

# AQA Chemistry A-Level

## 3.1.1: Atomic Structure

### Detailed Notes





### 3.1.1.1 - Fundamental Particles

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

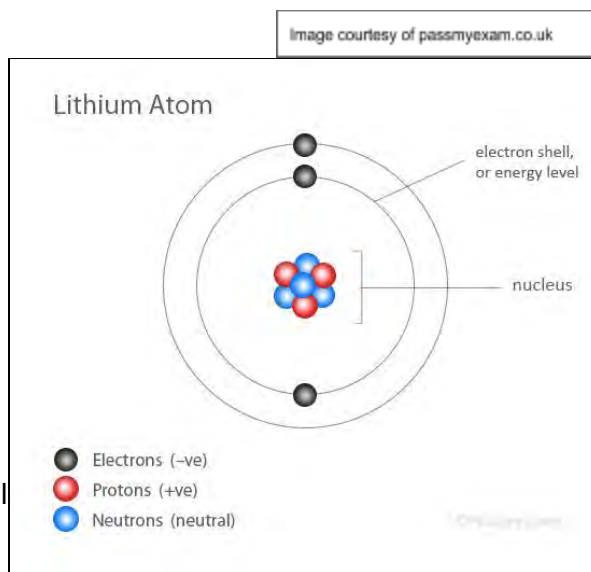
#### Plum Pudding Model

It was initially thought that atoms consisted of a **sphere of positive charge**, with small **negative charges distributed evenly** within it.

#### Electron Shell Model

It is now known that 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. It contains almost the entire **mass** of the atom. 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:

$$\text{Electrons in shell 2} = 2(2^2) = 8 \text{ electrons}$$

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





### 3.1.1.2 - Mass Number and Isotopes

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.

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

*Example:*

7
<b>N</b>
Nitrogen
14.007

Image courtesy of thegreenchalkboard.com

**Atomic number = 7**

**Mass number = 14**

**Proton number = 7**

**Neutron number = 14 - 7  
= 7**

**Relative atomic mass ( $A_r$ )** is defined as:

**The mean mass of an atom of an element, divided by one twelfth of the mean mass of an atom of the carbon-12 isotope.**

This takes the **relative abundances** of the different **isotopes** of an element into account.

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

### 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 number 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

## Ions

Ions are formed when an atom **loses or gains electrons** meaning it is no longer neutral and will have an **overall charge**.

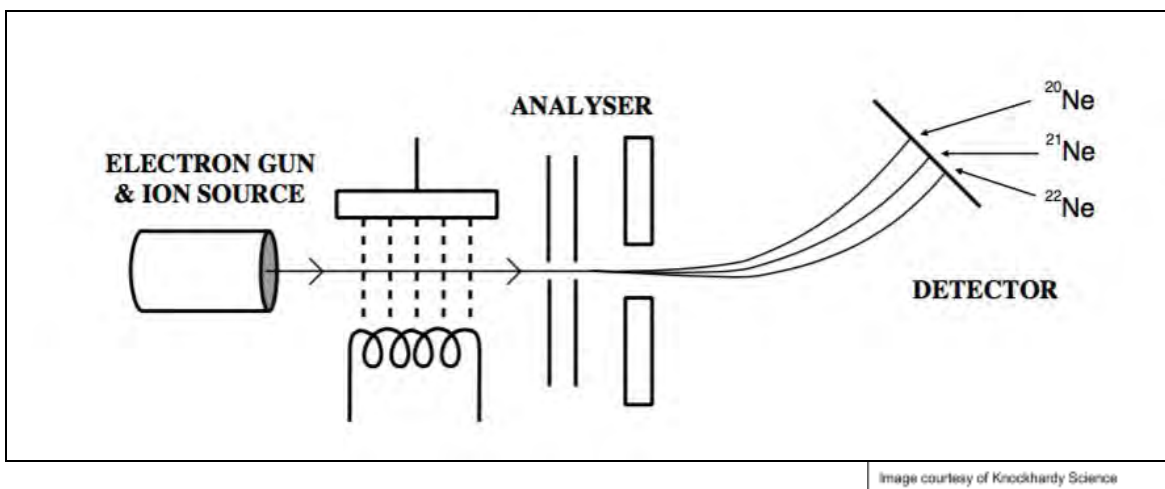
## Mass Spectrometry

This is an **analytical technique** used to identify different isotopes and find the overall relative atomic mass of an element.

### Time of Flight (TOF) Mass Spectrometry

This form of 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**.

1. **Ionisation** - A sample of an element is **vapourised** and injected into the mass spectrometer where a **high voltage** is passed over the chamber. This causes electrons to be removed from the atoms (it is ionised) leaving **+1 charged ions** in the chamber.
2. **Acceleration** - These positively charged ions are then **accelerated** towards a negatively charged **detection plate**.
3. **Ion Drift** - The ions are then deflected by a **magnetic field** into a **curved path**. The radius of their path is dependant on the charge and mass of the ion.

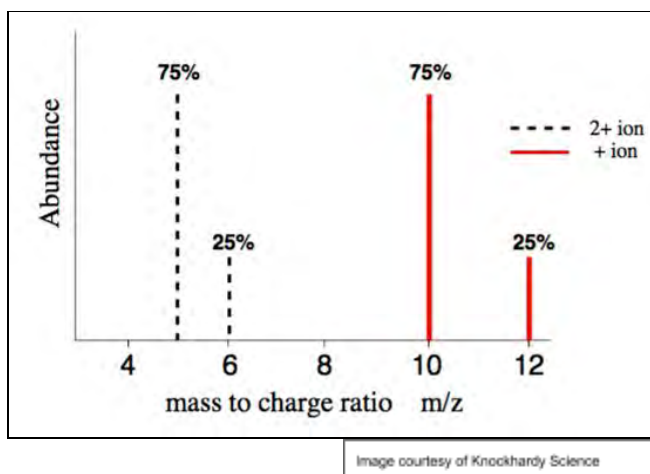




4. **Detection** - When the positive ions hit the negatively charged detection plate, they **gain an electron** producing a **flow of charge**. The greater the abundance, the greater the current produced.
5. **Analysis** - These current values are then used in combination with the **flight times** to produce a **spectra print-out** with the relative abundance of each isotope displayed.

During the ionisation process, a **2+ charged ion** may be produced. This means it will be affected more by the magnetic field producing a curved path of **smaller radius**. As a result, its mass to charge ratio ( $m/z$ ) is halved and this can be seen on spectra as a trace at **half the expected  $m/z$  value**.

*Example:*



Using this spectra, the  **$A_r$  can be calculated:**

$$A_r = \frac{m/z \times \text{abundance}}{\text{Total abundance}}$$

*Example:*

$$A_r = \frac{(10 \times 75) + (12 \times 25)}{(75 + 25)} = 10.5$$

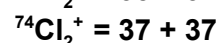
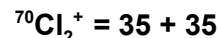
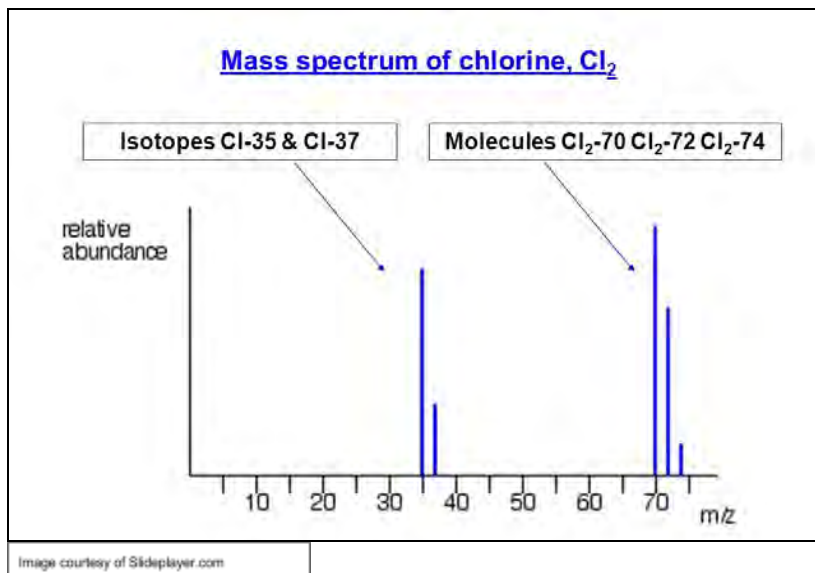




## Chlorine Spectra

Spectra produced by the mass spectrometry of chlorine display a **characteristic pattern** in a **3:1 ratio for  $\text{Cl}^+$  ions** and a **3:6:9 ratio for  $\text{Cl}_2^+$  ions**. This is because one isotope is more common than the other and the chlorine molecule can form in different combinations.

Example:



### 3.1.1.3 - Electron Configuration

#### Electron Orbitals

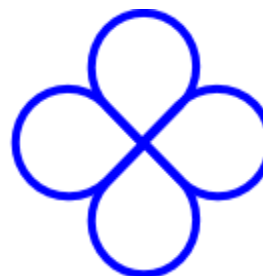
Electrons are held in **clouds of negative charge** called **orbitals**. There are different types of orbital; **s**, **p**, **d** and **f**. Each one has a different shape:



s-orbital  
(spherical)



p-orbital  
(dumbbell)

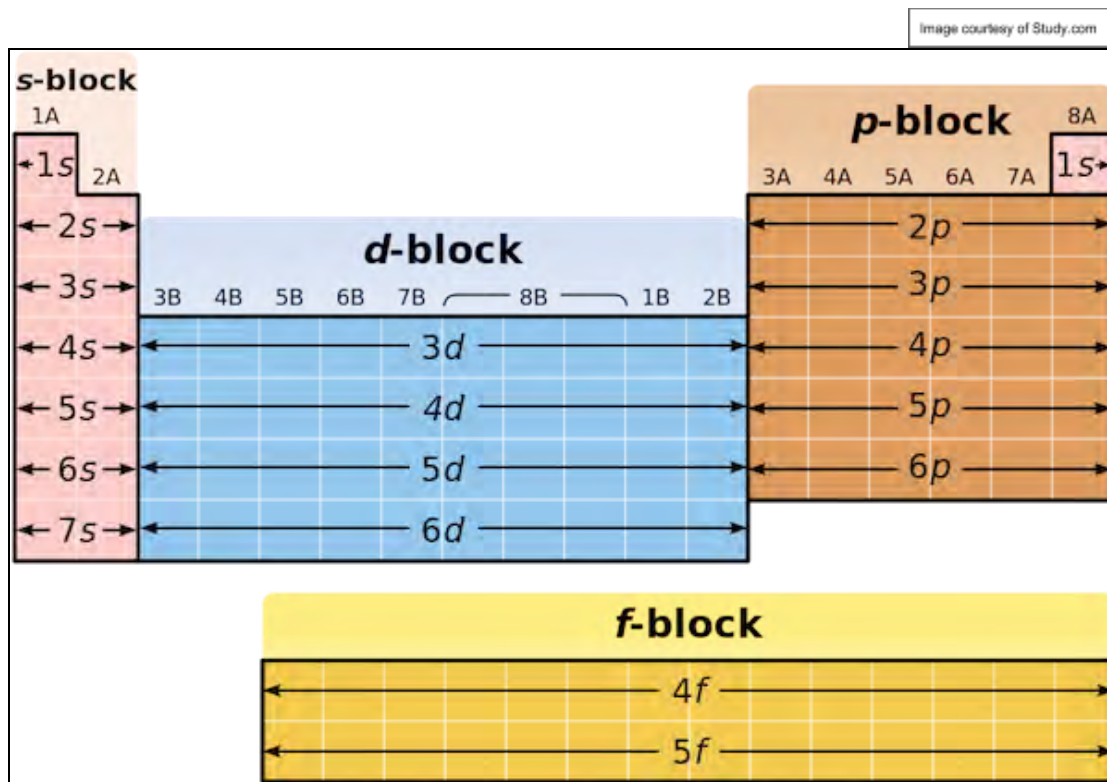


d-orbital





These orbitals correspond with **blocks** on the Periodic Table. Each element in the block has **outer electrons in that orbital**.



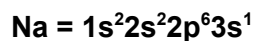
Each orbital can hold a different number of electrons before the next one is filled:

- s-orbital = 2 electrons**
- p-orbital = 6 electrons**
- d-orbital = 10 electrons**

The **energy** of the orbitals **increases from s to d** meaning the orbitals are **filled in this order**. Each orbital is filled before the next one is used to hold electrons.

*Example:*

**Sodium has 11 electrons. These would be written in the following configuration:**



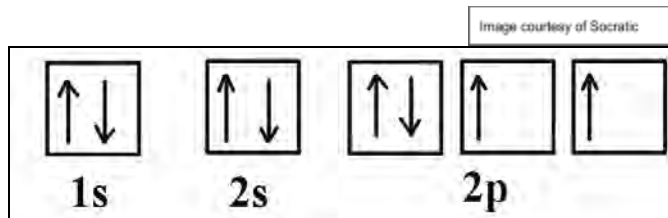
**It has 3 energy levels and 4 orbitals holding the 11 electrons.**



## Spin

Within an orbital, electrons **pair up with opposite spin** so that the atom is as **stable** as possible. Electrons in the **same orbital must have opposite spin**. Spin is represented by **arrows**.

*Example:*



Overall there are **three rules** for writing out electron configurations:

1. The lowest energy orbital is filled first.
2. Electrons with the same spin fill up an orbital first before pairing begins.
3. No single orbital holds more than 2 electrons.

The following table (courtesy of Ellesmere Chemistry) shows the electron configuration and orbital diagrams for Period 2 elements:

**Electron Configurations of Several Lighter Elements**

Element	Total Electrons	Orbital Diagram				Electron Configuration
		1s	2s	2p	3s	
Li	3	$\uparrow\downarrow$	$\uparrow$	$\square \square \square$	$\square$	$1s^2 2s^1$
Be	4	$\uparrow\downarrow$	$\uparrow\downarrow$	$\square \square \square$	$\square$	$1s^2 2s^2$
B	5	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow \square \square$	$\square$	$1s^2 2s^2 2p^1$
C	6	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow \uparrow \square$	$\square$	$1s^2 2s^2 2p^2$
N	7	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow \uparrow \uparrow$	$\square$	$1s^2 2s^2 2p^3$
NE	10	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	$\square$	$1s^2 2s^2 2p^6$
Na	11	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	$\uparrow$	$1s^2 2s^2 2p^6 3s^1$







## Exceptions to the Rules

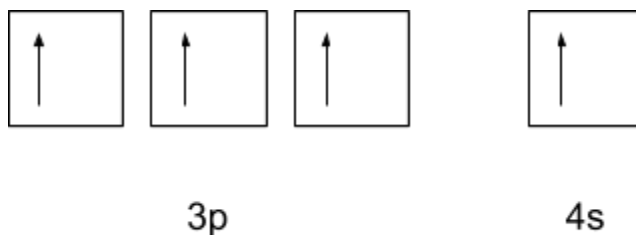
If electron spins are **unpaired** and therefore **unbalanced**, it produces a **natural repulsion** between the electrons making the atom very **unstable**. If this is the case, the electrons may take on a **different arrangement** to improve stability.

*Example:*

The  $3p^4$  orbital contains a single pair of electron with opposite spin making it unstable:



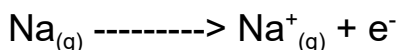
Therefore the electron configuration changes to become  $3p^3 4s^1$  which is a much more stable arrangement:



## Ionisation Energy

Ionisation energy is defined as:

**the minimum energy required to remove one mole of electrons from one mole of atoms in a gaseous state. It is measured in  $\text{kJmol}^{-1}$ .**



**Successive ionisation energies** occur when further electrons are removed. This usually requires **more energy** because as electrons are removed the **electrostatic force of attraction** between the positive nucleus and the negative outer electron **increases**. More energy is therefore needed to **overcome this attraction** so ionisation energy increases.

First ionisation energy follows **trends** within the Periodic Table.

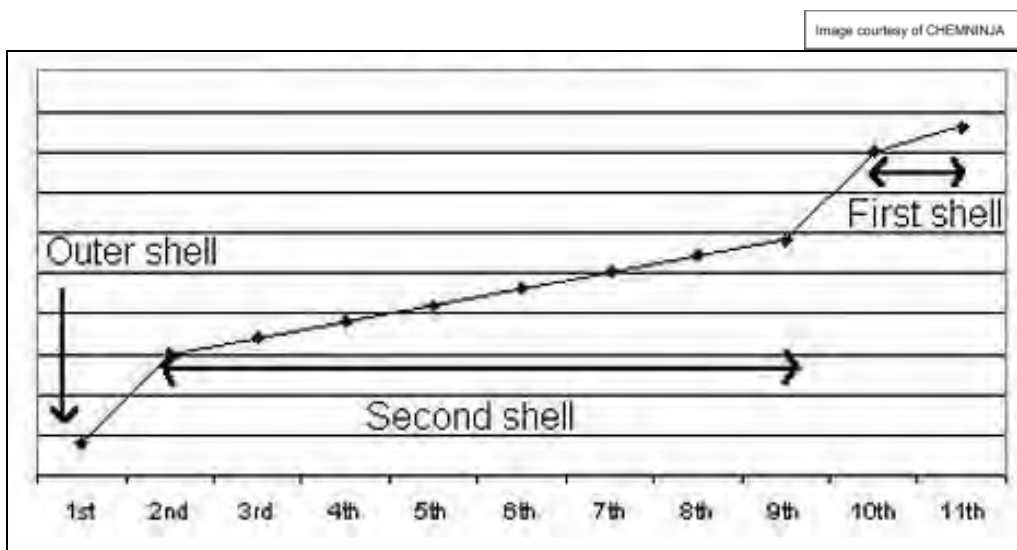
**Along a Period** - first ionisation energy **increases** due to a **decreasing atomic radius** and greater electrostatic **forces of attraction**.

**Down a Group** - first ionisation energy **decreases** due to an **increasing atomic radius** and **shielding** which reduces the effect of the electrostatic forces of attraction.





When successive ionisation energies are plotted on a graph, a **sudden large increase** indicates a **change in energy level**. This is because the electron is being removed from an orbital **closer to the nucleus** so **more energy is required** to do so.



This large energy increase provides **supporting evidence for the atomic orbital theory**.

The first ionisation energy of **aluminium** is **lower than expected** due to a single pair of electrons with **opposite spin**. As a result there is a **natural repulsion** which reduced the amount of energy needed to be put in to remove the outer electron.

