SL IB Chemistry

Your notes

Electronic Configurations

Contents

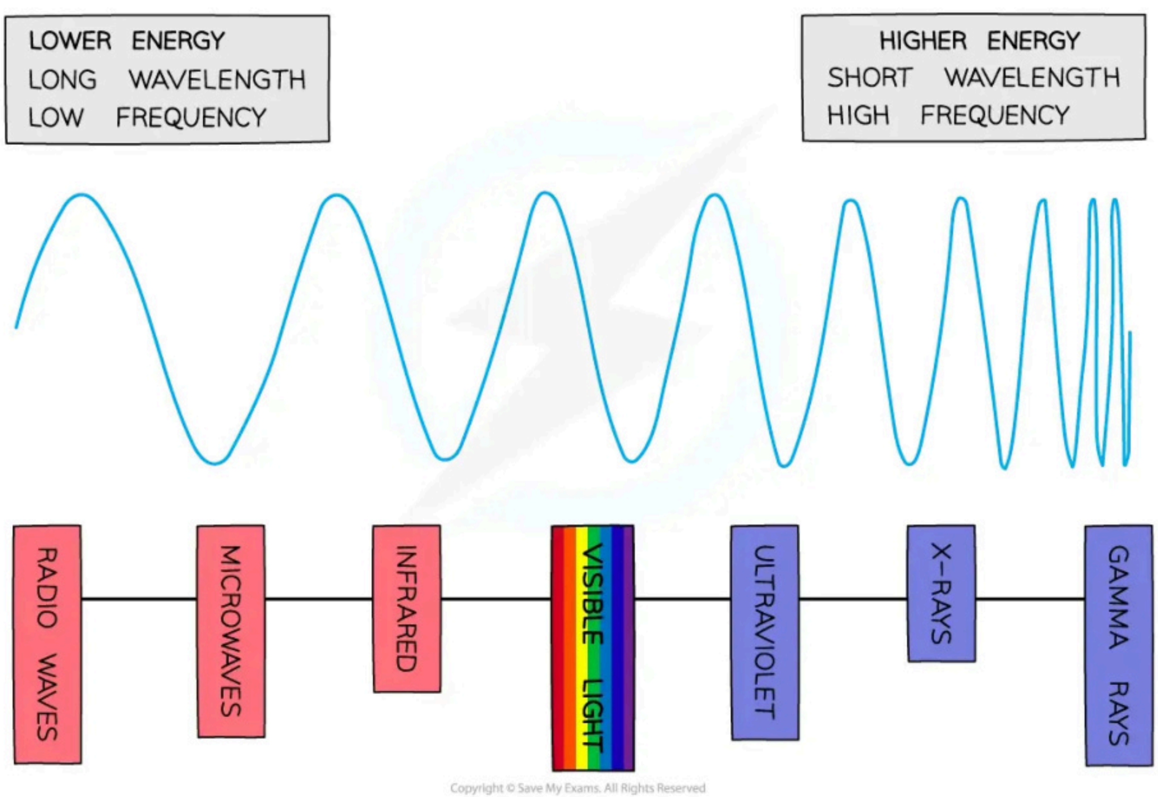
The Electromagnetic Spectrum

Your notes

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

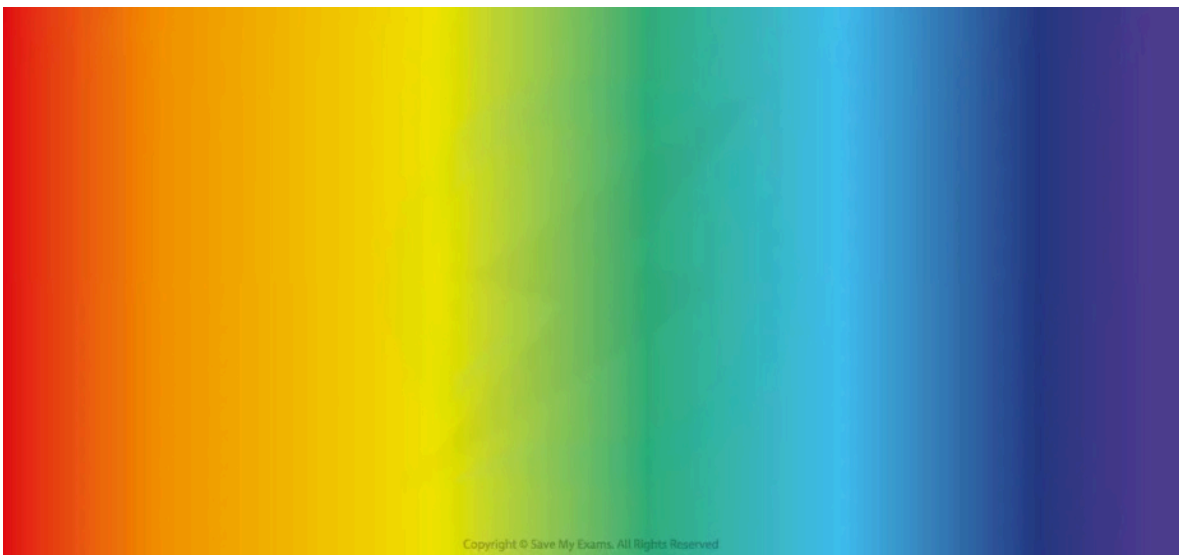
- All light waves travel at the same speed; what distinguishes them is their different frequencies

- The speed of light (symbol '**c**') is constant and has a value of **3.00×10^8 ms^{-1}**
- As you can see from the spectrum, frequency (symbol '**f**') is inversely proportional to wavelength (symbol '**λ**')
  - In other words, the higher the frequency, the shorter the wavelength
- The equation that links them is **$c = f\lambda$**
- 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

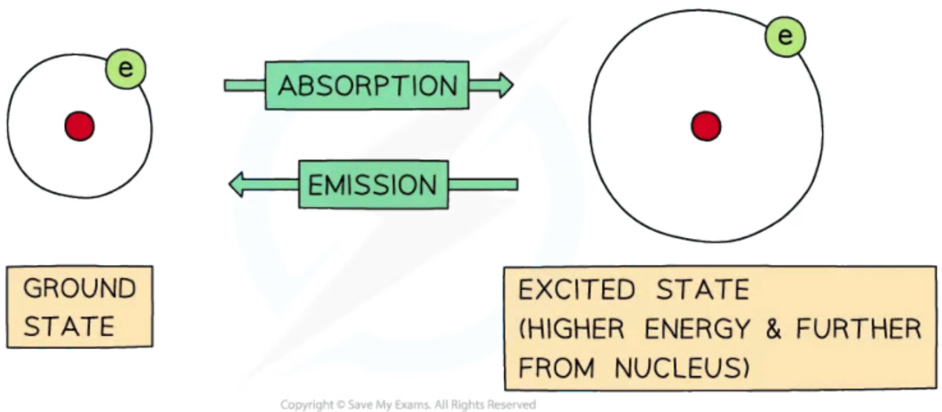
Your notes

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

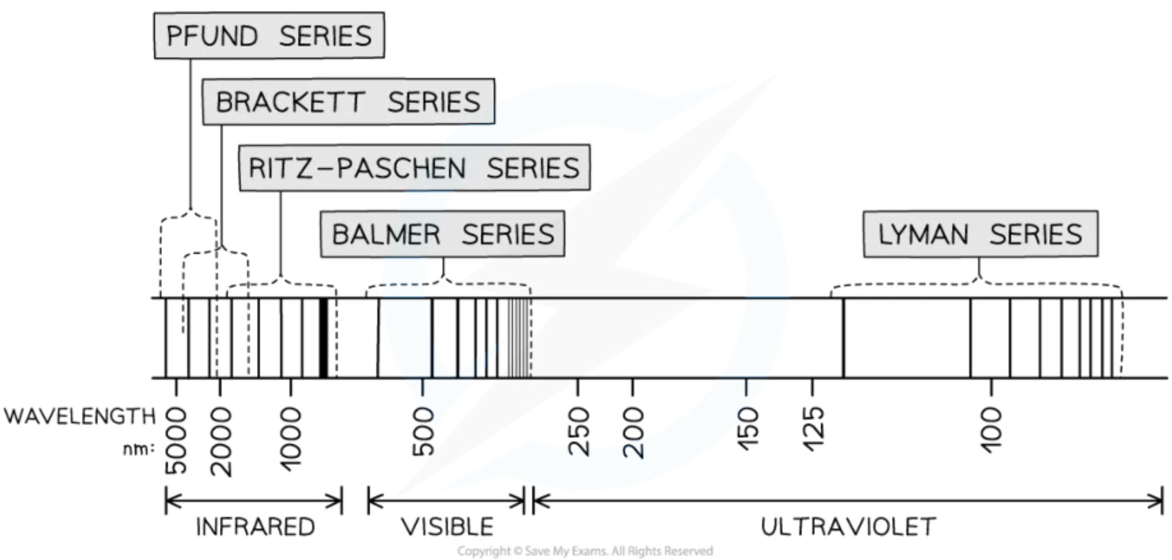
Spectrum of hydrogen diagram

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



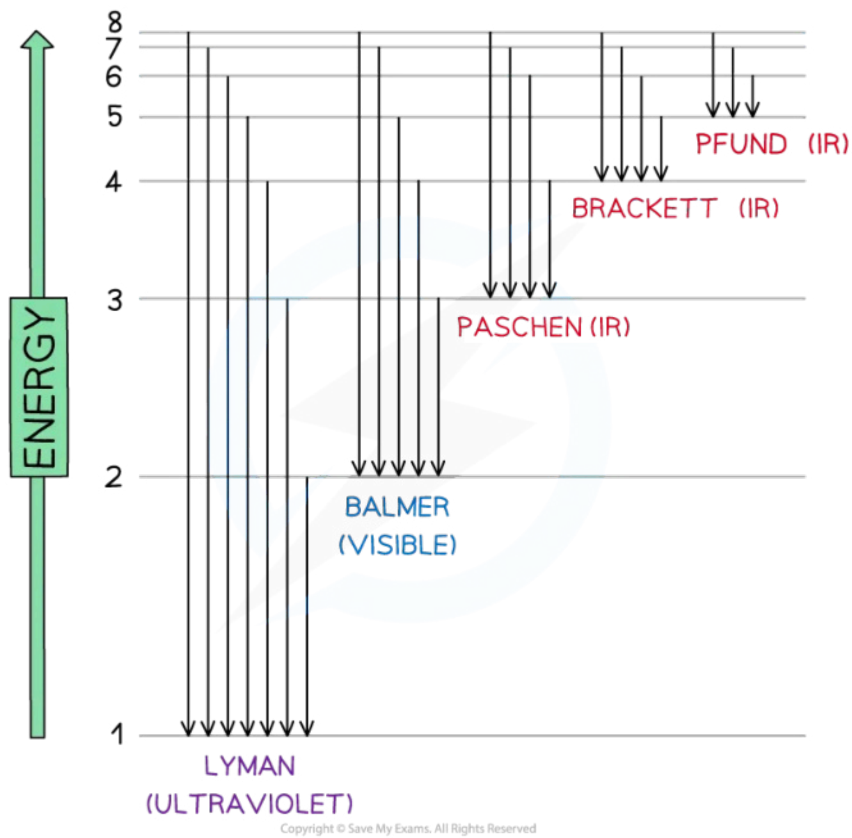
The full hydrogen spectrum

- 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

Your notes

Your notes



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

Your notes

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

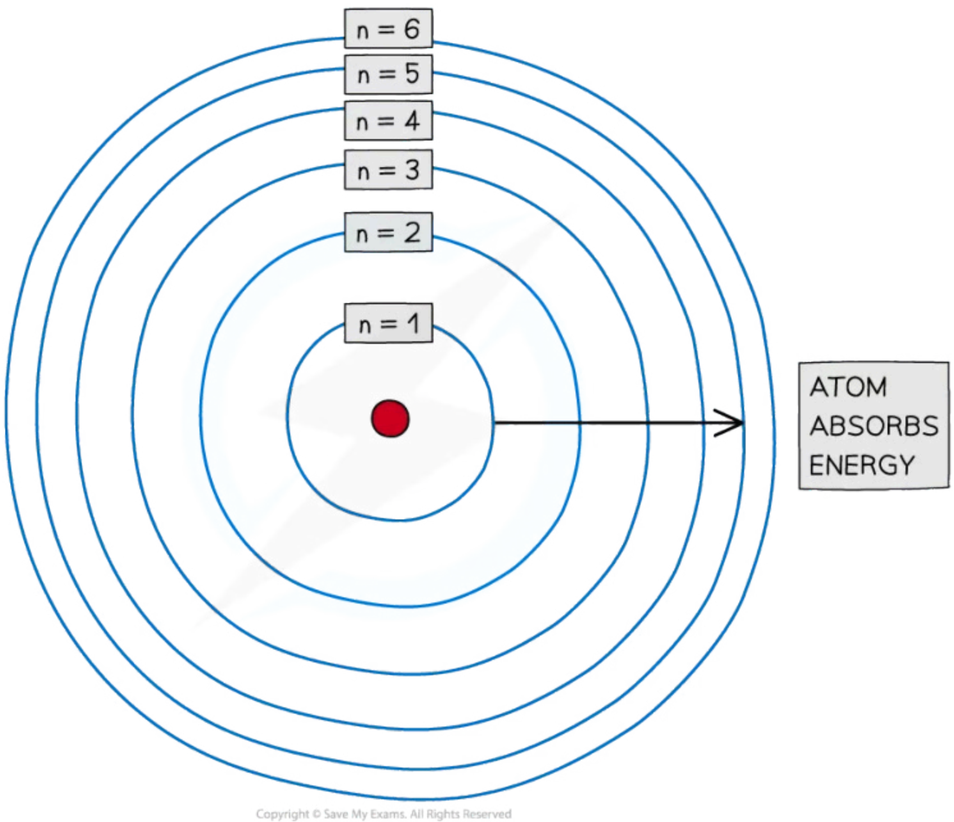
Energy Levels

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 x (3^2) = 18

Principle quantum shells

Your notes

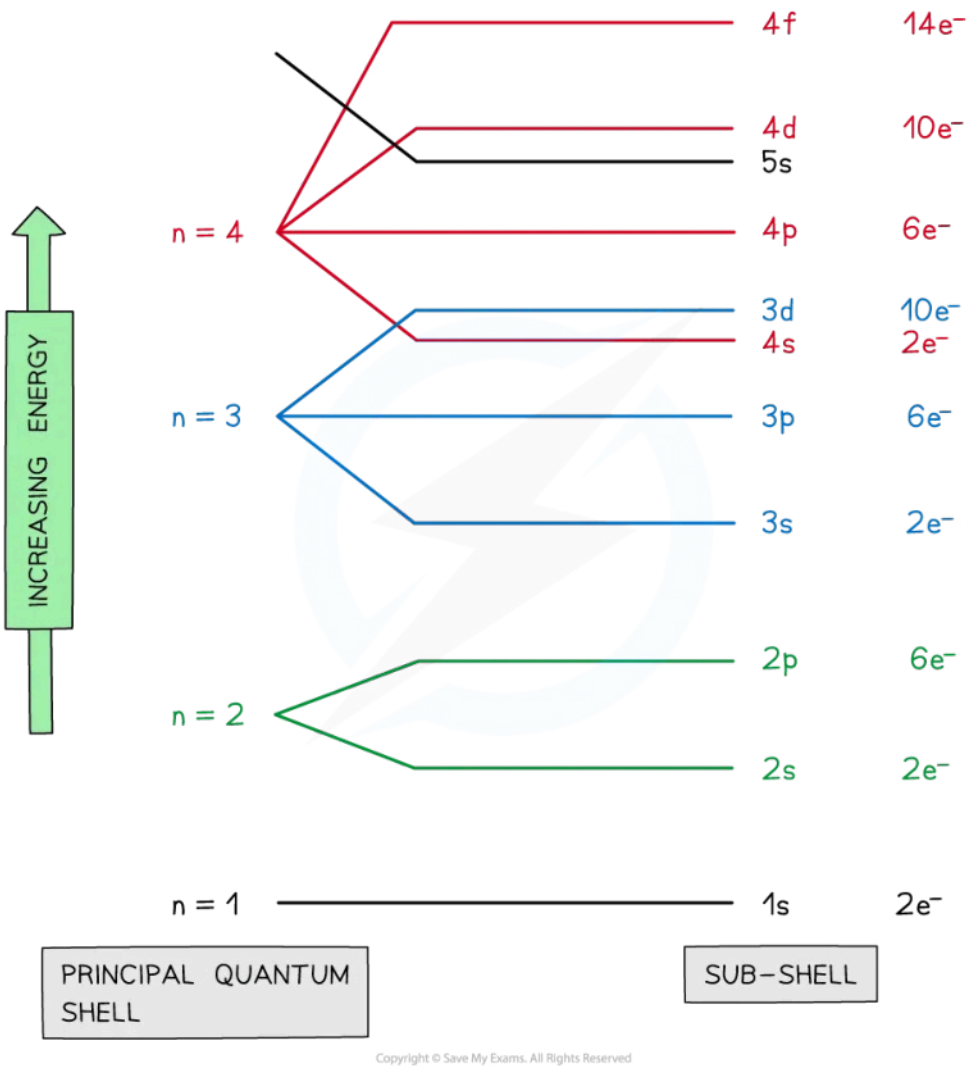


Electrons are arranged in principal quantum shells, which are numbered by principal quantum numbers

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



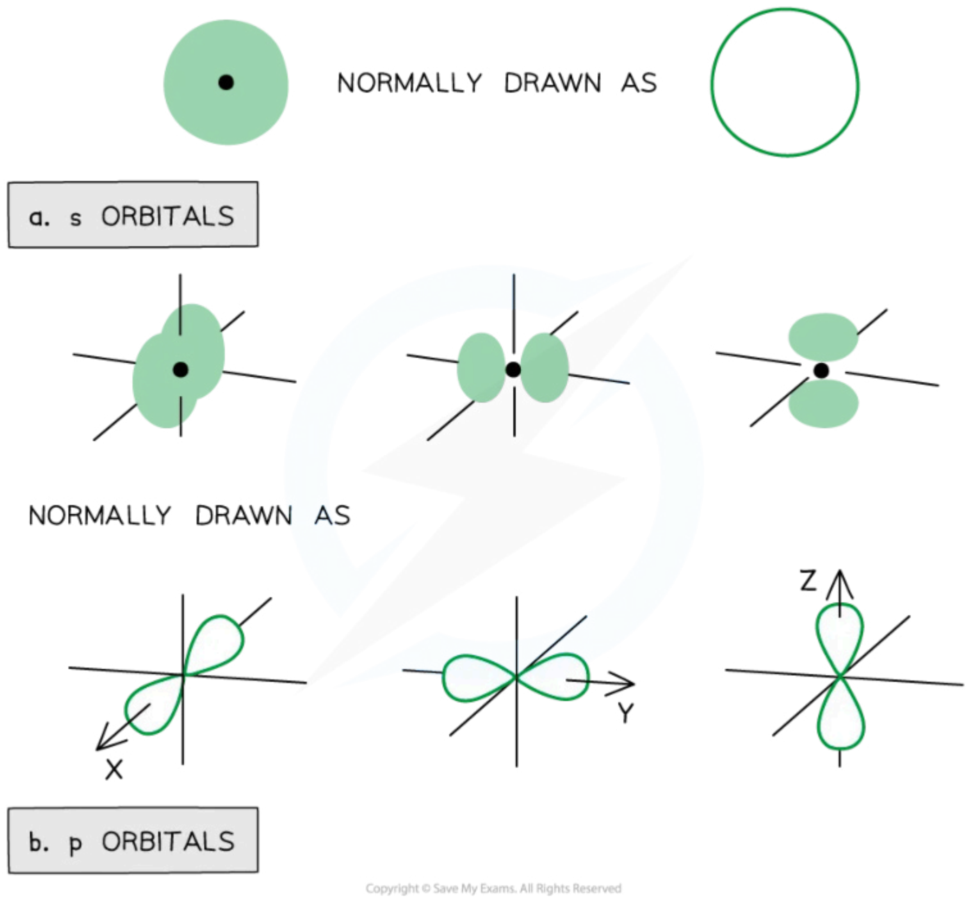
Electrons are arranged in principal quantum shells, which are numbered by principal quantum numbers

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

Your notes

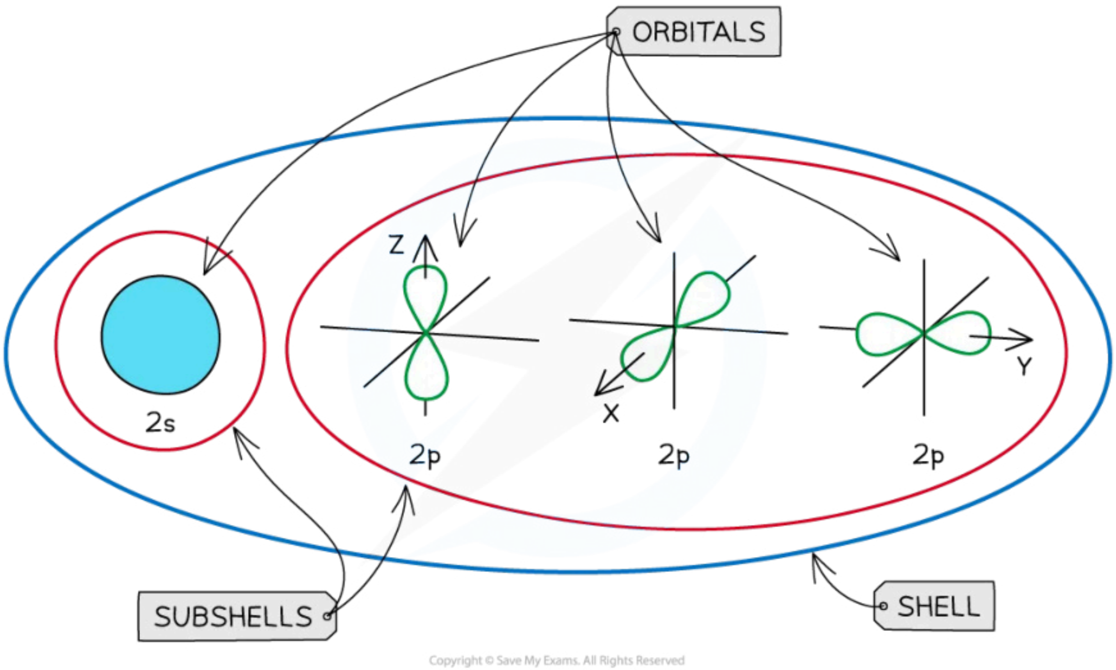


Representation of orbitals (the dot represents the nucleus of the atom) showing spherical s orbitals (a), p orbitals containing 'lobes' along the x, y and z axis

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

Summary of s and p orbitals

Your notes



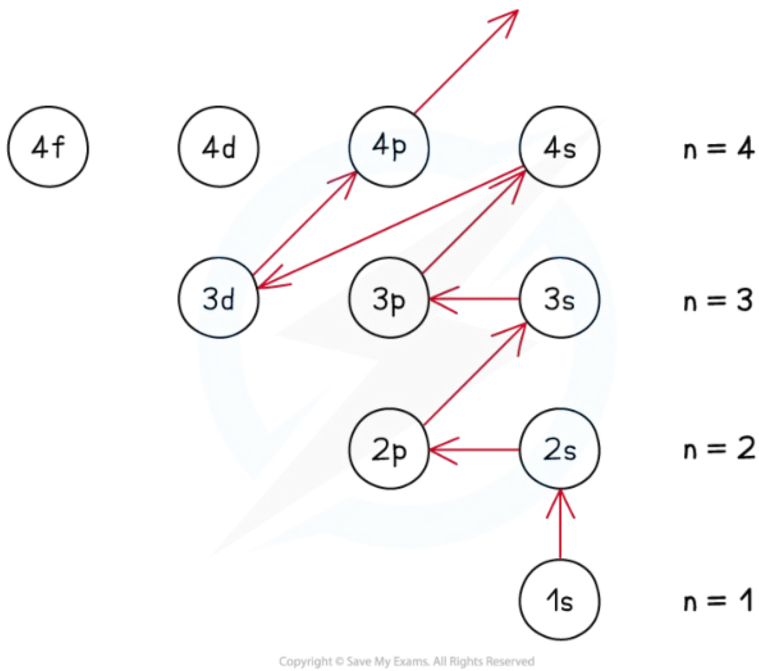
An overview of the shells, subshells and orbitals in an atom

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

Your notes



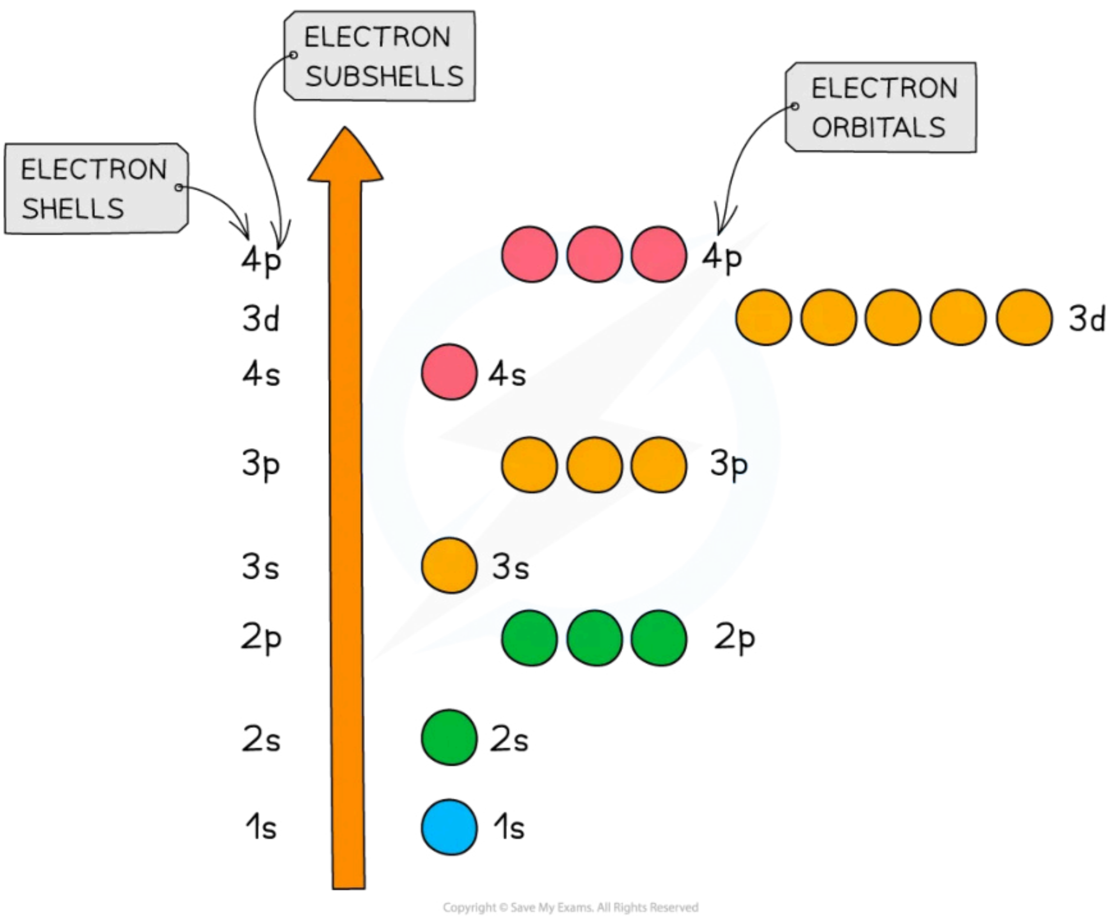
The Aufbau Principle – following the arrows gives you the filling order

Your notes

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



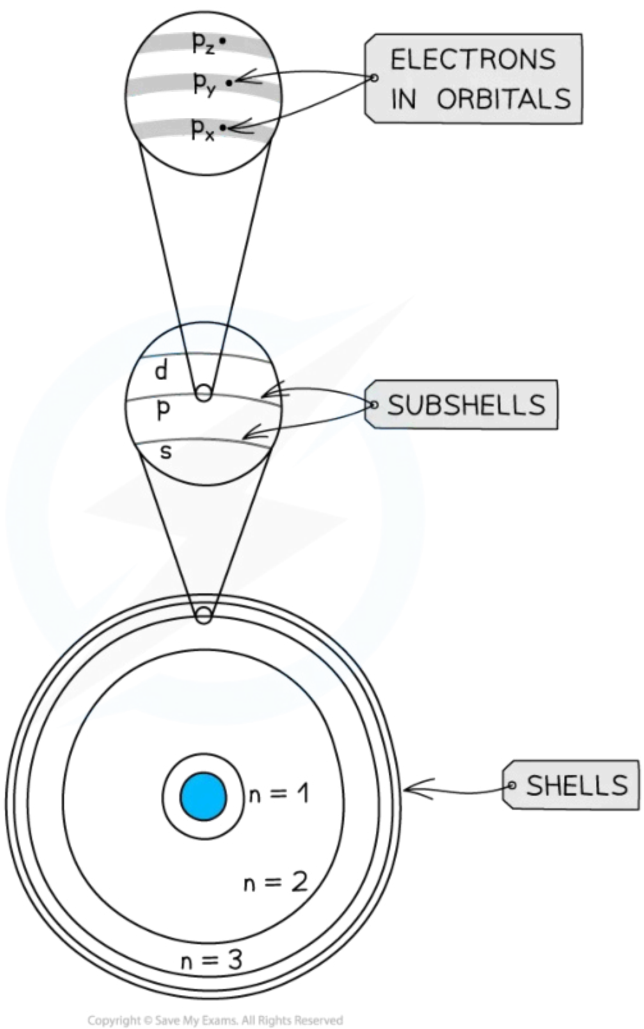
Relative energies of the shells and subshells

- 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

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 x 2 = total of 2 electrons
  - p : 3 x 2 = total of 6 electrons
  - d : 5 x 2 = total of 10 electrons
  - f : 7 x 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 px orbital is the same as a p_y orbital

Division of Shells Diagram



Shells are divided into subshells which are further divided into orbitals

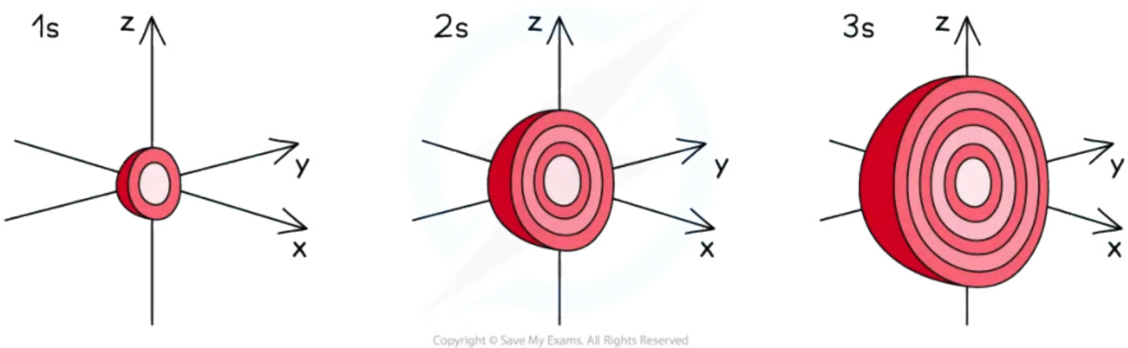
Summary of the Arrangement of Electrons in Atoms Table

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

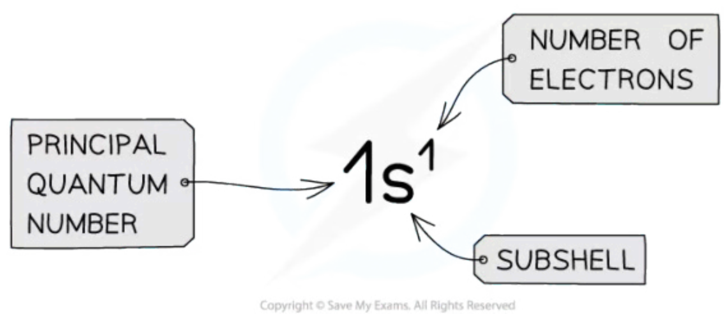
Your notes

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

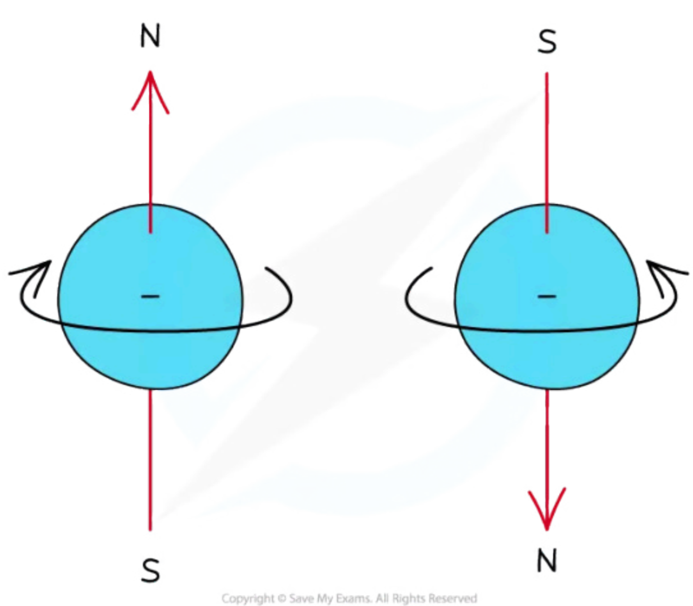
Electron Configuration Key



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**

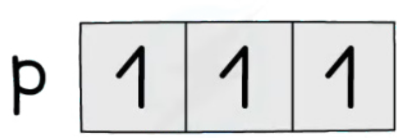
Spin pair repulsion diagram



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

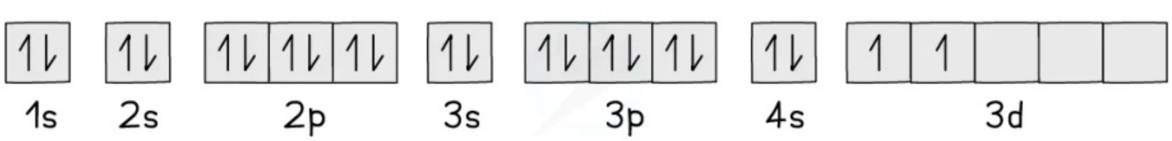


Electron configuration: three electrons in a p subshell

- 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 - the 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

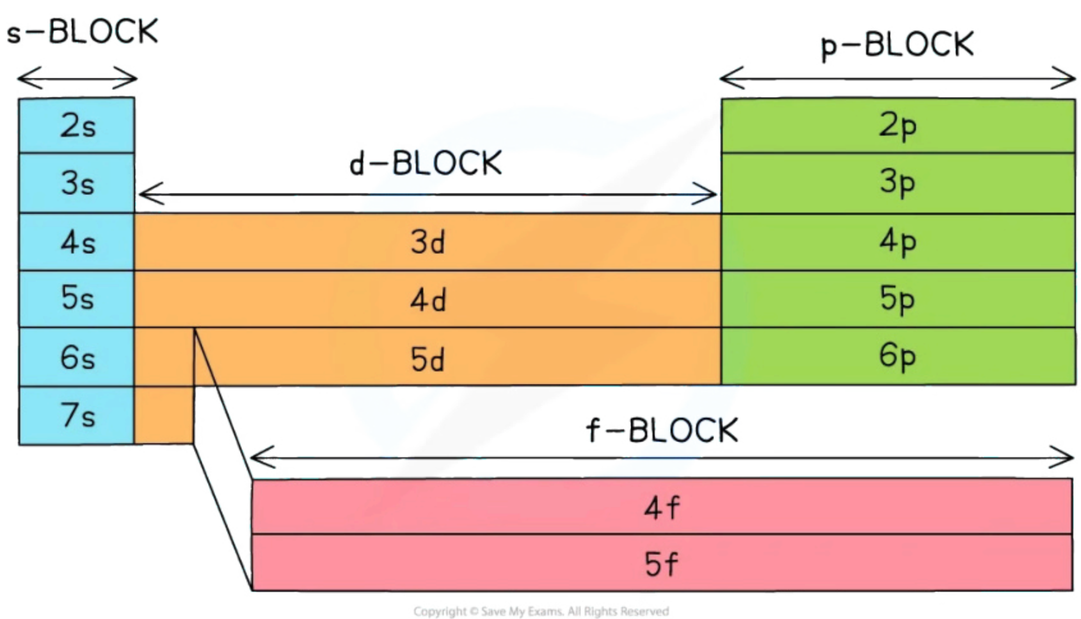


Your notes

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



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 [Ar] $3d^5$ $4s^1$ **not** [Ar] $3d^4$ $4s^2$
  - Cu is [Ar] $3d^{10}$ $4s^1$ **not** [Ar] $3d^9$ $4s^2$
- This is because the [Ar] $3d^5$ $4s^1$ and [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. 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:
  - [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 [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**: [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 Ca^{2+} ion is identical to that of argon:
  - **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 [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