Chapter 4: Calculations
Knowledge organiser

Formula mass

Every substance has a **formula mass**, M_r.

formula mass M_r = sum (relative atomic mass of all the atoms in the formula)

Avogadro's constant (HT only)

One mole of a substance contains 6.02×10^{23} atoms, ions, or molecules. This is **Avogadro's constant**.

One mole of a substance has the same mass as the M_r of the substance. For example, the M_r (H_2O) = 18, so 18 g of water molecules contains 6.02×10^{23} molecules, and is called one mole of water.

You can write this as: $moles = \dfrac{mass}{M_r}$

Theoretical yield

The **theoretical yield** of a chemical reaction is the mass of a product that you expect to be produced.

Even though no atoms are gained or lost during a chemical reaction, it is not always possible to obtain the theoretical yield because

- some of the product can be lost when it is separated from the reaction mixture
- there can be unexpected side reactions between reactants that produce different products
- the reaction may be reversible.

Percentage yield

The **yield** is the amount of product that you actually get in a chemical reaction.

Percentage yield is the actual yield as a proportion of the theoretical yield:

$percentage\ yield = \dfrac{actual\ yield}{theoretical\ yield} \times 100$

Atom economy

The **atom economy** of a reaction tells you the proportion of atoms that you started with that are part of *useful* products.

High atom economies are more sustainable, as they mean fewer atoms are being wasted in products that are not useful.

The percentage atom economy is calculated by:

$atom\ economy = \dfrac{M_r\ of\ useful\ product}{M_r\ of\ all\ products} \times 100$

Using balanced equations (HT only)

In a balanced symbol equation the sum of the M_r of the reactants equals the sum of the M_r of the products.

If you are asked what mass of a product will be formed from a given mass of a specific reactant, you can use the steps below to calculate the result.

1 balance the symbol equation
2 calculate moles of the substance with a known mass using $moles = \dfrac{mass}{M_r}$
3 using the balanced symbol equation, work out the number of moles of the unknown substance
4 calculate the mass of the unknown substance using $mass = moles \times M_r$

If you are asked to balance an equation, you can use the steps below to work out the answer.

1 work out M_r of all the substances
2 calculate the number of moles of each substance in the reaction using $moles = \dfrac{mass}{M_r}$
3 convert to a whole number ratio
4 balance the symbol equation

Concentration

Concentration is the amount of solute in a volume of solvent.

The unit of concentration is g/dm^3. Concentration can be calculated using:

$concentration\ (g/dm^3) = \dfrac{mass\ (g)}{volume\ (dm^3)}$

Sometimes volume is measured in cm^3:

$volume\ (dm^3) = \dfrac{volume\ (cm^3)}{1000}$

- lots of solute in little solution = high concentration
- little solute in lots of solution = low concentration

Concentration in mol/dm³

Concentration can also be measured in mol/dm^3.

$concentration\ of\ solution\ (mol/dm^3) = \dfrac{number\ of\ moles\ of\ solute}{volume\ of\ solution\ (dm^3)}$

You can use this formula and $mass = moles \times M_r$ to calculate the mass of solute dissolved in a solution.
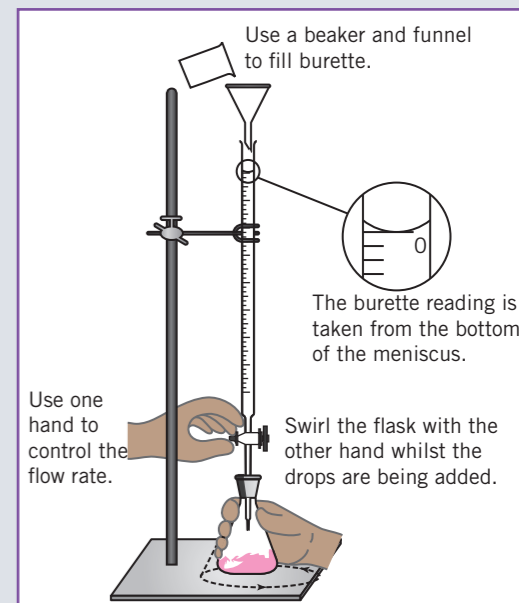
- The greater the mass of solute in solution, the greater the number of moles of solute, and therefore the greater the concentration.
- If the same number moles of solute is dissolved in a smaller volume of solution, the concentration will be greater.

mol is a the unit of moles

Moles of gases (HT only)

At any given temperature and pressure, the same number of moles of a gas will occupy the same volume.

At room temperature (25 °C) and pressure (1 atm), one mole of *any* gas will occupy $24\ dm^3$.

To calculate the number of moles of a gas:

$moles\ of\ a\ gas = \dfrac{volume\ (dm^3)}{24\ dm^3}$
or
$moles\ of\ a\ gas = \dfrac{volume\ (cm^3)}{24\,000\ cm^3}$

Calculating concentration

To calculate the concentration of the unknown solution (the solution in the conical flask):

1 Write a balanced symbol equation for the reaction.
2 Calculate the moles used from the known solution using:
$moles = concentration\ (mol/dm^3) \times volume\ (dm^3)$
3 Use the ratio from the balanced symbol equation to deduce the number of moles present in the unknown solution.
4 Calculate the concentration of the unknown solution using:
$concentration\ (mol/dm^3) = \dfrac{moles}{volume\ (dm^3)}$

Excess and limiting reactants (HT only)

In a chemical reaction between two or more reactants, often one of the reactants will run out before the others. You then have some of the other reactants left over. The reactant that is left over is in **excess**. The reactant that runs out is the **limiting reactant**.

To work out which reactants are in excess and which is the limiting reactant, you need to:

1 write the balanced symbol equation for the reaction
2 pick one of the reactants and its quantity as given in the question
3 use the ratio of the reactants in the balanced equation to see how much of the other reactant you need
4 compare this value to the quantity given in the question
5 determine which reactant is in excess and which is limiting.

Titration

Titration is an experimental technique to work out the concentration of an unknown solution in the reaction between an acid and an alkali.

1 Use a pipette to extract a known volume of the solution with an unknown concentration. A pipette measures a fixed volume only.
2 Add the solution of unknown concentration to a conical flask and put the conical flask on a white tile.
3 Add a few drops of a suitable indicator to the conical flask.
4 Add the other solution with a known concentration to the burette.
5 Carry out a rough titration to find out approximately what volume of solution in the burette needs to be added to the solution in the conical flask. Add the solution from the burette to the solution in the conical flask 1 cm³ at a time until the end point is reached.
6 The end point is when the indicator just changes colour.
7 Record the volume of the end point as your rough value.
8 Now repeat steps 1–7, but as you approach the end point add the solution from the burette drop-by-drop. Swirl the conical flask in between drops.
9 Record the volume of the end point.

Use a beaker and funnel to fill burette.

The burette reading is taken from the bottom of the meniscus.

Use one hand to control the flow rate.

Swirl the flask with the other hand whilst the drops are being added.

Key terms

Make sure you can write a definition for these key terms.

atom economy   burette   concordant   end point
excess reactant   formula mass   limiting reactant
percentage yield   pipette   room temperature and pressure
theoretical yield   titration   titre   useful   yield

Chapter 4: Calculations
Retrieval questions

Learn the answers to the questions below then cover the answers column
with a piece of paper and write as many as you can. Check and repeat.

	C4 questions	Answers
1	What is a mole?	mass of a substance that contains 6.02×10^{23} particles
2	Give the value for Avogadro's constant.	6.02×10^{23}
3	Which formula is used to calculate the number of moles from mass and M_r?	$\text{moles} = \dfrac{\text{mass}}{M_r}$
4	Which formula is used to calculate the mass of a substance from number of moles and M_r?	$\text{mass} = \text{moles} \times M_r$
5	What is a limiting reactant?	the reactant that is completely used up in a chemical reaction
6	What is a unit for concentration?	g/dm^3 or mol/dm^3
7	Which formula is used to calculate concentration from mass and volume?	$\text{concentration (g/dm}^3) = \dfrac{\text{mass (g)}}{\text{volume (dm}^3)}$
8	Which formula is used to calculate volume from concentration and mass?	$\text{volume (dm}^3) = \dfrac{\text{mass (g)}}{\text{concentration (g/dm}^3)}$
9	Which formula is used to calculate mass from concentration in g/dm^3 and volume?	$\text{mass (g)} = \text{concentration (g/dm}^3) \times \text{volume (dm}^3)$
10	How can you convert a volume reading in cm^3 to dm^3?	divide by 1000
11	If the amount of solute in a solution is increased, what happens to its concentration?	increases
12	If the volume of water in a solution is increased, what happens to its concentration?	decreases
13	What is the yield of a reaction?	mass of product obtained from the reaction
14	What is the theoretical yield of a reaction?	maximum mass of the product that could have been produced
15	Why is the actual yield always less than the theoretical yield?	• reaction may be reversible • some of the product can be lost on separation • unexpected side reactions between reactants
16	What is the percentage yield?	actual yield as a proportion of theoretical yield
17	How is percentage yield calculated?	$\dfrac{\text{actual yield}}{\text{theoretical yield}} \times 100$
18	What is atom economy?	measure of how many atoms of the reactants end up as useful products
19	Why is a high atom economy desirable?	results in less waste/is more sustainable
20	How is percentage atom economy calculated?	$\dfrac{M_r \text{ of useful product}}{M_r \text{ of all products}} \times 100$
21	How can concentration in mol/dm^3 be calculated?	$\dfrac{\text{moles of solute}}{\text{volume (dm}^3)}$
22	What is a titration?	method used to calculate the concentration of an unknown solution
23	What is the end-point?	the point at which the reaction is complete (when the indicator changes colour) and no substance is in excess
24	How should solution be added from the burette close to the end point?	drop by drop, swirling in between
25	Why is a white tile used in titration?	to see the colour change better
26	What is a titre?	volume of solution added from the burette
27	What volume does one mole of any gas occupy at room temperature and pressure?	$24\,dm^3$ or $24\,000\,cm^3$

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