



# HL IB Chemistry

  
Your notes

## Electronic Configurations

### Contents

- \* The Electromagnetic Spectrum
- \* Emission Spectra
- \* Energy Levels, Sublevels & Orbitals
- \* Writing Electron Configurations
- \* Ionisation Energy from an Emission Spectrum (HL)
- \* Successive Ionisation Energies (HL)



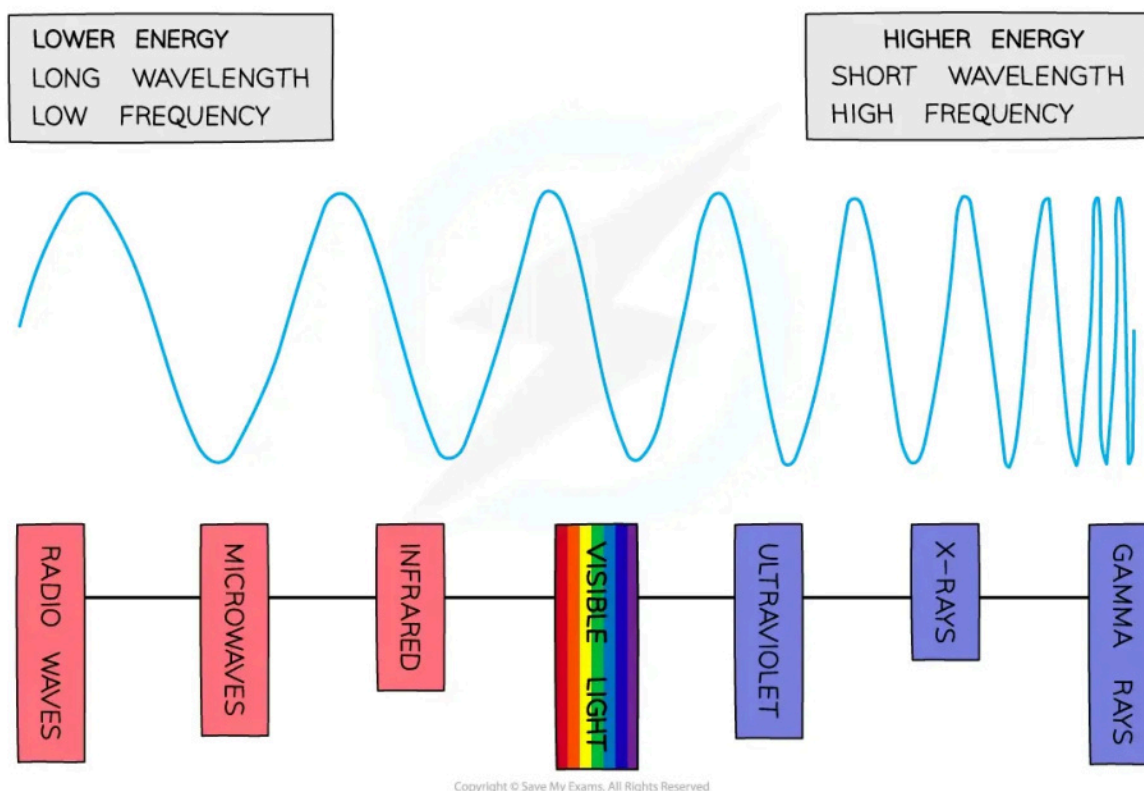
Your notes

## The Electromagnetic Spectrum

### The Electromagnetic Spectrum

- The **electromagnetic spectrum** is a range of **frequencies** that covers all electromagnetic radiation and their respective **wavelengths** and **energy**
- It is divided into bands or regions, and is very important in analytical chemistry.
- The spectrum shows the relationship between **frequency**, **wavelength** and **energy**
- **Frequency** is how many waves pass per second, and **wavelength** is the distance between two consecutive peaks on the wave
- **Gamma rays**, **X-rays** and **UV** radiation are all dangerous - you can see from that end of the spectrum that it is high frequency and high energy, which can be very damaging to your health

#### The electromagnetic spectrum diagram



*The electromagnetic spectrum spans a broad spectrum from very long radio waves to very short gamma rays*

- All light waves travel at the same speed; what distinguishes them is their different frequencies



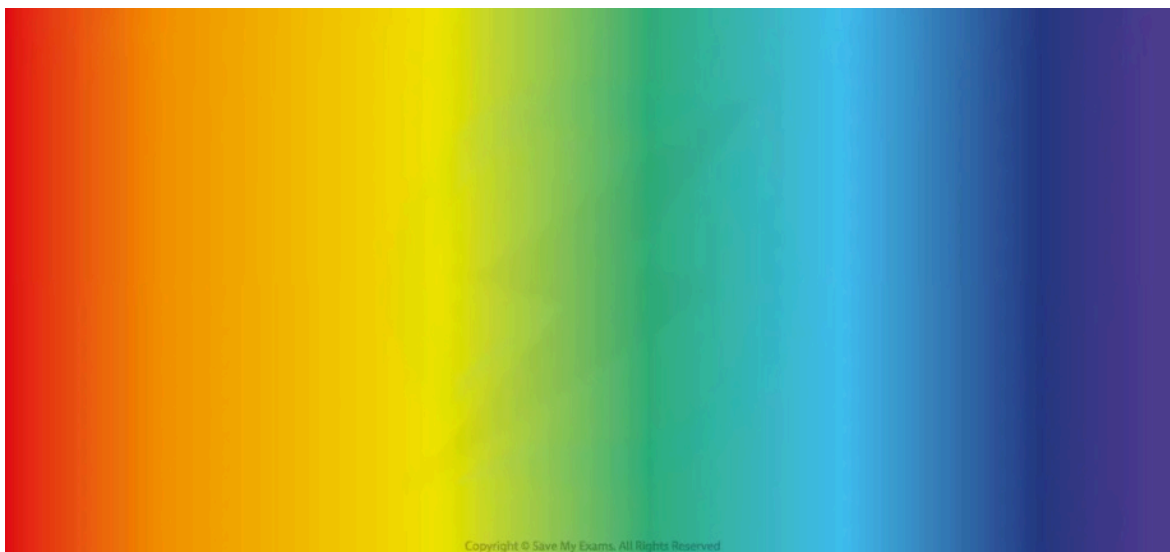
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- The speed of light (symbol ' $c$ ') is constant and has a value of  $3.00 \times 10^8 \text{ ms}^{-1}$
- As you can see from the spectrum, frequency (symbol ' $f$ ') is inversely proportional to wavelength (symbol ' $\lambda$ ')
  - In other words, the higher the frequency, the shorter the wavelength
- The equation that links them is  $c = f\lambda$
- Since  $c$  is constant you can use the formula to calculate the frequency of radiation given the wavelength, and vice versa

## Continuous versus line spectrum

- A continuous spectrum in the visible region contains all the colours of the spectrum
- This is what you are seeing in a rainbow, which is formed by the refraction of white light through a prism or water droplets in rain

### Continuous spectrum diagram



*A continuous spectrum shows all frequencies of light*

- However, a line spectrum only shows certain frequencies

### Helium spectrum diagram



*The line spectrum of helium which shows only certain frequencies of light*

- This tells us that the emitted light from atoms can only be certain fixed frequencies – it is **quantised** (quanta means 'little packet')

- Electrons can only possess certain amounts of energy - they cannot have any energy value

 **Examiner Tip**

- The formula that relates frequency and wavelength is printed in Section 1 of the IB Chemistry Data Booklet so you don't need to learn it
- You will also find the speed of light and other useful constants in Section 2



Your notes



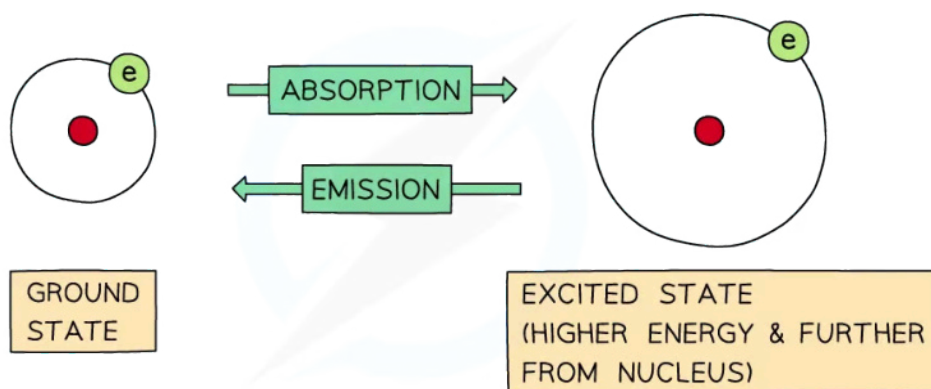
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## Emission Spectra

### Emission Spectra

- Electrons move rapidly around the nucleus in energy shells
- If their energy is increased, then they can jump to a higher energy level
- The process is reversible, so electrons can return to their original energy levels
  - When this happens, they emit energy
- The frequency of energy is exactly the same, it is just being emitted rather than absorbed:

#### Absorption and Emission diagram



*The difference between absorption and emission depends on whether electrons are jumping from lower to higher energy levels or the other way around*

- The energy they emit is a mixture of different frequencies
- This is thought to correspond to the many possibilities of electron jumps between energy shells
- If the emitted energy is in the visible region, it can be analysed by passing it through a diffraction grating
- The result is a **line emission spectrum**

### Line emission spectra

#### Spectrum of hydrogen diagram

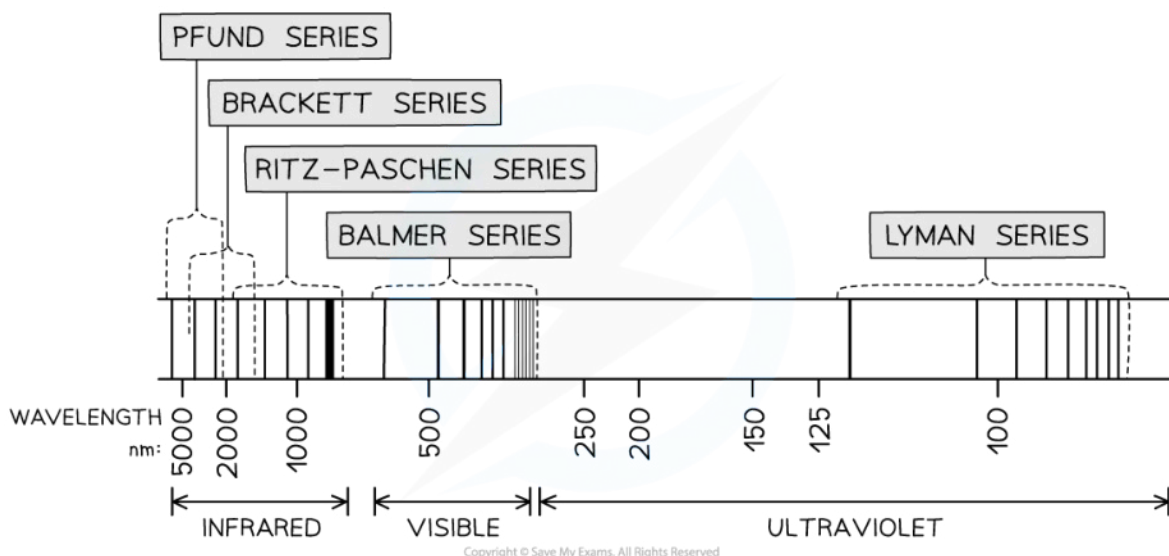


*The line emission (visible) spectrum of hydrogen*

- Each line is a specific energy value
  - This suggests that electrons can only possess a limited choice of allowed energies
- These packets of energy are called '**quanta**' (plural **quantum**)
- What you should notice about this spectrum is that the lines get closer together towards the blue end of the spectrum
- This is called **convergence** and the set of lines is **converging** towards the higher energy end, so the electron is reaching a maximum amount of energy
- This maximum corresponds to the **ionisation energy** of the electron
- These lines were first observed by the Swiss school teacher Johannes **Balmer**, and they are named after him
- We now know that these lines correspond to the electron jumping from higher levels down to the **second** or  $n = 2$  energy level

- A larger version of the hydrogen spectrum from the infrared to the ultraviolet region looks like this

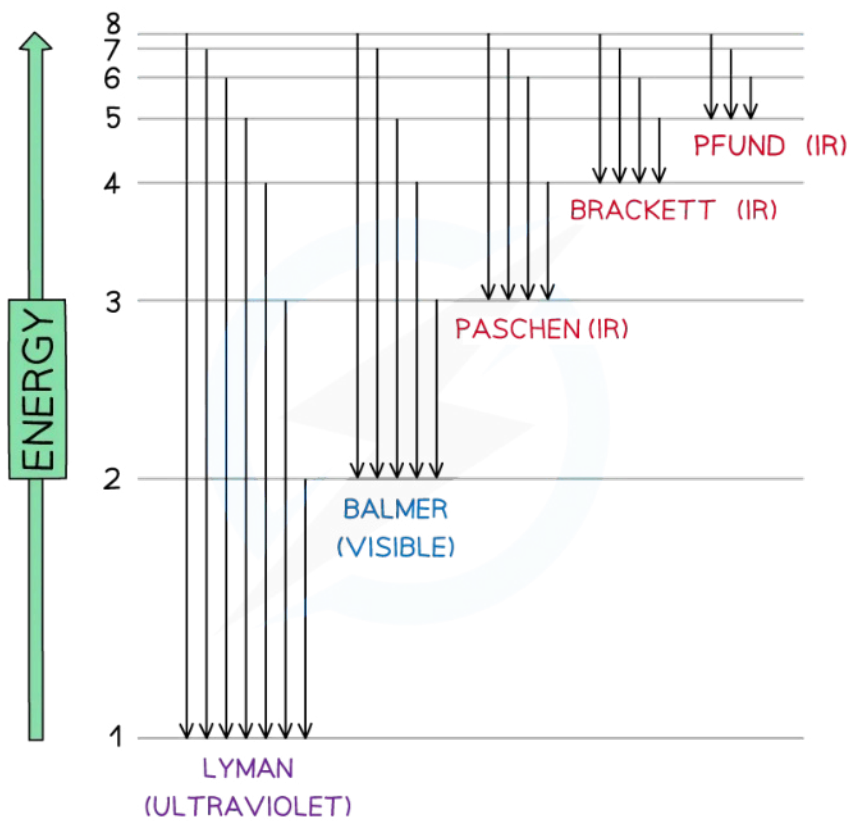
### Full hydrogen spectrum diagram



*The full hydrogen spectrum*

- In the spectrum, we can see sets or families of lines
- Balmer could not explain why the lines were formed - an explanation had to wait until the arrival of Planck's **Quantum Theory** in 1900
- Niels Bohr applied the **Quantum Theory** to electrons in 1913, and proposed that electrons could only exist in fixed energy levels
- The line emission spectrum of hydrogen provided evidence of these energy levels and it was deduced that the families of lines corresponded to electrons jumping from higher levels to lower levels

### Diagram to show the energy transitions for the hydrogen atom



**Electron jumps in the hydrogen spectrum**

- The findings helped scientists to understand how electrons work and provided the backbone to our knowledge of energy levels, sublevels and orbitals
- The jumps can be summarised as follows:

**Electron Jumps & Energy Table**

Jumps	Region	Energy
$n^\infty \rightarrow n_3$	Infrared	Low
$n^\infty \rightarrow n_2$	Visible	↓
$n^\infty \rightarrow n_1$	Ultraviolet	High

 **Worked example**

Which electron transition in the hydrogen atom emits visible light?

- A.  $n = 1$  to  $n = 2$
- B.  $n = 2$  to  $n = 3$
- C.  $n = 2$  to  $n = 1$
- D.  $n = 3$  to  $n = 2$

**Answer**

Option **D** is correct

- Emission in the visible region occurs for an electron jumping from any higher energy level to  **$n = 2$**



Your notes



## Energy Levels, Sublevels & Orbitals



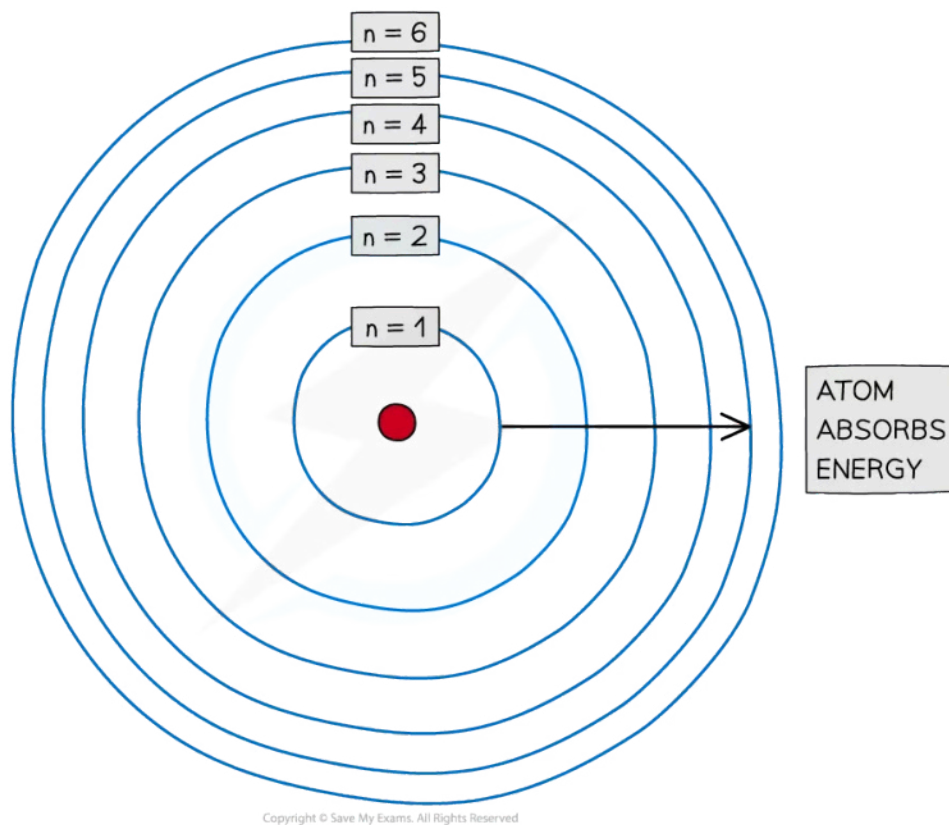
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### Energy Levels

#### What are electron shells?

- The arrangement of electrons in an atom is called the **electronic configuration**
- Electrons are arranged around the nucleus in **principal energy levels** or **principal quantum shells**
- **Principal quantum numbers (n)** are used to number the energy levels or quantum shells
  - The **lower** the principal quantum number, the closer the shell is to the nucleus
  - The **higher** the principal quantum number, the greater the energy of the electron within that shell
- Each principal quantum number has a **fixed** number of electrons it can hold
  - $n = 1$  : up to 2 electrons
  - $n = 2$  : up to 8 electrons
  - $n = 3$  : up to 18 electrons
  - $n = 4$  : up to 32 electrons
- There is a pattern here - the mathematical relationship between the number of electrons and the principal energy level is  $2n^2$ 
  - So for example, in the third shell  $n = 3$  and the number of electrons is  $2 \times (3^2) = 18$

#### Principle quantum shells

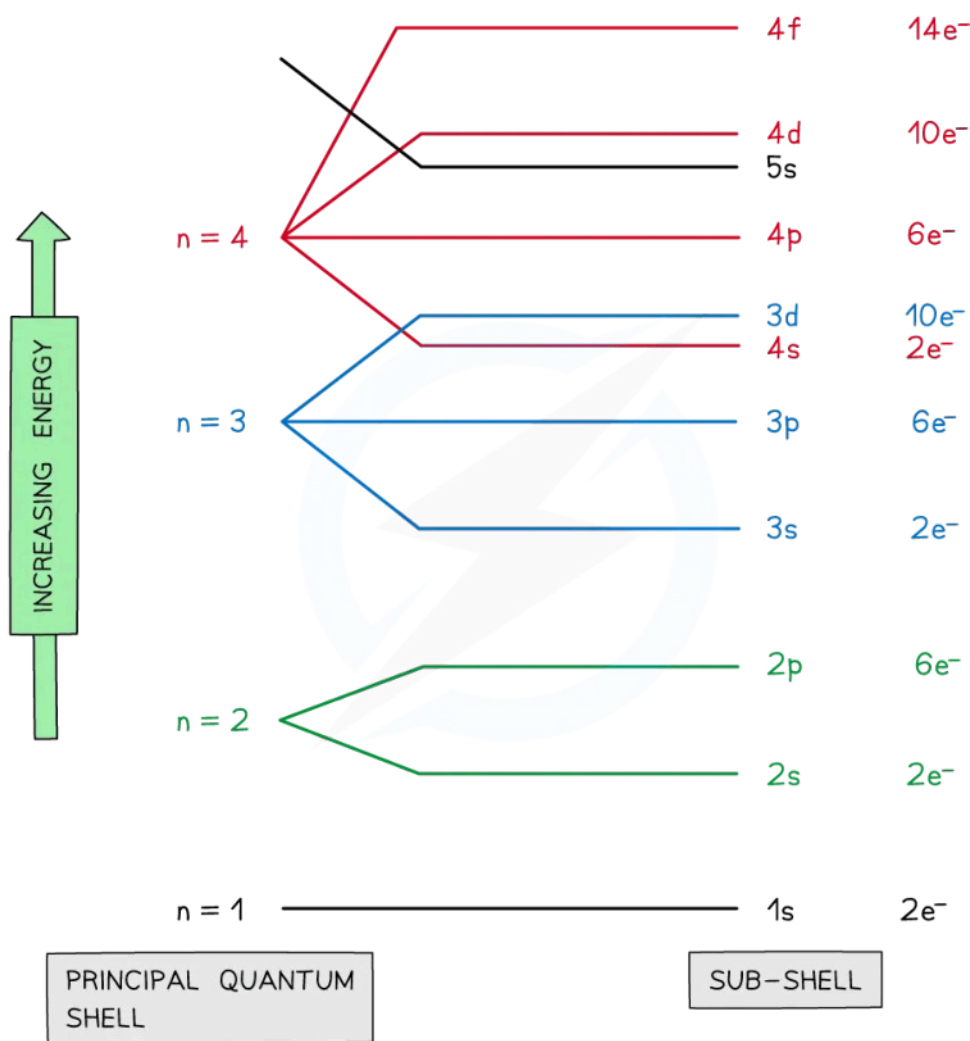


*Electrons are arranged in principal quantum shells, which are numbered by principal quantum numbers*

### What are subshells?

- The principal quantum shells are split into subshells which are given the letters s, p and d
  - Elements with more than 57 electrons also have an f subshell
  - The energy of the electrons in the subshells increases in the order  $s < p < d$
- The order of subshells overlap for the higher principal quantum shells as seen in the diagram below:

### Principle Quantum Number and Sub-Shells



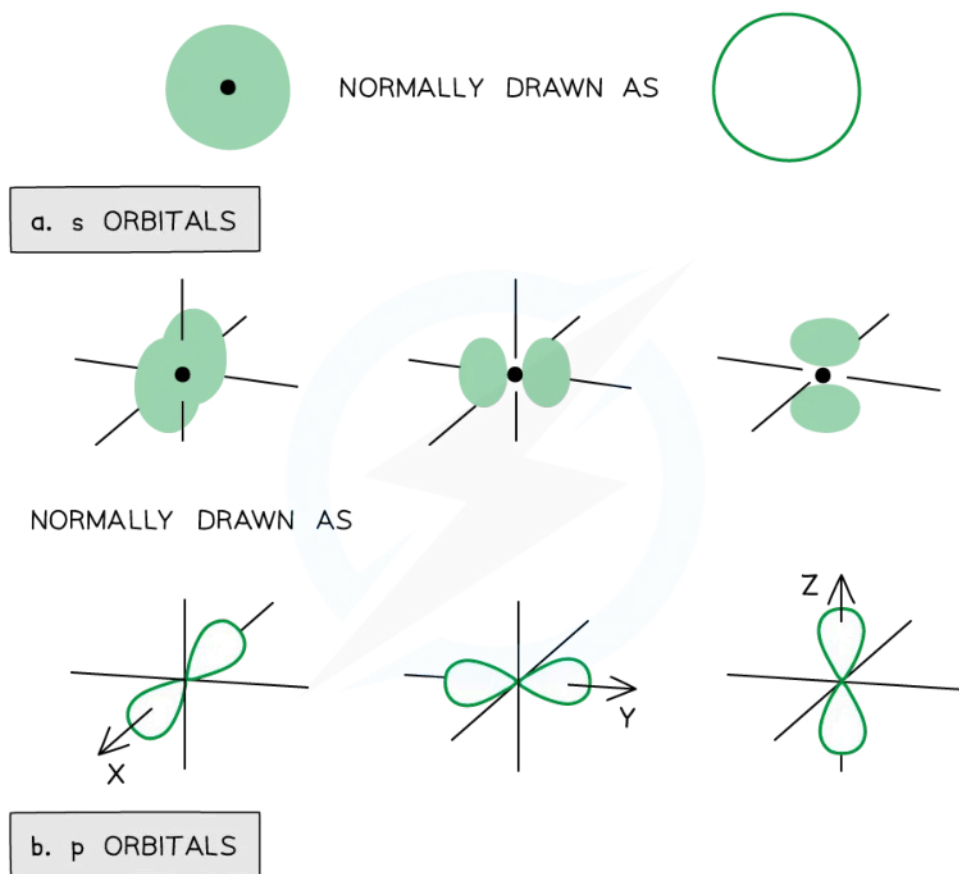
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Electrons are arranged in principal quantum shells, which are numbered by principal quantum numbers

### What are orbitals?

- The subshells contain one or more **atomic orbitals**
- Orbitals exist at **specific** energy levels and electrons can only be found at these specific levels, not in between
  - Each atomic orbital can be occupied by a maximum of two electrons
- The orbitals have specific 3D shapes:

#### The shape of s and p orbitals

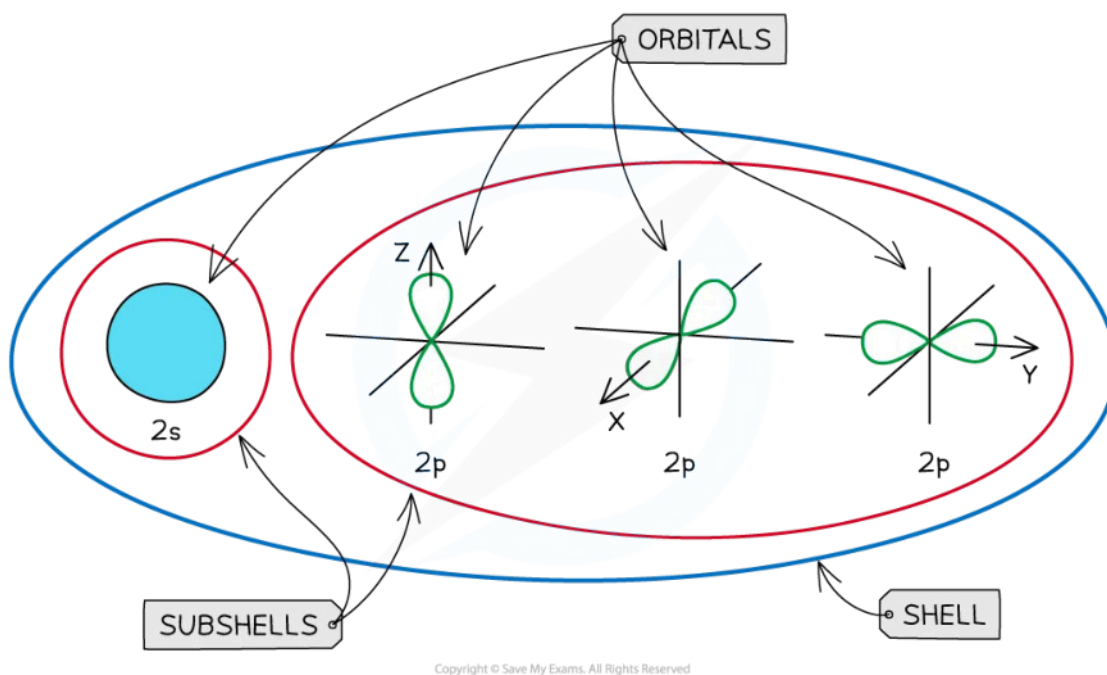


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**Representation of orbitals (the dot represents the nucleus of the atom) showing spherical s orbitals (a), p orbitals containing 'lobes' along the x, y and z axis**

- Note that the shape of the d orbitals is not required for IB Chemistry

### Summary of s and p orbitals



*An overview of the shells, subshells and orbitals in an atom*

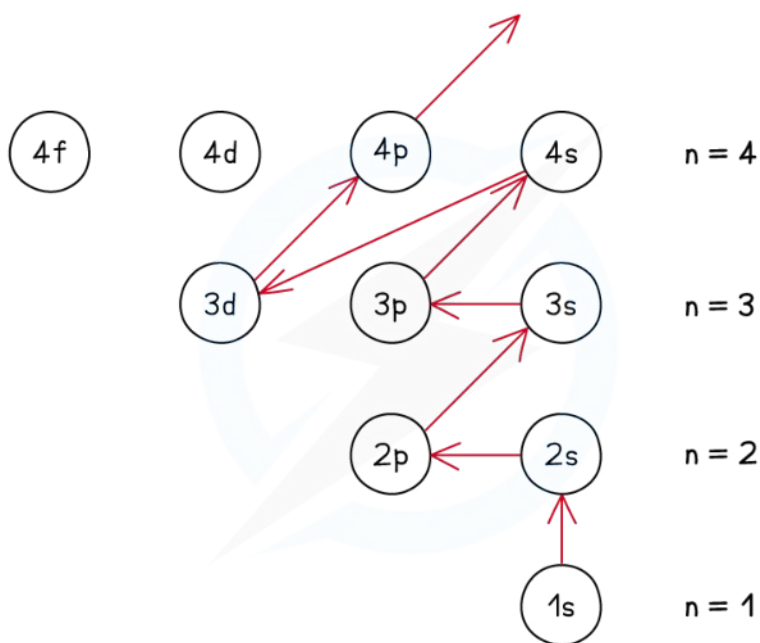
## Ground state

- The **ground state** is the **most stable electronic configuration** of an atom which has the **lowest amount of energy**
- This is achieved by filling the subshells of energy with the lowest energy first (1s)
  - This is called the **Aufbau Principle**
- The order of the subshells in terms of increasing energy does **not** follow a regular pattern at  $n = 3$  and higher

## The Aufbau Principle



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**The Aufbau Principle - following the arrows gives you the filling order**

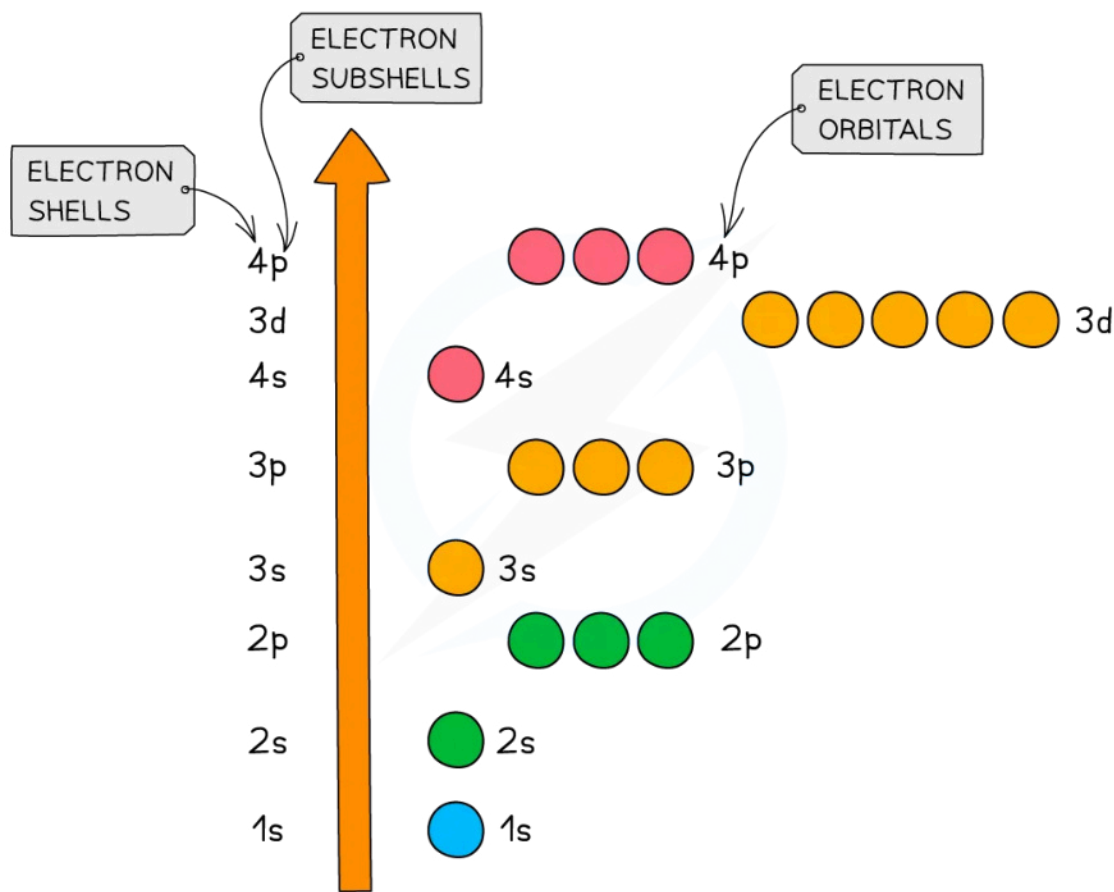


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## Sublevels & Orbitals

- The **principal quantum shells** increase in energy with increasing **principal quantum number**
  - E.g.  $n = 4$  is higher in energy than  $n = 2$
- The **subshells** increase in energy as follows:  $s < p < d < f$ 
  - The only exception to these rules is the 3d orbital which has slightly higher energy than the 4s orbital, so the 4s orbital is filled before the 3d orbital

### Energy Levels



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### Relative energies of the shells and subshells

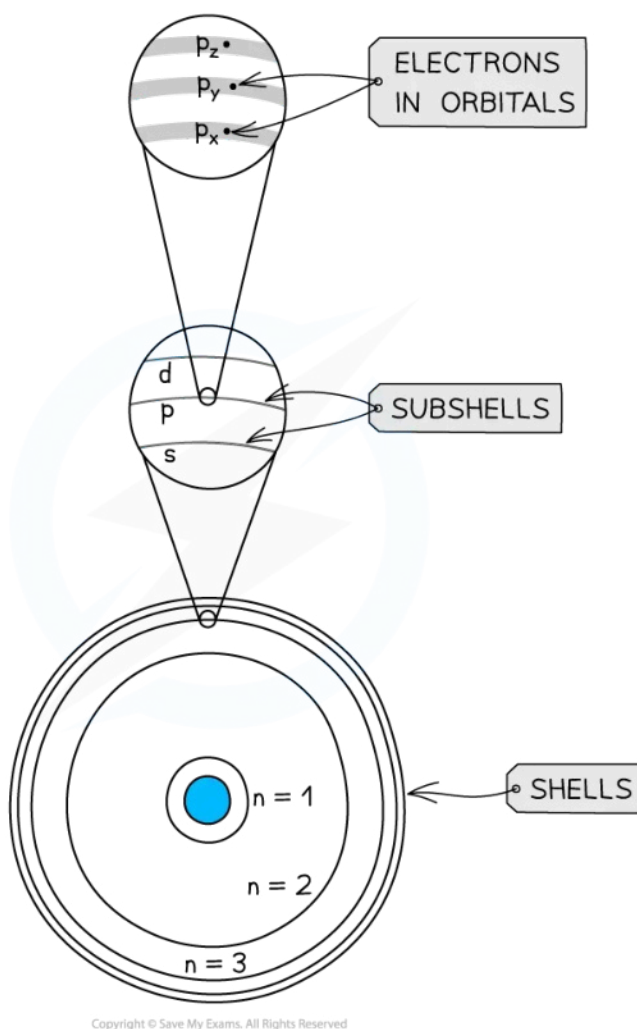
- Each shell can be divided further into **subshells**, labelled **s**, **p**, **d** and **f**
- Each subshell can hold a specific number of orbitals:
  - s subshell : 1 orbital
  - p subshell : 3 orbitals labelled  $p_x$ ,  $p_y$  and  $p_z$
  - d subshell : 5 orbitals
  - f subshell : 7 orbitals



Your notes

- Each orbital can hold a maximum number of 2 electrons so the maximum number of electrons in each subshell is as follows:
  - s:  $1 \times 2 =$  total of 2 electrons
  - p:  $3 \times 2 =$  total of 6 electrons
  - d:  $5 \times 2 =$  total of 10 electrons
  - f:  $7 \times 2 =$  total of 14 electrons
- In the ground state, orbitals in the same subshell have the same energy and are said to be degenerate, so the energy of a  $p_x$  orbital is the same as a  $p_y$  orbital

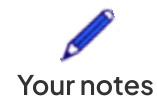
### Division of Shells Diagram



*Shells are divided into subshells which are further divided into orbitals*

### Summary of the Arrangement of Electrons in Atoms Table



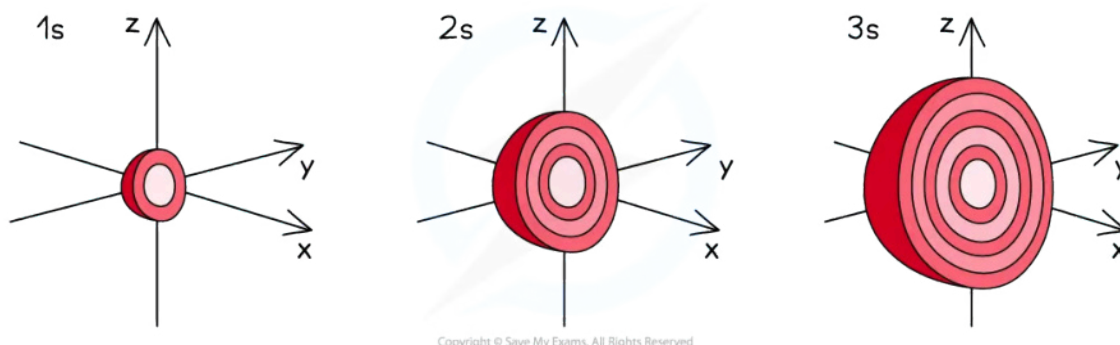


Principle quantum number, $n$ (shell)	Subshells possible (s, p, d, f)	Orbitals per subshell	Orbitals per principle quantum number	Electrons per subshell	Electrons per shell
1	s	1	1	2	2
2	s	1	4	2	8
	p	3		6	
3	s	1	9	2	18
	p	3		6	
	d	5		10	
4	s	1	16	2	32
	p	3		6	
	d	5		10	
	f	7		14	

### What is the shape of an s orbital?

- The s orbitals are **spherical** in shape
- The **size** of the s orbitals increases with increasing shell number
  - E.g. the s orbital of the **third** quantum shell ( $n = 3$ ) is bigger than the s orbital of the **first** quantum shell ( $n = 1$ )

#### s orbital diagram

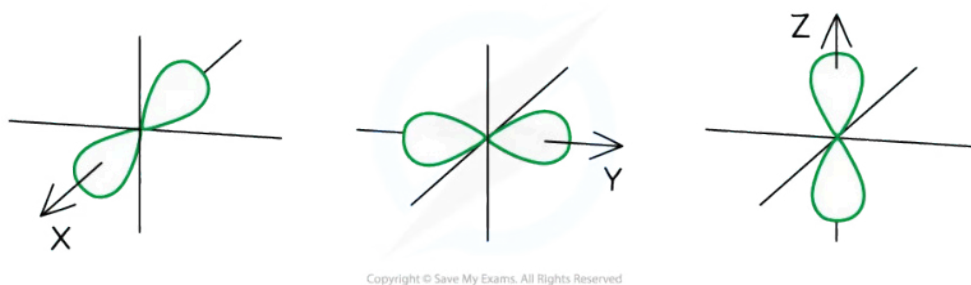


*The s orbitals become larger with increasing principal quantum number*

### What is the shape of a p orbital?

- The p orbitals are **dumbbell-shaped**
- Every shell has three p orbitals except for the first one ( $n = 1$ )
- The p orbitals occupy the x, y and z axes and point at right angles to each other, so are oriented **perpendicular** to one another
- The lobes of the p orbitals become **larger** and **longer** with increasing shell number

### p orbital diagram



*The p orbitals become larger and longer with increasing principal quantum number*



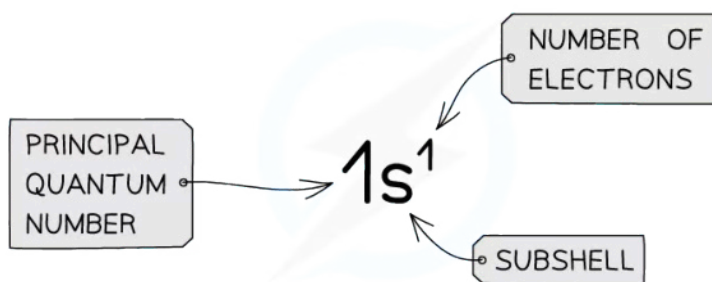
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## Writing Electron Configurations

### Writing Electron Configurations

- The **electron configuration** gives information about the number of electrons in each **shell**, **subshell** and **orbital** of an atom
- The subshells are filled in order of increasing energy

#### Electron Configuration Key

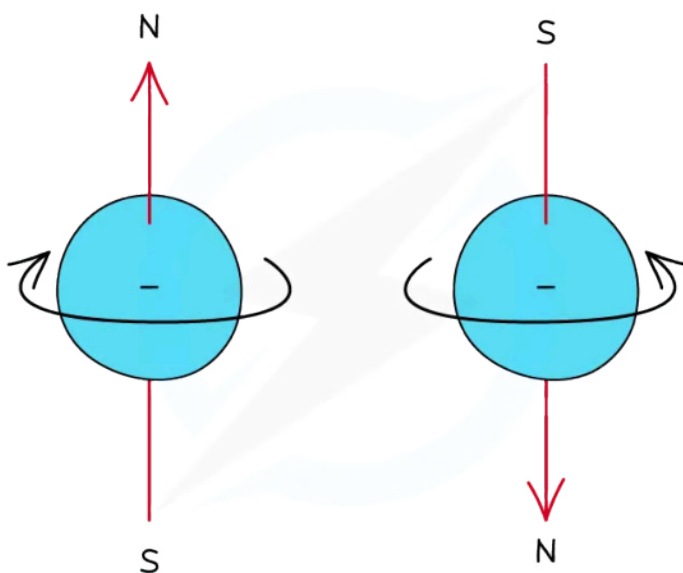


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*The electron configuration shows the number of electrons occupying a subshell in a specific shell*

- Electrons can be imagined as small **spinning charges** which rotate around their own axis in either a **clockwise** or **anticlockwise** direction

#### Spin pair repulsion diagram



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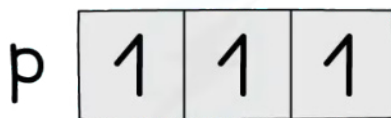


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*Electrons can spin either in a clockwise or anticlockwise direction around their own axis. The spin creates a tiny magnetic field with N-S pole pointing up or down, although you are not required to know this for the exam*

- Electrons with the same **spin** repel each other which is also called **spin-pair repulsion**
  - Therefore, electrons will occupy separate orbitals in the same subshell first to minimise this repulsion and have their **spin** in the same direction
  - They will then pair up, with a second electron being added to the first p orbital, with its spin in the **opposite** direction
- This is known as **Hund's Rule**
  - E.g. if there are three electrons in a **p subshell**, one electron will go into each  $p_x$ ,  $p_y$  and  $p_z$  orbital

### Hund's Rule

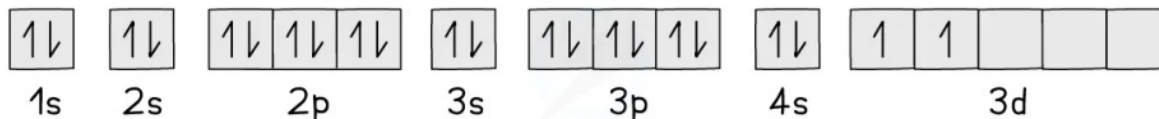


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### Electron configuration: three electrons in a p subshell

- The principal quantum number indicates the energy level of a particular shell but also indicates the energy of the electrons in that shell
  - A 2p electron is in the second shell and therefore has an energy corresponding to  $n = 2$
- Even though there is repulsion between negatively charged electrons, they occupy the same region of space in orbitals
- An orbital can only hold two electrons and they must have opposite spin - this is known as the **Pauli Exclusion Principle**
- This is because the energy required to jump to a higher empty orbital is **greater** than the inter-electron repulsion
- For this reason, they pair up and occupy the lower energy levels first
- The **electron configuration** can also be represented using the **orbital spin diagrams**
- Each box represents an **atomic orbital**
- The boxes are arranged in order of **increasing** energy from lower to higher (i.e. starting from closest to the nucleus)
- The electrons are represented by opposite arrows to show the **spin** of the electrons
  - E.g. the box notation for titanium is shown below

### Electron box notation for titanium diagram



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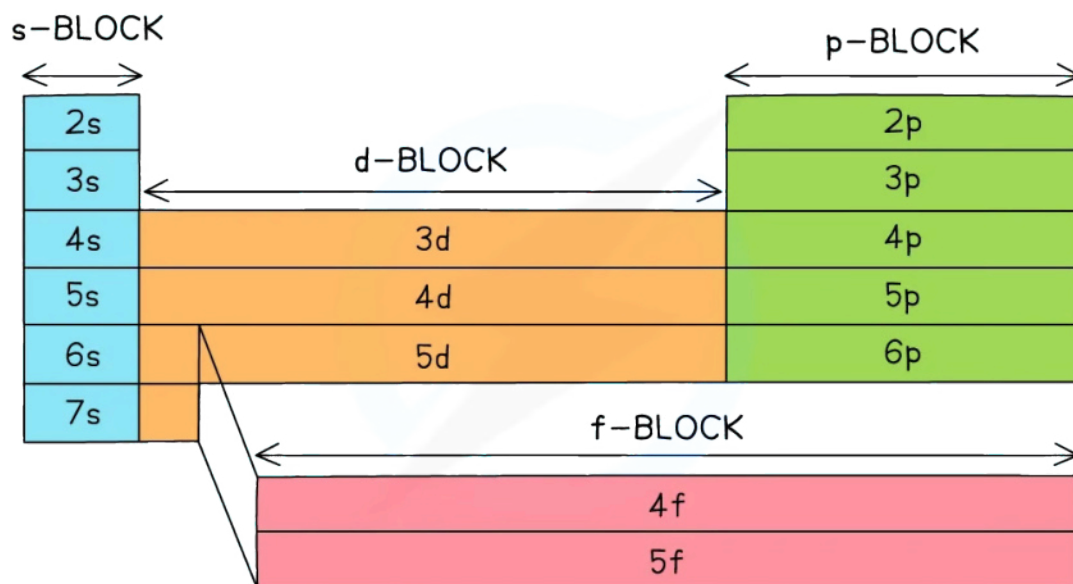


Your notes

The electrons in titanium are arranged in their orbitals as shown. Electrons occupy the lowest energy levels first before filling those with higher energy

- Writing out the **electronic configuration** tells us how the electrons in an atom or ion are arranged in their shells, subshells and orbitals
- This can be done using the **full** electron configuration or the **shorthand** version
  - The **full** electron configuration describes the arrangement of all electrons from the 1s subshell up
  - The **shorthand** electron configuration includes using the symbol of the nearest preceding **noble gas** to account for however many electrons are in that noble gas, followed by the rest of the electron configuration
- Ions** are formed when atoms **lose** or **gain** electrons
  - Negative ions are formed by **adding** electrons to the outer subshell
  - Positive ions are formed by **removing** electrons from the outer subshell
  - The transition metals **fill** the 4s subshell before the 3d subshell, but they also **lose** electrons from the 4s first rather than from the 3d subshell
- The Periodic Table is split up into four main blocks depending on their electronic configuration:
  - s block elements (valence electron(s) in s orbital)
  - p block elements (valence electron(s) in p orbital)
  - d block elements (valence electron(s) in d orbital)
  - f block elements (valence electron(s) in f orbital)

### s, p, d and f blocks in the Periodic Table



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The elements can be divided into four blocks according to their outer shell electron configuration

### Exceptions to the Aufbau Principle



Your notes

- Chromium and copper have the following electron configurations:
  - Cr is  $[\text{Ar}] 3d^5 4s^1$  **not**  $[\text{Ar}] 3d^4 4s^2$
  - Cu is  $[\text{Ar}] 3d^{10} 4s^1$  **not**  $[\text{Ar}] 3d^9 4s^2$
- This is because the  $[\text{Ar}] 3d^5 4s^1$  and  $[\text{Ar}] 3d^{10} 4s^1$  configurations are **energetically favourable**
- By promoting an electron from 4s to 3d, these atoms achieve a half full or full d-subshell, respectively

### Worked example

Write down the full and shorthand electron configuration of the following elements:

- Potassium
- Calcium
- Gallium
- $\text{Ca}^{2+}$

#### Answer 1:

- Potassium has 19 electrons so the **full electronic configuration** is:
  - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
- The 4s orbital is lower in energy than the 3d subshell and is therefore filled first
- The nearest preceding noble gas to potassium is **argon** which accounts for 18 electrons so the **shorthand electron configuration** is:
  - $[\text{Ar}] 4s^1$

#### Answer 2:

- Calcium has 20 electrons so the **full electronic configuration** is:
  - $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
- The 4s orbital is lower in energy than the 3d subshell and is therefore filled first
- The **shorthand** version is  $[\text{Ar}] 4s^2$  since argon is the nearest preceding noble gas to calcium which accounts for 18 electrons

#### Answer 3:

- Gallium has 31 electrons so the **full electronic configuration** is:
  - Full:**  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^1$
  - Shorthand:**  $[\text{Ar}] 3d^{10} 4s^2 4p^1$

#### Answer 4:

- If you ionise calcium and remove two of its outer electrons, the electronic configuration of the  $\text{Ca}^{2+}$  ion is identical to that of argon:
  - $\text{Ca}^{2+}$**  is  $1s^2 2s^2 2p^6 3s^2 3p^6$
  - Ar** is also  $1s^2 2s^2 2p^6 3s^2 3p^6$  so the shorthand version is  $[\text{Ar}]$

### Examiner Tip

- Orbital spin diagrams can be drawn horizontally or vertically, going up or down the page - there is no hard and fast rule about this
- The important thing is that you label the boxes and have the right number of electrons shown
- The arrows you use for electrons can be full or half-headed arrows, but they must be in opposite directions in the same box.



Your notes



Your notes

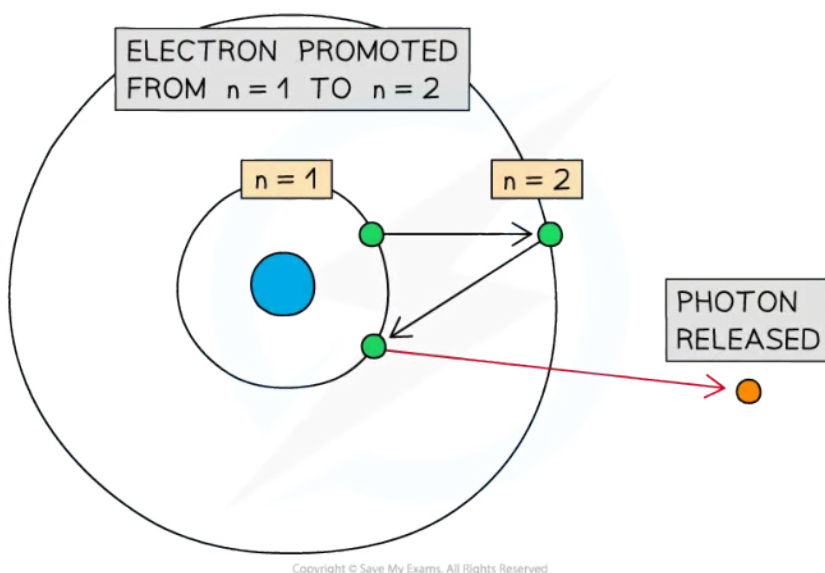
## Ionisation Energy from an Emission Spectrum (HL)

### Ionisation Energy from an Emission Spectrum

#### Emission Spectra

- Electrons move rapidly around the nucleus in energy shells
- Heat or electricity can be used to excite an electron to a higher main energy level
- These range from  $n = 1$  (ground state) to  $n = \infty$
- When the electrons 'fall' back down they must lose the energy difference between the two energy levels. This loss of energy is performed by releasing electromagnetic energy in the form of infrared, visible light or ultraviolet radiation.
- When the electron falls back to  $n = 1$  (ground state) the energy released is in the ultraviolet region of the spectrum
- This corresponds to the **Lyman series**

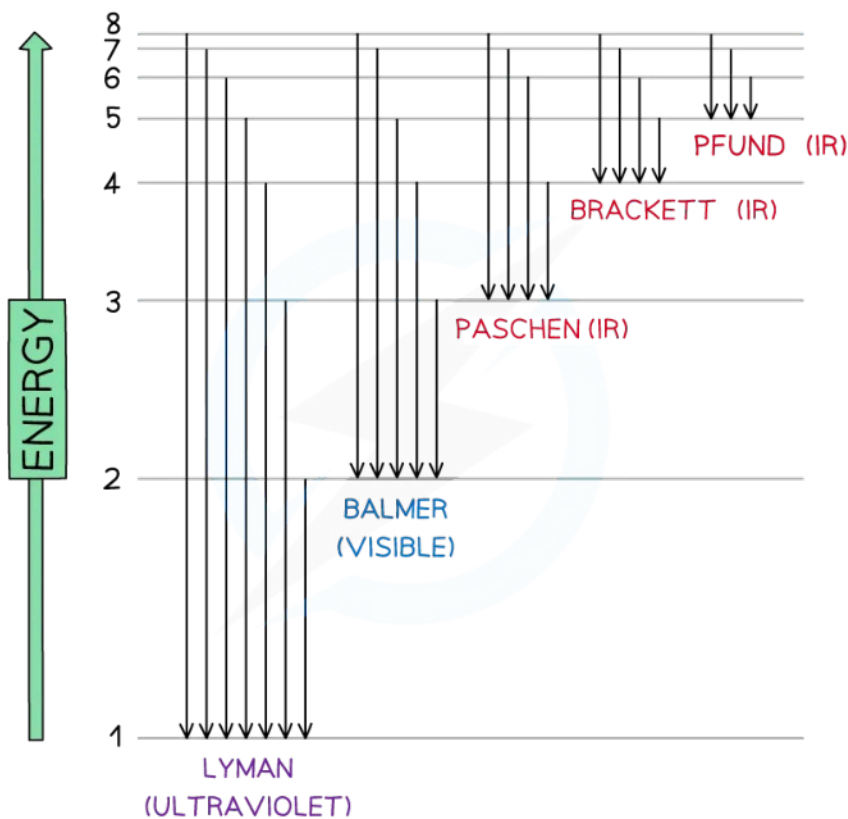
**Diagram to show the release of a photon when an electron is promoted**



*Promotion of an electron from the ground state ( $n=1$ ) to  $n=2$*

**Jumps in the hydrogen spectrum diagram**





### Electron jumps in the hydrogen spectrum

- This gives evidence for Bohr's model which is the idea that electrons exist in discrete energy levels so an exact amount of energy is required for an electron to 'jump' an energy level, a little like a ladder
- There are however limitations to this model
  - Assumes positions of electrons are fixed
  - Assumes energy levels are spherical in nature
  - Bohr limited calculations to hydrogen only, so does not explain the line spectra of other elements containing more than one electron

### The Limit of Convergence

As the line spectra is produced the lines will become closer together

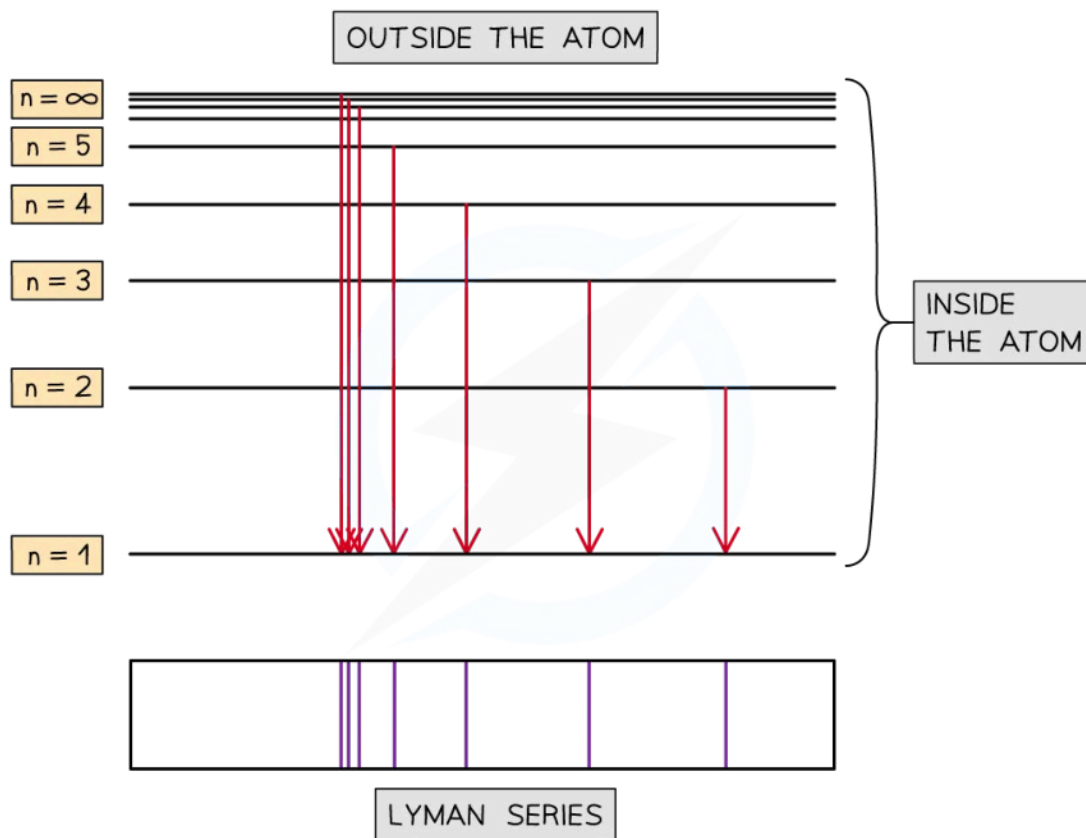
- Where the lines appear to meet is called the **limit of convergence**
- The convergence limit is the frequency at which the spectral lines converge
- The energy required for an electron to escape the atom, or reach the upper limit of convergence, is the ionisation energy
- The frequency of the radiation in the emission spectrum at the limit of convergence can be used to determine the first ionisation energy or  $IE_1$



Your notes

- In the **Lyman series** for the hydrogen atom (UV region), the frequency at the limit of convergence relates to the energy given out when an electron falls from  $n = \infty$  to  $n = 1$
- For hydrogen, the lines converge to a limit with a wavelength of 91.16 nm or  $91.16 \times 10^{-9}$  m

### Limit of Convergence diagram for hydrogen



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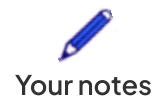
**Lyman series (ultra-violet radiation) corresponds to transitions between higher shells and the ground state ( $n=1$ )**

### Calculating First Ionisation Energy

- When dealing with the Lyman series, the largest transitions represent the fall from the infinite level to  $n=1$
- In reverse, it can be considered to be equal to the ionisation energy (note that ionisation energy is given per mole of atoms)
- Therefore, the first ionisation energy ( $IE_1$ ) of an atom can be calculated using the frequency (or wavelength) of the **convergence limit**
- We can do this by using the following equations

$$\Delta E = h\nu$$

$$c = \nu\lambda$$



- In order to calculate the first ionisation energy, ( $I E_1$ ), we must first calculate the **frequency** using the given data and rearranging:

$$c = \nu \lambda$$

as

$$\nu = c \div \lambda$$

- Once we know the frequency, we can use this to calculate the ionisation energy
  - $E$  = Energy (J)
  - $h$  = Planck's constant ( $6.63 \times 10^{-34}$  J s)
  - $\nu$  = frequency ( $s^{-1}$ )
  - $\lambda$  = wavelength (m)
  - $c$  = speed of light ( $3.00 \times 10^8$  m  $s^{-1}$ )

### Worked example

The convergence limit for the sodium atom has a frequency of  $1.24 \times 10^{15} s^{-1}$ . Calculate the first ionisation energy of sodium in  $kJ mol^{-1}$ .

**Answer:**

**Step 1:** Write out the equation to calculate the first ionisation energy ( $I E_1$ )

$$\Delta E = h \nu$$

**Step 2:** Substitute in numbers from question and data booklet to give energy change **per atom**

$$I E_1 = 6.63 \times 10^{-34} \times 1.24 \times 10^{15}$$

$$I E_1 = 8.22 \times 10^{-19} \text{ J atom}^{-1}$$

**Step 3:** Calculate the first ionisation energy per mole by multiplying by **Avogadro's constant**

$$I E_1 = 8.22 \times 10^{-19} \times 6.02 \times 10^{23}$$

$$I E_1 = 494\,916 \text{ J mol}^{-1}$$

**Step 4:** Convert  $J mol^{-1}$  to  $kJ mol^{-1}$  by dividing by 1000

$$I E_1 = 495 \text{ kJ mol}^{-1}$$

So the first ionisation energy ( $I E_1$ ) of sodium has been calculated as **495  $kJ mol^{-1}$**



Your notes

### Worked example

The convergence limit for the hydrogen atom has a wavelength of 91.16 nm. Calculate the ionisation energy for hydrogen in  $\text{kJ mol}^{-1}$ .

**Answer:**

**Step 1:** Calculate the frequency of the convergence limit, **converting wavelength into m (nm to m =  $\times 10^{-9}$ )**

$$c = \nu \lambda$$

$$\nu = c \div \lambda$$

$$\nu = 3.00 \times 10^8 \div 91.16 \times 10^{-9}$$

$$\nu = 3.29 \times 10^{15} \text{ s}^{-1}$$

**Step 2:** Substitute into the equation to calculate  $IE_1$  for one atom of hydrogen in  $\text{J mol}^{-1}$

$$\Delta E = h \nu$$

$$IE_1 = 6.63 \times 10^{-34} \times 3.29 \times 10^{15}$$

$$IE_1 = 2.18 \times 10^{-18} \text{ J atom}^{-1}$$

**Step 3:** Calculate  $IE_1$  for 1 mole of hydrogen atoms

$$IE_1 = 2.18 \times 10^{-18} \times 6.02 \times 10^{23}$$

$$IE_1 = 1\,313\,491 \text{ J mol}^{-1}$$

**Step 4:** Convert  $\text{J mol}^{-1}$  to  $\text{kJ mol}^{-1}$

$$IE_1 = 1313 \text{ kJ mol}^{-1}$$

So the first ionisation energy ( $IE_1$ ) of hydrogen has been calculated as  **$1313 \text{ kJ mol}^{-1}$**

### Examiner Tip

- These equations are found in the data booklet so you don't need to learn them
- Also, be careful to calculate the first ionisation energy ( $IE_1$ ) per mole by using **Avogadro's constant ( $N_A$ )**  $6.02 \times 10^{23}$  and converting units to  $\text{kJ mol}^{-1}$
- Finally, when working through calculations, keep the numbers in your calculator to avoid rounding up too early.



Your notes

## Successive Ionisation Energies (HL)

### Successive Ionisation Energies

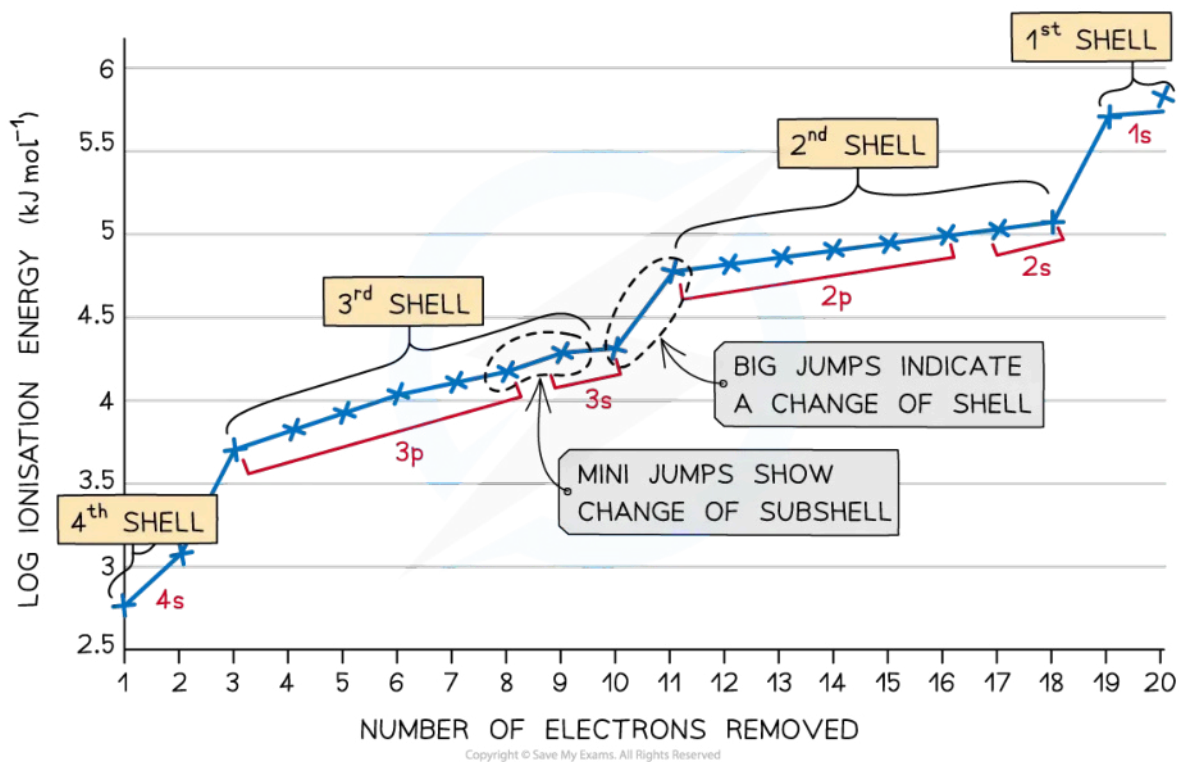
#### Successive ionisation energies of an element

- The **successive** ionisation energies of an element **increase**
- This is because once you have removed the outer electron from an atom, you have formed a **positive ion**
- Removing an electron from a positive ion is **more difficult** than from a neutral atom
- As more electrons are removed, the **attractive forces increase** due to decreasing shielding and an increase in the proton to electron ratio
- The increase in ionisation energy, however, is not constant and is dependent on the atom's electronic configuration
- Taking calcium as an example:

**Ionisation Energies of Calcium Table**

Electronic Configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$	$1s^2 2s^2 2p^6 3s^2 3p^6$	$1s^2 2s^2 2p^6 3s^2 3p^5$
IE	First	Second	Third	Fourth
IE (kJ mol <sup>-1</sup> )	590	1150	4940	6480

#### Successive Ionisation Energies of Calcium



Graph to show the successive ionisation energies for the element calcium

- The **first** electron removed has a low  $IE_1$  as it is easily removed from the atom due to the spin-pair repulsion of the electrons in the 4s orbital
- The **second** electron is more difficult to remove than the first electron as there is no **spin-pair repulsion**
- The **third** electron is much more difficult to remove than the second one corresponding to the fact that the third electron is in a **principal quantum** shell which is closer to the nucleus (3p)
- Removal of the **fourth** electron is more difficult as the orbital is no longer full, and there is less **spin-pair repulsion**
- The graph shows there is a large increase in successive ionisation energy as the electrons are being removed from an increasingly positive ion
- The big jumps on the graph show the change of **shell** and the small jumps are the change of **subshell**
- **Successive ionisation data** can be used to:
  - Predict or confirm the simple electronic configuration of elements
  - Confirm the number of electrons in the outer shell of an element
  - Deduce the group an element belongs to in the Periodic Table
- By analysing where the large jumps appear and the number of electrons removed when these large jumps occur, the **electron configuration** of an atom can be determined
- Na, Mg and Al will be used as examples to deduce the electronic configuration and positions of elements in the Periodic Table using their successive ionisation energies

#### Successive Ionisation Energies Table



Your notes

Element	Atomic Number	Ionisation Energy (kJ mol <sup>-1</sup> )			
		First	Second	Third	Fourth
Na	11	494	4560	6940	9540
Mg	12	736	1450	7740	10500
Al	13	577	1820	2740	11600

## Sodium

- For sodium, there is a huge **jump** from the **first** to the **second** ionisation energy, indicating that it is much easier to remove the first electron than the second
- Therefore, the first electron to be removed must be the last electron in the **valence shell** thus Na belongs to group I
- The large jump corresponds to moving from the 3s to the full 2p subshell
  - Na  $1s^2 2s^2 2p^6 3s^1$

## Magnesium

- There is a huge increase from the **second** to the **third** ionisation energy, indicating that it is far easier to remove the first two electrons than the third
- Therefore the **valence shell** must contain only two electrons indicating that magnesium belongs to group II
- The large jump corresponds to moving from the 3s to the full 2p subshell
  - Mg  $1s^2 2s^2 2p^6 3s^2$

## Aluminium

- There is a huge increase from the **third** to the **fourth** ionisation energy, indicating that it is far easier to remove the first three electrons than the fourth
- The 3p electron and 3s electrons are relatively easy to remove compared with the 2p electrons which are located closer to the nucleus and experience greater **nuclear charge**
- The large jump corresponds to moving from the **third shell** to the **second shell**
  - Al  $1s^2 2s^2 2p^6 3s^2 3p^1$



Your notes

### Worked example

Values for the successive  $IE$ s of an unknown element are:

- $IE_1 = 899 \text{ kJ mol}^{-1}$ ,
- $IE_2 = 1757 \text{ kJ mol}^{-1}$ ,
- $IE_3 = 14850 \text{ kJ mol}^{-1}$ ,
- $IE_4 = 21005 \text{ kJ mol}^{-1}$

Deduce which group of the periodic table of elements you would expect to find the unknown element.

**Answer:**

The largest jump is between  $IE_2$  and  $IE_3$  which will correspond to a change in energy level. Therefore, the unknown element must be in **group 2**.

### Worked example

The table shows successive ionisation energies for element **X** in period 2.

#### Successive Ionisation Energies of Unknown Element

Ionisation number	1	2	3	4	5	6	7	8
Ionisation energy ( $\text{kJ mol}^{-1}$ )	1314	3388	5301	7469	1089	13327	71337	84080

Identify element **X**.

**Answer:**

- The largest jump in ionisation energy is between  $IE_6$  and  $IE_7$  meaning that the 7th electron is being removed from an energy level closer to the nucleus
- Therefore, element **X** must be group 16 (6)
- If element **X** is in group 16 (6) and in period 2, it must be **oxygen**

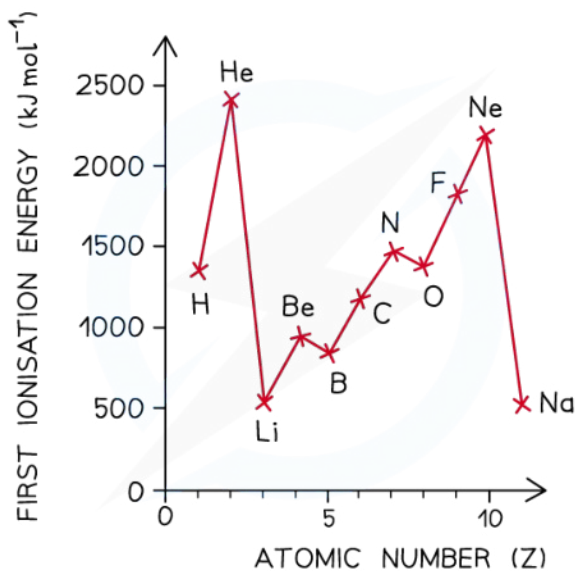
- Ionisation energies show **periodicity** – a trend across a period of the Periodic Table
- As could be expected from their electron configuration, the Group 1 metals have a relatively low ionisation energy, whereas the noble gases have very high ionisation energies
- The size of the first ionisation energy is affected by four factors:
  - **Size of the nuclear charge**
  - **Distance of outer electrons from the nucleus**
  - **Shielding effect of inner electrons**
  - **Spin-pair repulsion**
- First ionisation energy **increases** across a period and **decreases** down a group





Your notes

### Ionisation Energies of Hydrogen to Sodium



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*A graph showing the ionisation energies of the elements hydrogen to sodium*

### Ionisation energy across a period

- The ionisation energy across a period generally **increases** due to the following factors:
  - Across a period the **nuclear charge increases**
  - This causes the **atomic radius** of the atoms to **decrease**, as the outer shell is pulled closer to the nucleus, so the distance between the nucleus and the outer electrons **decreases**
  - The **shielding** by inner shell electrons remain reasonably constant as electrons are being added to the same shell
  - It becomes **harder to remove an electron** as you move across a period; **more energy** is needed
  - So, the ionisation energy increases

### Dips in the trend

- There is a slight **decrease** in  $I_{E1}$  between **beryllium** and **boron** as the fifth electron in boron is in the 2p subshell, which is further away from the nucleus than the 2s subshell of beryllium
  - Beryllium** has a first ionisation energy of  $900 \text{ kJ mol}^{-1}$  as its electron configuration is  $1s^2 2s^2$
  - Boron** has a first ionisation energy of  $800 \text{ kJ mol}^{-1}$  as its electron configuration is  $1s^2 2s^2 2p_x^1$
- There is a slight **decrease** in  $I_{E1}$  between **nitrogen** and **oxygen** due to **spin-pair repulsion** in the  $2p_x$  orbital of oxygen
  - Nitrogen** has a first ionisation energy of  $1400 \text{ kJ mol}^{-1}$  as its electron configuration is  $1s^2 2s^2 2p_x^1 2p_y^1 2p_z^1$
  - Oxygen** has a first ionisation energy of  $1310 \text{ kJ mol}^{-1}$  as its electron configuration is  $1s^2 2s^2 2p_x^2 2p_y^1 2p_z^1$

- In oxygen, there are 2 electrons in the  $2p_x$  orbital, so the repulsion between those electrons makes it slightly easier for one of those electrons to be removed

### From one period to the next

- There is a large **decrease** in ionisation energy between the **last** element in one period, and the **first** element in the next period
- This is because:
  - There is increased **distance** between the nucleus and the outer electrons as you have added a new shell
  - There is increased **shielding** by inner electrons because of the added shell
  - These two factors outweigh the increased **nuclear charge**



Your notes