Cambridge (CIE) IGCSE Chemistry

Your notes

The Mole & the Avogadro Constant

Contents

The mole & the Avogadro Constant

Extended tier only

- Chemical amounts are measured in moles
- The mole, symbol mol, is the SI unit of **amount of substance**
- One mole of a substance contains the same number of the stated particles
  - This can be atoms, molecules or ions
- One mole contains **6.02×10^{23}** particles; this number is known as the **Avogadro Constant**
- For example:
  - One mole of sodium (Na) contains 6.02×10^{23} atoms of sodium
  - One mole of hydrogen (H_2) contains 6.02×10^{23} molecules of hydrogen
  - One mole of sodium chloride (NaCl) contains 6.02×10^{23} formula units of sodium chloride
- The mass of 1 mole of a substance is known as the **molar mass**
  - For an element, it is the same as the **relative atomic mass** written in grams
  - For a compound, it is the same as the **relative molecular** or **formula mass** in grams

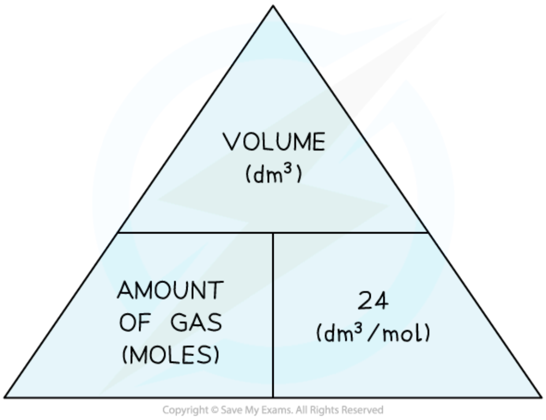
The mole & volume of gas

Extended tier only

Molar volumes of gas

- **Avogadro's Law** states that at the same **temperature** and **pressure**, equal amounts of gases occupy the **same volume** of space
  - e.g. 1 mole of hydrogen gas occupies the same volume as 1 mole of methane gas
- At room temperature and pressure, the volume occupied by one mole of any gas was found to be **24 dm^3** or **24,000 cm^3**
  - This is known as the **molar gas volume at RTP**
  - RTP stands for "room temperature and pressure" and the conditions are **20 °C** and **1 atmosphere** (atm)
- From the molar gas volume, the following formula triangles can be derived:

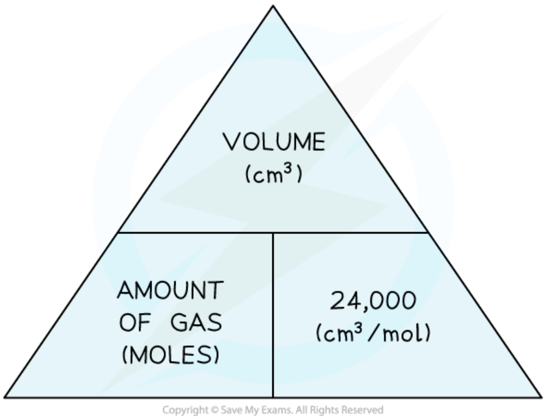
Molar gas volume (dm^3) formula triangle



This shows the relationship between moles of gas, volume in dm^3 and the molar volume

- If the volume is given in cm^3 instead of dm^3, then divide by 24,000 instead of 24:

Molar gas volume (cm^3) formula triangle



This shows the relationship between moles of gas, volume in cm^3 and the molar volume

- The formula can be used to calculate the number of moles of gases from a given volume or vice versa
  - Simply cover the one you want and the triangle tells you what to do
- For example, to find the volume of a gas:
  - **Volume = Moles x Molar Volume**

Examples of Converting Moles to Volume Table

Gas	Amount (moles)	Volume
Hydrogen	3	(3 x 24) = 72 dm^3 (3 x 24000) = 72000 cm^3

Carbon dioxide	0.25	(0.25 x 24) = 6 dm^3 (0.25 x 24000) = 6000 cm^3
Oxygen	5.4	(5.4 x 24) = 129.6 dm^3 (5.4 x 24000) = 129600 cm^3
Ammonia	0.02	(0.02 x 24) = 0.48 dm^3 (0.02 x 24000) = 480 cm^3

- For example, to find the number of moles of a gas:
  - **Moles = Volume ÷ Molar Volume**

Examples of Converting Volume to Moles Table

Gas	Volume	Moles
Methane	225.6 dm^3	(225.6 ÷ 24) = 9.4 mol
Carbon monoxide	7.2 dm^3	(7.2 ÷ 24) = 0.3 mol
Sulfur dioxide	960 dm^3	(960 ÷ 24) = 40 mol
Oxygen	1200 cm^3	(1200 ÷ 24000) = 0.05 mol

Examiner Tips and Tricks

- You are not expected to know the value of Avogadro's constant
- But, you do need to know the equation as well as how to use and re-arrange it

Your notes

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Linking moles, mass & Mr

Extended tier only

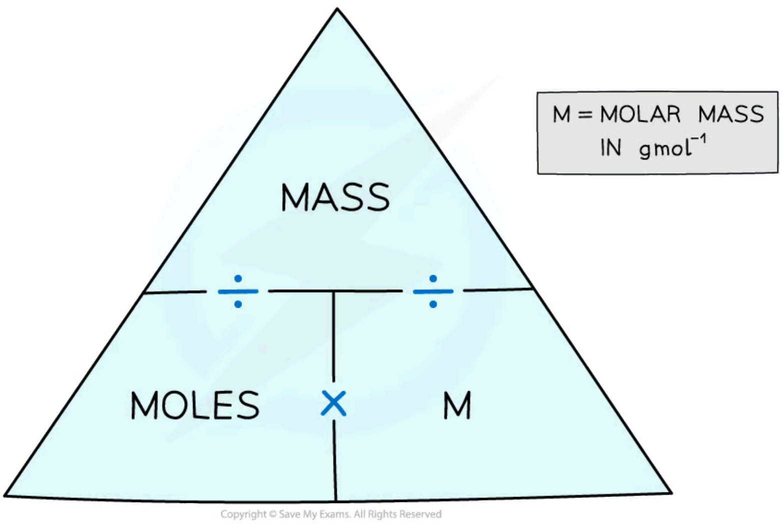
- One mole of any element is equal to the relative atomic mass of that element in **grams**
- If you had 1 mole of carbon atoms in your hand, that number of carbon atoms would have a mass of 12 g (because the A_r of carbon is 12)
  - So, one mole of helium atoms has a mass of 4 g (A_r of He is 4)
  - One mole of lithium has a mass of 7 g (A_r of Li is 7) and so on
- One mole of any compound is the **relative molecular mass** or relative formula mass in **grams**
- To find the mass of one mole of a compound, add up the relative atomic masses
  - For example, carbon dioxide has an *Mr* of:
    (1 x C) + (2 x O)
    (1 x 12) + (2 x 16) = 44

Moles, mass and relative mass

- The number of moles of any chemical can be calculated using:

$$\text{Moles} = \frac{\text{mass}}{M_r}$$

- We can use the following formula triangle to convert between moles, mass in grams and the molar mass:



Formula triangle for moles, mass and molar mass

- Calculating the number of moles of an element uses the same equation, but with relative atomic mass replacing M

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Worked Example

What is the mass of 0.250 moles of zinc?

Answer:

- From the Periodic Table, the relative atomic mass of Zn is 65
  - So, the molar mass is 65 g / mol
- The mass is calculated by **moles x molar mass**:
  - 0.250 mol x 65 g / mol = **16.25 g**

Worked Example

How many moles are in 2.64 g of sucrose, $C_{12}H_{22}O_{11}$ (M_r = 342)?

Answer:

- The molar mass of sucrose is 342 g / mol
- The number of moles is found by **mass ÷ molar mass**:
  - $\frac{2.64}{342}$ = **7.72×10^{-3} mol**

Examiner Tips and Tricks

Always show your workings in calculations as its easier to check for errors and you may pick up credit if you get the final answer wrong.

Calculating moles & masses

- Chemical amounts are measured in moles
- The mole, symbol mol, is the SI unit of **amount of substance**
- One mole of any substance contains the same number of the stated particles
  - This can be atoms, molecules or ions
- One mole contains **6.02×10^{23}** particles
  - This number is known as the **Avogadro constant**

- For example:
  - One mole of sodium (Na) contains 6.02×10^{23} atoms of sodium
  - One mole of hydrogen (H_2) contains 6.02×10^{23} molecules of hydrogen
  - One mole of sodium chloride (NaCl) contains 6.02×10^{23} formula units of sodium chloride

Your notes

Worked Example

For magnesium chloride, $MgCl_2$, calculate the number of:

1. Molecules in 1 mole
2. Atoms in 1 mole
3. Chloride ions in 1 mole
4. Magnesium ions in 2 moles

Answers:

1. The formula is $MgCl_2$, so 1 mole of $MgCl_2$ is:
   - $1 \times 6.02 \times 10^{23} = 6.02 \times 10^{23}$ molecules
2. There are 3 atoms in $MgCl_2$, so 1 mole of $MgCl_2$ contains:
   - $3 \times 6.02 \times 10^{23} = 18.06 \times 10^{23}$ atoms
3. There are 2 chloride ions in $MgCl_2$, so 1 mole of $MgCl_2$ contains:
   - $2 \times 6.02 \times 10^{23} = 12.04 \times 10^{23}$ chloride ions
4. There is 1 magnesium ion in $MgCl_2$, so 2 mole of $MgCl_2$ contains:
   - $2 \times (1 \times 6.02 \times 10^{23}) = 12.04 \times 10^{23}$ magnesium ions

Worked Example

In 15.7 g of water ($M_r = 18$):

1. How many molecules are there?
2. How many atoms are there?

Answers:

1. The number of molecules:
   - The molar mass of water is 18 g / mol
   - The number of moles is found by **mass ÷ molar mass**
     - 15.7 g ÷ 18 g / mol = **0.872 mol**
   - There are 6.02×10^{23} molecules of water in 1 mole of water
   - So, in 0.872 moles of water, there are:
     - $6.02 \times 10^{23} \times 0.872 = \mathbf{5.25 \times 10^{23}}$ molecules
2. The number of atoms:

- In each molecule of water, there are 3 atoms (2 hydrogen atoms, one oxygen atom)
- So, the number of atoms in 15.7 g = $3 \times 5.25 \times 10^{23}$ = **1.58×10^{24}** atoms

Your notes

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Reacting masses

Extended tier only

- Chemical / symbol equations can be used to calculate:
  - The **moles** of reactants and products
  - The **mass** of reactants and products
- To do this:
  - Information from the question is used to find the amount in moles of the substances being considered
  - Then, the **ratio** between the substances is identified using the balanced chemical equation
  - Once the moles have been determined they can then be converted into grams using the relative atomic or relative formula masses

Worked Example

Magnesium undergoes combustion to produce magnesium oxide.

The overall reaction that is taking place is shown in the equation below.

$$2Mg\ (s) + O_2\ (g) \longrightarrow 2\ MgO\ (s)$$

Calculate the mass of magnesium oxide that can be made by completely burning 6.0 g of magnesium in oxygen in the following reaction:

$A_r(O) = 16 \quad A_r(Mg) = 24$

Answer:

1. Calculate the moles of magnesium
   - Moles = $\frac{\text{mass}}{M_r} = \frac{6}{24} = 0.25$
2. Use the molar ratio from the balanced symbol equation
   - 2 moles of magnesium produce 2 moles of magnesium oxide
   - The ratio is 1 : 1
   - Therefore, 0.25 moles of magnesium oxide is produced
3. Calculate the mass of magnesium oxide
   - Mass = moles x M_r = 0.25 moles x (24 + 16) = 10 g

Your notes

Worked Example

In theory, aluminium could decompose as shown in the equation below.

$$2Al_2O_3 \longrightarrow 4Al + 3O_2$$

Calculate the maximum possible mass of aluminium, in tonnes, that can be produced from 51 tonnes of aluminium oxide.

$$A_r(O) = 16 \quad A_r(Al) = 27$$

Answer:

1. Calculate the moles of aluminium oxide
   - Mass = 51 tonnes x 10^6 = 51 000 000 g
   - M_r of aluminium oxide = (2 x 27) + (3 x 16) = 102
   - Moles = $\frac{\text{mass}}{M_r} = \frac{51\ 000\ 000}{102}$ = 500 000
2. Use the molar ratio from the balanced symbol equation
   - 2 moles of aluminium oxide produces 4 moles of aluminium
   - The ratio is 1 : 2
   - Therefore, 2 x 500 000 = 1 000 000 moles of aluminium is produced
3. Calculate the mass of aluminium
   - Mass = moles x M_r = 1 000 000 moles x 27 = 27 000 000 g
   - Mass in tonnes = $\frac{27\ 000\ 000}{10^6}$ = 27 tonnes

Examiner Tips and Tricks

Remember: The molar ratio of a balanced equation gives you the ratio of the amounts of each substance in the reaction.

Limiting reactants

- A chemical reaction stops when one of the reactants is used up
- The reactant that is used up first is the **limiting reactant**, as it limits the duration and hence the amount of product that a reaction can produce
  - The one that is remaining is the **excess** reactant
  - The limiting reagent is the reactant which is **not present in excess** in a reaction
- The amount of product is therefore **directly proportional** to the amount of the limiting reactant added at the beginning of a reaction

Determining the limiting reactant

- In order to determine which reactant is the limiting reagent in a reaction, we have to consider the amounts of each reactant used and the molar ratio of the balanced chemical equation
- When performing reacting mass calculations, the limiting reagent is always the number that should be used, as it indicates the maximum possible amount of product that can form
  - Once all of a limiting reagent has been used up, the reaction cannot continue
- The steps are:
  1. Convert the mass of each reactant into moles by dividing by the molar masses
  2. Write the balanced equation and determine the molar ratio
  3. Look at the equation and compare the moles

Worked Example

9.2 g of sodium is reacted with 8.0 g of sulfur to produce sodium sulfide, Na_2S.

Which reactant is in excess and which is the limiting reactant?

Relative atomic masses (A_r): Na = 23; S = 32

Answer:

1. Calculate the moles of each reactant
   - Moles = $\frac{\text{mass}}{M_r}$
   - Moles Na = $\frac{9.2}{23}$ = 0.40
   - Moles S = $\frac{8.0}{32}$ = 0.25
2. Write the balanced equation and determine the molar ratio
   - $2Na + S \rightarrow Na_2S$
   - So, the molar ratio of Na : S is 2 : 1
3. Compare the moles
   - To react completely 0.40 moles of Na requires 0.20 moles of S
   - Since there are 0.25 moles of sulfur:
     - S is in excess
     - Therefore, Na is the limiting reactant

Your notes

Calculating Concentration

Your notes

Units of concentration

- A **solute** is a solid substance that dissolves into a liquid
  - The amount of solute can be expressed in **grams (g)** or **moles (mol)**
- A **solvent** is the liquid that a solute dissolves in
  - The amount / volume of a solvent is measured in **cm^3** or **dm^3**
- Most chemical reactions occur between solutes which are dissolved in solvents, such as water or an organic solvent
- A **solution** is the mixture formed when a solute dissolves in a solvent
  - The amount / volume of a solution measured in **cm^3** or **dm^3**
- **Concentration** refers to the amount of solute there is in a specific volume of the solvent
  - The greater the amount of solute in a given volume, the greater the concentration
  - Concentration is sometimes commonly referred to as strength
    - For example, dissolving more coffee in hot water results in a stronger coffee
- Typically, concentration is expressed in terms of the amount of substance per dm^3
  - Therefore, the units of concentration are:
    - **g / dm^3**
    - **mol / dm^3**

Calculating concentration

Extended tier only

Calculating concentration using mass

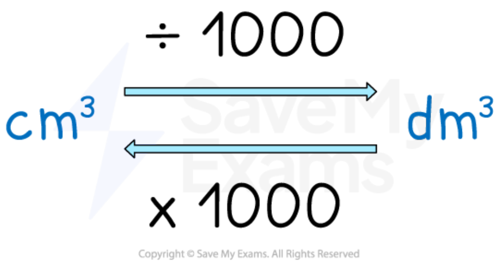
- The general formula to calculate the concentration in g / dm^3 is:

$$\text{concentration (g / dm}^3\text{)} = \frac{\text{mass of solute (g)}}{\text{volume of solution (dm}^3\text{)}}$$

- Concentration can also be measured in grams per cubic decimetre
  - 1 decimetre cubed (dm^3) = 1000 cm^3
  - 1 decimetre cubed (dm^3) is the same as 1 litre
- You may be given data in a question which needs to be converted from cm^3 to dm^3 or the other way around

Converting cm^3 and dm^3

Your notes



To go from cm^3 to dm^3 divide by 1000. To go from dm^3 to cm^3 multiply by 1000

Worked Example

A student dissolved 10 g of sodium hydroxide, NaOH, in 2 dm^3 of distilled water. Calculate the concentration of the solution in g / dm^3.

Answer:

- Write down the information you are given in the question:
  - Mass of solute: 10 g
  - Volume of solution: 2 dm^3
- Calculate the concentration:
  - Concentration = $\frac{\text{mass of solute (g)}}{\text{volume (dm}^3\text{)}}$
  - Concentration = $\frac{10 \text{ g}}{2 \text{ dm}^3}$ = **5 g / dm^3**

Calculating concentration using moles

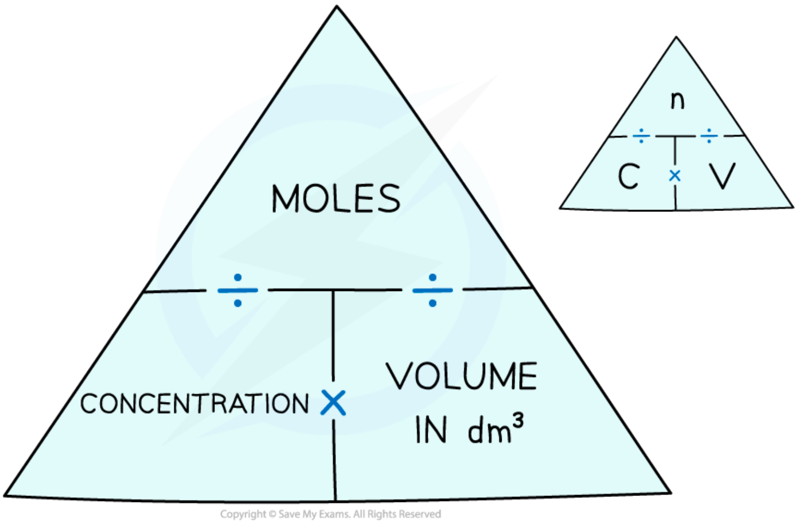
- It is more useful to a chemist to express concentration in terms of moles per unit volume rather than mass per unit volume
- Concentration can therefore be expressed in moles per decimetre cubed and calculated using the following equation:

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

- We can modify the concentration formula to include moles
  - The units in the answer can be written as mol / dm^3 (this can also be written as mol dm^{-3})
- You may have to convert from g / dm^3 into mol / dm^3 and vice versa depending on the question
- To go from g / dm^3 to mol / dm^3
  - Divide by the molar mass in grams

Your notes

- To go from mol / dm^3 to g / dm^3
  - Multiply by the molar mass in grams
- Some students find formula triangles help them to understand the relationship:



The concentration-moles formula triangle can help you solve these problems

Worked Example

Calculate the amount of solute, in moles, present in 2.5 dm^3 of a solution whose concentration is 0.2 mol / dm^3.

Answer:

- Write down the information you are given in the question:
  - Concentration of solution: 0.2 mol / dm^3
  - Volume of solution: 2.5 dm^3
- Calculate the number of moles:
  - Moles = concentration x volume
  - Moles = 0.2 x 2.5 = **0.5 mol**

Worked Example

Calculate the concentration of a solution of sodium hydroxide, NaOH, in mol / dm^3, when 80 g is dissolved in 500 cm^3 of water.

Relative atomic masses, A_r: Na = 23; H = 1; O = 16

Answer:

- Calculate the M_r of NaOH:
  - 23 + 16 + 1 = 40
- Determine the number of moles of NaOH:
  - 40 g = 1 mole
  - So, 80 g = 2 moles
- Convert cm^3 to dm^3:
  - $\frac{500}{1000}$ = 0.5 dm^3
- Calculate the concentration:
  - Concentration = $\frac{\text{moles}}{\text{volume}}$
  - Concentration = $\frac{2}{0.5}$ = 4 mol / dm^3

Your notes

Worked Example

25.0 cm^3 of 0.050 mol / dm^3 sodium carbonate was completely neutralised by 20.00 cm^3 of dilute hydrochloric acid. Calculate the concentration in mol / dm^3 of the hydrochloric acid.

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

Answer:

- Calculate the moles of sodium carbonate:
  - Moles of Na_2CO_3 = concentration x volume
    - **Remember:** The volume needs to be in dm^3
  - Moles of Na_2CO_3 = 0.05 x $\frac{25.0}{1000}$ = 0.00125
- Calculate the moles of hydrochloric acid:
  - The balanced symbol equation shows that 1 mole of Na_2CO_3 reacts with 2 moles of HCl
  - So, 0.00125 moles of Na_2CO_3 reacts with 0.00250 moles of HCl
- Calculate the concentration of hydrochloric acid:
  - Concentration = $\frac{\text{moles}}{\text{volume}}$
    - **Remember:** The volume needs to be in dm^3
    - 20 cm^3 ÷ 1000 = 0.02 dm^3
  - Concentration = $\frac{0.00250}{0.02}$ = 0.125 mol / dm^3

Your notes

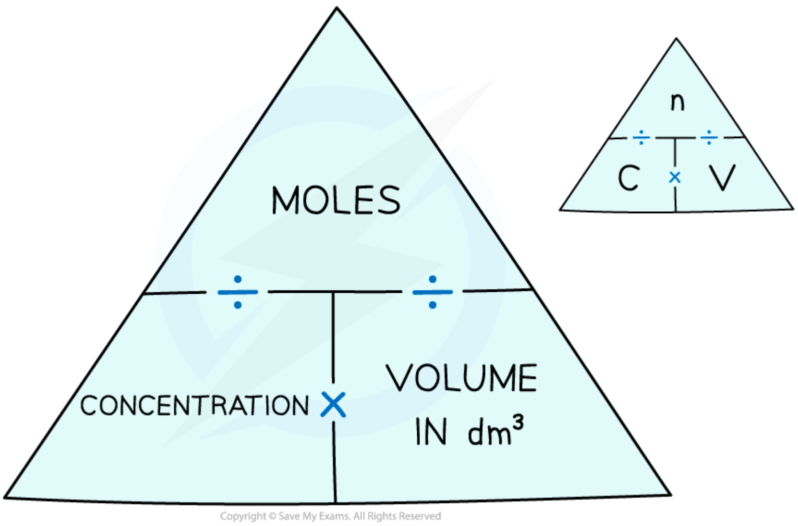
Examiner Tips and Tricks

Remember: Always convert the units from cm^3 to dm^3 by dividing by 1000.

Titration calculations

Extended tier only

- Titrations are a method of analysing the **concentration** of solutions
    - Acid-base titrations are one of the most important kinds of titrations
- Titrations can determine exactly how much alkali is needed to neutralise a quantity of acid – and vice versa
- You may be asked to calculate:
    - The **moles** present in a given amount
    - The **concentration** or **volume** required to **neutralise** an acid or a base
- Once a titration is completed and the average titre has been calculated, you can calculate the unknown variable using the formula triangle as shown below



Formula triangle showing the relationship between concentration, number of moles and volume of liquid

Worked Example

A solution of 25.0 cm^3 of hydrochloric acid was titrated against a solution of 0.100 mol/dm^3 NaOH.

12.1 cm^3 of NaOH was required for a complete reaction.

Determine the concentration of the acid.

Your notes

Answer:

- **Step 1:** Write the equation for the reaction:
  - **$HCl\ (aq) + NaOH\ (aq) \rightarrow NaCl\ (aq) + H_2O\ (l)$**
- **Step 2:** Calculate the number of moles of the NaOH
  - Moles = $(\frac{\text{volume}}{1000})$ x concentration
  - Moles of NaOH = 0.012 dm^3 x 0.100 mol / dm^3 = 1.21×10^{-3} mol
- **Step 3:** Deduce the number of moles of the acid
  - Since the acid reacts in a 1:1 ratio with the alkali, the number of moles of HCl is also 1.21×10^{-3} mol
  - This is present in 25.0 cm^3 of the solution (25.0 cm^3 = 0.025 dm^3)
- **Step 4:** Find the concentration of the acid
  - Concentration = $\frac{\text{moles}}{\text{volume (dm}^3)}$
  - Concentration of HCl = $\frac{1.21 \times 10^{-3}\ \text{mol}}{0.025\ \text{dm}^3}$ = **0.0484 mol/dm^3**

Worked Example

25.00 cm^3 of 0.15 mol / dm^3 barium hydroxide, $Ba(OH)_2$, was required to neutralise 12.80 cm^3 of nitric acid, HNO_3, during a titration. Calculate the concentration of HNO_3 that was used. Give your answer to 2 decimal places.

$Ba(OH)_2\ (aq) + 2HNO_3\ (aq) \rightarrow Ba(NO_3)_2\ (aq) + 2H_2O\ (l)$

Answer:

- **Step 1:** Calculate the number of moles of barium hydroxide
  - Moles of barium hydroxide = concentration x volume (dm^3) = 0.15 x 0.025 = 3.75×10^{-3} mols
- **Step 2:** Using the equation, calculate the number of moles of nitric acid
  - Moles of nitric acid = $3.75 \times 10^{-3} \times 2 = 7.5 \times 10^{-3}$
  - The number of moles must be multiplied by 2 due to the 1:2 ratio
- **Step 3:** Calculate the concentration of nitric acid
  - Concentration of nitric acid = $\frac{7.5 \times 10^{-3}}{0.0128}$ = **0.59 mol / dm^3 to 2 dp**
- Remember to convert cm^3 to dm^3 by dividing by 1000

Worked Example

Your notes

Calculating volume

Calculate the volume of 0.50 mol / dm^3 nitric acid, HNO_3, required to neutralise 25.00 cm^3 of 0.80 mol / dm^3 potassium hydroxide, KOH. Give your answer in cm^3.

$$KOH\ (aq) + HNO_3\ (aq) \rightarrow KNO_3\ (aq) + H_2O\ (l)$$

Answer:

- **Step 1:** Calculate the number of moles of potassium hydroxide
  - Moles of potassium hydroxide = concentration x volume (dm^3) = 0.80 x 0.025 = 0.02 mols
- **Step 2:** Using the equation, calculate the number of moles of nitric acid
  - Moles of nitric acid = 0.02 mols
  - The ratio is 1:1 so the number of moles of nitric acid is the same
- **Step 3:** Calculate the volume of nitric acid in cm^3
  - Volume of nitric acid = $\frac{\text{moles}}{\text{concentration}} = \frac{0.02}{0.50}$ = 0.040 dm^3
  - Volume of nitric acid = 0.040 dm^3 x 1000 = 40 cm^3

Your notes

Calculating empirical & molecular formulae

Extended tier only

- As previously discussed in Empirical Formulae & Formulae of Ionic Compounds:
- The **empirical formula** is the simplest whole number ratio of the atoms of each element present in one molecule or formula unit of the compound
  - E.g. the empirical formula of ethanoic acid is CH_2O

How to calculate empirical formulae

- Empirical formula calculations are very methodical
- Use a table and the following steps to complete an empirical formula calculation:

1. Write the element
2. Write the value given for each element
   - This may be given as a mass, in g, or as a percentage
   - There are exam questions where you are required to calculate the value of one of the elements
3. Write the relative atomic mass of each element
4. Calculate the moles of each element
   - Moles = $\frac{\text{mass}}{A_r}$
5. Calculate the ratio of elements
   - Divide all the moles by the smallest number of moles
   - If you get a ratio that does not have whole numbers, you multiply by an appropriate number to make all the values into whole numbers
6. Write the final empirical formula

Worked Example

A sample of a compound was found to contain 10 g of hydrogen and 80 g of oxygen.

Calculate the empirical formula of this compound.

A_r (H) = 1 A_r (O) = 16

Your notes

Answer:

1. Element	H	O
2. Value	10	80
3. Relative atomic mass	1	16
4. Moles = $\frac{\text{mass}}{A_r}$	$\frac{10}{1}$ = 10	$\frac{80}{16}$ = 5
5. Ratio (divide by smallest)	$\frac{10}{5}$ = 2	$\frac{5}{5}$ = 1
6. Answer	The empirical formula is H_2O	

Worked Example

Carbohydrate **X** was analysed and found to contain 31.58% carbon and 5.26% hydrogen by mass.

Find the empirical formula of carbohydrate **X**.

A_r(H) = 1 A_r(C) = 12 A_r(O) = 16

Answer:

A carbohydrate contains carbon, hydrogen and oxygen

The percentages do not add up to 100%, which means that you need to calculate the percentage of oxygen needs to be calculated

Percentage of oxygen = 100 – 31.58 – 5.26 = 63.16%

1. Element	C	H	O
2. Value	31.58	5.26	63.16
3. Relative atomic mass	12	1	16
4. Moles = $\frac{\text{mass}}{A_r}$	$\frac{31.58}{12}$ = 2.63	$\frac{5.26}{1}$ = 5.26	$\frac{63.16}{16}$ = 3.95
5. Ratio (divide by smallest)	$\frac{2.63}{2.63}$ = 1	$\frac{5.26}{2.63}$ = 2	$\frac{3.95}{2.63}$ = 1.5
5. Whole number ratio	1 x 2 = 2	2 x 2 = 4	1.5 x 2 = 3
6. Answer	The empirical formula is $C_2H_4O_3$		

Your notes

Examiner Tips and Tricks

The molar ratio must be a whole number.

If you don't get a whole number when calculating the ratio of atoms in an empirical formula, such as 1.5, multiply that and the other ratios to achieve whole numbers.

How to calculate molecular formula

- Molecular formula gives the **actual numbers of atoms of each element** present in the formula of the compound

Table showing the relationship between empirical and molecular formulae

Compound	Empirical formula	Molecular formula
Methane	CH_4	CH_4
Ethane	CH_3	C_2H_6
Ethene	CH_2	C_2H_4
Benzene	CH	C_6H_6

- To calculate the molecular formula:
  1. Find the relative formula mass of the empirical formula
     - Add the relative atomic masses of all the atoms in the empirical formula
  2. Use the following equation:
     - $\frac{\text{relative formula mass of molecular formula}}{\text{relative formula mass of empirical formula}}$
  3. Multiply the number of each element present in the empirical formula by the number from step 2 to find the molecular formula

Worked Example

The empirical formula of **X** is $C_4H_{10}S_1$

The relative formula mass (M_r) of **X** is 180.

Calculate the molecular formula of **X**.

$A_r(C) = 12 \quad A_r(H) = 1 \quad A_r(S) = 32$

Answer:

1. Calculate the relative formula mass of the empirical formula:
   - M_r = (12 x 4) + (1 x 10) + (32 x 1) = 90
2. Divide the relative formula mass of **X** by the relative formula mass of empirical formula:
   - 180 / 90 = 2
3. Multiply for the molecular formula:
   - The number of atoms of each elements should be multiplied by 2
   - $(C_{4 \times 2}) + (H_{10 \times 2}) + (S_{1 \times 2})$
   - Molecular formula of **X** = $C_8H_{20}S_2$

Your notes

Deducing formulae of hydrated salts

- A hydrated salt is a crystallised salt that contains water molecules as part of its structure
- The formula of a hydrated salt shows the water molecules, e.g. $CuSO_4{\bullet}2H_2O$
  - The • symbol shows that the water present is water of crystallisation
- The formula of hydrated salts can be determined experimentally by:
  - Weighing a sample of the hydrated salt
  - Heating it until the water of crystallisation has been driven off
    - This is achieved by heating until a constant mass
  - Re-weighing the anhydrous salt
- From the results, you can determine the mass of anhydrous salt and the mass of the water of crystallisation
- Applying a similar approach to deducing empirical formulae, the formula of the hydrated salt can be calculated

How to calculate water of crystallisation

- The steps for empirical formula can be adapted for hydrated salt / water of crystallisation calculations
  - Instead of writing elements, write the two components of a hydrated salt
    - The salt
    - Water
  - Instead of writing relative atomic mass, write the relative molecular / formula mass of the salt and water
- Use a table and the following steps to complete the calculation:
  1. Write the salt and water
  2. Write the value given for the salt and water

- There are exam questions where you are required to calculate one of these values

3. Write the relative molecular / formula mass of the salt and water

4. Calculate the moles of the salt and water
   - Moles = $\frac{\text{mass}}{M_r}$

5. Calculate the ratio salt : water
   - Divide all the moles by the smallest number of moles
   - The calculation should give a ratio of **1** salt : ***x*** water

6. Write the final hydrated salt formula

Your notes

Worked Example

11.25 g of hydrated copper sulfate, $CuSO_4.xH_2O$, is heated until it loses all of its water of crystallisation.

It is re-weighed and its mass is 7.19 g.

Calculate the formula of the hydrated copper(II) sulfate.

A_r(Cu) = 63.5 A_r(S) = 32 A_r(O) = 16 A_r(H) = 1

Answer:

1. Salt and water	$CuSO_4$	H_2O
2. Value	7.19	11.25 - 7.19 = 4.06
3. M_r	63.5 + 32 + (16 x 4) = 159.5	(1 x 2) + 16 = 18
4. Moles = $\frac{\text{mass}}{M_r}$	$\frac{7.19}{159.5}$ = 0.045	$\frac{4.06}{18}$ = 0.226
5. Salt : water ratio	$\frac{0.045}{0.045}$ = 1	$\frac{0.226}{0.045}$ = 5
6. Formula of hydrated salt	The formula is $CuSO_4$•**5**H_2O	

Examiner Tips and Tricks

The specification is not clear about whether deducing the formula of hydrated salts is required.

However, it is an application of deducing empirical formulae so it is worth knowing how to do this.

Your notes

Your notes

Calculating percentage yield, percentage by mass & percentage purity

Extended tier only

Percentage yield

- **Yield** is the term used to describe the amount of **product** you get from a reaction
- For economic reasons, the objective of every chemical producing company is to have as high a percentage yield as possible to increase profits and reduce costs and waste
- In practice, you **never** get 100% yield in a chemical process for several reasons
- These include:
  - Some reactants may be left behind in the **equipment**
  - The reaction may be **reversible** and in these reactions a high yield is never possible as the products are continually turning back into the reactants
  - Some products may also be lost during **separation** and **purification** stages such as filtration or distillation
  - There may be **side reactions** occurring where a substance reacts with a gas in the air or an **impurity** in one of the reactants
  - Products can also be lost during **transfer** from one container to another

How to calculate percentage yield

- **Percentage yield** compares the actual yield to the theoretical yield
- The equation for percentage yield is:

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

- **Actual yield** is the recorded amount of product obtained
- **Theoretical yield** is the amount of product that would be obtained under perfect practical and chemical conditions
  - Typically, this involves a reacting mass calculation based on the balanced symbol equation

Worked Example

Copper(II) sulfate may be prepared by the reaction of dilute sulfuric acid with copper(II) oxide. A student prepared 1.6 g of dry copper(II) sulfate crystals.

Calculate the percentage yield if the theoretical yield is 2.0 g.

Answer

- Actual yield of copper(II) sulfate = 1.6 g
- Percentage yield of copper(II) sulfate = $\frac{1.6}{2.0}$ x 100 = **80%**

Examiner Tips and Tricks

- You are expected to remember the equation for percentage yield
- If you remember it incorrectly and get a percentage yield greater than 100%, then you have made an error!
- The most common error is to divide the theoretical yield by the actual yield
  - In this case, you just need to swap the numbers around in your calculation

How to calculate percentage composition by mass

- The percentage composition of any compound is a way to express the mass of each element as a percentage of the total mass of the compound
- The equation for percentage composition is:

percentage composition of an element =

$$\frac{\textbf{total mass of the element in the compound}}{\textbf{relative formula mass of the compound}} \times 100$$

- For example, in water:
  - Water is a simple molecule with the chemical formula H_2O
  - So, water is made of two hydrogen (H) atoms and one oxygen (O) atom
  - From the Periodic Table, the relative atomic mass of:
  - Hydrogen = 1
  - Oxygen = 16
- Therefore, the total mass of water is:
  - (2 x 1) + 16 = 18
- To find the percentage composition of hydrogen:
  - Percentage of hydrogen = $\frac{2 \times 1}{18}$ x 100 = 11.1%
- Similarly, the percentage composition of oxygen is:

Your notes

- Percentage of oxygen = $\frac{1 \times 16}{18} \times 100 = 88.9\%$
- **Note:** The total percentage by mass of all the elements should add up to 100%, e.g. 11.1% + 88.9% = 100%

Your notes

Worked Example

Calculate the percentage by mass of iron in iron(III) oxide, Fe_2O_3.

Answer:

- From the Periodic Table, the relative atomic masses are:
  - Fe = 56
  - Oxygen = 16
- The total mass of iron in iron(III) oxide is:
  - 2 x 56 = 112
- The total mass of iron(III) oxide is:
  - (2 × 56) + (3 × 16) = 160
- The equation for percentage composition is:
  - Percentage composition = $\frac{\text{total mass of element}}{\text{total mass of compound}} \times 100$
- So, the percentage composition of iron in iron(III) oxide is:
  - Percentage of iron = $\frac{112}{160} \times 100 = 70\%$

Worked Example

The chemical formula of the fertiliser ammonium nitrate is NH_4NO_3. Calculate the percentage by mass of nitrogen in ammonium nitrate.

Answer:

- From the Periodic Table, the relative atomic masses are:
  - Nitrogen = 14
  - Hydrogen = 1
  - Oxygen = 16
- **Careful:** There are **two** nitrogen atoms in ammonium nitrate
- The total mass of nitrogen in ammonium nitrate is:
  - 2 x 14 = 28
- The total mass of ammonium nitrate is:
  - (1 x 14) + (4 × 1) + (1 x 14) + (3 × 16) = 80
- The equation for percentage composition is:

- Percentage Composition = $\frac{\text{total mass of element}}{\text{total mass of compound}} \times 100$

- So, the percentage composition of nitrogen in ammonium nitrate is:
- Percentage of nitrogen = $\frac{(2 \times 14)}{80} \times 100 = 35\%$

Your notes

Examiner Tips and Tricks

- Make sure you calculate the percentage composition using the **total mass** of the element.
  - For example, a common mistake with ammonium nitrate is doing the calculation for only one atom of nitrogen.
  - This would lose a mark in an exam
- Show ALL your working out. If you make a mistake in the calculation, you could still score a mark for your workings.

How to calculate percentage purity

- A pure substance has nothing else mixed with it
- Often, the product you are trying to obtain may become contaminated with unwanted substances such as unreacted reactants, catalysts and other impurities
- To equation to calculate percentage purity is:

$$\textbf{percentage purity} = \frac{\textbf{mass of pure substance}}{\textbf{total mass of substance}} \textbf{ x 100}$$

Worked Example

A sample of lead(II) bromide was made. It weighed 15 g.

The sample was found to be impure and only contained 13.5 g of lead(II) bromide.

Calculate the percentage purity of the lead(II) bromide.

Answer:

- The mass of the pure substance is 13.5 g
- The total mass of the substance is 15 g
- Percentage purity = $\frac{\text{mass of pure substance}}{\text{total mass of substance}} \text{ x } 100$
- Percentage purity = $\frac{13.5}{15} \times 100 = \mathbf{90\%}$

Your notes

Examiner Tips and Tricks

- All of these calculations are to find a percentage so don't forget to multiply by 100 to convert your answer to a percentage.