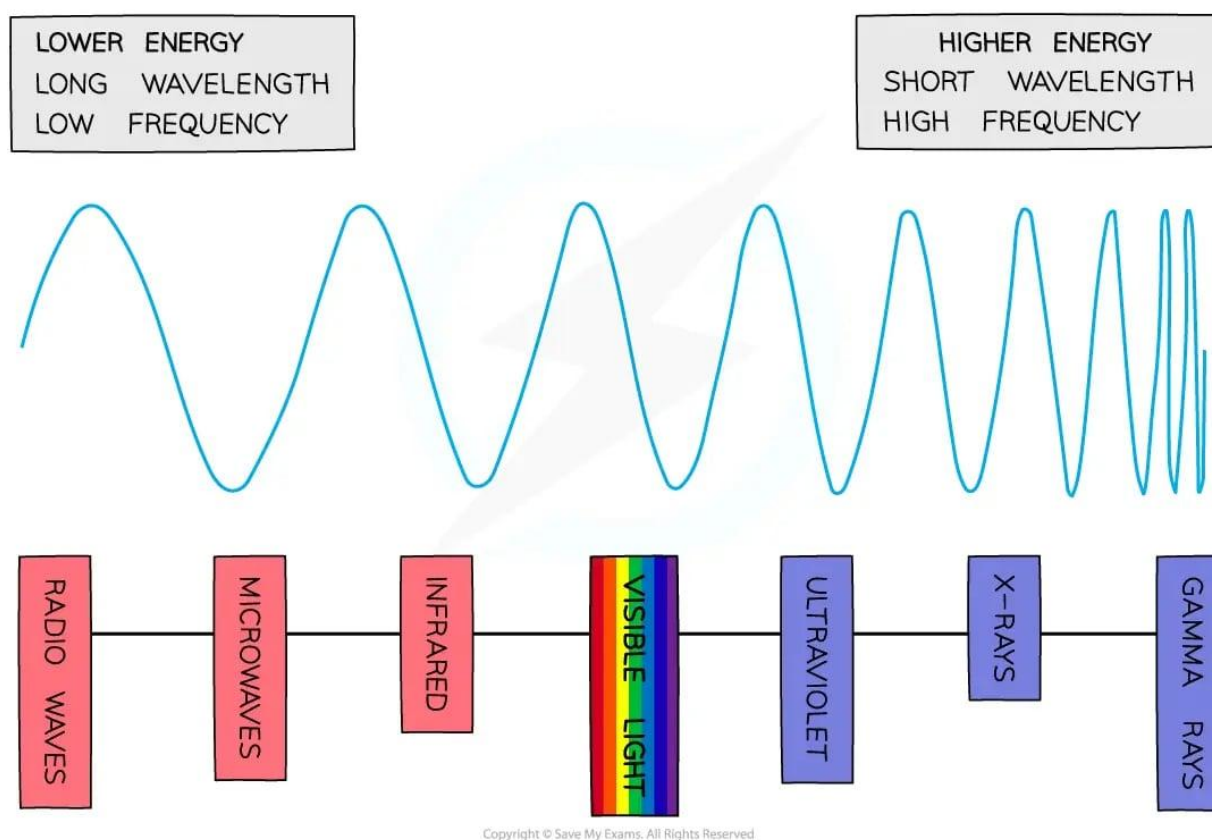


The Electromagnetic Spectrum

- 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

- 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 'v') is inversely proportional to wavelength (symbol ' λ ')
 - In other words, the higher the frequency, the shorter the wavelength
- The equation that links them is $c = v\lambda$
- 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

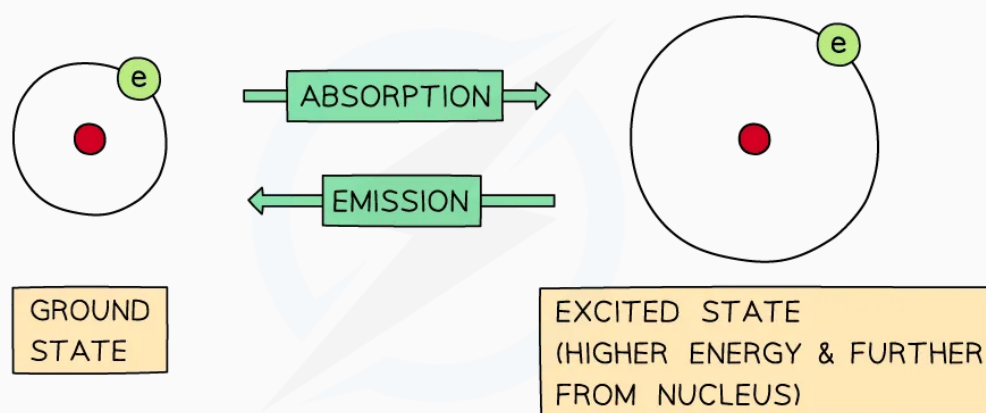
Exam Tip

- 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

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



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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

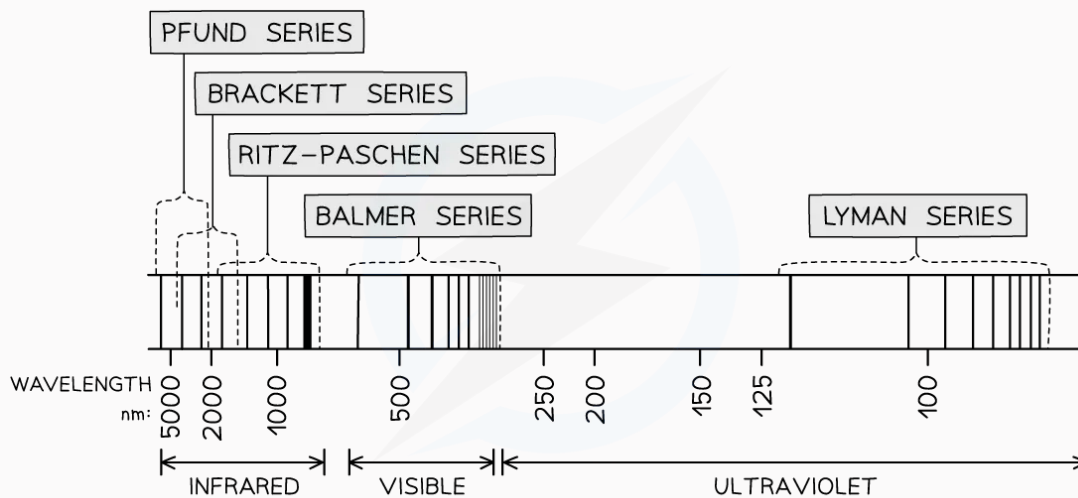


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The line emission (visible) spectrum of hydrogen

- 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



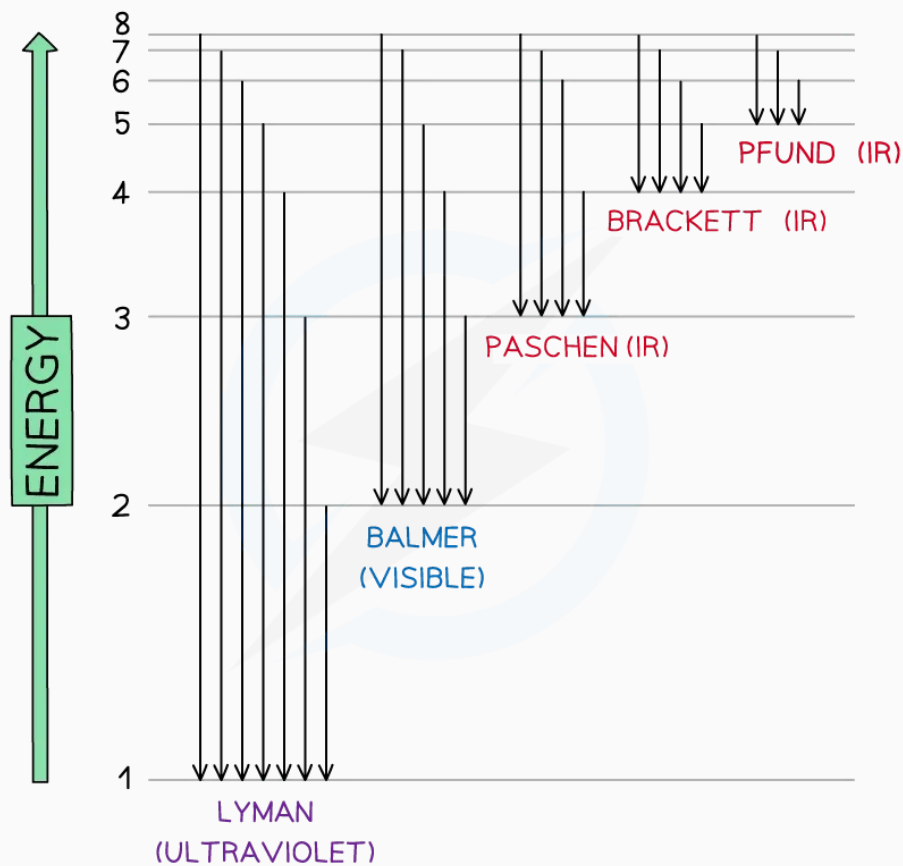
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The full hydrogen spectrum

- 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 $n = 2$

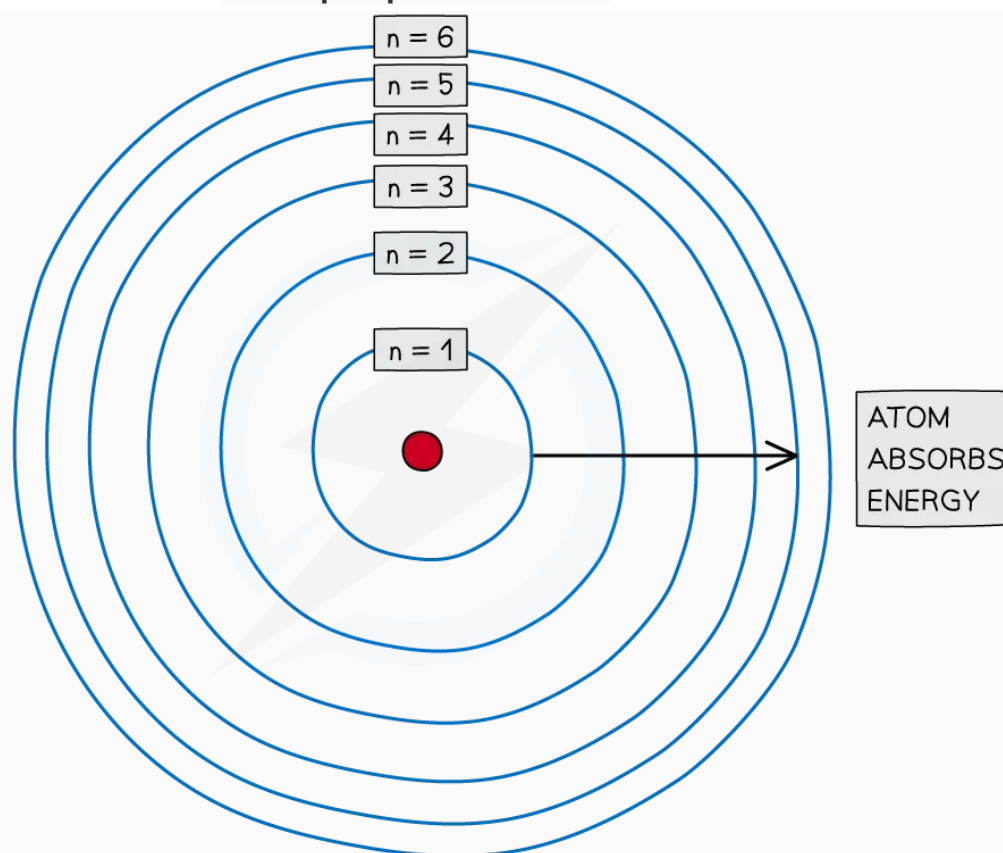
Energy Levels

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



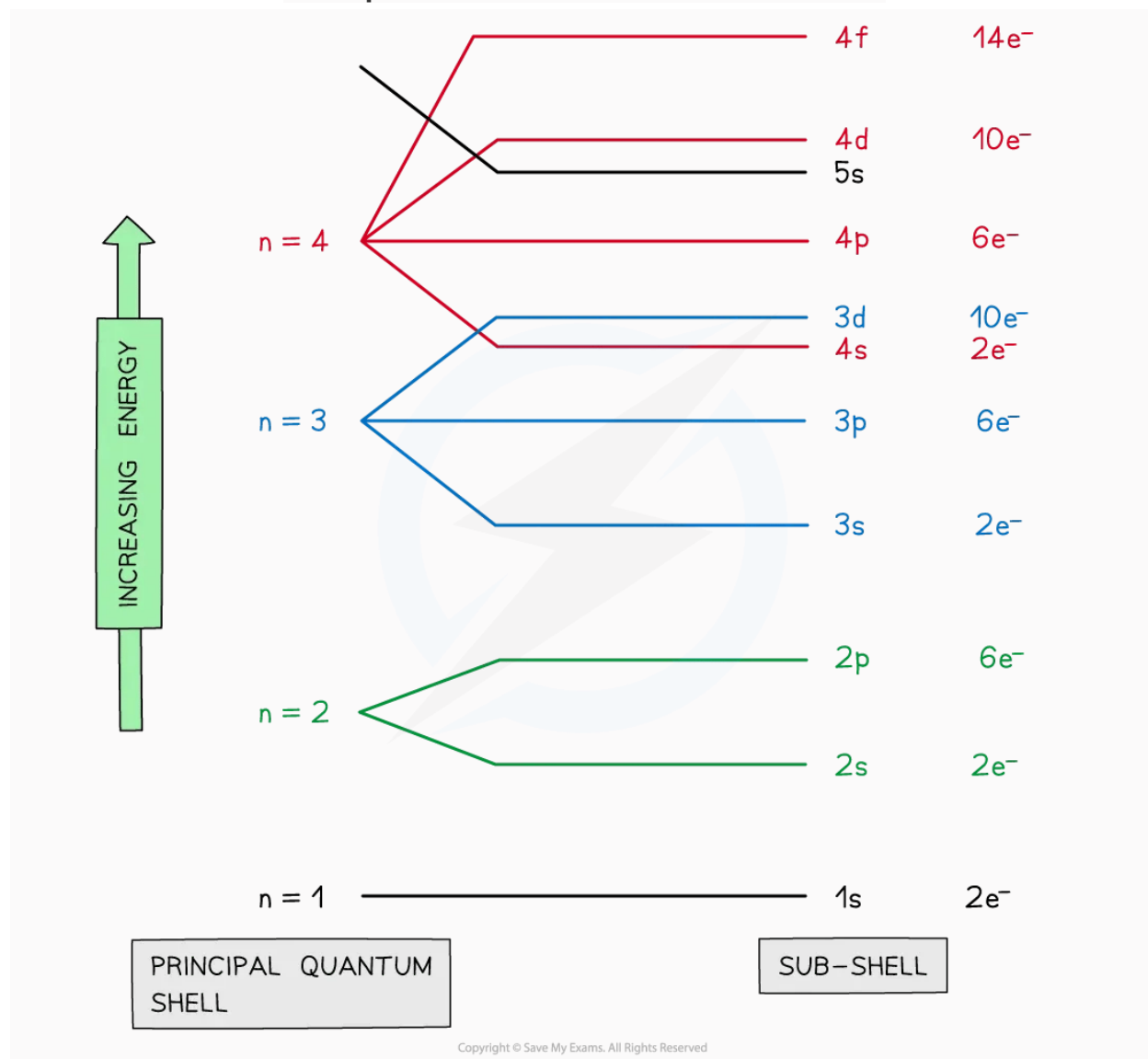
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Electrons are arranged in principal quantum shells, which are numbered by principal quantum numbers

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

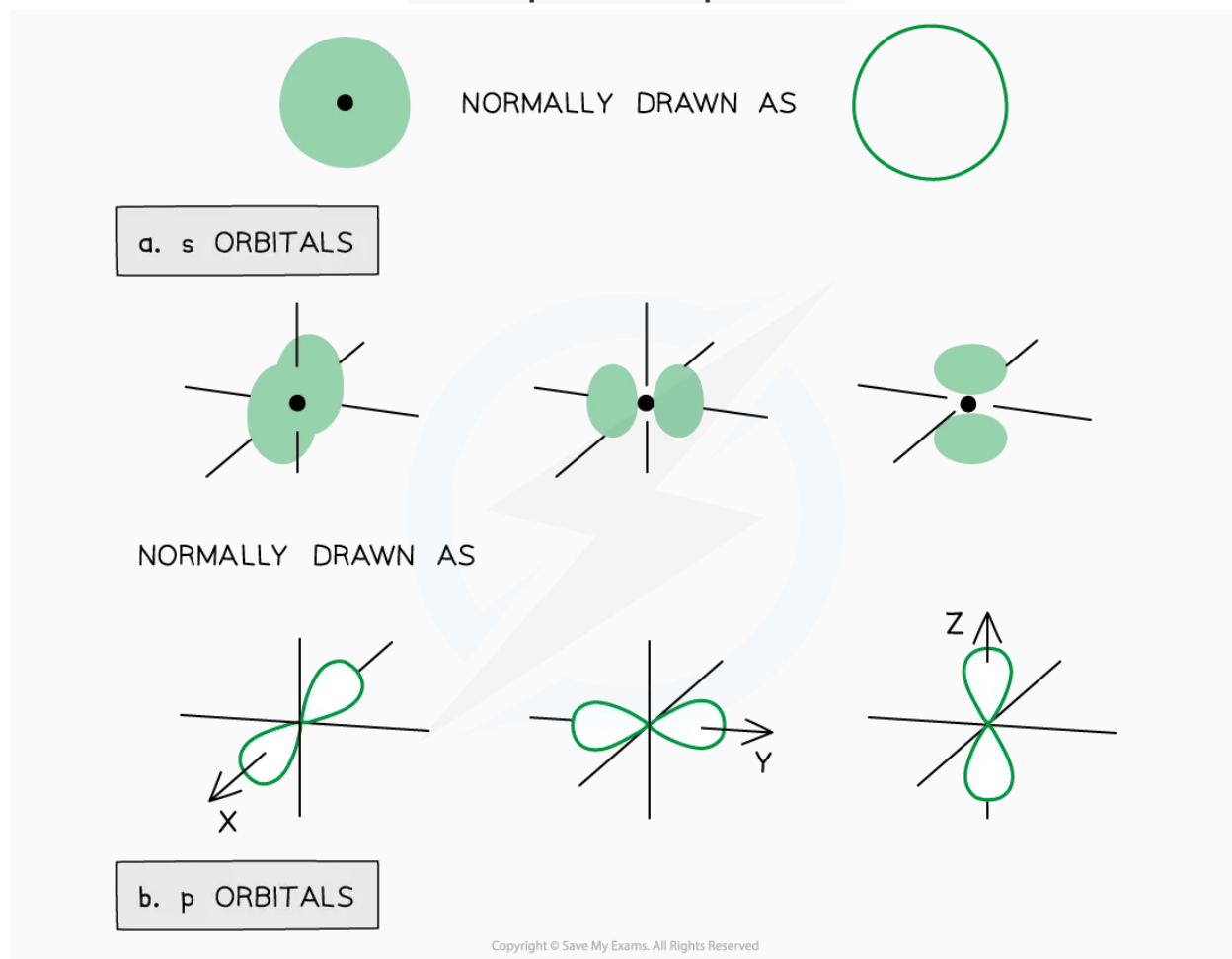


Electrons are arranged in principal quantum shells, which are numbered by principal quantum numbers

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:

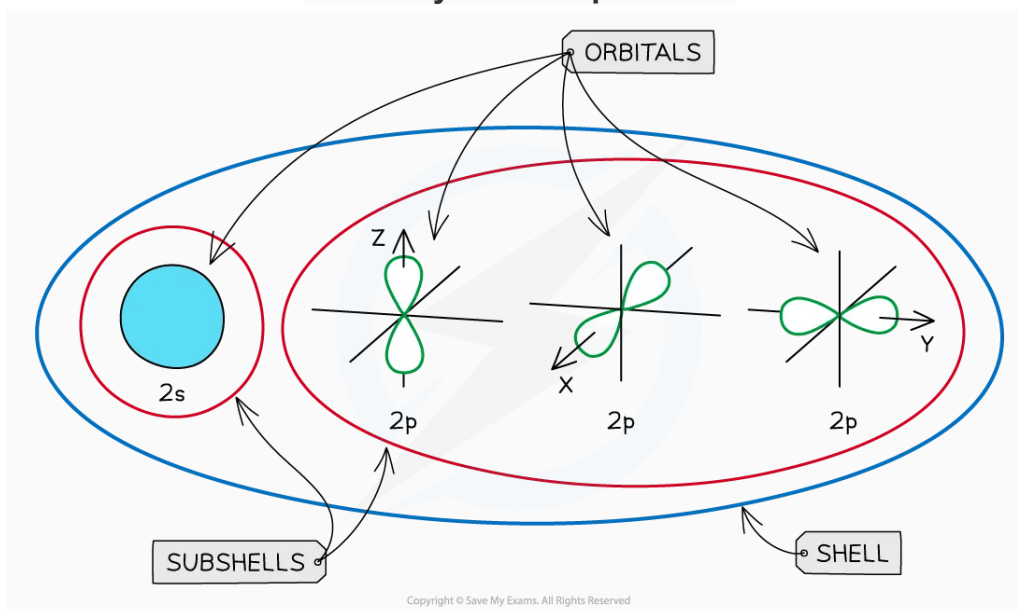
The shape of s and p orbitals



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

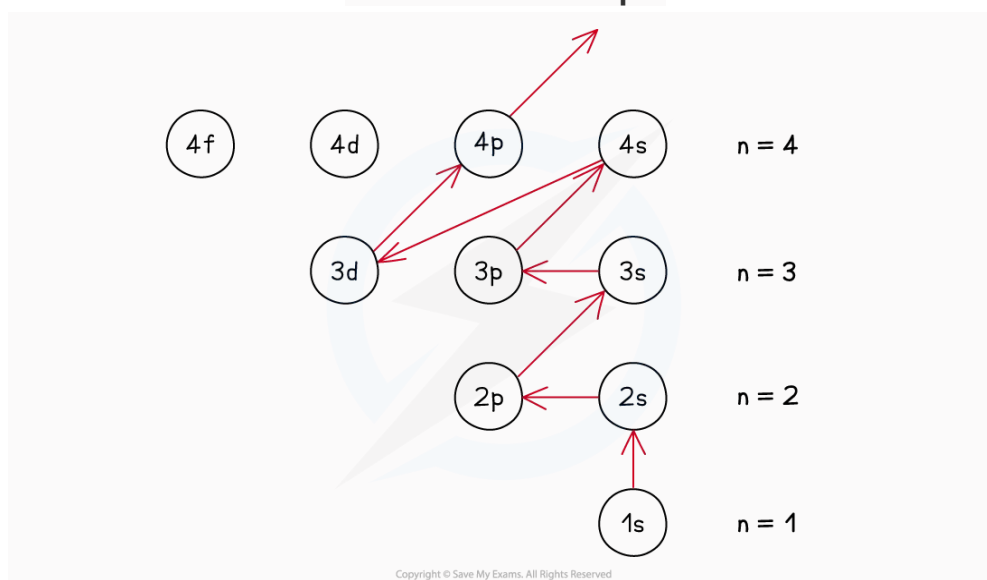


An overview of the shells, subshells and orbitals in an atom

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

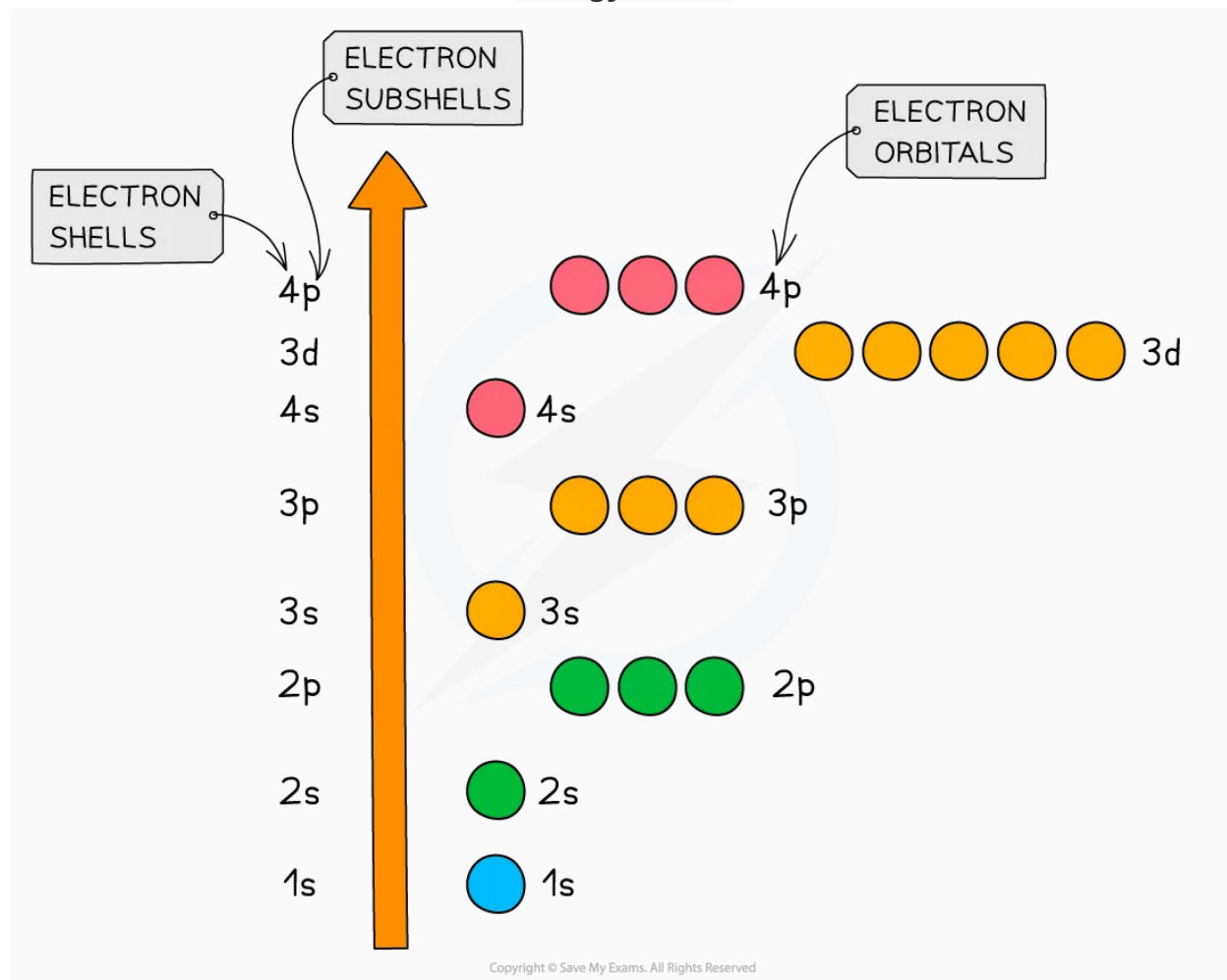


The Aufbau Principle - following the arrows gives you the filling order

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

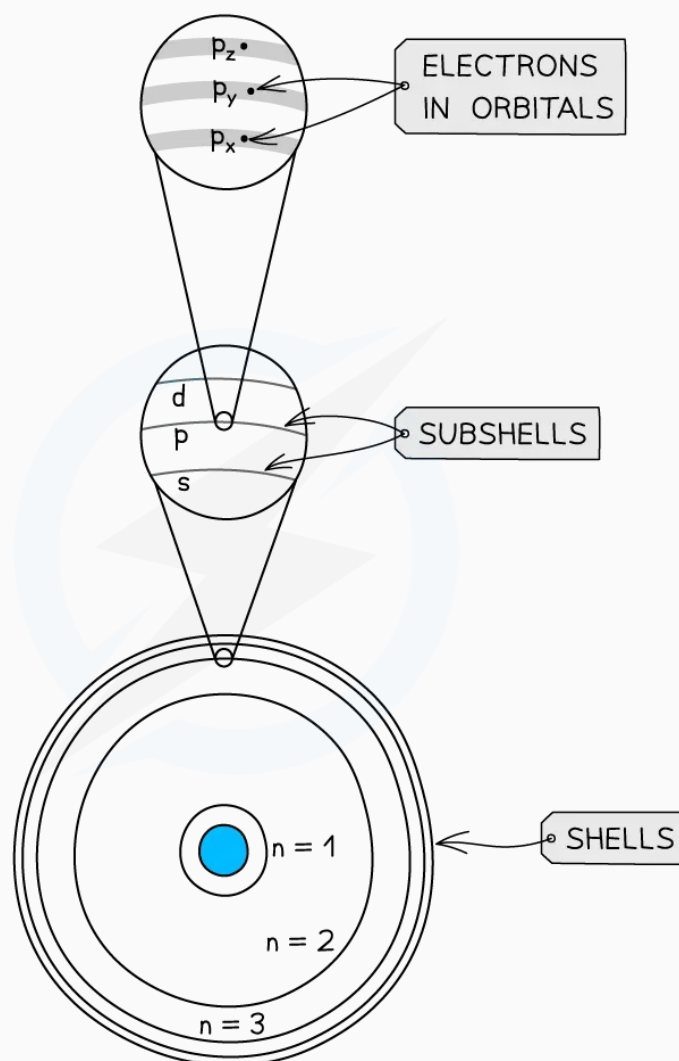


Relative energies of the shells and subshells

- 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

- 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



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Shells are divided into subshells which are further divided into orbitals

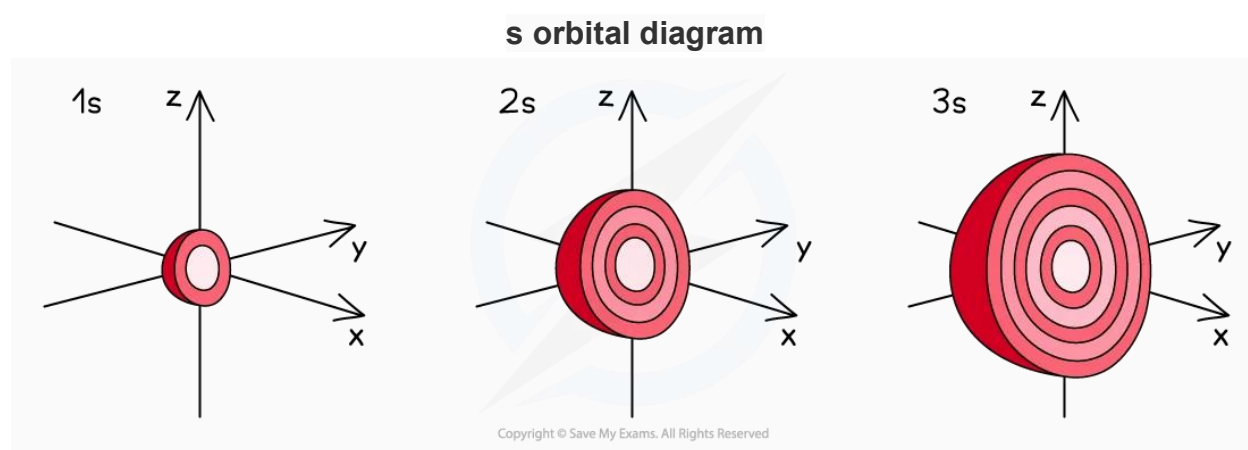
Summary of the Arrangement of Electrons in Atoms Table

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 ($n = 1$)

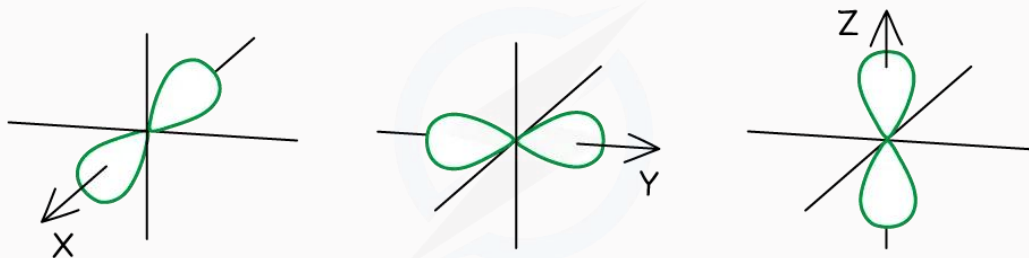


The s orbitals become larger with increasing principal quantum number

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



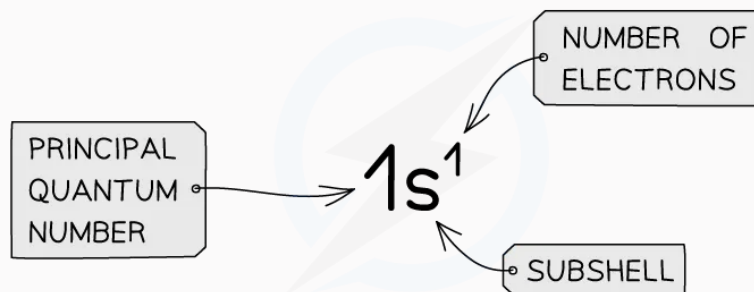
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The p orbitals become larger and longer with increasing principal quantum number

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

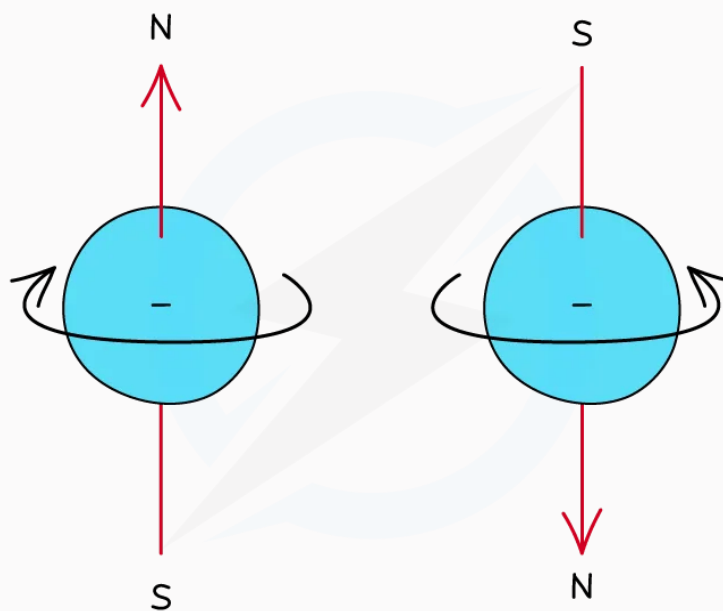


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The electron configuration shows the number of electrons occupying a subshell in a specific shell

- 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

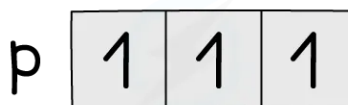


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Electrons can spin either in a clockwise or anticlockwise direction around their own axis. The spin creates a tiny magnetic field with N-S pole pointing up or down, although you are not required to know this for the exam

- 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



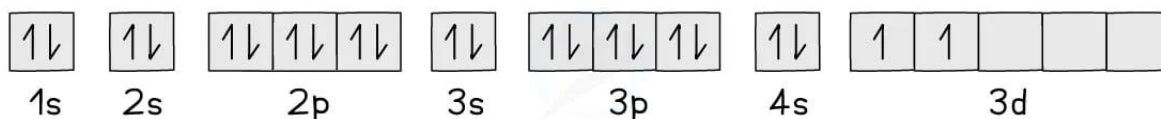
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Electron configuration: three electrons in a p subshell

- 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



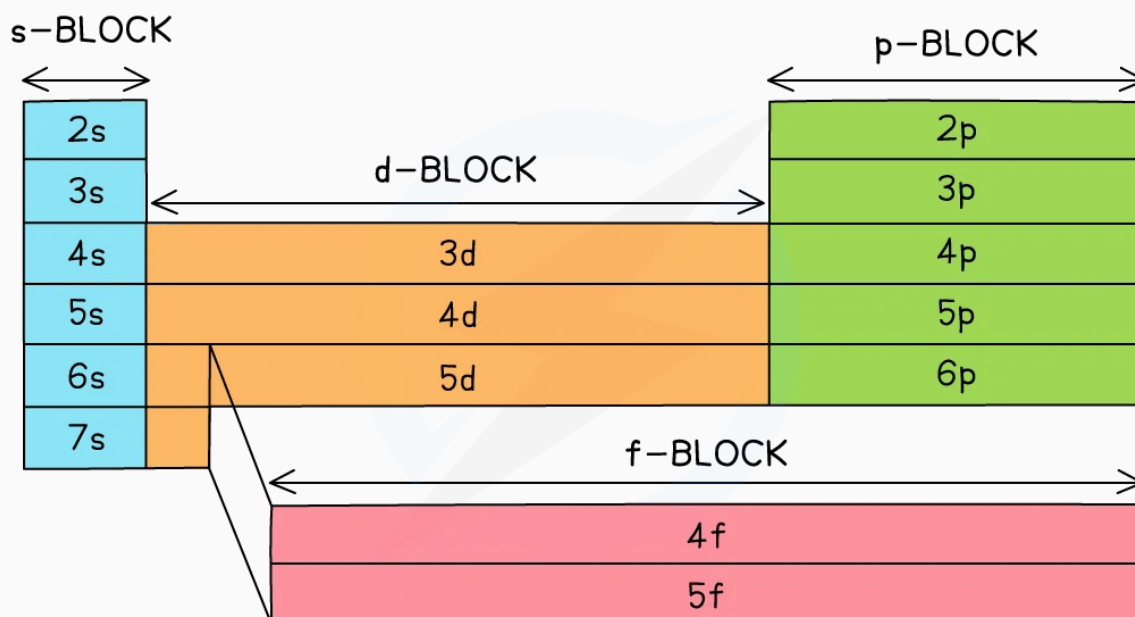
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The electrons in titanium are arranged in their orbitals as shown. Electrons occupy the lowest energy levels first before filling those with higher energy

- 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

- 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:

1. Potassium
2. Calcium
3. Gallium
4. Ca²⁺

Answer 1:

- Potassium has 19 electrons so the full electronic configuration is:
 - 1s² 2s² 2p⁶ 3s² 3p⁶ 4s¹
- 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:
 - [Ar] 4s¹

Answer 2:

- Calcium has 20 electrons so the full electronic configuration is:
 - 1s² 2s² 2p⁶ 3s² 3p⁶ 4s²
- The 4s orbital is lower in energy than the 3d subshell and is therefore filled first
- The shorthand version is [Ar] 4s² 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: 1s² 2s² 2p⁶ 3s² 3p⁶
 - Shorthand: [Ar] 3d¹⁰ 4s² 4p¹

Answer 4:

- If you ionise calcium and remove two of its outer electrons, the electronic configuration of the Ca²⁺ ion is identical to that of argon:
 - Ca²⁺ is 1s² 2s² 2p⁶ 3s² 3p⁶
 - Ar is also 1s² 2s² 2p⁶ 3s² 3p⁶ so the shorthand version is [Ar]

Exam 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

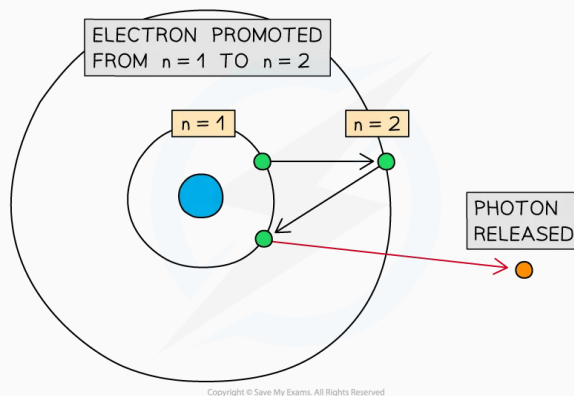
- The arrows you use for electrons can be full or half-headed arrows, but they must be in opposite directions in the same box.

Ionisation Energy from an Emission Spectrum

Emission Spectra

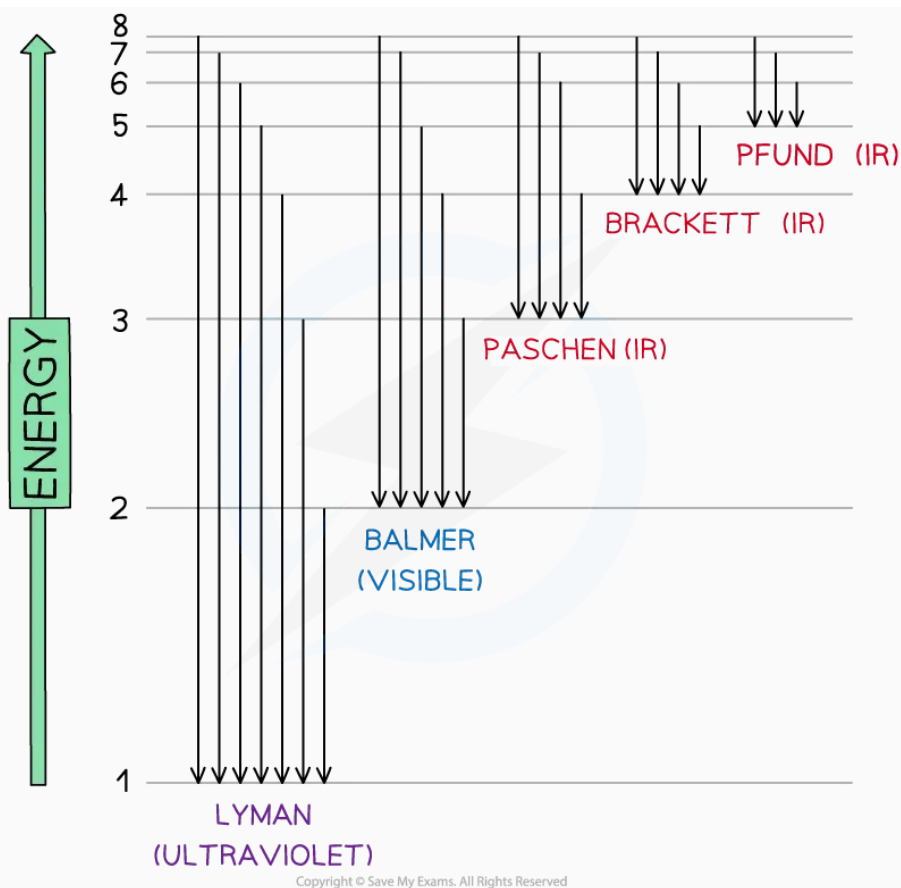
- Electrons move rapidly around the nucleus in energy shells
- Heat or electricity can be used to excite an electron to a higher main energy level
- These range from $n = 1$ (ground state) to $n = \infty$
- When the electrons 'fall' back down they must lose the energy difference between the two energy 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

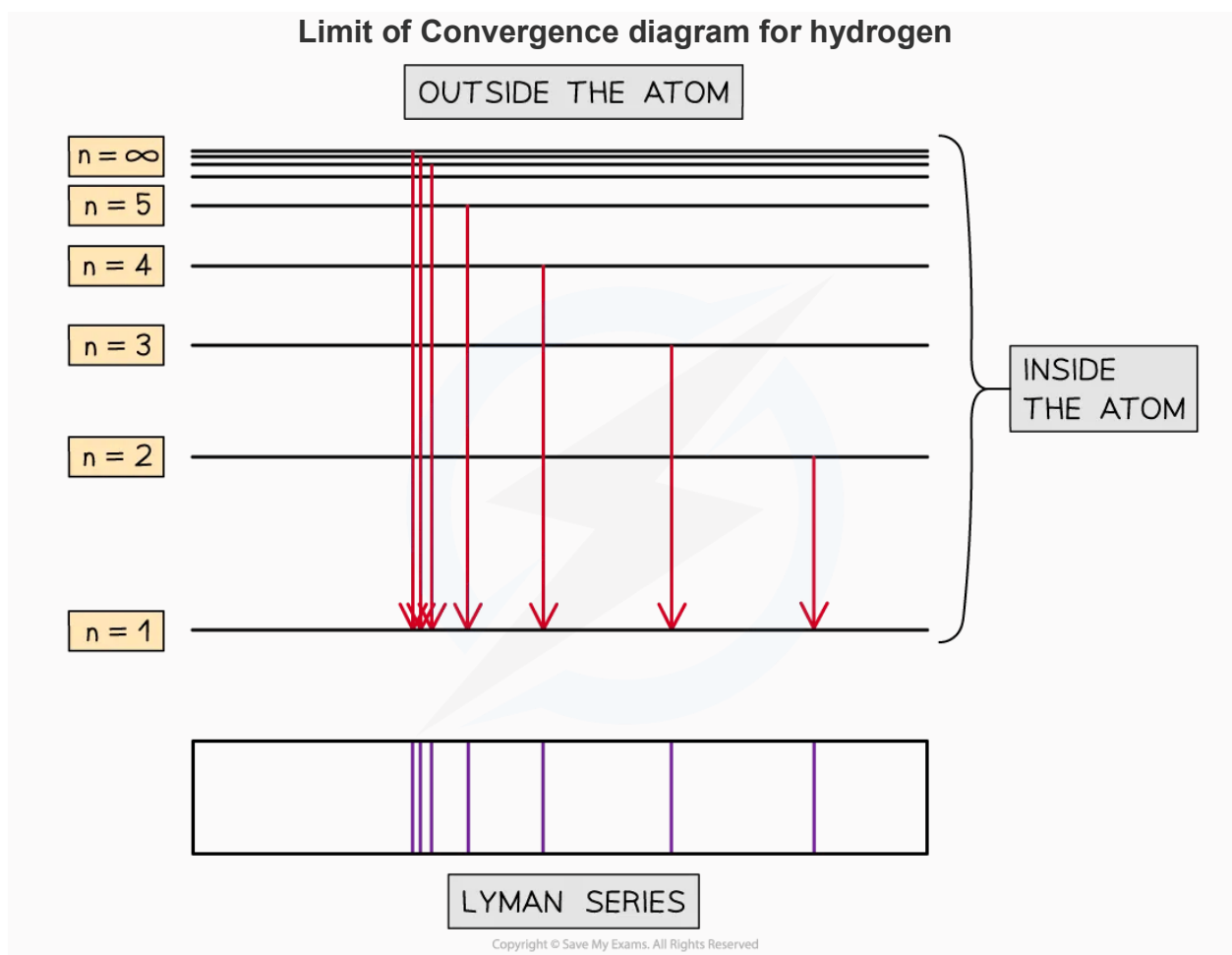
- This gives evidence for Bohr's model which is the idea that electrons exist in discrete energy levels so an exact amount of energy is required for an electron to 'jump' an energy level, a little like a ladder
- There are however limitations to this model
 - Assumes positions of electrons are fixed
 - 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
- 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 $91.16 \times 10^{-9} \text{ m}$



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, (IE_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 (6.63×10^{-34} J s)
 - ν = frequency (s^{-1})
 - λ = wavelength (m)
 - c = speed of light (3.00×10^8 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 (IE_1)

$$\Delta E = h \nu$$

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

$$IE_1 = 6.63 \times 10^{-34} \times 1.24 \times 10^{15}$$

$$IE_1 = 8.22 \times 10^{-19} \text{ J atom}^{-1}$$

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

$$IE_1 = 8.22 \times 10^{-19} \times 6.02 \times 10^{23}$$

$$IE_1 = 494\,916 \text{ J mol}^{-1}$$

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

$$IE_1 = 495 \text{ kJ mol}^{-1}$$

So the first ionisation energy (IE_1) of sodium has been calculated as 495 kJ mol^{-1}

Worked example

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

Answer:

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

$$c = \nu \lambda$$

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

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

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

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

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

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

Exam 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) 6.02×10^{23} and converting units to kJ mol^{-1}
- Finally, when working through calculations, keep the numbers in your calculator to avoid rounding up too early.

Successive Ionisation Energies

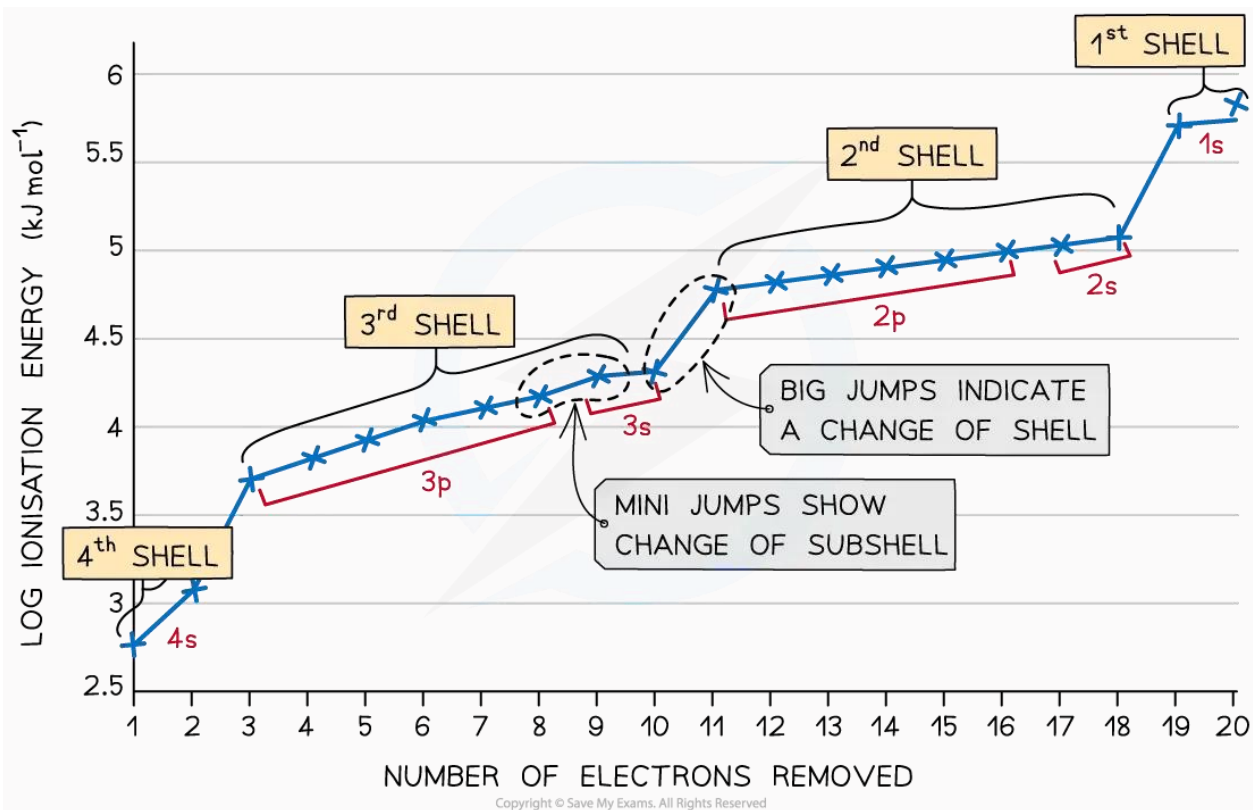
Successive ionisation energies of an element

- 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^{-1})	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

Element	Atomic Number	Ionisation Energy (kJ mol ⁻¹)			
		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 1s² 2s² 2p⁶ 3s¹

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 $1s^2 2s^2 2p^6 3s^2 3p^1$

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

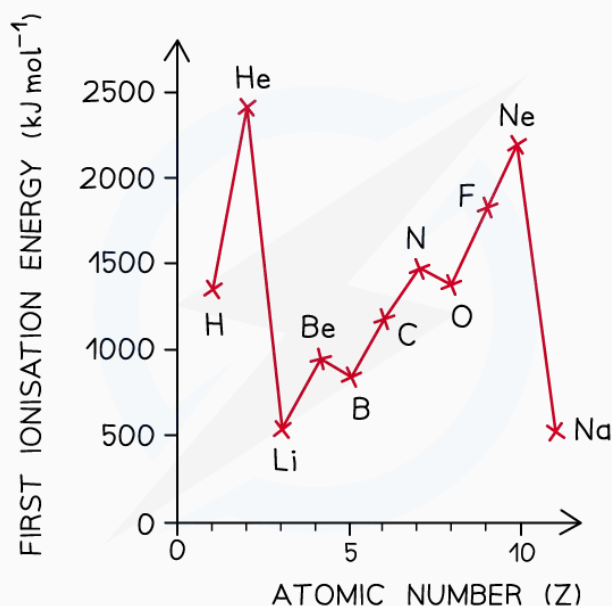
Ionisation number	1	2	3	4	5	6	7	8
Ionisation energy (kJ mol ⁻¹)	1314	3388	5301	7469	1089	13327	71337	84080

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

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 IE_1 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 kJ mol⁻¹ as its electron configuration is $1s^2 2s^2$
 - Boron has a first ionisation energy of 800 kJ mol⁻¹ as its electron configuration is $1s^2 2s^2 2p_x^1$
- There is a slight decrease in IE_1 between nitrogen and oxygen due to spin-pair repulsion in the 2p_x orbital of oxygen
 - Nitrogen has a first ionisation energy of 1400 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 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