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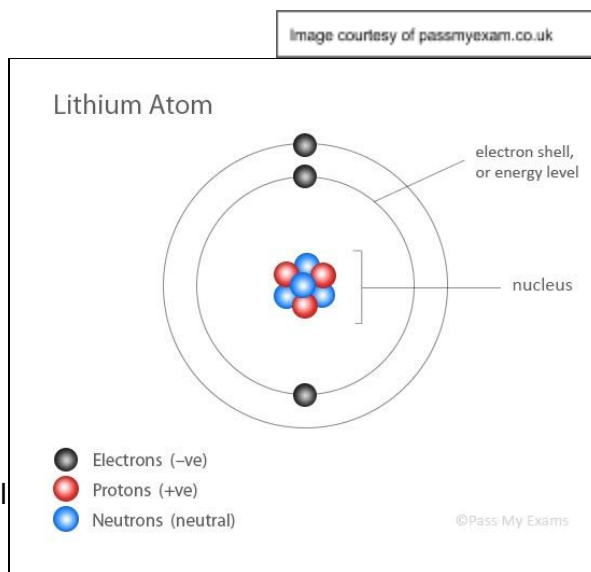
Plum Pudding Model
It was initially thought that atoms consisted of a **sphere of positive charge**, with small **negative** charges **distributed evenly** within it.

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.

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Lithium Atom

electron shell, or energy level

nucleus

Electrons (–ve)
Protons (+ve)
Neutrons (neutral)

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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
N
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 (*Ar*) 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.

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

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 0 neutrons**
Deuterium	**= 1 proton and 1 neutrons**
Tritium	**= 1 proton and 2 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 dependent on the charge and mass of the ion.

Image courtesy of Knockhardy Science
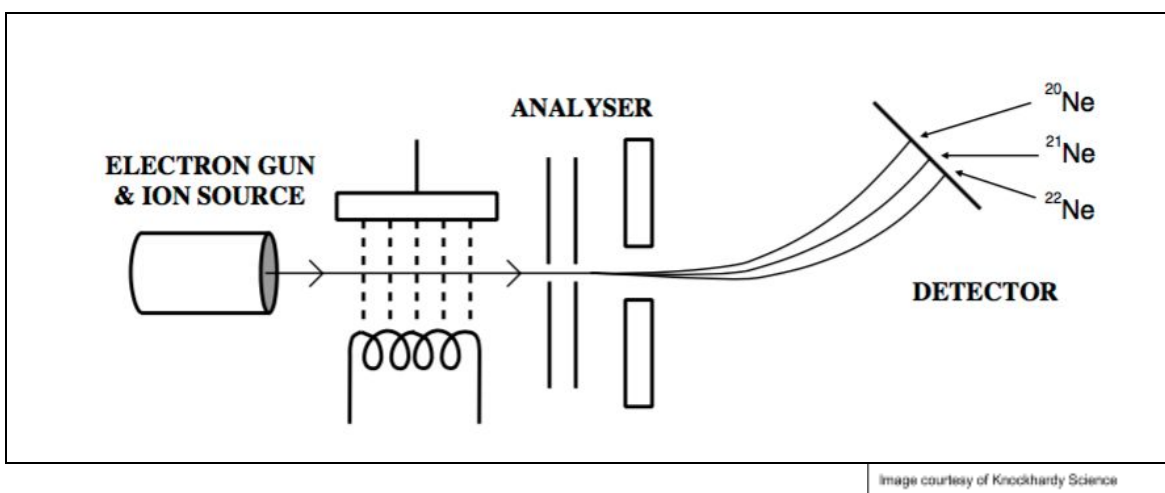
4. **Detection** - When the positive ions hit the negatively charged detection plate, they **gain an electron** producing a **flow of charge**. The greater the abundance, the greater the current produced.

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:

Image courtesy of Knockhardy Science
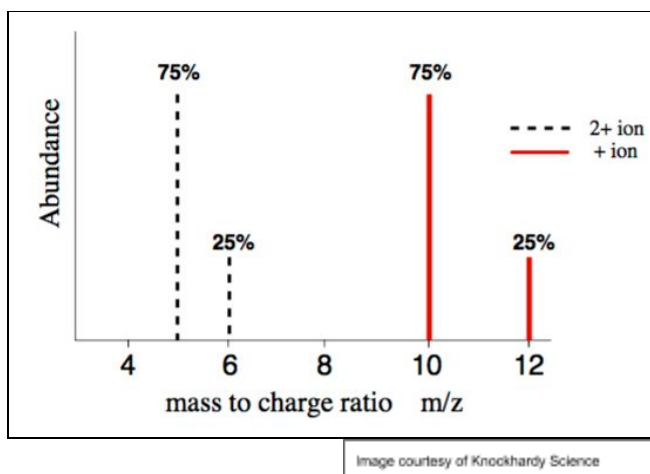
Using this spectra, the *Ar* **can be calculated**:

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

Example:

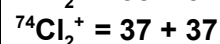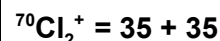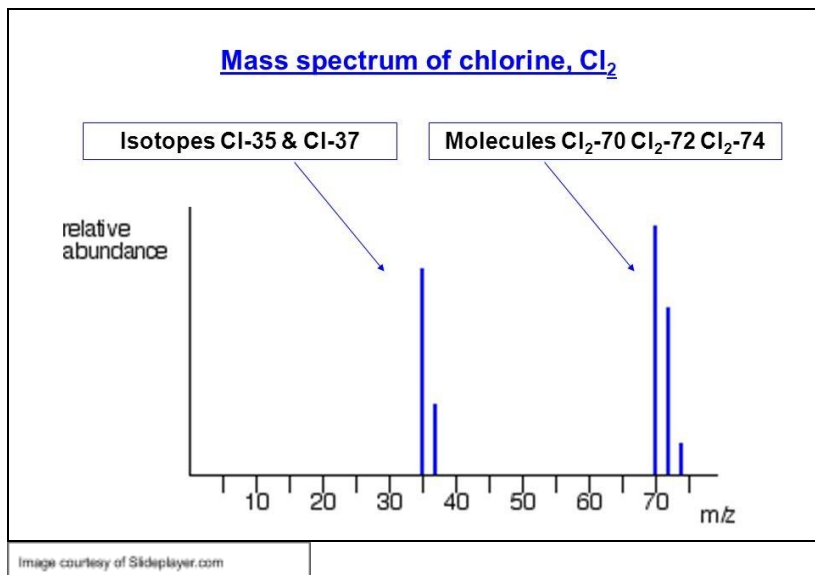**Ar = $\frac{(10 \times 75) + (12 \times 25)}{(75 + 25)}$ = 10.5**

Chlorine Spectra

Spectra produced by the mass spectrometry of chlorine display a **characteristic pattern** in a **3:1 ratio for Cl$^+$ ions** and a **3:6:9 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.

Example:

Mass spectrum of chlorine, Cl$_2$

Isotopes Cl-35 & Cl-37

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

relative abundance

$$10 \quad 20 \quad 30 \quad 40 \quad 50 \quad 60 \quad 70$$
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
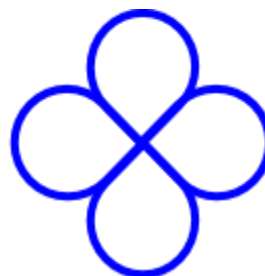
3.1.1.3 - Electron Configuration

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:
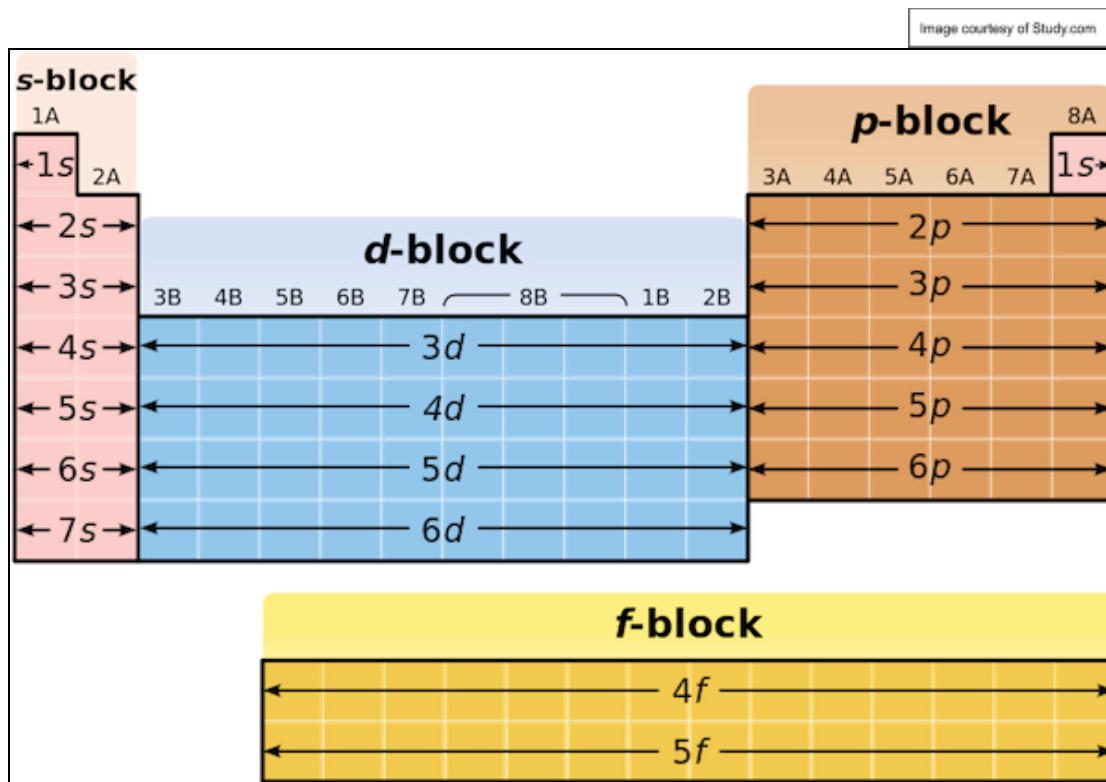
s-orbital
(spherical)

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**.


Image courtesy of Study.com

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:

Na = $1s^2 2s^2 2p^6 3s^1$
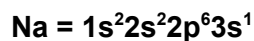
It has 3 energy levels and 4 orbitals holding the 11 electrons.
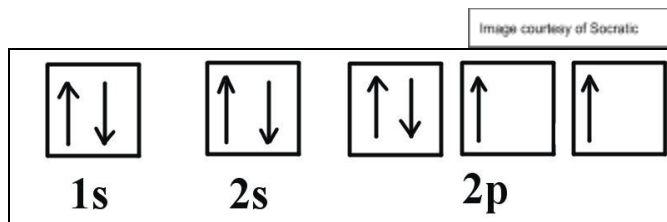
Spin

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	Obital Diagram					Electron Configuration
		1s	2s	2p		3s	
Li	3	↑↓	↑				$1s^2 2s^1$
Be	4	↑↓	↑↓				$1s^2 2s^2$
B	5	↑↓	↑↓	↑			$1s^2 2s^2 2p^1$
C	6	↑↓	↑↓	↑ ↑			$1s^2 2s^2 2p^2$
N	7	↑↓	↑↓	↑ ↑ ↑			$1s^2 2s^2 2p^3$
NE	10	↑↓	↑↓	↑↓ ↑↓ ↑↓			$1s^2 2s^2 2p^6$
Na	11	↑↓	↑↓	↑↓ ↑↓ ↑↓		↑	$1s^2 2s^2 2p^6 3s^1$

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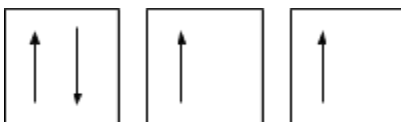
Therefore the electron configuration changes to become 3p^{3}4s^1 which is a much more stable arrangement:
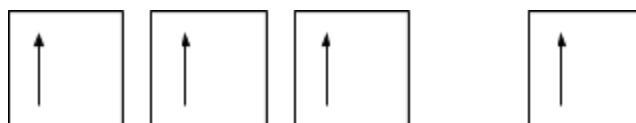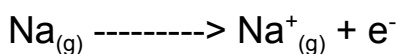

3p   4s

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 kJmol^{-1}.

$$Na_{(g)} \text{---------> } Na^+_{(g)} + e^-$$

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.

Image courtesy of CHEMNINJA
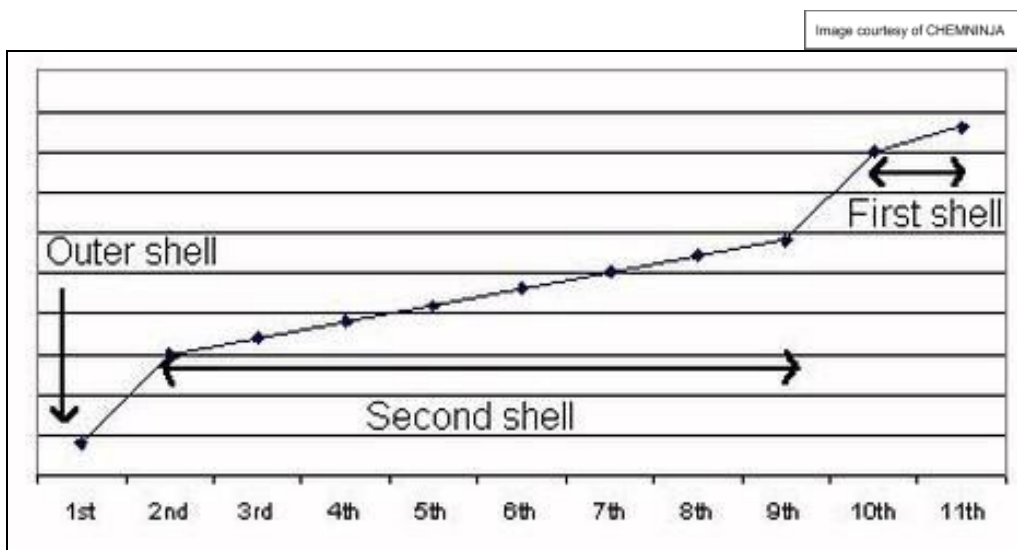
This large energy increase provides **supporting evidence for the atomic orbital theory**.

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 reduces the amount of energy needed to be put in to remove the outer electron.