C4: Chemical Calculations: Chemistry Specification

Conservation of Mass

The law of conservation of mass says that no atoms are lost or made during a chemical reaction. This means that the mass of the products equals the mass of the reactants.

Relative Formula Mass

The relative formula mass is represented by the symbol M_r. RFM is the sum of the relative atomic masses of the atoms in the formula. In a balanced chemical equation, the total of the relative formula masses of the reactants equals the total of the relative formula masses of the products in the quantities shown.

Mass Changes when Products or Reactants are Gases

Some reactions may appear to have a change in mass but this can is because a reactant or product is a gas and its mass has not been taken into account. For example if a gas is made in a chemical reaction and escapes into the atmosphere the mass will appear to decrease.

Use of amount of substance in relation to volumes of gases

1 mole of any gas occupy the same volume under the same conditions of temperature and pressure. The volume of one mole of any gas at room temperature (20°C) and pressure (1 atmosphere pressure) is $24dm^3$. The number of mole of gas can be calculated using the formula:

No of moles of gas = volume of gas (dm^3) / $24dm^3$

Or

No of moles of gas = volume of gas (cm^3) / $24000cm^3$

Using Moles to Balance Equations

In a chemical reaction involving two reactants you would use an excess of one of the reactants to make sure that all of the other reactant is used up. The reactant that is completely used up is called the limiting reactant because it limits the amount of products that can be made.

Amount of Substances in Equations

The masses of reactants and products can be calculated from balanced symbol equations and chemical equations can be interpreted in terms of moles. For example:

$$2H_2 + O_2 \rightarrow 2H_2O$$

This shows that 2 moles of hydrogen react with 1 mole of oxygen to make 2 moles of water.

Concentration of Solutions

Lots of chemical reactions take place in solutions. The concentration of a solution is measured in mass per given volume of solution and so the units are g/dm^3.

Titrations

The volumes of acid and alkali solutions that react with each other can be measured by titration using a suitable indicator. For example if you had a known concentration of acid and wanted to know the volume to neutralise $25cm^3$ of sodium hydroxide you would carry out a titration. You would add an indicator such as phenolphthalein, methyl orange or litmus to sodium hydroxide in a conical flask and you would add the acid from a burette. When the end point is near start swirling the conical flask and add the acid drop by drop until the indicator changes colour. Record the volume of acid added. In titration calculations you will need to use and rearrange the formula:

Number of moles = concentration x volume

Using Concentrations of Solutions

The concentration of a solution is measured in mol/dm^3. The amount in moles of solute or its mass in grams in a given volume of solution can be calculated from its concentration. If the volumes of two solutions that react completely are known and the concentration of one solution is known, the concentration of the other solution can be calculated. To find the concentration of a substance use the formulas:

Concentration (g/dm^3) = mass of solute (g) / volume of solution (dm^3)

Concentration (g/dm^3) = (mass of solute (g) / volume of solution (cm^3)) x 1000

Moles

Chemical amounts are measured in moles. The symbol for mole is mol. The mass of 1 mole of a substance in grams is equal to its relative formula mass. For example water has an RFM of 18 and 1 mole of water has a mass of 18g. 1 mole of any substance contains the same number of particles as one mole of any other substance. This number is known as the Avogadro constant. The value of the Avogadro constant is 6.02×10^{23} per mole.

Number of Moles = Mass / RFM

Percentage Yield

In theory no atoms are lost of gained in a chemical reaction but often in a chemical reaction we do not obtain all the product that we should. This could be because the reaction was reversible and did not go to completion, some of the products was lost when it was made or separated from the mixture or some of the reactants did not react in the way expected. The amount of a product obtained is known as the actual yield. Theoretical yield is how much of the product should be made. When the actual yield is compared with the theoretical amount as a percentage, it is called the percentage yield. It is calculated using the formula:

% Yield = (Actual Yield / Theoretical Yield) × 100

Atom Economy

The atom economy is a measure of the amount of reactants that end up as useful products. For sustainable development and for economic reasons it is important to use reactions with high atom economy. Atom economy can be calculated with the equation:

% atom economy = (RFM of desired product / RFM of all reactants) x 100

C4: Chemical Calculations: Chemistry Specification: Worked Examples

Relative Formula Mass

To calculate RFM of a substance you:

1. Identify the different types of atoms.
2. Identify how many of these atoms you have.
3. Identify the atomic mass for each of these atoms.
4. Multiply the atomic mass for each atom by the number of atoms.
5. Add the totals together.

For example: RFM of C_2H_6

C x 2 = 12 x 2 = 24
H x 6 = 1 x 6 = 6

RFM = 30

Percentage Yield

To calculate the percentage yield you:

1. Calculate the RFM of the substances involved.
2. Use this to calculate theoretical yield.
3. Write in the formula % Yield = (Actual Yield / Theoretical Yield) × 100
4. Substitute numbers.
5. Do the working out.
6. Round to appropriate number of s.f and add units.

For example:

Calcium Carbonate → Calcium Oxide + Carbon Dioxide

$CaCO_3 \rightarrow CaO + CO_2$

100kg of calcium carbonate is broken down and 45kg of calcium oxide is made. Calculate the % yield.

Step 1:

RFM of $CaCO_3$ = 100
RFM of CaO = 56

Step 2:

10kg of $CaCO_3$ should make 56kg of CaO

Steps 3 to 6:

% Yield = (Actual Yield / Theoretical Yield) × 100
= (45/ 56) × 100
= 0.8035714286 × 100
= 80.3571428571
= 80%

Moles

To calculate number of moles you:

1. Calculate the RFM of the substance.
2. Write in the formula Number of Moles = Mass / RFM
3. Substitute numbers.
4. Do the working out.
5. Round to appropriate number of s.f and add units

For example: How many moles of hydrochloric acid molecules are there in 8.2g of acid?

RFM of HCl is = 36.5
Number of moles = mass / RFM
=8.2 / 36.5
=0.2246575342
=0.25mol

C4: Chemical Calculations: Chemistry Specification: Worked Examples

Use of amount of substance in relation to volumes of gases

To calculate volume of gas you:

1. Identify if the volume you have been given is in cm^3 or dm^3
2. Write in the formula.
3. Substitute numbers.
4. Do the working out.
5. Round to appropriate number of s.f
6. Add units.

For example: A balloon is filled with $100cm^3$ of helium gas. How many moles of helium is this?

No of moles of gas = volume of gas (cm^3) / $24000cm^3$

= 100/ 24000

=0.004166666667

=0.0042mol

Titrations

For titration calculates you:

1. Identify the number of moles involved in the reaction.
2. Identify the ratio of reacting moles.
3. Convert cm^3 into dm^3 by dividing by 1000
4. Calculate the number of moles in the solution with a known concentration and volume using the formula no of moles = concentration x volume
5. Identify the number of moles for the other reactant using your ratio and number of moles you have already calculated.
6. Calculate the concentration using the rearranged formula: Concentration = no. of moles / volume

For example: $25cm^3$ of KOH is neutralised by $6.25cm^3$ of HCl which has a concentration of $2.00mol/dm^3$. Calculate the concentration of KOH.

$$KOH + HCl \rightarrow KCl + H_2O$$

Step 1: 1 mole of KOH and 1 mole of HCl

Step 2: 1: 1 ratio

Step 3: $25cm^3 = 0.025dm^3$ $6.25cm^3 = 0.00625cm^3$

Step 4: no of moles = concentration x volume

no of moles = 2 x 0.0625

no of moles = 0.0125mol

Step 5: 1: 1 ratio so 0.0125mol of KOH also.

Step 6: Concentration = no. of moles / volume

Concentration = 0.0125/ 0.025

Concentration = $0.5mol/dm^3$

Atom Economy

To calculate the atom economy you:

1. Balance the equation if needed.
2. Calculate the RFM of all the reactants.
3. Calculate the RFM of the desired product.
4. Write in the formula % atom economy = (RFM of desired product / RFM of all reactants) x 100
5. Substitute numbers.
6. Do the working out.
7. Round to appropriate number of s.f
8. Add units

For example:

Iron Oxide + Carbon → Iron + Carbon Dioxide

$$2Fe_2O_3 + 3C \rightarrow 4Fe + 3CO_2$$

Calculate the % atom economy for this process that forms iron.

Steps 1 and 2:

RFM of $2Fe_2O_3$ = 320

RFM of 3C = 36

RFM of 4Fe = 224

Step 3: RFM of all reactants = 320 + 36 = 356

Steps 4 to 8:

% atom economy = (RFM of desired product / RFM of all reactants) x 100

= (224/ 356) x 100

= 0.6292134831 x 100

= 62.9213483146

= 62.9%

Using Concentrations of Solutions

To calculate concentration you:

1. Identify if the volume you have been given is in cm^3 or dm^3
2. Write in the formula.
3. Substitute numbers.
4. Do the working out.
5. Round to appropriate number of s.f
6. Add units.

For example: 25g of sodium chloride is dissolved into $200cm^3$ of water. Calculate the concentration.

Concentration (g/dm^3) = (mass of solute (g) / volume of solution (cm^3)) x 1000

= (25/ 200) x 1000

= 0.125 x 1000

= $125g/dm^3$