4.3 Quantitative chemistry

Chemists use quantitative analysis to determine the formulae of compounds and the equations for reactions. Given this information, analysts can then use quantitative methods to determine the purity of chemical samples and to monitor the yield from chemical reactions.

Chemical reactions can be classified in various ways. Identifying different types of chemical reaction allows chemists to make sense of how different chemicals react together, to establish patterns and to make predictions about the behaviour of other chemicals. Chemical equations provide a means of representing chemical reactions and are a key way for chemists to communicate chemical ideas.

4.3.1 Chemical measurements, conservation of mass and the quantitative interpretation of chemical equations

4.3.1.1 Conservation of mass and balanced chemical equations

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

This means that chemical reactions can be represented by symbol equations which are balanced in terms of the numbers of atoms of each element involved on both sides of the equation.

Students should understand the use of the multipliers in equations in normal script before a formula and in subscript within a formula.

4.3.1.2 Relative formula mass.

The relative formula mass (M_r) of a compound is the sum of the relative atomic masses of the atoms in the numbers shown in the formula.

In a balanced chemical equation, the sum of the relative formula masses of the reactants in the quantities shown equals the sum of the relative formula masses of the products in the quantities shown.

4.3.1.3 Mass changes when a reactant or product is a gas

Some reactions may appear to involve a change in mass but this can usually be explained because a reactant or product is a gas and its mass has not been taken into account. For example: when a metal reacts with oxygen the mass of the oxide produced is greater than the mass of the metal or in thermal decompositions of metal carbonates carbon dioxide is produced and escapes into the atmosphere leaving the metal oxide as the only solid product.

Students should be able to explain any observed changes in mass in non-enclosed systems during a chemical reaction given the balanced symbol equation for the reaction and explain these changes in terms of the particle model.

4.3.1.4 Chemical measurements

Whenever a measurement is made there is always some uncertainty about the result obtained.

Students should be able to:

- represent the distribution of results and make estimations of uncertainty
- use the range of a set of measurements about the mean as a measure of uncertainty.

4.3.2 Use of amount of substance in relation to masses of pure substances

4.3.2.1 Moles (HT only)

Chemical amounts are measured in moles. The symbol for the unit mole is mol.

The mass of one mole of a substance in grams is numerically equal to its relative formula mass.

One mole of a substance contains the same number of the stated particles, atoms, molecules or ions as one mole of any other substance.

The number of atoms, molecules or ions in a mole of a given substance is the Avogadro constant. The value of the Avogadro constant is 6.02×10^{23} per mole.

Students should understand that the measurement of amounts in moles can apply to atoms, molecules, ions, electrons, formulae and equations, for example that in one mole of carbon (C) the number of atoms is the same as the number of molecules in one mole of carbon dioxide (CO₂).

Students should be able to use the relative formula mass of a substance to calculate the number of moles in a given mass of that substance and vice versa.

4.3.2.2 Amounts of substances in equations (HT only)

The masses of reactants and products can be calculated from balanced symbol equations.

Chemical equations can be interpreted in terms of moles. For example:

$$Mg + 2 HCI \rightarrow MgCl_2 + H_2$$

shows that one mole of magnesium reacts with two moles of hydrochloric acid to produce one mole of magnesium chloride and one mole of hydrogen gas.

Students should be able to:

- calculate the masses of substances shown in a balanced symbol equation
- calculate the masses of reactants and products from the balanced symbol equation and the mass of a given reactant or product.

4.3.2.3 Using moles to balance equations (HT only)

The balancing numbers in a symbol equation can be calculated from the masses of reactants and products by converting the masses in grams to amounts in moles and converting the numbers of moles to simple whole number ratios.

Students should be able to balance an equation given the masses of reactants and products.

Students should be able to change the subject of a mathematical equation.

4.3.2.4 Limiting reactants (HT only)

In a chemical reaction involving two reactants, it is common to use an excess of one of the reactants to ensure that all of the other reactant is used. The reactant that is completely used up is called the limiting reactant because it limits the amount of products.

Students should be able to explain the effect of a limiting quantity of a reactant on the amount of products it is possible to obtain in terms of amounts in moles or masses in grams.

4.3.2.5 Concentration of solutions

Many chemical reactions take place in solutions. The concentration of a solution can be measured in mass per given volume of solution, eg grams per dm³ (g/dm³).

Students should be able to:

- calculate the mass of solute in a given volume of solution of known concentration in terms of mass per given volume of solution
- (HT only) explain how the mass of a solute and the volume of a solution is related to the concentration of the solution.

4.3.3 Yield and atom economy of chemical reactions (chemistry only)

4.3.3.1 Percentage yield

Even though no atoms are gained or lost in a chemical reaction, it is not always possible to obtain the calculated amount of a product because:

- the reaction may not go to completion because it is reversible
- some of the product may be lost when it is separated from the reaction mixture
- some of the reactants may react in ways different to the expected reaction.

The amount of a product obtained is known as the yield. When compared with the maximum theoretical amount as a percentage, it is called the percentage yield.

Students should be able to:

- calculate the percentage yield of a product from the actual yield of a reaction
- (HT only) calculate the theoretical mass of a product from a given mass of reactant and the balanced equation for the reaction.

4.3.3.2 Atom economy

The atom economy (atom utilisation) is a measure of the amount of starting materials that end up as useful products. It is important for sustainable development and for economic reasons to use reactions with high atom economy.

The percentage atom economy of a reaction is calculated using the balanced equation for the reaction as follows:

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Relative formula mass of desired product from equation _{Sum\ of\ relative\ formula\ masses\ of\ all\ reactants\ from\ equation} \times 100
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Students should be able to:

- calculate the atom economy of a reaction to form a desired product from the balanced equation
- (HT only) explain why a particular reaction pathway is chosen to produce a specified product given appropriate data such as atom economy (if not calculated), yield, rate, equilibrium position and usefulness of by-products.

4.3.4 Using concentrations of solutions in mol/dm³ (chemistry only) (HT only)

The concentration of a solution can be measured in mol/dm³.

The amount in moles of solute or the mass in grams of solute in a given volume of solution can be calculated from its concentration in mol/dm³.

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.

Students should be able to explain how the concentration of a solution in mol/dm³ is related to the mass of the solute and the volume of the solution.

4.3.5 Use of amount of substance in relation to volumes of gases (chemistry only) (HT only)

Equal amounts in moles of gases occupy the same volume under the same conditions of temperature and pressure.

The volume of one mole of any gas at room temperature and pressure (20°C and 1 atmosphere pressure) is 24 dm³.

The volumes of gaseous reactants and products can be calculated from the balanced equation for the reaction.

Students should be able to:

- calculate the volume of a gas at room temperature and pressure from its mass and relative formula mass
- calculate volumes of gaseous reactants and products from a balanced equation and a given volume of a gaseous reactant or product
- change the subject of a mathematical equation.