Edexcel IAL Chemistry A-Level

Topic 2: Atomic Structure and the Periodic Table

Detailed Notes

Fundamental Particles

The atomic structure model 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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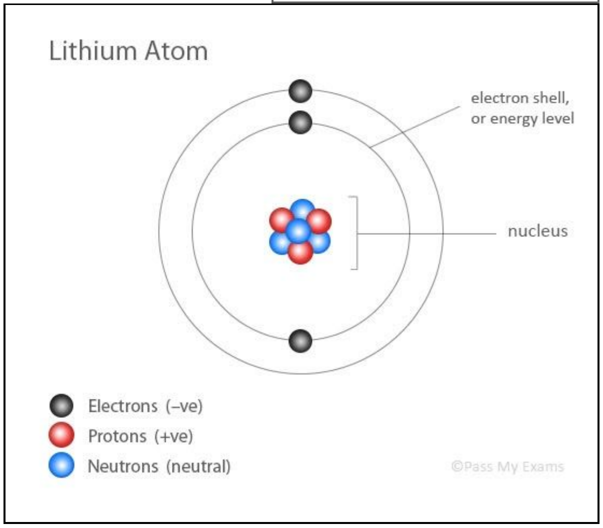


Particle	Proton	Neutron	Electron
Relative Charge	+1	0	-1
Relative Mass	1	1	1/1840

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:

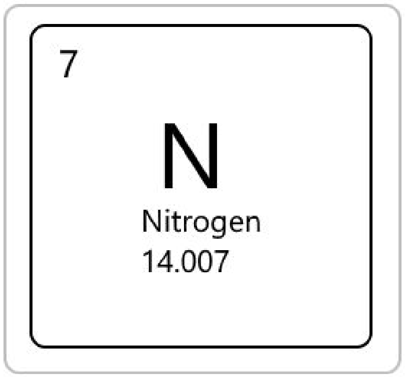


Image courtesy of thegreenchalkboard.com

Atomic number = 7
Mass number = 14

Number of protons = 7
Number of electrons = 7
Number of neutrons = 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** because 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 - the following are all isotopes of hydrogen:

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.

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

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:

$$\begin{aligned} \text{Mr of } H_2O &= 2 \times 1.0 \\ &\quad + 1 \times 16.0 \\ &= 18.0 \end{aligned}$$

Calculating the relative molecular mass can be used to identify the molecules present in a sample.

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 (they are 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 the path is dependent on the charge and mass of the ion.

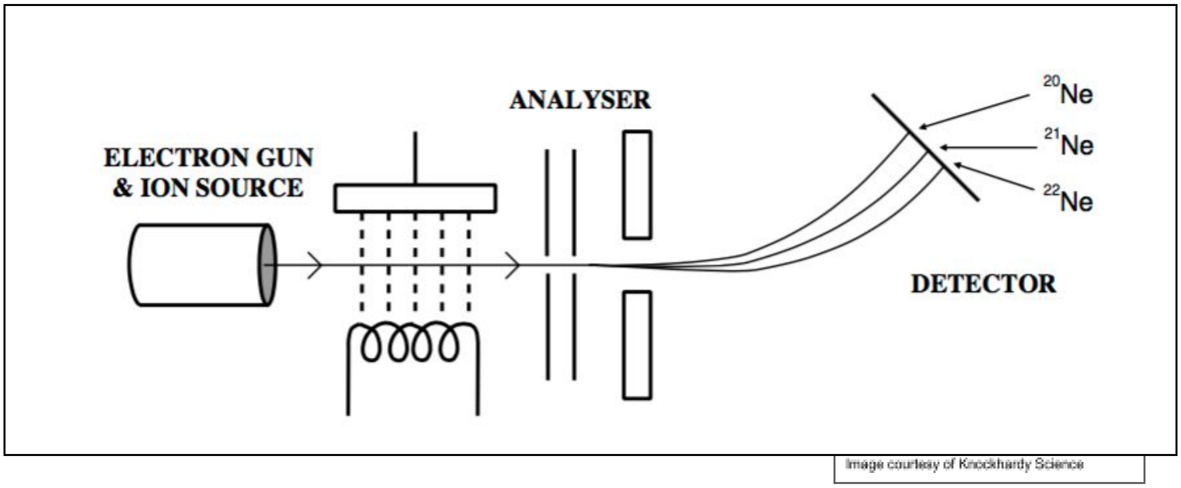


Image courtesy of Knockhardy Science

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

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. This can be seen on spectra as a trace at **half the expected m/z value**.

Example:

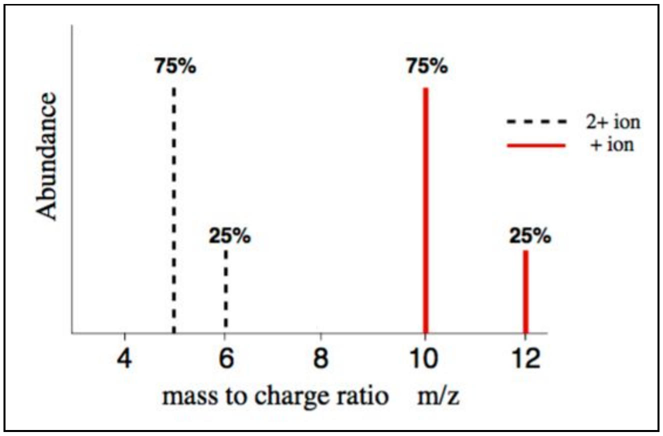


Image courtesy of Knockhardy Science

Using this print-out spectra, the ***Ar*** (relative atomic mass) **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.

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

Example:

From the spectra above,

$$\mathbf{Ar = \frac{(10x75) + (12x25)}{(75 + 25)} = 10.5}$$

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

Predicting Mass Spectra

If you know the **abundances** of an isotope you can generate the mass spectra for its molecules, including **relative peak heights**.

Example:

The relative abundance of ^{35}Cl atoms is 75% and ^{37}Cl atoms is 25%. In other words, for every 100 atoms of chlorine, 25 would be ^{35}Cl and 75 would be ^{37}Cl.

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.

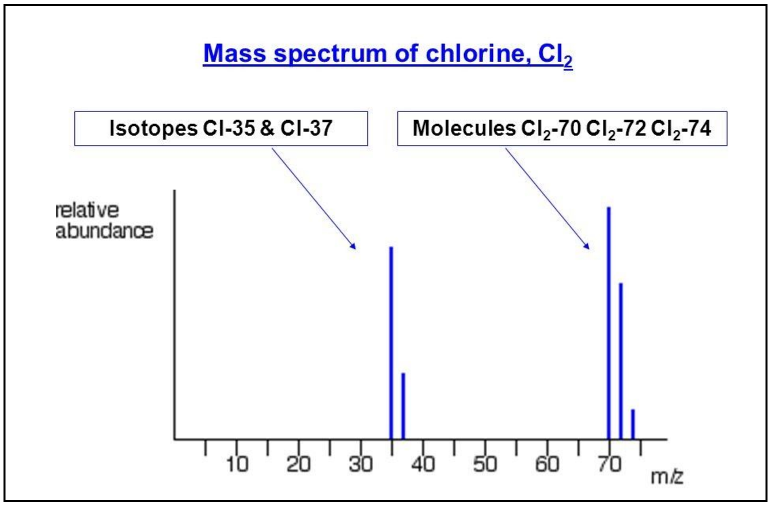


Image courtesy of Slideplayer.com

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

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

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,** causing ionisation energy to increase. All ionisation energies are **endothermic**, as the removal of electrons requires an **energy input.**

The **second ionisation energy** is defined as:

The minimum energy required to remove one mole of electrons from one mole of 1+ ions in a gaseous state. It is measured in kJmol^{-1}.

$$Na^+_{(g)} \rightarrow Na^{2+}_{(g)} + e^-$$

This definition can be used to define **successive ionisation energies.**

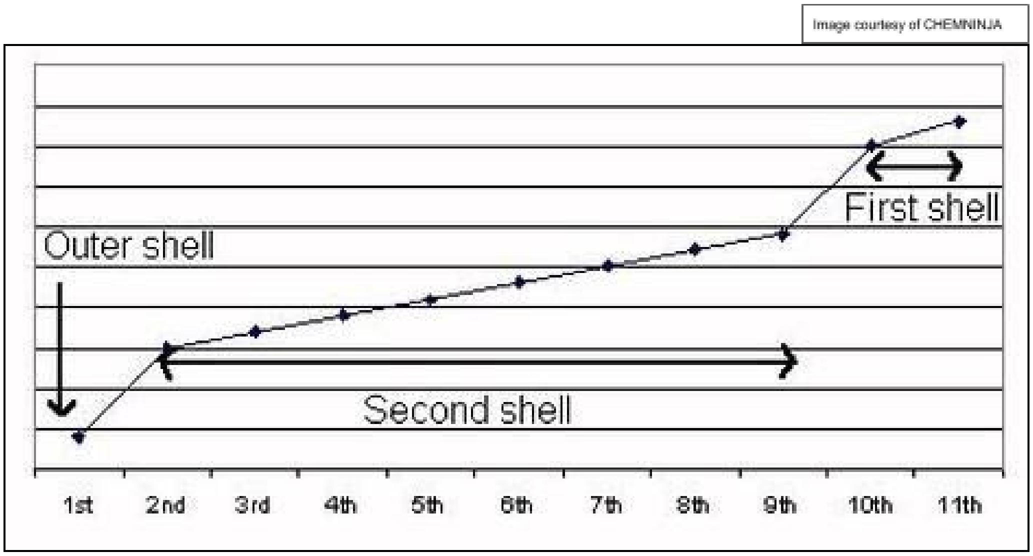
Ionisation energy is influenced by 3 factors:

1. The number of **protons.**
2. The **electron shielding.**
3. The **subshell** from which the electron is removed.

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**. Electrostatic forces of attraction increase since there is an increasing number of protons.

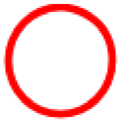
Down a Group - first ionisation energy **decreases** due to an **increasing atomic radius** and **electron shielding** which reduces the effect of the electrostatic forces of attraction. When successive ionisation energies are plotted on a graph, a **sudden large increase** indicates a **change in energy level**. This is because the electron is being removed from an orbital **closer to the nucleus** so **more energy is required** to do so.



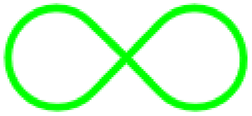
This large energy increase provides **supporting evidence for the atomic orbital theory**. The first ionisation energy of **Aluminium** is **lower than expected** due to a single pair of electrons with **opposite spin**. As a result there is a **natural repulsion** which reduces the amount of energy needed to be put in to remove the outer electron.

Electron Orbitals

Electrons are held in **clouds of negative charge** called **orbitals**. There are different types of orbital; ***s, p, d* and *f*.** Each orbital can hold 0, 1 or 2 electrons. When an orbital holds 2 electrons the electrons must have opposite spins. Orbitals have different shapes:



s-orbital
(spherical)



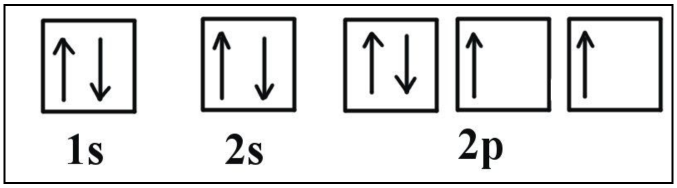
p-orbital
(dumbbell)

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:

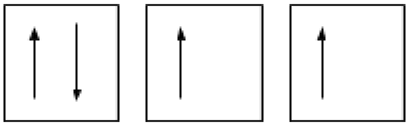
1. The lowest energy orbital is filled first.
2. Electrons with the same spin fill up an orbital first before pairing begins.
3. No single orbital holds more than 2 electrons.

Exceptions to the Rules

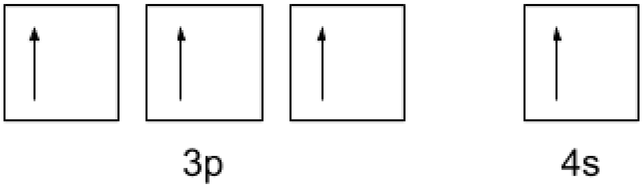
If electron spins are **unpaired** and therefore **unbalanced**, it produces a **natural repulsion** between the electrons making the atom very **unstable**. If this is the case, the electrons may take on a **different arrangement** to improve stability.

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:

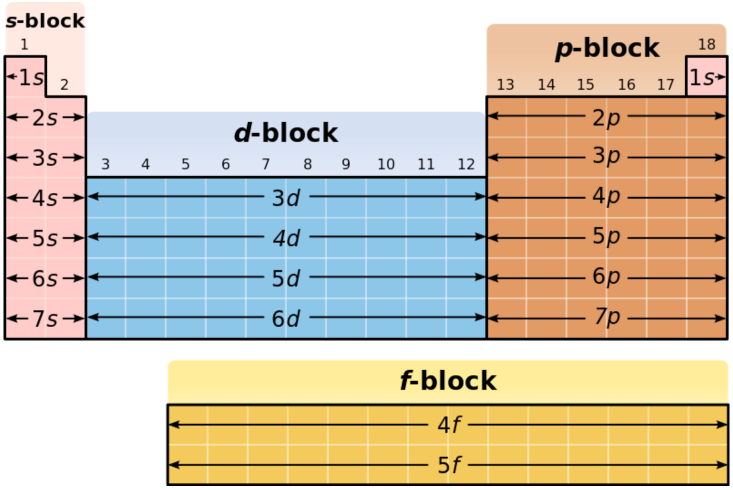


Electron Configurations

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

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

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



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 = $1s^22s^22p^63s^1$
It has 3 energy levels and 4 orbitals holding the 11 electrons.

There are two main **exceptions** to electron configuration. A completely full or half full d sublevel is more stable than a partially filled d sublevel, so an electron from the 4s orbital is excited to the 3d orbital.

Chromium: $1s^22s^22p^63s^23p^63d^54s^1$
Copper: $1s^22s^22p^63s^23p^63d^{10}4s^1$

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.

Periodicity Data

The trends of properties like **melting point, atomic radius** and **ionisation energy** can be represented on a graph. These trends are known as **periodic properties.**

Ionisation energies may be shown on a logarithmic graph, which has a scale where a **one unit** increase represents an increase by a **factor of 10**. For instance, the numbers 10 and 100 would be the same distance apart as the numbers 100 and 1000. This enables you to plot data that has a **large range.**

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.

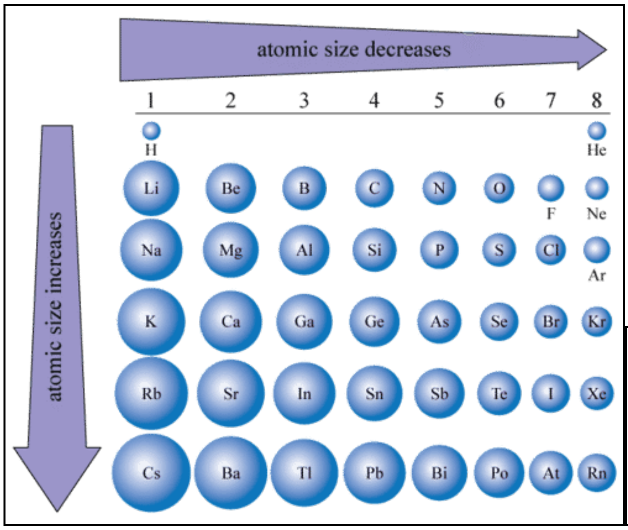


Image courtesy of ck12.org

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 amount of **shielding** means less energy is required to remove the outer electron.

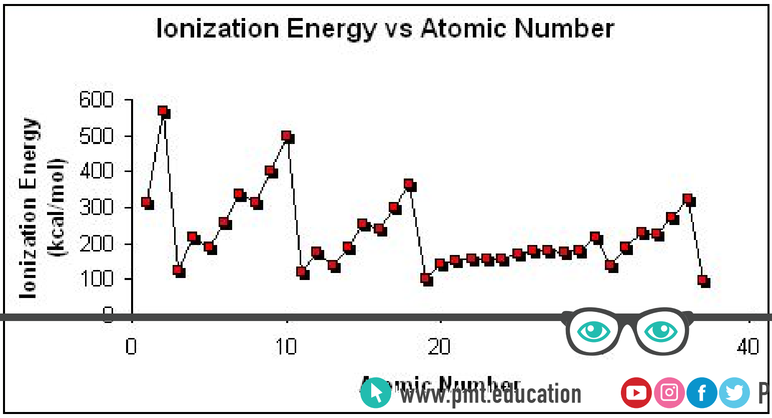


Image courtesy of Science with Mrs Welch

Physical Properties of Period 2

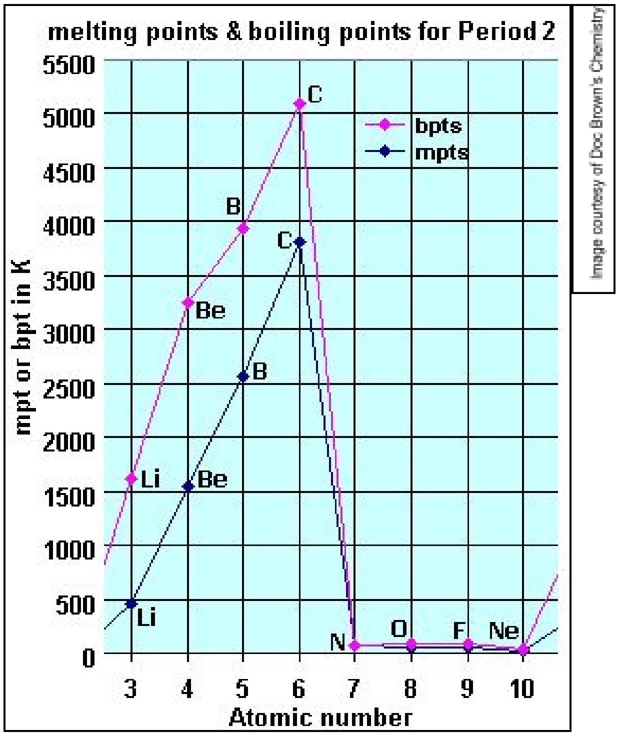
Melting Points

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 **positively 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.

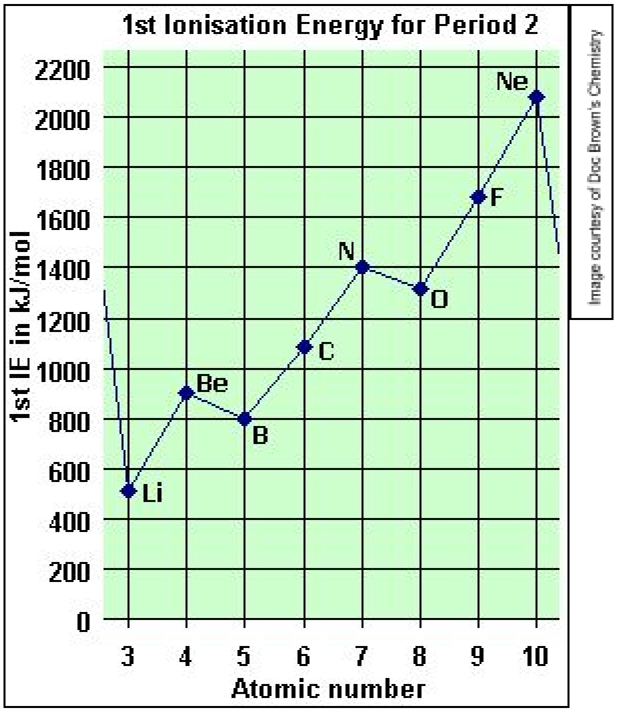
Nitrogen, oxygen, fluorine and neon are all **small**, **simple covalent molecules** held with weak **van der waals** forces. These intermolecular forces don't require much energy to overcome so these molecules have relatively similar, low melting points.



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. Between beryllium and boron, electrons start to be added to a 2p orbital rather than 2s. The 2p orbital has a slightly **higher energy level** than the 2s orbital so this electron is found slightly further from the nucleus. This means it can be removed more easily (less energy required). Between nitrogen and oxygen, electrons start to pair in the 2p orbitals. The paired electrons are both negatively charged so they repel each other. This **repulsion** allows an electron to be removed with less energy than expected.



Physical Properties of Period 3

Melting Points

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

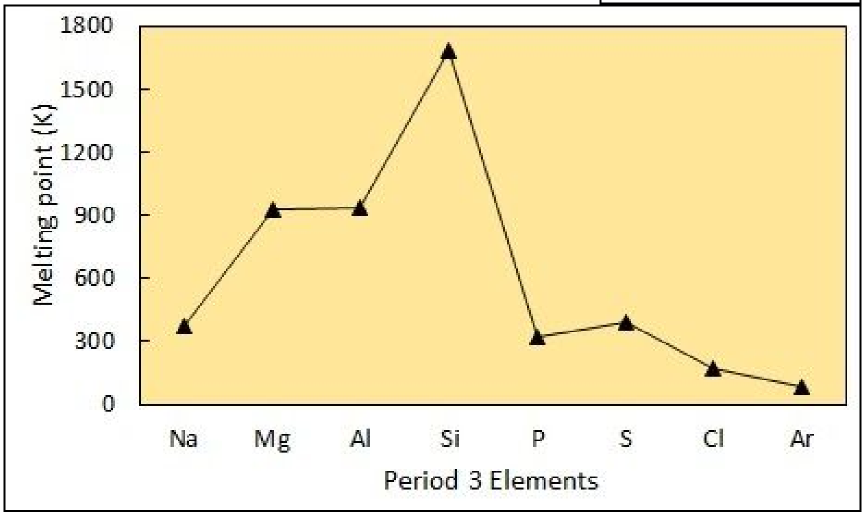
Sodium, magnesium and aluminium are all metals with **metallic bonding**. Their melting points increase due to greater **positively charged ions** (Na = +1, Mg = +2, Al = +3). This also means **more electrons are released** as free electrons, so the attractive electrostatic forces increase from Na to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

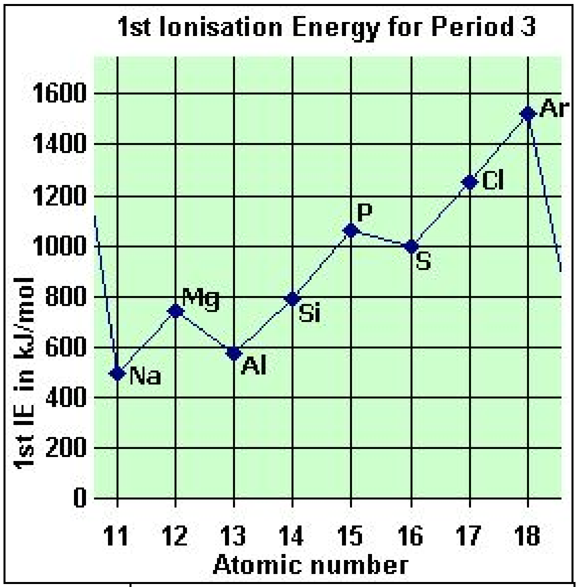


Ionisation Energies

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. Between magnesium and aluminium, electrons start to be added to a 3p orbital rather than 3s. The 3p orbital has a slightly **higher energy level** than the 3s orbital so this electron is found slightly further from the nucleus. This means it can be removed more easily (less energy required).

Between phosphorus and sulfur, electrons start to pair in the 3p orbitals. The paired electrons are both negatively charged so they repel each other. This **repulsion** allows an electron to be removed with less energy than expected.



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