Edexcel Chemistry A-Level

Topic 1: Atomic Structure and the Periodic Table

Detailed Notes

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. 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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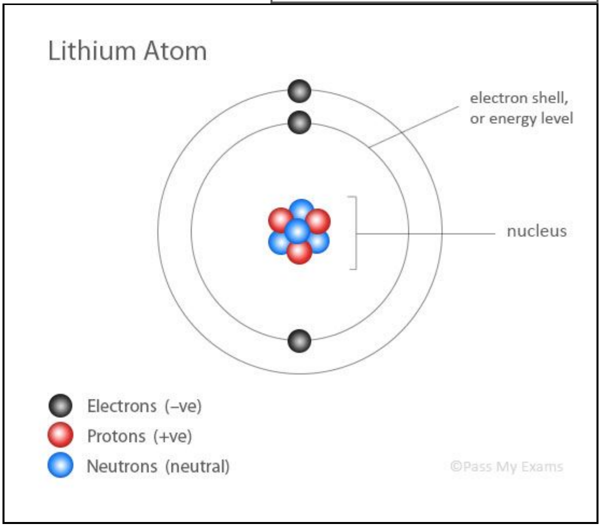


Particle	Proton	Neutron	Electron
Relative Charge	+1	0	-1
Relative Mass	1	1	1/1840

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, hence it can be referred to as proton number.

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

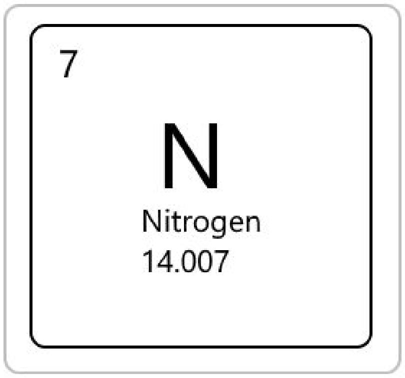


Image courtesy of thegreenchalkboard.com

Atomic number = 7
Mass number = 14

Proton number = 7

Neutron number = 14 - 7
= 7

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

Relative Masses

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

The mean mass of an atom of an element, relative to 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.

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

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

It can be calculated for a molecule by adding together the separate Ar values of the component elements.
Example:

$$\begin{array}{lcl} \text{Mr of } H_2O & = & 2 \times 1.0 \\ & & \underline{1 \times 16.0} \\ & = & 18.0 \end{array}$$

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

Ions and Mass Spectrometry

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

They are very useful in the **analytical technique** of **mass spectrometry**. It is 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.

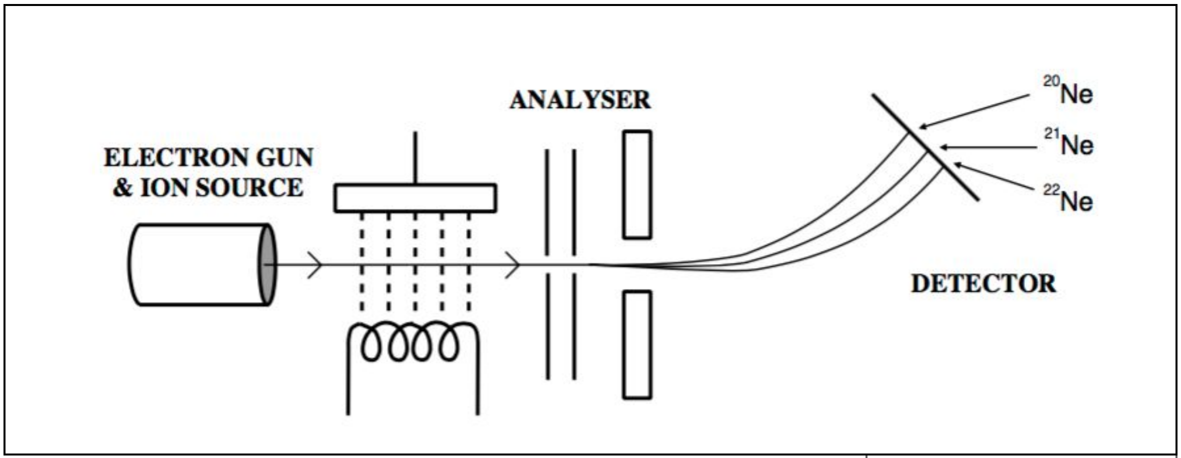


Image courtesy of Knockhardy Science

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:

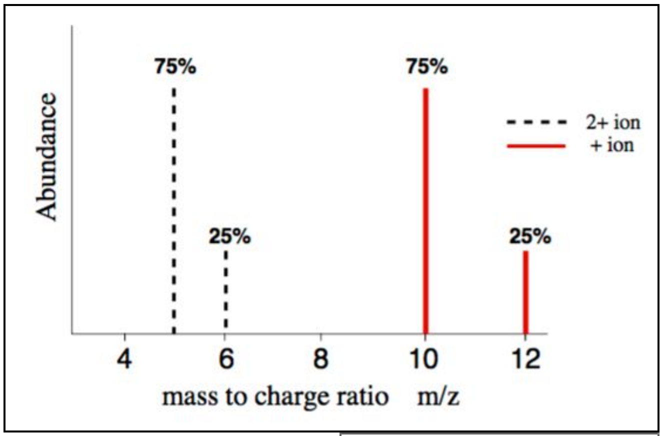


Image courtesy of Knockhardy Science

Using this print-out 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.

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

Example:

From the spectra above.

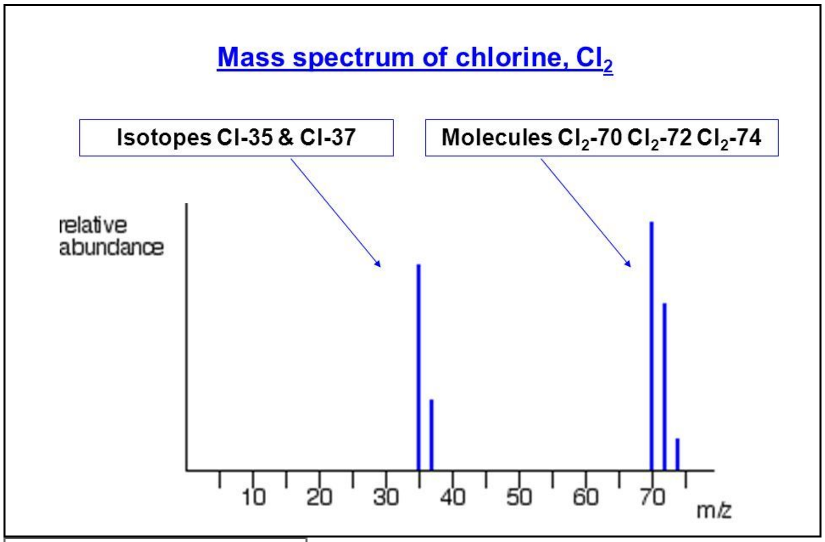
$$\mathbf{Ar} = \frac{(10\times75) + (12\times25)}{(75 + 25)} = 10.5$$

Using this calculated value of 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 **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:



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$^{70}Cl_2^+ = 35 + 35$

$^{72}Cl_2^+ = 35 + 37$ OR $= 37 + 35$

$^{74}Cl_2^+ = 37 + 37$

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}.

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

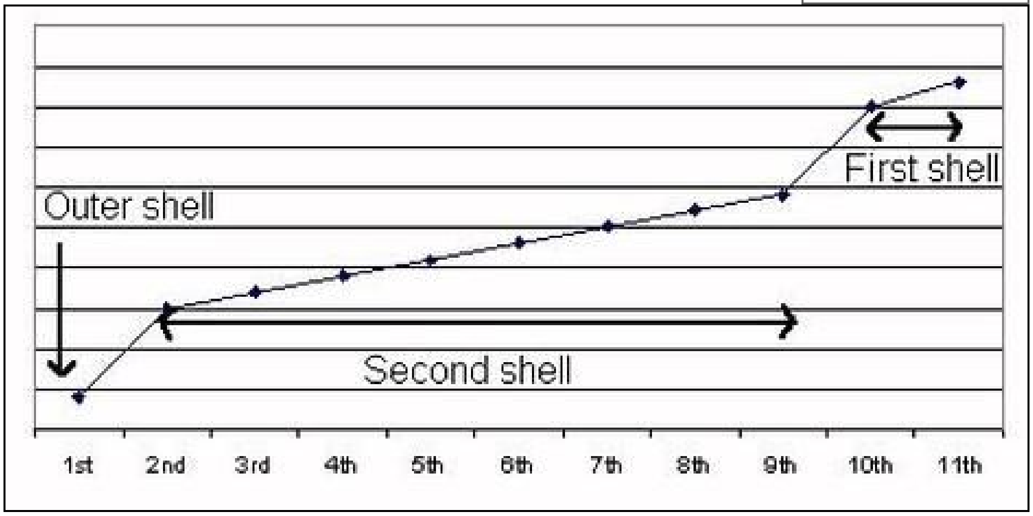
Successive ionisation energies occur when further electrons are removed. This usually requires **more energy** because as electrons are removed, the **electrostatic force of attraction** between the positive nucleus and the negative outer electron **increases**. More energy is therefore needed to **overcome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

First ionisation energy follows **trends** within the Periodic Table as they are influenced by proton-electron forces of attraction and electron shielding.

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 **electron 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.

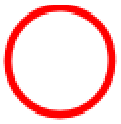
Electron Configurations

Scientific ideas on electronic configurations have **developed over time** as new discoveries are made. The current, accepted model has based on a series evidence:

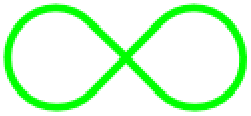
1. **Emission spectra** provide evidence for the existence of **quantum shells**.
2. **Successive ionisation energies** provide evidence for quantum shells within atoms and the suggest the **group** to which the element belongs.
3. **First ionisation energy** of successive elements provides evidence for **electron subshells**.

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 holds two electrons and has a different shape:



s-orbital
(spherical)



p-orbital
(dumbbell)

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

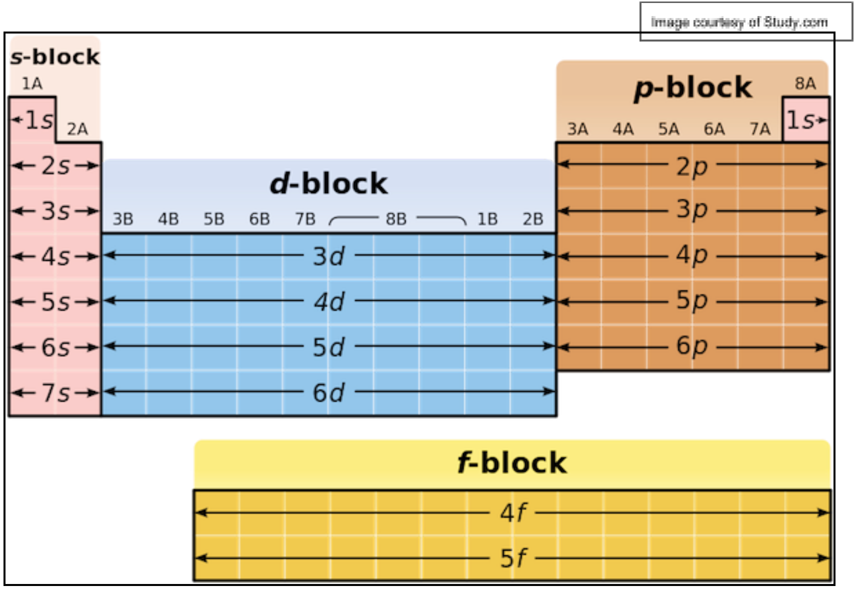


Image courtesy of Study.com

Each subshell has a different number of orbitals and therefore can hold a different number of electrons before the next one is filled:

s-subshell = 2 electrons
p-subshell = 6 electrons
d-subshell = 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 spins**. Spin is represented by opposite **arrows**.
Example:

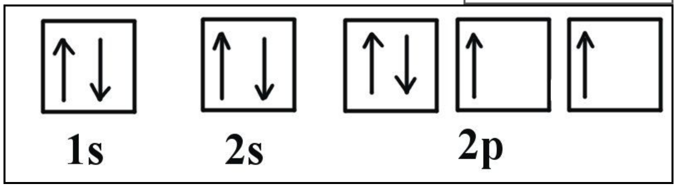


Image courtesy of Socratic

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

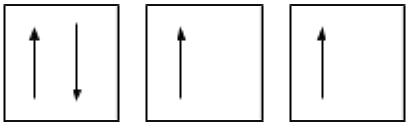
1. The lowest energy orbital is filled first.
2. Electrons with the same spin fill up an orbital first before pairing begins.
3. No single orbital holds more than 2 electrons.

Exceptions to the Rules

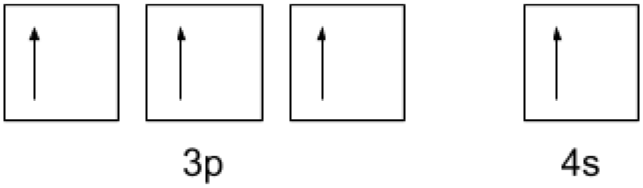
If electron spins are **unpaired** and therefore **unbalanced**, it produces a **natural repulsion** between the electrons making the atom very **unstable**. If this is the case, the electrons may take on a **different arrangement** to improve stability.

Example:

The 3p^4 orbital contains a single pair of electrons with opposite spins making it unstable:



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



Periodicity

Periodicity refers to the study of patterns of physical, atomic and chemical properties within the Periodic Table that repeat regularly.

The Periodic Table arranges the known elements according to **proton number**. All the elements along a **period** have the same number of **electron shells**. All the elements down a **group** have the same number of **outer electrons**, this number is indicated by the group number.

Elements are classified into **blocks** within the Periodic Table that show electron configuration:

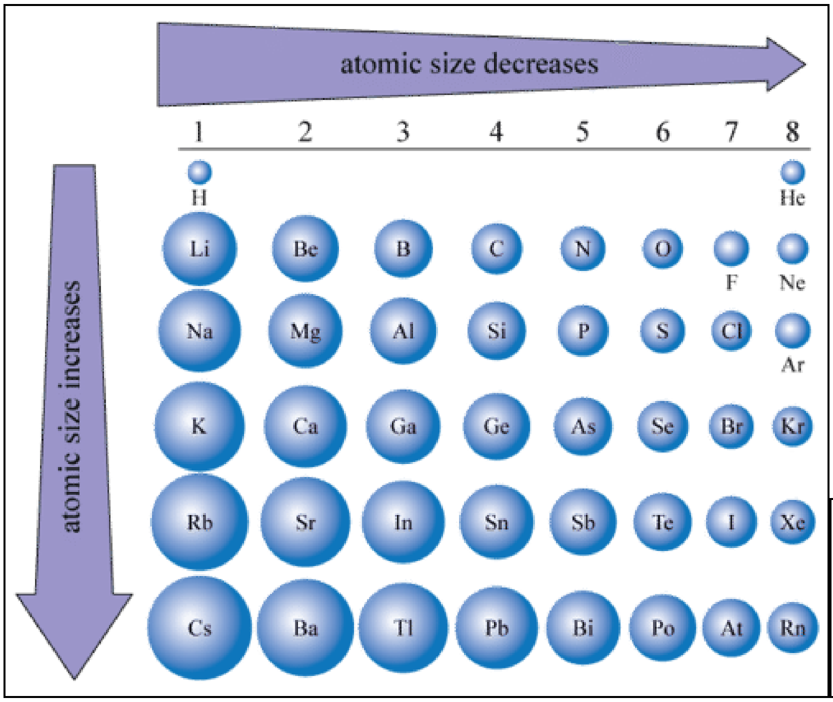
s-block = groups 1 and 2
p-block = groups 3 to 0
d-block = transition metals
f-block = radioactive elements

These different electron configurations are often **linked to other trends** within the Periodic Table. Periodicity is the study of these trends.

Atomic Radius

Along a **period**, atomic radius **decreases**. This is due to an **increased nuclear charge** for the same number of electron shells. The outer electrons are pulled in closer to the nucleus as the increased charge produces a **greater attraction**. As a result, the atomic radius for that element is reduced.

Down a **group**, atomic radius **increases**. With each increment down a group, an electron shell is added each time. This increases the distance between the outer electrons and the nucleus, **reducing the power of attraction**. More shells also increases electron **shielding** where the inner shells create a ‘barrier’ that blocks the attractive forces. Therefore the **nuclear attraction is reduced** further and atomic radius increases.



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Ionisation Energy

Along a **period**, ionisation energy **increases**. The decreasing atomic radius and increasing nuclear charge means that the outer electrons are **held more strongly** and therefore **more energy is required** to remove the outer electron and ionise the atom.

Down a **group**, ionisation energy **decreases**. The **nuclear attraction** between the nucleus and outer electrons reduces and increasing amounts of **shielding** means less energy is required to remove the outer electron.

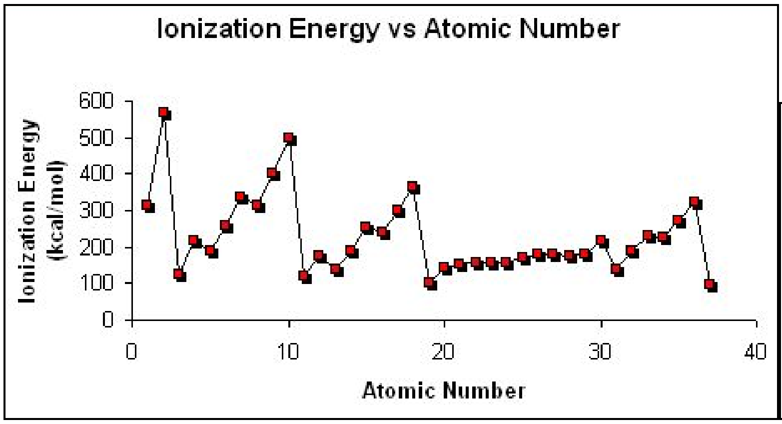


Image courtesy of Science with Mrs Welch

Physical Properties of Period 2

Melting Points

The melting points of the period two elements peaks towards the middle of the period due to the different **bond strength and structures**:

Lithium and Beryllium have **metallic bonding**. Their melting points increase due to greater **positive charged ions** (Li = +1, Be = +2). This also means **more electrons are released** as free electrons in the Beryllium lattice so the attractive electrostatic forces are greater than for Lithium.

Boron and Carbon form giant covalent lattices with **very strong covalent bonds** in up to three dimensions. These covalent bonds require a lot of energy to break giving them very high melting points.

Nitrogen, Oxygen, Fluorine and Neon are all **small**, **simple covalent molecules** held with weak **van der waals** forces. These intermolecular forces don't require much energy to overcome so these molecules have relatively low, similar melting points.

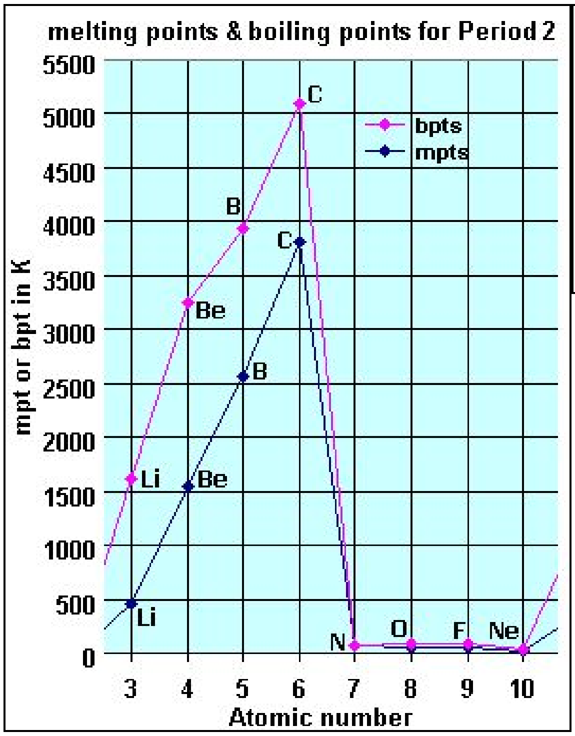
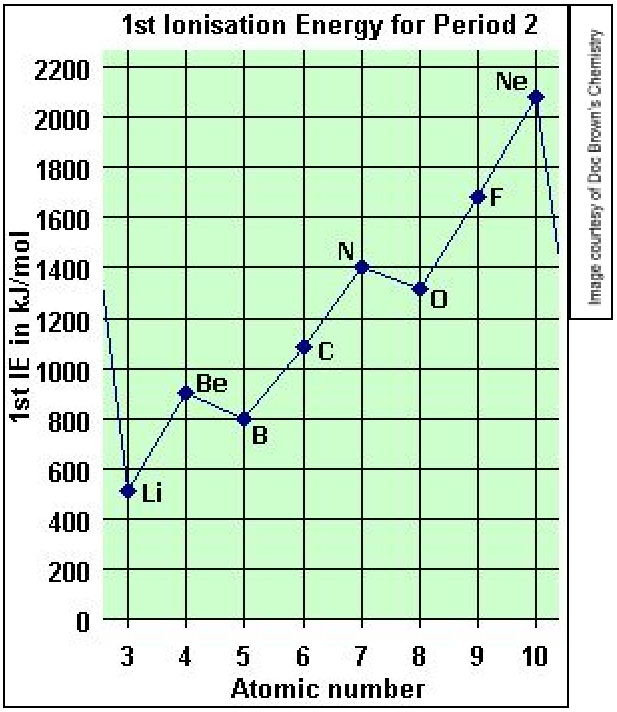


Image courtesy of Doc Brown's Chemistry

Ionisation Energies

First ionisation energies follow a general increasing trend along period 2. This is due to the decreasing atomic radius and increasing nuclear charge so outer electrons are **held more strongly**.

Boron and Oxygen are exceptions to this trend due to the quantum behaviour of the electrons. The electron configurations of these elements contain **unpaired electrons** that require less energy to remove resulting in a **lower first ionisation energy**.



Physical Properties of Period 3

Melting Points

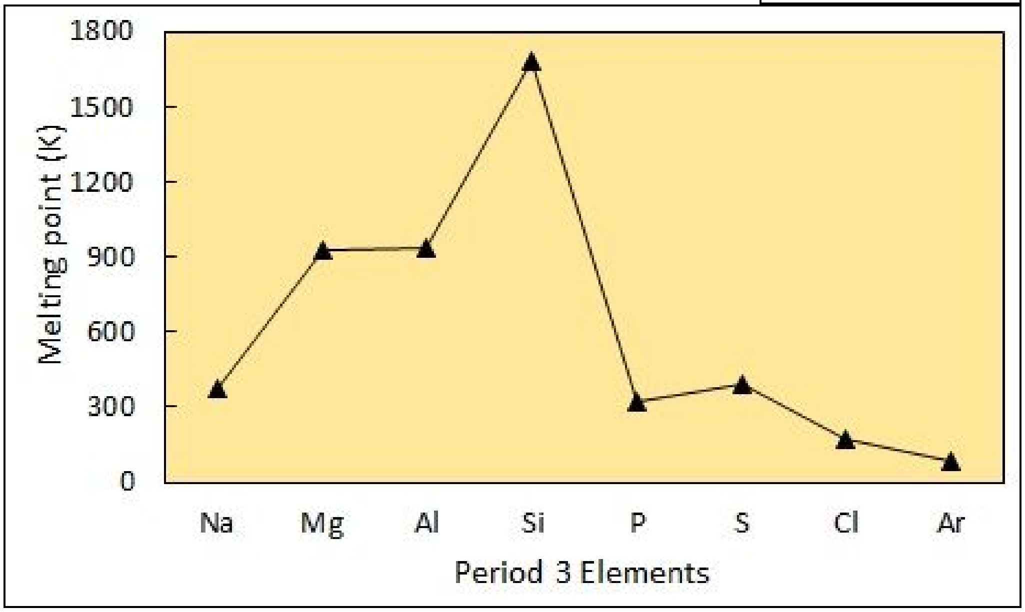
The melting points of the period three elements is linked to the **bond strength and structure**:

Sodium, Magnesium and Aluminium are all metals with **metallic bonding**. Their melting points increase due to greater **positive charged ions** (Na = +1, Mg = +2, Al = +3). This also means **more electrons are released** as free electrons so the attractive electrostatic forces increase from Na to Al.

Silicon is macromolecular meaning it has a **very strong covalent structure**. These covalent bonds require a lot of energy to break giving it a very high melting point.

Phosphorus, Sulphur and Chlorine are all **simple covalent molecules** held with weak **van der waals** forces. These intermolecular forces don't require much energy to overcome so these molecules have relatively low, similar melting points.
Argon is a noble gas that exists as **individual atoms** with a **full outer shell of electrons**. This makes the atom **very stable** and the van der waals forces between them very weak. As a result, the melting point of Argon is very low and it exists as a gas at room temperature.

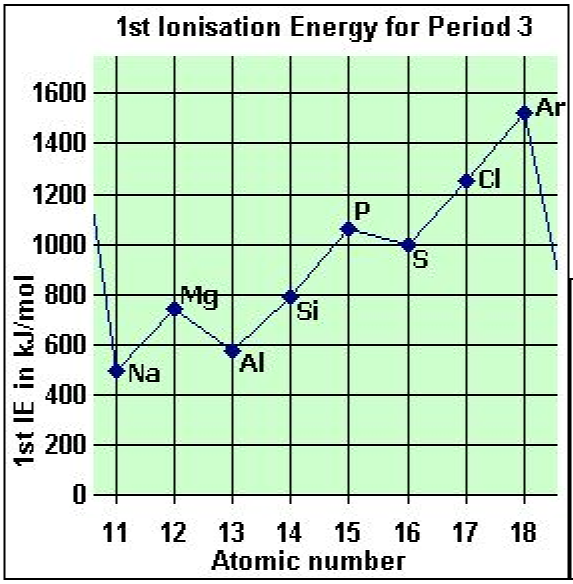
Image courtesy of CapeChemistry



Ionisation Energies

First ionisation energies follow a general increasing trend along period 3. This is due to the decreasing atomic radius and increasing nuclear charge so outer electrons are **held more strongly**.

Aluminium and Sulfur are exceptions to this trend due to the quantum behaviour of the electrons. The electron configurations of these elements contain **unpaired electrons** that require less energy to remove resulting in a **lower first ionisation energy**.



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