Edexcel International AS Chemistry

Your notes

Amount of Substance

Contents

Your notes

Concentration Calculations

Amount of substance calculations

- As previously discussed, the amount of substance can be defined as the number of particles in a substance, *n*, measured in moles (often abbreviated to mol)
- In reality, amount of substance is used as a blanket term to cover most chemical calculations, especially those that involve moles
- The two main calculations for amount of substance are:

$$\text{Moles, } n = \frac{mass,\ m}{molar\ mass,\ M}$$

$$\text{Moles, } n = \text{concentration x volume}$$

- Other common calculations for amount of substance include:

$$\text{Moles, } n = \frac{number\ of\ particles}{Avogadro's\ constant}$$

$$\text{Moles, } n = \frac{PV}{RT} \text{ from the ideal gas equation } (PV = nRT)$$

Concentration calculations

- Concentration can be defined as the amount of a substance dissolved in a quantity of liquid
- When a mass concentration is calculated, the units are usually g dm^{-3}
  - Other units are possible such as g cm^{-3}, kg m^{-3} and sometimes in medicines you might see them as mg / ml
  - The equation to calculate mass concentration is:

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

- When a molar concentration is calculated, the units are mol dm^{-3}
  - Calculating molar concentrations requires the use of two equations:

$$\text{number of moles (or amount)} = \frac{\text{mass}}{\text{molar mass}}$$

- Molar mass is the mass per mole of a substance in g mol^{-1}

molar concentration in mol dm^{-3} = $\dfrac{\text{number of moles (or amount)}}{\text{volume of solution in dm}^3}$

Your notes

Worked Example

Mass concentration calculations

1. What is the mass concentration when 6.34 g of sodium chloride is dissolved into a 0.250 dm^3 solution?
2. A sodium carbonate solution has a mass concentration of 5.2 g dm^{-3}. What is the volume of the solution made when 250 g of sodium carbonate is used?
3. The mass concentration of a solution is 26.7 g dm^{-3}. What is the mass of sodium bromide in 500 cm^3 of solution?

Answer 1

- Mass concentration $= \dfrac{\text{mass (g)}}{\text{volume (dm}^3)} = \dfrac{6.34}{0.250} =$ 25.4 g dm^{-3} (to 3 s.f.)

Answer 2

- Volume of solution $= \dfrac{\text{mass (g)}}{\text{mass concentration (g dm}^3)} = \dfrac{250}{5.2} =$ 48 dm^3
  - This answer should be given to 2 s.f. as there is a value in the question with only 2 significant figures

Answer 3

- Mass = mass concentration (g dm^{-3}) x volume of solution (dm^3) = 26.7 x 0.5 = 13.4 g (to 3 s.f.)
  - The 500 cm^3 in the question has to be converted into dm^3
  - $\dfrac{500}{1000}$ = 0.5 dm^3

Worked Example

Molar concentration calculations

1. What is the molar concentration when 6.34 g of sodium chloride is dissolved into a 250 cm^3 solution?
2. A sodium carbonate solution has a molar concentration of 1.25 mol dm^{-3}. What is the volume of the solution made when 250 g of sodium carbonate is used?
3. The molar concentration of a sodium bromide solution is 0.250 mol dm^{-3}. What is the mass of sodium bromide in 500 cm^3 of this solution?

Answer 1

- Number of moles of NaCl $= \frac{\text{mass}}{\text{molar mass}} = \frac{6.34}{(23.0 + 35.5)} =$ 0.1084 moles
  - Molar concentration in mol dm^{-3} $= \frac{\text{number of moles (or amount)}}{\text{volume of solution in dm}^3} = \frac{0.1084}{0.250} =$ 0.434 mol dm^{-3}

Answer 2

- Number of moles of Na_2CO_3 $= \frac{\text{mass}}{\text{molar mass}} = \frac{250}{(23.0 \times 2) + 12.0 + (16.0 \times 3)} =$ 2.358 moles
  - Volume of solution in dm^3 $= \frac{\text{number of moles (or amount)}}{\text{Molar concentration in mol dm}^{-3}} = \frac{2.358}{1.25} =$ 1.89 dm^3

Answer 3

- Number of moles of NaBr = molar concentration x volume of solution = 0.250 x 0.500 = 0.125 moles
- Mass of NaBr = number of moles of NaBr x molar mass = 0.125 x (23.0 + 79.9) = 12.9 g

Parts per million

- When expressing extremely low concentrations a unit that can be used is **parts per million** or **ppm**
- This is useful when giving the concentration of a pollutant in water or the air when the absolute amount is tiny compared the the volume of water or air
- **1 ppm** is defined as
  - A mass of **1 mg** dissolved in **1 dm^3** of water
- Since 1 dm^3 weighs 1 kg we can also say it is
  - A mass of **1 mg** dissolved in **1 kg** of water, or 10^{-3} g in 10^3 g which is the same as saying the concentration is **1 in 10^6** or **1 in a million**

Worked Example

The concentration of chlorine in a swimming pool should between between 1 and 3 ppm. Calculate the maximum mass, in kg, of chlorine that should be present in an olympic swimming pool of size 2.5 million litres.

Answer:

Step 1: calculate the total mass in mg assuming 3ppm(1 litre is the same as 1 dm^3)

Your notes

- $3 \times 2.5 \times 10^6 = 7.5 \times 10^6$ mg

Step 2: convert the mass into kilograms (1 mg = 10^{-6} kg)

- $7.5 \times 10^6 \times 10^{-6}$ kg = **7.5 kg**

Your notes

Atmospheric gas concentration

- The concentration of atmospheric gases, particularly pollutants, can be measured in **parts per million, ppm**
- Instead of using mass, the comparison of gas is done by volume
  - You might see the values quoted in **ppmv** - the v shows that the value relates to concentration by volume
- A concentration of 1 ppmv means that there is 1 cm^3 of a particular gas in 1000000cm^3 or 1000 dm^3
- The equation to calculate the concentration of a gas in ppm is:

$$\text{concentration in ppm} = \frac{\text{volume of gas} \times 1000000}{\text{volume of air}}$$

- The volumes can be given in any units but they must be the same units, otherwise one of them will need to be converted

Worked Example

Atmospheric gas concentration calculations

Calculate the concentration, in ppm, of the following:

1. A volume of 2.5 dm^3 of carbon dioxide in 10000 dm^3 of air
2. A volume of 2.5 dm^3 of sulfur dioxide in 4000 dm^3 of air
3. A volume of 152 cm^3 of ozone in 112 dm^3 of air

Answer 1

- Concentration in ppm

$$= \frac{\text{volume of gas} \times 1000000}{\text{volume of air}} = \frac{2.5 \times 1000000}{10000} = \text{250 ppm}$$

Answer 2

- Concentration in ppm

$$= \frac{\text{volume of gas} \times 1000000}{\text{volume of air}} = \frac{2.5 \times 1000000}{4000} = \text{625 ppm}$$

Answer 3

A volume of 152 cm^3 of ozone in 112 dm^3 of air

- Concentration in ppm

$$= \frac{\text{volume of gas} \times 1000000}{\text{volume of air}} = \frac{0.152 \times 1000000}{112.0} = 1360 \text{ ppm}$$

Your notes

Examiner Tips and Tricks

When completing atmospheric gas calculations, the gas involved does not affect the calculation as shown by worked examples 1 and 2

Reacting Mass Calculations

- Chemical equations can be used to calculate the **moles** or **masses** of reactants and products
- To do this, information given in 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

Example 1

Calculate the maximum mass of magnesium oxide that can be produced by completely burning 7.5 g of magnesium in oxygen.

magnesium + oxygen → magnesium oxide

Answer:

1. Write the balanced chemical equation:

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

2. Determine the relative atomic and formula masses:
   - Magnesium, Mg = 24.3 g mol^{-1}
   - Oxygen, O_2 = 32.0 g mol^{-1}
   - Magnesium oxide, MgO = 40.3 g mol^{-1}
3. Calculate the moles of magnesium used in the reaction:

$$n(\text{Mg}) = \frac{7.5\ \text{g}}{24.3\ \text{g mol}^{-1}} = 0.3086 \text{ moles}$$

4. Deduce the number of moles of magnesium oxide, using the balanced chemical equation:
   - 2 moles of magnesium form 2 moles of magnesium oxide
     - The ratio is 1 : 1
   - Therefore, n(MgO) = 0.3086 moles
5. Calculate the mass of magnesium oxide:

$$\text{Mass} = \text{moles} \times M_r$$

$$\text{Mass} = 0.3086 \text{ mol} \times 40.3 \text{ g mol}^{-1} = 12.4 \text{ g}$$

6. Therefore, the mass of magnesium oxide produced is **12.4 g**

Your notes

Worked Example

Example 2

Calculate the mass of aluminium, in tonnes, that can be produced from 51 tonnes of aluminium oxide. The equation for the reaction is:

aluminium oxide ⟶ aluminium + oxygen

Answer:

1. Write the balanced chemical equation:

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

2. Determine the relative atomic and formula masses:

- Aluminium oxide, Al_2O_3 = 102.0 g mol^{-1}
- Aluminium, Al = 27.0 g mol^{-1}
- Oxygen, O_2 = 32.0 g mol^{-1}

3. Calculate the mass, in g, of aluminium oxide used in the reaction:

$$51 \text{ tonnes} \times 10^6 = 51\,000\,000 \text{ g}$$

4. Calculate the moles of aluminium oxide used in the reaction:

$$n(Al_2O_3) = \frac{51000000 \text{ g}}{102.0 \text{ g mol}^{-1}} = 500\,000 \text{ mol}$$

5. Deduce the number of moles of aluminium, using the balanced chemical equation:

- 2 moles of aluminium oxide form 4 moles of aluminium
  - The ratio is 1:2
- Therefore, n(Al) = 500 000 x 2 = 1 000 000 mol

6. Calculate the mass of aluminium:

$$\text{mass} = \text{moles} \times M_r$$

$$\text{mass} = 1\,000\,000 \text{ mol} \times 27.0 \text{ g mol}^{-1} = 27\,000\,000 \text{ g}$$

7. Convert the mass to tonnes:

$$\text{mass} = \frac{27000000}{10^6}$$

mass = **27 tonnes**

Examiner Tips and Tricks

As long as you are consistent it doesn't matter whether you work in grams or tonnes or any other mass unit as the reacting masses will always be in proportion to the balanced equation.

Your notes

Balancing Equations using Reacting Masses

- If the masses of reactants and products of a reaction are known then we can use them to write a balanced equation for that reaction
- This is done by converting the **masses** to **moles** and simplifying to find the **molar ratios**

Worked Example

Example 3

A student reacts 1.2 g of carbon with 16.2 g of zinc oxide. The resulting products are 4.4 g of carbon dioxide and 13.0 g of zinc.

Determine the balanced equation for the reaction.

Answer:

1. Write the unbalanced chemical equation:

$$C + ZnO \rightarrow Zn + CO_2$$

2. Determine the relative atomic and formula masses:
   - Carbon, C = 12.0 g mol^{-1}
   - Zinc, Zn = 65.4 g mol^{-1}
   - Zinc oxide, ZnO = 81.4 g mol^{-1}
   - Carbon dioxide, CO_2 = 44.0 g mol^{-1}
3. Calculate the moles of each substance

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

$$n(\text{C}) = \frac{1.2}{12.0} = 0.1 \text{ mol}$$

$$n(\text{Zn}) = \frac{13.0}{65.4} = 0.2 \text{ mol}$$

$$n(\text{ZnO}) = \frac{16.2}{81.4} = 0.2 \text{ mol}$$

$$n(\text{CO}_2) = \frac{4.4}{44.0} = 0.1 \text{ mol}$$

4. Determine the ratio (divide by the smallest value)

Your notes

$$C = \frac{0.1}{0.1} = 1$$

$$Zn = \frac{0.2}{0.1} = 2$$

$$ZnO = \frac{0.2}{0.1} = 2$$

$$CO_2 = \frac{0.1}{0.1} = 1$$

5. Apply the values to the unbalanced equation:

$$\mathbf{1}C + \mathbf{2}ZnO \rightarrow \mathbf{2}Zn + \mathbf{1}CO_2$$

6. Simplify:

$$C + \mathbf{2}ZnO \rightarrow \mathbf{2}Zn + CO_2$$

Examiner Tips and Tricks

These questions look hard but they are actually quite easy to do, as long as you follow the steps and organise your work neatly.

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

Your notes

Reacting Volume Calculations

- Reacting volume calculations are commonly associated with the reactions of gases
- All gases occupy the same volume under the same conditions
  - At room temperature and pressure (r.t.p.), the **molar gas volume** of any gas is 24.0 dm^3
    - Room temperature and pressure are 293 K / 20 °C and 101.3 kPa respectively
  - At standard temperature and pressure (s.t.p.), the molar gas volume of any gas is 22.4 dm^3
    - Standard temperature and pressure are 273 K / 0 °C and 101.3 kPa respectively
- The equation to calculate the number of moles for any volume of gas is:

$$\text{Number of moles} = \frac{\text{Volume of gas }(dm^3)}{\text{Molar gas volume }(dm^3)}$$

Worked Example

Molar gas volume calculations

Calculate the number of moles present in 4.5 dm^3 of carbon dioxide at:

1. Room temperature and pressure
2. Standard temperature and pressure

Answers

1. $\text{Number of moles} = \frac{\text{Volume of gas }(dm^3)}{\text{Molar gas volume }(dm^3)} = \frac{4.5}{24} =$ 0.1875 moles
2. $\text{Number of moles} = \frac{\text{Volume of gas }(dm^3)}{\text{Molar gas volume }(dm^3)} = \frac{4.5}{22.4} =$ 0.201 moles

   (to 3 s.f.)

- Volumes of gas can also be calculated using
  - Number of moles calculations
  - Volume calculations
- This can help determine the size of the equipment that you use in an experiment

Your notes

Worked Example

Calculating gas volumes from moles

Calculate the volume of gas produced when 1.50 g of sodium reacts with water at standard temperature and pressure.

Answer

Step 1: Write the balanced equation for the reaction

- $2Na (s) + 2H_2O (l) \rightarrow 2NaOH (aq) + H_2 (g)$

Step 2: Calculate the number of moles of sodium

- Number of moles $= \frac{\text{mass (g)}}{\text{molar mass (g mol}^{-1})} = \frac{1.5}{23.0} =$ 0.0652 moles (to 3s.f.)

Step 3: Use the stoichiometry of the equation to calculate the number of moles of hydrogen

- The stoichiometric ratio of Na : H_2 is 2 : 1
  - Therefore, the number of moles of hydrogen is $\frac{0.0652}{2} =$ 0.0326 moles

Step 4: Calculate the volume of hydrogen gas evolved

- Volume of gas = number of moles x molar gas volume
  - Volume of gas = 0.0326 x 22.4 = 0.730 dm^3 (to 3s.f.)

Worked Example

Calculating gas volumes from other volumes

Calculate the total volume of gas produced when 6.50 dm^3 of propane combusts completely

Answer

Step 1: Write the balanced equation for the reaction

- $C_3H_8 (g) + 5O_2 (g) \rightarrow 3CO_2 (g) + 4H_2O (g)$

Step 2: Determine the number of moles of gas produced

- One mole of propane produces 3 moles of carbon dioxide and 4 moles of water
  - Therefore, one mole of propane produces a total of 7 moles of gas

Step 3: Calculate the volume of gas that is produced

- 6.50 dm^3 of propane will produce 7 x 6.50 dm^3 of gas = 45.5 dm^3 gas

The Ideal Gas Expression

Kinetic theory of gases

Your notes

- **The kinetic theory of gases** states that molecules in gases are constantly moving
- The theory makes the following assumptions:
  - That gas molecules are moving very fast and randomly
  - That molecules hardly have any volume
  - That gas molecules do not attract or repel each other (**no intermolecular forces**)
  - No kinetic energy is lost when the gas molecules collide with each other (**elastic collisions**)
  - The temperature of the gas is related to the average kinetic energy of the molecules
- Gases that follow the kinetic theory of gases are called **ideal gases**
- However, in reality gases do not fit this description exactly **but** may come very close and are called **real gases**

Ideal gas equation

- The **ideal gas equation** shows the relationship between pressure, volume, temperature and number of moles of gas of an ideal gas:

PV = nRT

- P = pressure (pascals, Pa)
  - V = volume (m^3)
  - n = number of moles of gas (mol)
  - R = gas constant (8.31 J K^{-1} mol^{-1})
  - T = temperature (kelvin, K)

Worked Example

Calculating the volume of a gas

Calculate the volume occupied by 0.781 mol of oxygen at a pressure of 220 kPa and a temperature of 21 °C

Answer

Step 1: Rearrange the ideal gas equation to find volume of gas

$$V = \frac{nRT}{P}$$

Step 2: Calculate the volume the oxygen gas occupies

- P = 220 kPa = 220 000 Pa
  - n = 0.781 mol
  - R = 8.31 J K^{-1} mol^{-1}
  - T = 21 °C = 294 K

$$V = \frac{0.781 \times 8.31 \times 294}{220000} = 0.00867\ m^3 = 8.67\ dm^3$$

Worked Example

Calculating the molar mass of a gas

A flask of volume 1000 cm^3 contains 6.39 g of a gas. The pressure in the flask was 300 kPa and the temperature was 23 °C.

Calculate the relative molecular mass of the gas.

Answer

Step 1: Rearrange the ideal gas equation to find the number of moles of gas

$$n = \frac{PV}{RT}$$

Step 2: Calculate the number of moles of gas

- P = 300 kPa = 300 000 Pa
  - V = 1000 cm^3 = 1 dm^3 = 0.001 m^3
  - R = 8.31 J K^{-1} mol^{-1}
  - T = 23 °C = 296 K

$$n = \frac{300000 \times 0.001}{8.31 \times 296} = 0.12\ mol$$

Step 3: Calculate the molar mass using the number of moles of gas

$$n = \frac{mass}{molar\ mass}$$

$$\text{molar mass} = \frac{6.39}{0.12} = 53.25\ g\ mol^{-1}$$

Examiner Tips and Tricks

To calculate the temperature in **Kelvin**, add 273 to the Celsius temperature, e.g. 100 °C is 373 Kelvin.

Your notes

You must be able to rearrange the ideal gas equation to work out all parts of it.

The **units** are incredibly important in this equation - make sure you know what units you should use, and do the necessary conversions when doing your calculations!

Your notes

Calculating Yield & Atom Economy

Percentage yield

- In a lot of reactions, not all reactants react to form products which can be due to several factors:
  - Other reactions take place simultaneously
  - The reaction does not go to **completion**
  - Products are **lost** during separation and purification
- The **percentage yield** shows how much of a particular product you get from the reactants compared to the maximum theoretical amount that you can get:

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

- The **actual yield** is the number of moles or mass of product obtained **experimentally**
  - The **theoretical yield** is the number of moles or mass obtained by a reacting mass calculation

Worked Example

In an experiment to displace copper from copper(II) sulfate, 6.5 g of zinc was added to an excess of copper(II) sulfate solution. The resulting copper was filtered off, washed and dried. The mass of copper obtained was 4.8 g.

Calculate the percentage yield of copper.

Answer:

Step 1: The balanced symbol equation is:

Zn (s) + CuSO4 (aq) → ZnSO4 (aq) + Cu (s)

Step 2: Calculate the amount of zinc reacted in moles

$$number\ of\ moles = \frac{6.5\ g}{65.4\ g\ mol^{-1}} = 0.10\ mol$$

Step 3: Calculate the maximum amount of copper that could be formed from the molar ratio: *Since the ratio of Zn(s) to Cu(s) is 1:1 a maximum of 0.10 moles can be produced*

Step 4: Calculate the maximum mass of copper that could be formed (theoretical yield)

$$\text{mass} = \text{mol} \times M$$

$$\text{mass} = 0.10 \text{ mol} \times 63.55 \text{ g mol-1}$$

$$\text{mass} = 6.4 \text{ g (2 sig figs)}$$

Step 5: Calculate the percentage yield of copper

$$percentage\ yield\ =\ \frac{4.8\ g}{6.4\ g}\ \times\ 100\ =\ 75\%$$

Examiner Tips and Tricks

It is possible to calculate a percentage yield that is greater than 100%. This would be an error which could occur when preparing crystals due to:

- The crystals may still be dry when weighed
- There are impurities in the crystals
- The mass of the filter paper or container could mistakingly be included in the total mass of the product

Atom economy

- The atom economy of a reaction shows how many of the atoms used in the reaction become the desired product
    - The rest of the atoms or mass is wasted
- It is found directly from the balanced equation by calculating the M_r of the desired product

$$Atom\ economy\ =\ \frac{molecular\ mass\ of\ desired\ product}{sum\ of\ molecular\ masses\ of\ ALL\ reactants}\ \times\ 100$$

In addition reactions, the atom economy will always be 100% because all of the atoms are used to make the desired product Whenever there is only one product, the atom economy will always be 100% For example, in the reaction between ethene and bromine:

$$CH_2{=}CH_2 + Br_2 \rightarrow CH_2BrCH2Br$$

- The atom economy could also be calculated using mass, instead or M_r
    - In this case, you would divide the mass of the desired product formed by the total mass of all reactants, and then multiply by 100
- Questions about atom economy often ask in qualitative or quantitative terms

Worked Example

Qualitative atom economy Ethanol can be produced by various reactions, such as:

Your notes

Your notes

Hydration of ethene: $C_2H_4 + H_2O \rightarrow C_2H_5OH$

Substitution of bromoethane: $C_2H_5Br + NaOH \rightarrow C_2H_5OH + NaBr$

Explain which reaction has a higher atom economy.

Answer

Hydration of ethene has a higher atom economy (of 100%) because all of the reactants are converted into products, whereas the substitution of bromoethane produces NaBr as a waste product

Worked Example

Quantitative atom economy

The blast furnace uses carbon monoxide to reduce iron(III) oxide to iron.

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

Calculate the atom economy for this reaction, assuming that iron is the desired product. (A_r / M_r data: Fe_2O_3 = 159.6, CO = 28.0, Fe = 55.8, CO_2 = 44.0)

Answer

Step 1: Write the equation:

$$Atom\ economy\ =\ \frac{molecular\ mass\ of\ desired\ product}{sum\ of\ molecular\ masses\ of\ ALL\ reactants} \times 100$$

Step 2: Substitute values and evaluate:

$$Atom\ economy = \frac{2 \times 55.8}{159.6 + (3 \times 28.0)} \times 100 = 45.9\%$$

Examiner Tips and Tricks

Careful: Sometimes a question may ask you to show your working when calculating atom economy.

In this case, even if it is an addition reaction and it is obvious that the atom economy is 100%, you will still need to show your working.