT} = \frac{100 000 \times 0.0005}{(8.31 \times 293)} = 0.0205 \text{ mol}
\]

Mass = moles \times Mr
\[
= 0.0205 \times (35.5 \times 2) = 1.46 \text{ g}
\]

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\(^\circ\)C at a pressure of 100kPa and a volume of 80.0cm\(^3\) was measured. Calculate the \( Mr \) of the volatile liquid (\( R = 8.31 \))

\[
\text{moles} = \frac{PV}{RT} = \frac{100 000 \times 0.00008}{(8.31 \times 343)} = 0.00281 \text{ mol}
\]

\( Mr = \frac{\text{mass}}{\text{moles}} \)
\[
= \frac{0.15}{0.00281} = 53.4 \text{ g mol}^{-1}
\]

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.
**Example 19**

40 cm³ of oxygen and 60 cm³ of carbon dioxide, each at 298 K and 100 kPa, were placed into an evacuated flask of volume 0.50 dm³. What is 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 \( \frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2} \) as on right.

Can do this as moles of gas do not change.

As Temperature is the same can make the above equation \( P_1V_1 = P_2V_2 \)

\[
P_2 = \frac{P_1V_1}{V_2} = \frac{100000 \times 1 \times 10^{-4}}{5 \times 10^{-4}} = 20000 \text{ Pa}
\]

**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 is monatomic).

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

**Example 20** If one burnt 500 cm³ of methane at 1 atm and 300K what volume of Oxygen would be needed and what volume of CO₂ would be given off under the same conditions?

\[
\text{CH}_4(g) + 2 \text{O}_2(g) \rightarrow \text{CO}_2(g) + 2 \text{H}_2\text{O}(l)
\]

1 mole 2 mole 1 mole

500 cm³ 1 dm³ 500 cm³

Simply multiply gas volume x2

**Example 21** An important reaction which occurs in the catalytic converter of a car is

\[
2\text{CO}(g) + 2\text{NO}(g) \rightarrow 2\text{CO}_2(g) + \text{N}_2(g)
\]

In this reaction, when 500 cm³ of CO reacts with 500 cm³ of NO at 650 °C and at 1 atm.

Calculate the total volume of gases produced at the same temperature and pressure?

\[
\begin{align*}
\text{total volume of gases produced} &= 750 \text{cm}^3 \\
\end{align*}
\]
Converting quantities between different substances using a balanced equation

\[ N_2 + 3H_2 \rightarrow 2NH_3 \]

The balancing (stoichiometric) numbers are mole ratios

\( 1 \) 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 above three equations can be used.

1. For pure solids, liquids and gases
   \[ \text{moles} = \frac{\text{mass}}{\text{Mr}} \]

2. For gases
   \[ PV = nRT \]

3. For solutions
   \[ \text{Concentration} = \frac{\text{moles}}{\text{volume}} \]

Example 22: Calculate the mass of carbon dioxide produced from heating 5.50 g of sodium hydrogencarbonate.  
\[ 2\text{NaHCO}_3 \rightarrow \text{Na}_2\text{CO}_3 + \text{CO}_2 + \text{H}_2\text{O} \]

Step 1: calculate moles of sodium hydrogencarbonate
   \[ \text{Moles} = \frac{\text{mass}}{\text{Mr}} = \frac{5.50}{84} = 0.0655 \text{ mol} \]

Step 2: use balanced equation to give moles of \( \text{CO}_2 \)
   \[ 2 \text{NaHCO}_3 : 1 \text{mol CO}_2 \]
   So \( 0.0655 \text{ HNO}_3 : 0.0328 \text{mol CO}_2 \)

Step 3: calculate mass of \( \text{CO}_2 \)
   \[ \text{Mass} = \text{moles} \times \text{Mr} = 0.0328 \times 44.0 = 1.44 \text{g} \]

Example 23: 23.6 cm\(^3\) of \( \text{H}_2\text{SO}_4 \) neutralised 25.0 cm\(^3\) of 0.150M NaOH. Calculate the concentration of the \( \text{H}_2\text{SO}_4 \)
\[ \text{H}_2\text{SO}_4 + 2\text{NaOH} \rightarrow \text{Na}_2\text{SO}_4 + 2\text{H}_2\text{O} \]

Step 1: calculate moles of sodium hydroxide
   \[ \text{Moles} = \text{conc} \times \text{vol} = 0.150 \times 0.025 = 0.00375 \text{ mol} \]

Step 2: use balanced equation to give moles of \( \text{H}_2\text{SO}_4 \)
   \[ 2 \text{moles NaOH} : 1 \text{moles H}_2\text{SO}_4 \]
   So \( 0.00375 \text{ NaOH} : 0.001875 \text{ mol } \text{H}_2\text{SO}_4 \)

Step 3 calculate concentration of \( \text{H}_2\text{SO}_4 \)
   \[ \text{conc} = \frac{\text{moles}}{\text{Volume}} = \frac{0.001875}{0.0236} = 0.0794 \text{ mol dm}^{-3} \]

Example 24: 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?
\[ 2\text{Mg (NO}_3)_2 (s) \rightarrow 2 \text{MgO (s)} + 4\text{NO}_2 (g) + \text{O}_2 (g) \]

Step 1: calculate moles of magnesium nitrate
   \[ \text{Moles} = \frac{\text{mass}}{\text{Mr}} = \frac{0.651}{148.3} = 0.00439 \text{ mol} \]

Step 2: use balanced equation to give moles of gas produced
   \[ 2 \text{moles Mg (NO}_3)_2 : 4\text{NO}_2 (g) + \text{O}_2 (g) \]
   i.e. 5 moles of gas
   So \( 0.00439 \text{ Mg (NO}_3)_2 : 0.01098( 0.00439 \times \frac{5}{2}) \text{ moles gas} \)

Step 3: calculate volume of gas
   \[ \text{Volume} = \frac{nRT}{P} = \frac{(0.01098 \times 8.31 \times 333)}{100000} = 0.00030\text{dm}^3 \]

Example 25: Calculate the mass of copper that reacts completely with 150 cm\(^3\) of 1.60 mol dm\(^{-3}\) nitric acid
\[ 3\text{Cu} + 8\text{HNO}_3 \rightarrow 3\text{Cu(NO}_3)_2 + 2\text{NO} + 4\text{H}_2\text{O} \]

Step 1: calculate moles of nitric acid
   \[ \text{Moles} = \text{conc} \times \text{vol} = 1.6 \times 0.15 = 0.24 \text{ mol} \]

Step 2: use balanced equation to give moles of Cu
   \[ 8 \text{moles HNO}_3 : 3 \text{moles Cu} \]
   So \( 0.24 \text{ HNO}_3 : 0.09 (0.24 \times \frac{1}{8}) \text{ mol Cu} \)

Step 3: calculate mass of Cu
   \[ \text{Mass} = \text{moles} \times \text{Mr} = 0.09 \times 63.5 = 5.71 \text{g} \]
Limiting and excess reactants

**Example 26** Calculate the maximum mass of titanium that could be produced from reacting 100 g of TiCl₄ with 80.0 g of sodium.

\[
\text{TiCl}_4 + 4 \text{ Na} \rightarrow 4 \text{ NaCl} + \text{ Ti}
\]

Step 1: calculate amount, in mol, TiCl₄
\[
\text{amount} = \frac{\text{mass}}{\text{Mr}} = \frac{100}{189.9} = 0.527 \text{ mol}
\]

Step 2 use balanced equation to work out which reactant is in excess
Using 1TiCl₄:4 Na ratio we can see that 0.527 mol of TiCl₄ 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 TiCl₄

Step 3: use balanced equation to calculate amount in mol of Ti formed
1 mol TiCl₄: 1 mole Ti
So 0.527 mol TiCl₄ produces 0.527 mole Ti

Step 4: calculate mass of Ti formed
\[
\text{Mass} = \text{amount} \times \text{Mr} = 0.527 \times 47.9 = 25.2 \text{ g}
\]

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

\[
\text{Fe}_2\text{O}_3 + 3\text{CO} \rightarrow 2\text{Fe} + 3 \text{ CO}_2
\]

% atom economy
\[
\frac{(2 \times 55.8)}{(2 \times 55.8 + 3 \times 16) + 3 \times (12+16)} \times 100
\]

= 45.8%

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

**Example 28:** 25.0g of Fe₂O₃ was reacted and it produced 10.0g of Fe. Calculate the percentage yield.

\[
\text{Fe}_2\text{O}_3 + 3\text{CO} \rightarrow 2\text{Fe} + 3 \text{ CO}_2
\]

First calculate maximum mass of Fe that could be produced

Step 1: work out moles of Iron oxide
\[
\text{Moles} = \frac{\text{mass}}{\text{Mr}} = \frac{25.0}{159.6} = 0.1566 \text{ mol}
\]

Step 2: use balanced equation to give moles of Fe
1 moles Fe₂O₃ : 2 moles Fe
So 0.1566 Fe₂O₃ : 0.313 moles Fe

Step 3: work out mass of Fe
\[
\text{Mass} = \text{moles} \times \text{Mr} = 0.313 \times 55.8 = 17.5 \text{ g}
\]

% yield
\[
\text{% yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100
\]

\[
= \frac{10}{17.5} \times 100 = 57.1\%
\]
Titrations

The method for carrying out the titration

• rinse equipment (burette with acid, pipette with alkali, conical flask with distilled water)
• pipette 25 cm³ 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.

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.

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

If 2 or 3 values are within 0.10 cm³ 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 cm³)

Common Titration Equations

CH₃CO₂H + NaOH → CH₃CO₂⁻Na⁺ + H₂O
H₂SO₄ + 2NaOH → Na₂SO₄ + 2H₂O
HCl + NaOH → NaCl + H₂O
NaHCO₃ + HCl → NaCl + CO₂ + H₂O
Na₂CO₃ + 2HCl → 2NaCl + CO₂ + H₂O

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 (NaHCO₃) and calcium carbonate (CaCO₃) 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 CO₂ 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.

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Example 29: A 25.0cm³ sample of vinegar was diluted in a 250cm³ volumetric flask. This was then put in a burette and 23.10cm³ of the diluted vinegar neutralised 25.0 cm³ of 0.100 M NaOH. What is the concentration of the vinegar in g dm⁻³?

CH₃CO₂H + NaOH → CH₃CO₂Na⁺ + H₂O

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 CH₃CO₂H
1 moles NaOH = 1 moles CH₃CO₂H
So 0.00250 NaOH : 0.00250 moles CH₃CO₂H

Step 3. Work out concentration of diluted CH₃CO₂H in 23.1 (and 250 cm³) in mol dm⁻³
conc = moles/Volume
= 0.00250 / 0.0231
= 0.108 mol dm⁻³

Step 4. Work out concentration of original concentrated CH₃CO₂H in 25cm³ in moldm⁻³
conc = 0.108 x 10 = 1.08 mol dm⁻³

Step 5. Work out concentration of CH₃CO₂H in original concentrated 25 cm³ in gdm⁻³
conc in gdm⁻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.

M₂CO₃(aq) + 2HCl(aq) → 2MCl(aq) + CO₂(g) + H₂O(l)

A 3.96 g sample of M₂CO₃ was dissolved in distilled water to make 250 cm³ of solution. A 25.0 cm³ portion of this solution required 32.8 cm³ of 0.175 mol dm⁻³ hydrochloric acid for complete reaction. Calculate the Mr of M₂CO₃ 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 M₂CO₃ in 25.0 cm³ put in conical flask
use balanced equation to give moles of M₂CO₃
2 mol HCl : 1 mol M₂CO₃
So 0. 00574 NaOH : 0.00287 mol M₂CO₃

3. Calculate the number of moles M₂CO₃ acid in original 250 cm³ of solution
Moles in 250cm³ = 0.00287 x 10
=0.0287 mol

4. Work out the Mr of M₂CO₃
Mr = mass / moles
= 3.96/ 0.0287= 138.0

5. Work out Ar of M = (138-12- 16x3)
2
Ar of M = 39 M= potassium

Example 31. 950 mg of impure calcium carbonate tablet was crushed. 50.0 cm³ 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 cm³ with distilled water. 10.0 cm³ of this solution was titrated with 11.1cm³ of 0.300 mol dm⁻³ sodium hydroxide solution. Calculate the percentage of CaCO₃ 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 cm³
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 cm³ of solution
Moles in 100cm³ = 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 cm³ of 1.00 mol dm⁻³ there is 0.05moles
moles of HCl that reacted with the indigestion tablet =0.0167 mol

5 Use balanced equation to give moles of CaCO₃
CaCO₃(s) + 2HCl(aq) → CaCl₂(aq) + CO₂(g) + H₂O(l)
2 mol HCl : 1 mol CaCO₃
So 0.0167 HCl : 0.00835 mol CaCO₃

6. Work out the mass of CaCO₃ in original tablet
mass= moles x Mr
= 0.00835 x 100 = 0.835 g

percentage of CaCO₃ by mass in the tablet = 0.835/0.950 x100 = 87.9 %

Common Titration Equations

CH₃CO₂H + NaOH → CH₃CO₂Na⁺ + H₂O
H₂SO₄ + 2NaOH → Na₂SO₄ +2H₂O
HCl + NaOH → NaCl +H₂O
NaHCO₃ + HCl → NaCl + CO₂ + H₂O
Na₂CO₃ + 2HCl → 2NaCl + CO₂ + H₂O
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

\[ \% \text{ uncertainty} = \frac{\text{uncertainty}}{\text{Measurement made on apparatus}} \times 100 \]

e.g. for burette

\[ \% \text{ uncertainty} = \frac{0.15}{\text{average titre result}} \times 100 \]

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

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.

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%

The uncertainty of a reading (one judgement) is at least ±0.1 of the smallest scale reading.
The uncertainty of a measurement (two judgements) is at least ±1 of the smallest scale reading.

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.

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

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.