OCR A Chemistry A-level

# Module 2.1: Atoms and Reactions

Detailed Notes

2.1.1 Atomic Structure and Isotopes

Fundamental Particles

The model for atomic structure has evolved over time as knowledge and scientific understanding changes.

The current, accepted model of the atom consists of a **small, dense central nucleus** surrounded by **orbiting electrons** in electron **shells**. This was discovered in the Rutherford scattering experiment in 1911.

The nucleus consists of **protons and neutrons** giving it an overall **positive** charge. The mass of the atom is concentrated at the nucleus. In a **neutral** atom, the number of electrons is equal to the number of protons due to the relative charges.
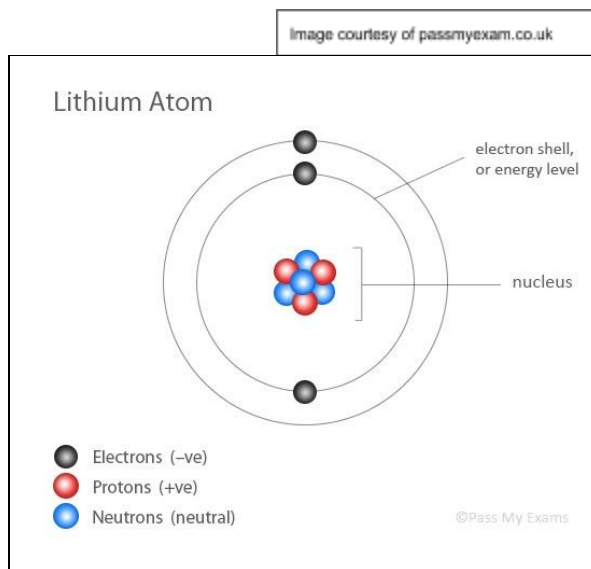
Particle	Proton	Neutron	Electron
Relative Charge	+1	0	-1
Relative Mass	1	1	1/1840

The **maximum** number of **orbiting** electrons that can be held by any single shell, depends on the number of the shell. This can be calculated using $2n^2$ where **n** is the number of the shell.

Example:

Electrons in shell 2 = 2(2^2) = 8 electrons

Each electron shell **must fill** before the next one can hold any electrons.

Atomic Number and Mass Number

Mass number is represented using *A* and can be calculated as the **sum of protons and neutrons** in an atom.

Atomic number is represented using *Z* and is **equal to the number of protons** in an atom. It is often referred to as the **proton number**.

Using these numbers, the quantity of each fundamental particle in an atom can be calculated.

Example: Calculating the number of neutrons in a nitrogen atom

7

N

Nitrogen

14.0

Atomic number = 7
Mass number = 14

Proton number = 7

Neutron number = 14 - 7
= 7

Ions are formed when an atom **loses or gains electrons** meaning it is no longer neutral and will have an **overall charge**. In an ion, the number of electrons is equal to the number of protons minus the ionic charge.

Example: Calculating the number of electrons in a lithium atom and a lithium ion

3

Li

Lithium

6.9
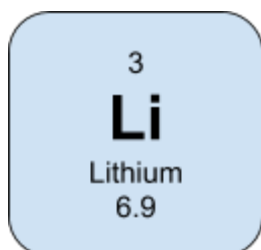
Li = **3 electrons**

Li$^+$ = (3 - 1) electrons = **2 electrons**

Isotopes

Isotopes are atoms of the same element with the **same atomic number**, but with a **different number of neutrons**, resulting in a **different mass number**.

Neutral atoms of isotopes will **react chemically in the same way** as their proton number and electron configuration is the same. The sharing and transfer of electrons is unaffected. However, the different mass numbers means they have **different physical properties**.

Example:

Hydrogen = 1 proton and 1 neutron
Deuterium = 1 proton and 2 neutrons
Tritium = 1 proton and 3 neutrons

Deuterium is used in heavy water (D_2O) to control nuclear processes.

Relative Mass

Relative atomic mass (*Ar*) is defined as:

The weighted mean mass of an atom of an element, relative to one twelfth of the mean mass of an atom of the carbon-12 isotope.

Relative atomic mass takes the **relative abundances** of the different **isotopes** of an element into account:

$$Ar = \frac{\text{mean mass of an atom of an element}}{1/12 \times \text{mean mass of C-12 isotope}}$$

Relative isotopic mass is defined as:

The isotopic mass of an isotope relative to one twelfth of the mean mass of an atom of the carbon-12 isotope.

Relative molecular mass (*Mr*) is defined as:

The weighted mean mass of a molecule of a compound, relative to one twelfth of the mean mass of an atom of the carbon-12 isotope.

Relative molecular mass can be calculated for a molecule by adding together the separate Ar values of the component elements.

Example:

$$Mr \text{ of } H_2O = \frac{\begin{array}{c} 2 \times 1.0 \\ 1 \times 16.0 \end{array}}{18.0}$$

Relative formula mass is similar to Mr but is used for compounds with giant structures.

Mass Spectrometry

Mass spectrometry is used to identify different isotopes and find the overall relative atomic mass of an element. Ions are very useful in the **analytical technique** of **mass spectrometry**.

Time of Flight (TOF) mass spectrometry records the time it takes for ions of each isotope to reach a detector. Using this, **spectra** can be produced showing **each isotope present**. The signals reflect the abundances of the isotopes present.

From a spectra, the *Ar* **can be calculated** by multiplying each **m/z** value by its **abundance** and adding each of these together, before dividing by the total abundance of all species present:
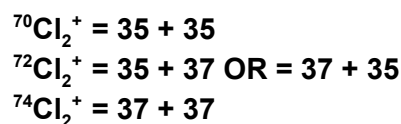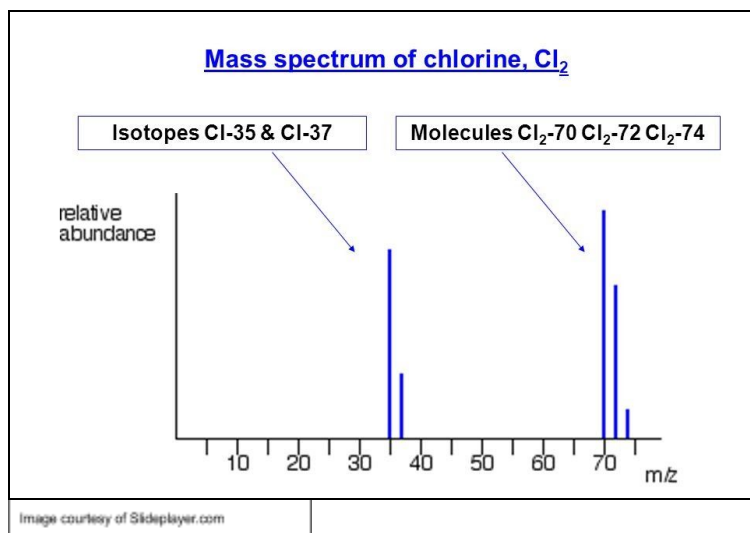
$$Ar = \frac{\text{Sum of (m/z x abundance)}}{\text{Total abundance}}$$

Using this calculated Ar, the element can be identified by referring to the Periodic Table.

Chlorine Spectra

Spectra produced by the mass spectrometry of chlorine display a **characteristic pattern** in a **3:1 ratio for Cl$^+$ ions** and a **9:6:1 ratio for Cl$_2$$^+$ ions**. This is because one isotope is more common than the other and the chlorine molecule can form in different combinations. There is a **chlorine-35** isotope and a **chlorine-37** isotope which both have different abundances:

Example:

Mass spectrum of chlorine, Cl$_2$

Isotopes Cl-35 & Cl-37

Molecules Cl$_2$-70 Cl$_2$-72 Cl$_2$-74

relative abundance

10 20 30 40 50 60 70 m/z

Image courtesy of Slideplayer.com

^{70}Cl$_2$$^+$ = 35 + 35
^{72}Cl$_2$$^+$ = 35 + 37 OR = 37 + 35
^{74}Cl$_2$$^+$ = 37 + 37

2.1.2 Compounds, Formulae and Equations

Formulae and Equations

Ionic bonding occurs between a **metal and a nonmetal**. Electrons are **transferred** from the metal to the non-metal to achieve full outer shells.

When the electrons are transferred, it creates **charged particles** called **ions**.

Binary compounds contain only 2 elements. To name these:
- Put the metal first.
- Change the ending of the second element to -ide.
- The ionic lattice should be neutral, so the charges must balance.

Example:

Calcium chloride contains calcium Ca^{2+} ions and chloride Cl^- ions.
To balance charges, 2 x Cl^- are needed for every Ca^{2+}.
So, the ionic formula is $CaCl_2$.

A **polyatomic** ion contains more than one atom. There are some key polyatomic ions that you should be aware of:

NO_3^- = nitrate ion
SO_4^{2-} = sulfate ion
CO_3^{2-} = carbonate ion
OH^- = hydroxide ion
NH_4^+ = ammonium ion

It is also possible to predict an element's ionic charge from its position in the **periodic table**:

- Group 1 metals lose an electron to **form 1+ ions.**
- Group 2 metals lose two electrons to **form 2+ ions.**
- Group 7 elements need to gain an electron to form a **1- ion.**
  Group 7 elements are known as the **halogens** and their negative ions are known as **halide ions**.

Chemical Equations

All chemical equations **must** be balanced. There should be the same total number of atoms of each element on each side of the equation. The charges must balance too.
Remember that **state symbols** should also be included for reactions.

2.1.3 Amount of Substance

The Mole

Amount of substance defines the number of particles in a substance. It is measured in **moles**.

The mole is a **unit of measurement** for substances. It always contains the **same number of particles**.

$$N_A = 6.02 \times 10^{23} \text{ particles}$$

This number is the **Avogadro Constant** (N_A) and is the number of particles per mole. It allows the number of particles present in a sample of a substance with known mass to be found:

$$\text{Number of particles} = n \times N_A$$

(n = moles)   (N_A = Avogadro constant)

The mole is a **very important unit of measurement** in many calculations:

$$\text{Moles} = \frac{\text{mass}}{Mr} = \frac{\text{concentration} \times \text{volume}}{1000}$$

(where concentration is in mol dm^{-3} and volume is in cm^3)

Molar mass is the mass per mole and has units g mol^{-1}.

Molar gas volume is the gas volume per mole and has units dm^3 mol^{-1}.

Definition of Formulae

Empirical formula is the simplest whole number ratio of atoms of each element present in a compound.

The empirical formula can be found by using the composition by mass or percentage composition by mass and the relative atomic masses of the elements present.

Molecular formula is the number and type of atoms of each element in a molecule. It is the true number of each atom in the molecule.

The molecular formula can be determined using the Mr of the empirical formula and the true Mr of the molecule. This gives a multiplier value which can be used to scale up the empirical formula.

$$\frac{\text{Mr of molecule}}{\text{empirical Mr}} = \text{multiplier}$$

Water of crystallisation is water that is part of the crystalline structure. The molecules are stoichiometrically chemically bonded into the crystal structure.

An **anhydrous** substance contains no water of crystallisation.

A **hydrated** substance contains water of crystallisation.

The formula of a hydrated salt can be calculated from experimental results or from a given percentage or mass composition.

Equations and Calculations

Chemical equations must be **balanced** before they can be used in calculations. This is because the **reacting ratios** must be correct. It can be useful to also include **state symbols** so it is clear what might be observed during the reaction, for example, bubbles of gas or a precipitate forming.

These balanced equations can then be used to calculate **reacting masses**, **percentage yield** and **atom economy**.

Concentration can be expressed in g dm⁻³ or mol dm⁻³. A 1 mol dm⁻³ solution contains 1 mol of solute dissolved in every 1 dm⁻³ of solution.

A **standard solution** is a solution of known concentration. This can be prepared by dissolving a known mass of solid in solvent and making it up to an exact volume.

The **limiting reagent** in a reaction is the reactant that is not in excess. It will be used up first, causing the reaction to stop. In calculations, you must use the moles of the limiting reagent along with the stoichiometric ratios of reactant to product to calculate the moles of product formed.

The Ideal Gas Equation

When under **standard conditions**, gases and volatile liquids follow certain trends:

Pressure is proportional to Temperature
Volume is proportional to Temperature
Pressure and Volume are inversely proportional

These relationships can be combined to give the **ideal gas equation**:

$$pV = nRT = \frac{mRT}{Mr}$$

In order to use this equation, the variables must be in the correct **standard units**:

p = pressure in Pascals, Pa

V = volume in m³

T = temperature in Kelvin, K

n = moles, mol

m = mass in grams, g

R is the **ideal gas constant**, equal to **8.31 JK⁻¹mol⁻¹**.

Percentage Yields and Atom Economy

Percentage Yield

$$\% \text{ yield} = \frac{\text{Experimental mass} \times 100}{\text{Theoretical mass}}$$

Experiments usually have a percentage yield **less than 100%**. This could be due to the reaction being **incomplete**, **loss** of products on equipment, or unwanted **side reactions**.

Atom Economy

$$\% \text{ atom economy} = \frac{\text{Mr of desired product} \times 100}{\text{Mr of reactants}}$$

In industrial chemical processes, it is desirable to have a **high atom economy** for a reaction. This means there is **little or no waste product**, only the desired product. Therefore, it means the process is more **economically viable** for industrial scale manufacture. It also helps to **preserve raw materials**.

Experimental techniques
Use a **digital mass balance** to measure mass. It is important to use a balance with a suitable **resolution** for your experiment.

Use a **measuring cylinder** to measure the volume of a solution. If you are making up a standard solution, you should use a **volumetric flask** of the required volume.

Use a **gas syringe** to measure the volume of gas produced in an experiment. Alternatively, measure the mass lost on a balance and use this value to calculate the moles of gas produced during the reaction.

2.1.4 Acids

Acids, Bases, Alkalis and Neutralisation

An **acid** releases H^+ ions in aqueous solution.

An **alkali** releases OH^- ions in aqueous solution. An alkali is a water-soluble base.

Common acids:

HCl - hydrochloric acid
H₂SO₄ - sulfuric acid
HNO₃ - nitric acid
CH₃COOH - ethanoic acid
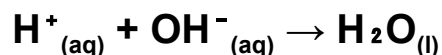
Common bases:

NaOH - sodium hydroxide
KOH - potassium hydroxide
NH₃ - ammonia

A **strong** acid fully dissociates in aqueous solution.

A **weak** acid partially dissociates in aqueous solution.

Neutralisation is the reaction of an acid with a base. In aqueous solution the ionic equation for the reaction is:

$$H^+_{(aq)} + OH^-_{(aq)} \rightarrow H_2O_{(l)}$$

Reactions with bases also form a **salt**:

acid + carbonate → salt + water + carbon dioxide
acid + metal oxide → salt + water

Acid-Base Titrations

A titration is a practical method where a **standard solution** of known concentration is reacted with a solution of **unknown concentration** in order to determine the concentration of this solution. For this, there is a standard method to make up the standard solution and carry out the titration.

Standard Solution - simple method

1. Weigh the sample bottle containing the solid on a (2 dp) balance.

2. Transfer solid to beaker and reweigh sample bottle.

3. Record the difference in mass.

4. Add distilled water and stir with a glass rod until all the solid has dissolved.

5. Transfer to a volumetric flask with washings.

6. Make up to the 250 cm^3 mark with distilled water.

7. Shake flask.

Common errors in this method include **systematic errors** on the balance, **lost substance** in transfer and **overfilling** of the volumetric flask. These can be reduced using **washing** methods and by reading volumes from the **bottom of the meniscus**.

Titration - simple method

1. Fill the burette with the standard solution of known concentration, ensuring the jet space in the burette is filled and doesn't contain air bubbles.

2. Use a pipette filler and pipette to transfer 25 cm^3 of the solution with unknown concentration into a conical flask.

3. Add two to three drops of indicator.

4. Record the initial burette reading.

5. Titrate the contents of the conical flask by adding the solution to it from the burette until the indicator undergoes a definite, permanent colour change.

6. Record the final burette reading and calculate the titre volume.

7. Repeat until at least two concordant results are obtained (within 0.1 cm^3 of each other).

The equipment used in a titration all comes with their own **uncertainty values**. These must be combined to find the overall uncertainty in the final answer.

The best way of reducing uncertainties in a titration is to **increase the titre volume needed** for the reaction. This can be done by increasing the volume and concentration of the substance in the conical flask or by decreasing the concentration of the substance in the burette.

It is also important to carry out a **risk assessment** before undertaking any practical work. This should analyse the **equipment,** the **lab environment** and the **chemicals** being used, and suggest methods for **reducing the risk** and what should be done if an accident occurs.

Diagram - Titration setup
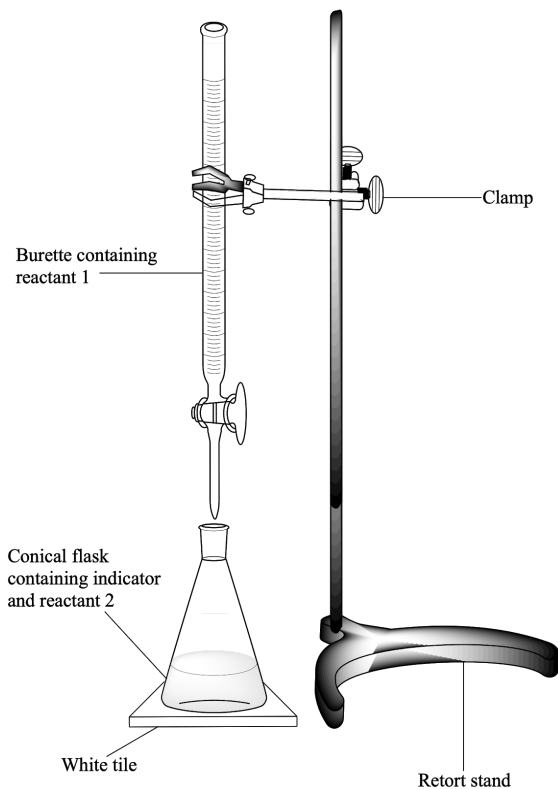
2.1.5 Redox

Oxidation Number

Oxidation number gives the **oxidation state** of an element or ionic substance. Allocation of oxidation number to a species follows a number of rules:

- Oxidation number of an **element is zero**.
- Oxidation numbers in a **neutral** compound add up to **zero**.
- Oxidation numbers in a charged compound add up to **the total charge**.
- **Hydrogen** has an oxidation number of **+1**.
- **Oxygen** has an oxidation number of **-2**.
- All **halogens** have an oxidation number of **-1**.
- **Group 1** metals have an oxidation number of **+1**.
- In **metal hydrides**, the oxidation number of hydrogen is **-1**.
- In **peroxides**, the oxidation number of oxygen is **-1**.

These rules can be used to work out the oxidation number of species or elements in a reaction.

Example:
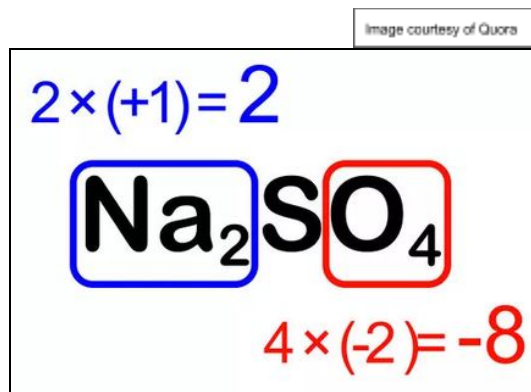
This compound is neutral, so the oxidation numbers must total zero. Therefore, using the rules above, the oxidation number of sulfur can be found.

$$2 - 8 + x = 0$$
$$-6 + x = 0$$
$$x = 6$$

Roman numerals are used to indicate the magnitude of an oxidation number. For example, iron has two common oxidation states, iron(II) and iron(III).

Redox Reactions

Oxidation involves the **loss of electrons. Reduction** involves the **gain of electrons.**

Oxidation results in the oxidation number becoming more **positive** whereas **reduction** results in the oxidation number becoming more **negative**.

Oxidation and reduction occur **simultaneously** in a reaction because one species loses electrons which are then donated and gained by the other species. Therefore, they are known as **redox** reactions (reduction - oxidation).

This redox rule is remembered using the acronym **OILRIG** (oxidation is loss, reduction is gain).

Oxidising and Reducing Agents

An oxidising agent **accepts electrons** from the species that is being oxidised. Therefore, it **gains electrons** and is **reduced**. This is seen as a **reduction** in oxidation number for the oxidising agent (gets less positive).

A reducing agent **donates electrons** to the species being reduced. Therefore, it **loses electrons** and is **oxidised**. This is seen as an **increase** in oxidation number for the reducing agent (gets more positive).

Disproportionation Reactions

In a **disproportionation reaction**, a species is both oxidised and reduced, seen as both an increase and a decrease in oxidation number for that species.
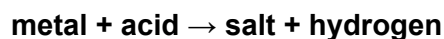
An example is seen when chlorine reacts with cold water to produce **chlorate(I) ions (ClO⁻)** and **chloride ions**. The oxidation state goes from zero to both **+1 and -1**.

Example:

$$Cl_2 + H_2O \longrightarrow ClO^- + Cl^- + 2H^+$$
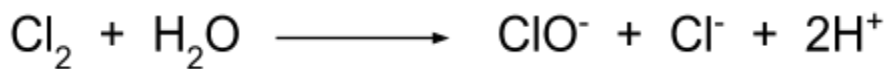
Redox Reactions with Metals

Metals react with **acids** to form **salts** in MASH reactions:

metal + acid → salt + hydrogen

You should use known oxidation numbers of species to work out the change in oxidation number for the metal.