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Chemistry

For the IB Diploma

> Chapter 3

Electron configurations

> The electromagnetic spectrum

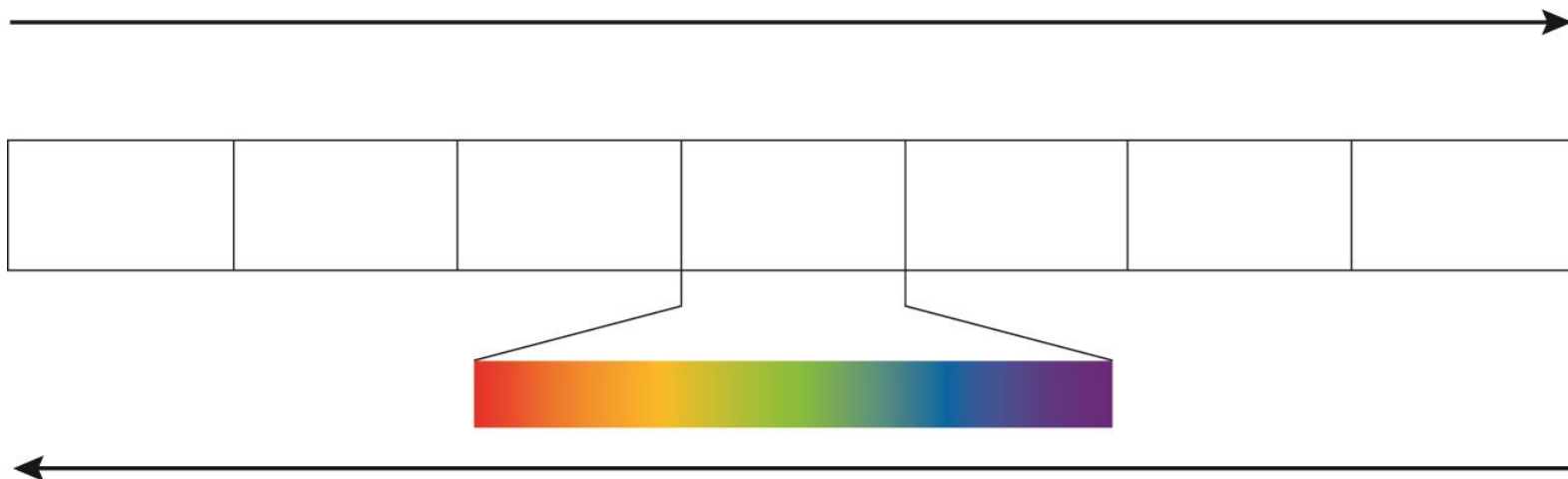


Figure 3.1: The electromagnetic spectrum.

$$\text{frequency} \propto \frac{1}{\text{wavelength}}$$

$$\text{frequency} \propto \text{energy}$$

$$\text{energy} \propto \frac{1}{\text{wavelength}}$$

> Hydrogen emission spectrum

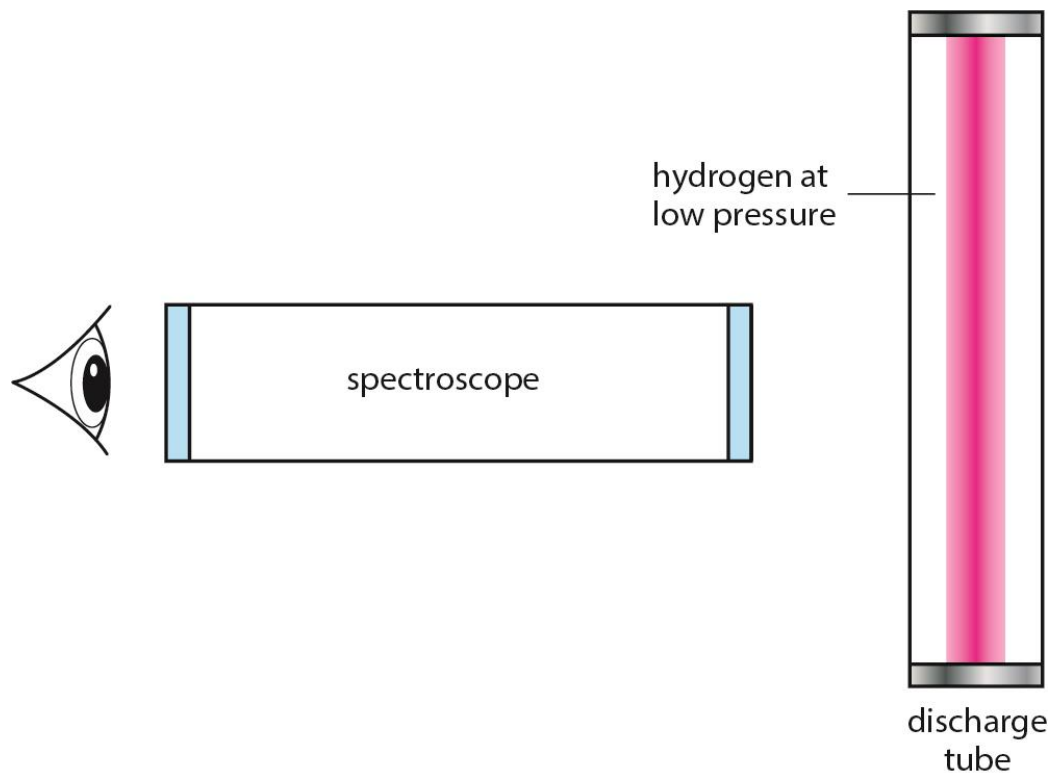


Figure 3.2: Observing the emission spectrum of hydrogen.

> How do the lines arise in the emission spectrum of hydrogen?

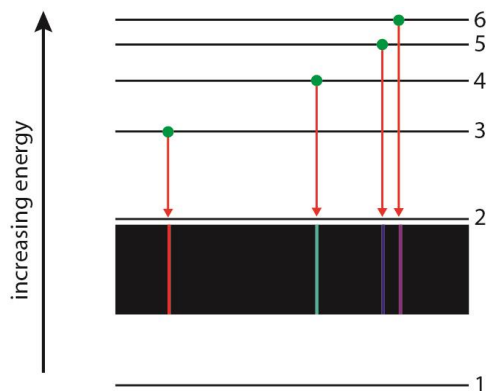


Figure 3.3: A representation of the atomic emission spectrum of hydrogen.

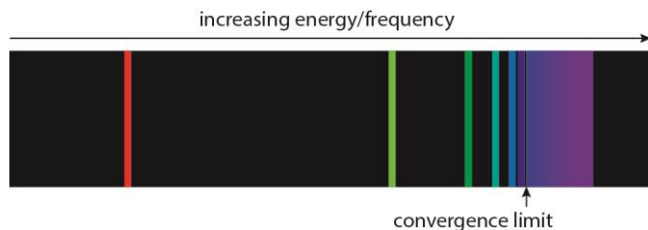


Figure 3.4: A representation of the Lyman series (electron falling to $n = 1$) of hydrogen in the ultraviolet region of the electromagnetic spectrum.

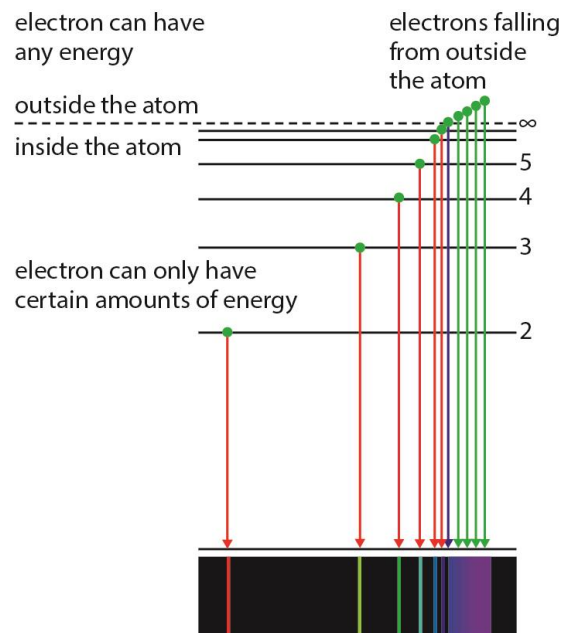


Figure 3.5: The purple arrow represents the transition giving rise to the convergence limit in the Lyman series (electron falling from just outside the atom to $n = 1$) for hydrogen.

➤ The sub-levels and number of electrons in each sub-level

Main energy level	Sub-levels				Number of electrons in each sub-level			
					s	p	d	f
1	1s				2			
2	2s	2p			2	6		
3	3s	3p	3d		2	6	10	
4	4s	4p	4d	4f	2	6	10	14
5	5s	5p	5d	5f	2	6	10	14

> The ordering of the energy levels and sub-levels within an atom

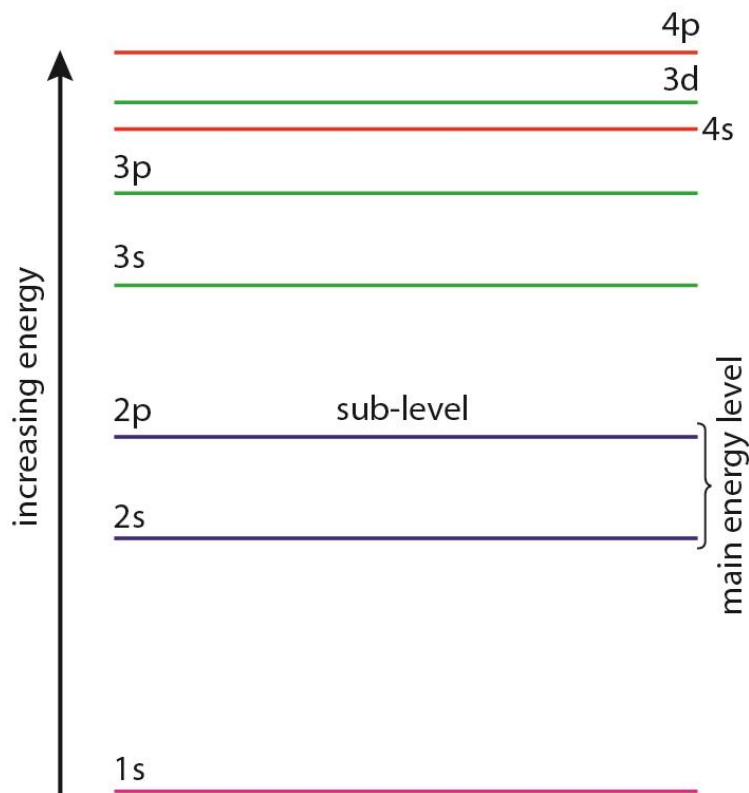
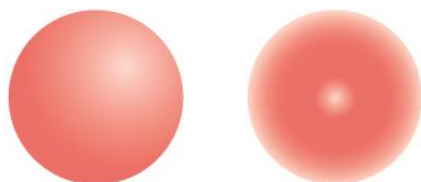


Figure 3.6: The ordering of the energy levels and sub-levels within an atom. The sub-levels within a main energy level are shown in the same colour.

> Orbital diagrams



a

b

Figure 3.7: **a** The shape of a 1s orbital; **b** the electron density in a 1s orbital.

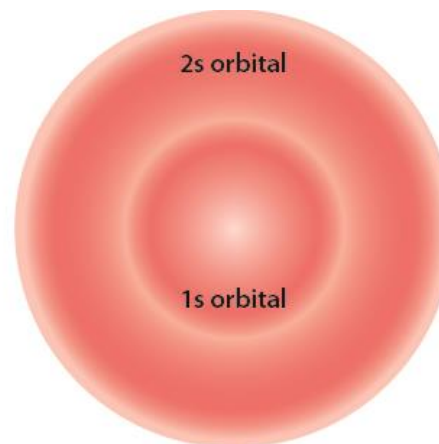
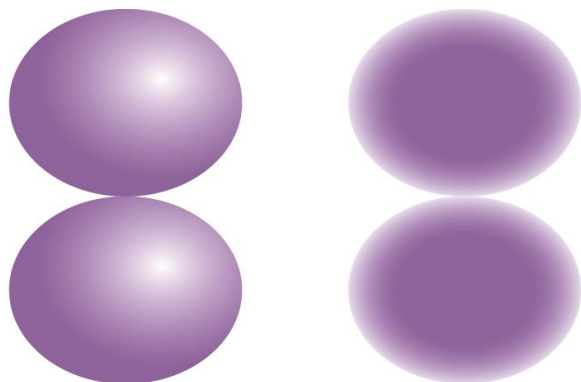


Figure 3.8: A cross section of the electron density of the 1s and 2s orbitals together.



a

b

Figure 3.9: **a** The shape of a 2p orbital; **b** the electron density in a 2p orbital.

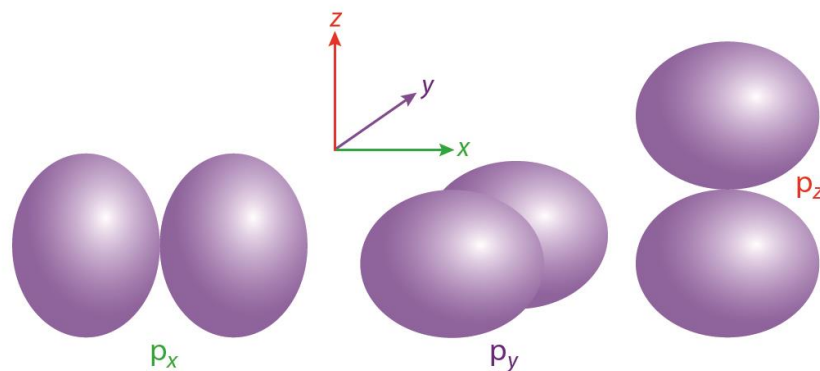


Figure 3.10: The three p orbitals that make up a p sub-level pointing at 90° to each other.

> The Aufbau principle

How do you work out the electron configurations of the elements?

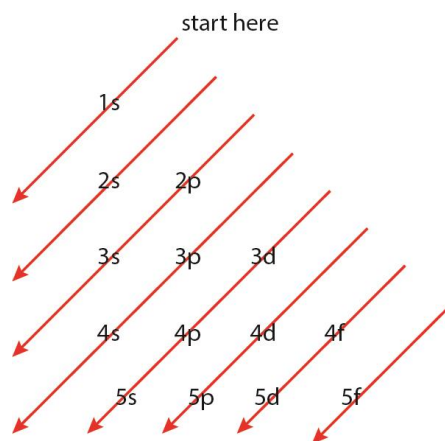


Figure 3.11: Follow the arrows to get the order in which sub-levels are filled.

		1	2	← number of electrons in outer shell										group number -10 = → 13 14 15 16 17 18																					
		1	<div>H</div>																	<div>He</div>															
																				→ 1s ²															
		1	2	← number of electrons in s sub-level										number of electrons in p sub-level → 1 2 3 4 5 6																					
period number gives number of highest main energy level occupied	2	Li	Be	→ 2s ²										B	C	N	O	F	Ne	→ 2p ⁶															
	3	Na	Mg	→ 3s ²										Al	Si	P	S	Cl	Ar	→ 3p ⁶															
	4	K	Ca	→ 4s ²										Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	→ 3d ¹⁰				Ga	Ge	As	Se	Br	Kr	→ 4p ⁶	
	5	Rb	Sr											Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd					In	Sn	Sb	Te	I	Xe		
	6	Cs	Ba											La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg					Tl	Pb	Bi	Po	At	Rn		
s block				d block										p block																					

Figure 3.12: Electron configurations can be worked out from the periodic table. Some exceptions to the general rules for filling sub-levels are highlighted in pink. Helium has the electron configuration 1s², and so, has no p electrons—despite this, it is usually put in the p block to be in the same group as the other noble gases (Group 18).

> Putting electrons into orbitals

Pauli exclusion principle: two electrons in the same orbital must have opposite spins.

Hund's rule: electrons fill orbitals of the same energy (degenerate orbitals) to give the maximum number of electrons with the same spin.

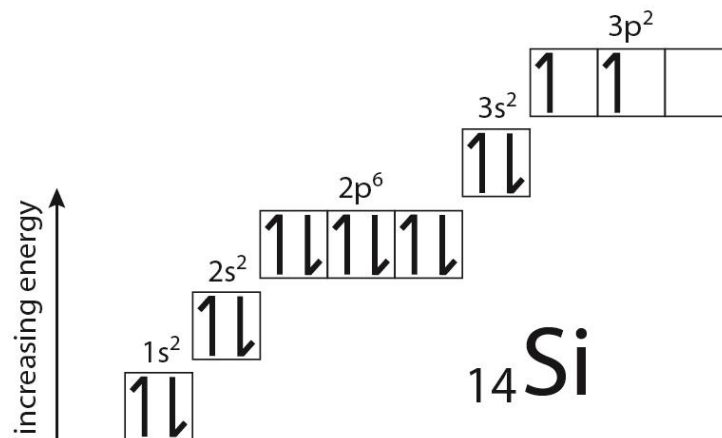


Figure 3.13: Electron configuration of silicon.

V	[Ar]	$4s^2$	$3d^3$
		$\uparrow\downarrow$	$\uparrow \uparrow \uparrow$
Cr	[Ar]	$4s^1$	$3d^5$
		\uparrow	$\uparrow \uparrow \uparrow \uparrow \uparrow$
Ni	[Ar]	$4s^2$	$3d^8$
		$\uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow$

Figure 3.14: Orbital diagrams for three transition metal atoms, showing how the electrons occupy the 4s and 3d orbitals.

> Ionisation

First ionisation energy



Second ionisation energy



nth ionisation energy



➤ Successive ionisation energies of potassium – last in, first out

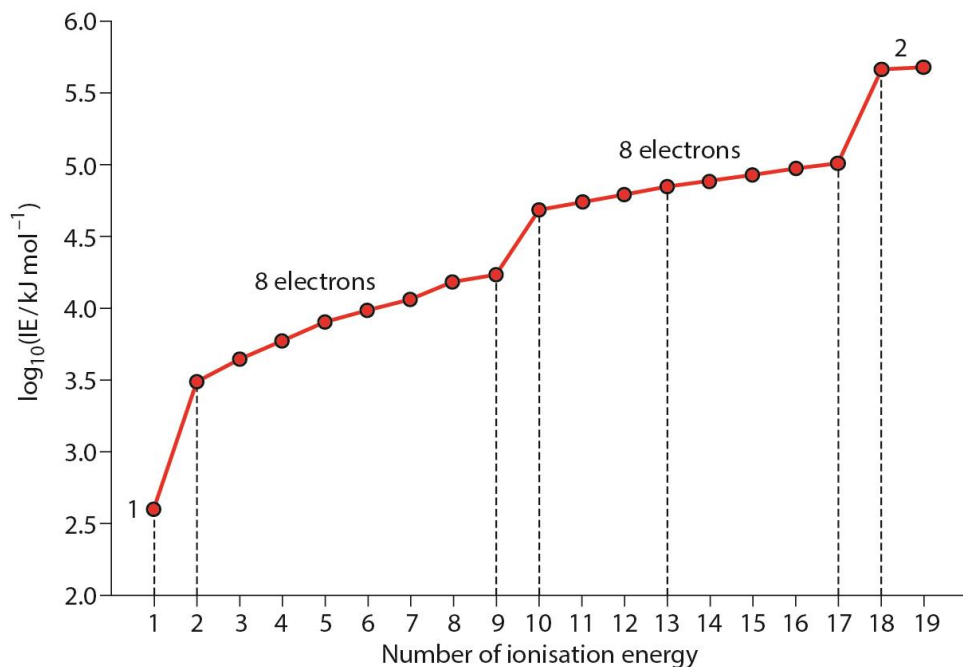


Figure 3.15: Successive ionisation energies (IEs) for potassium. Plotting \log_{10} of these numbers reduces the range. The 1st ionisation energy of potassium is 418 kJ mol^{-1} , whereas the 19th is $475\,000 \text{ kJ mol}^{-1}$. It would be very difficult to plot these values on a single graph.

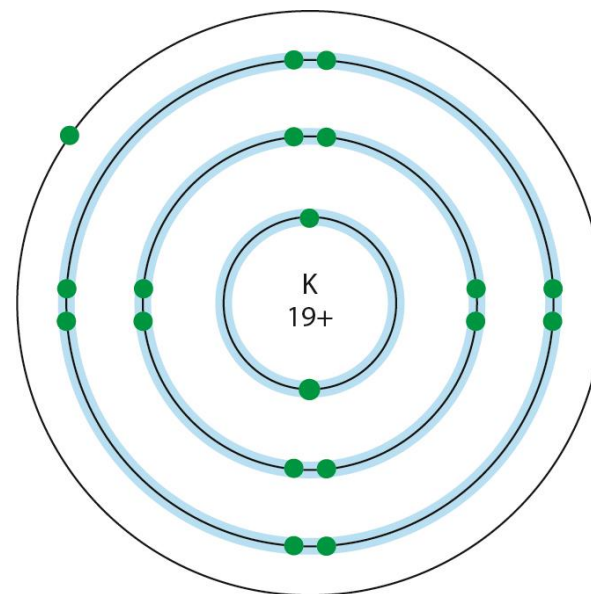


Figure 3.16: The outer electron in a potassium atom is shielded from the full attractive force of the nucleus by the inner shells of electrons (shaded in blue).

> The first 4 ionisation energies of silicon

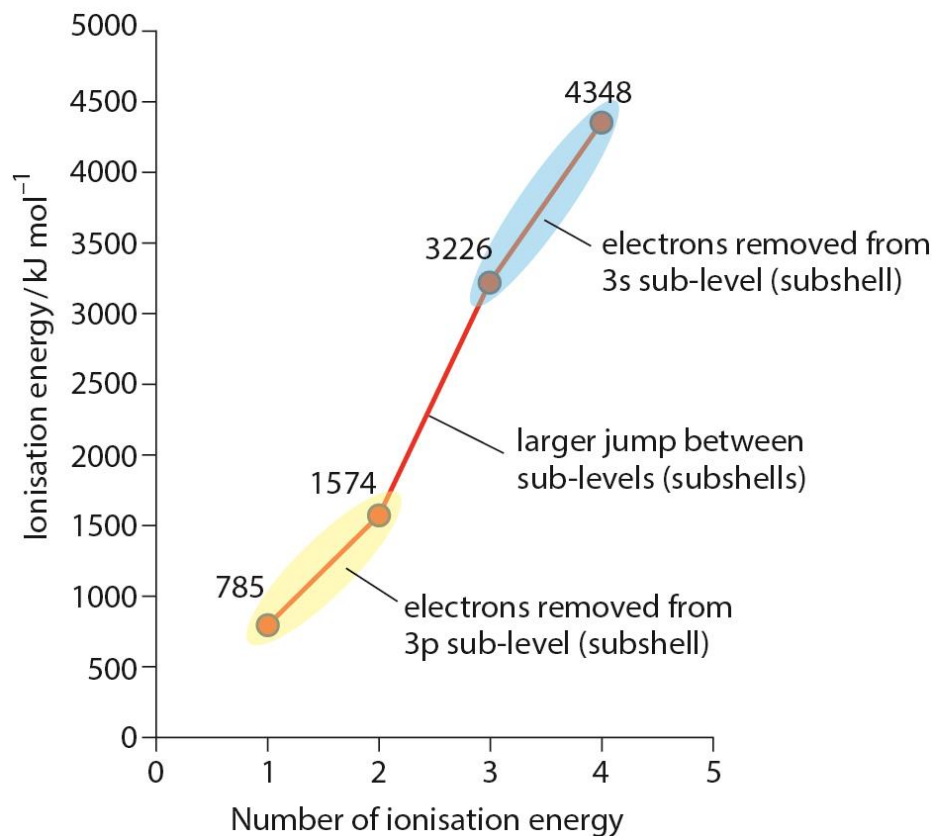


Figure 3.17: The first four ionisation energies of silicon.

> Variation of ionisation energy down a group

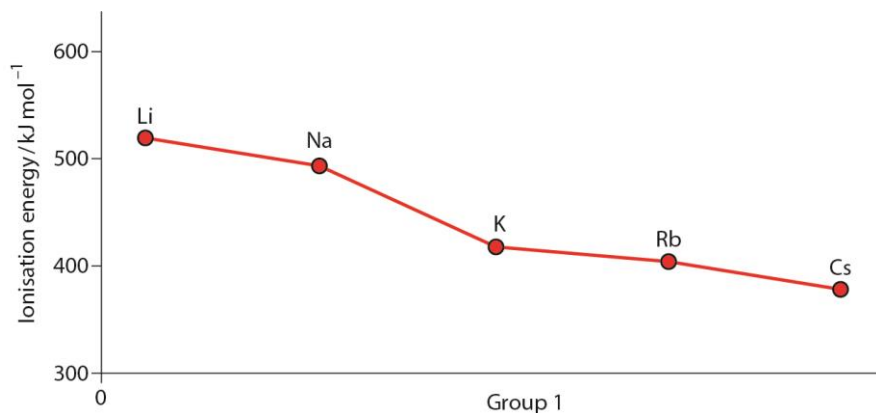


Figure 3.18: The variation in first ionisation energy down Group 1.

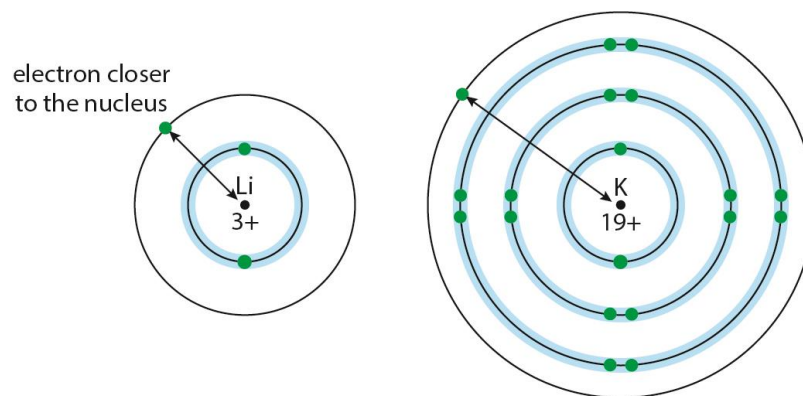


Figure 3.19: In a larger atom, the outer electron is further from the nucleus and, therefore, less attracted by it. The electrons that shield the outer electron are highlighted in blue.

> Variation of ionisation energy across a period

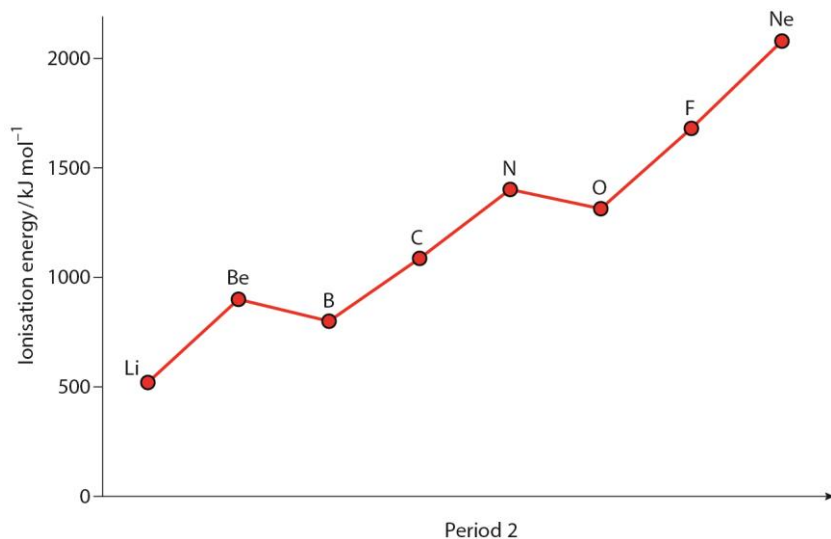


Figure 3.20: The first ionisation energies for the Period 2 elements.

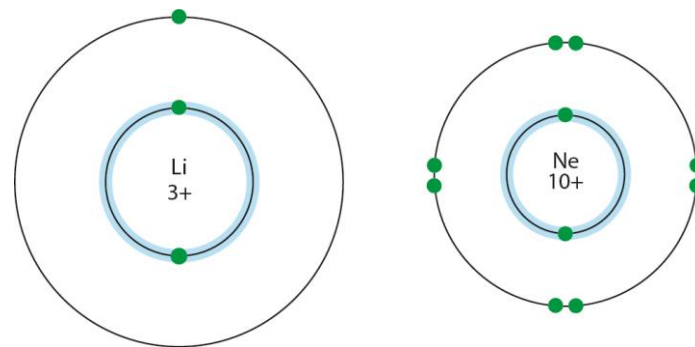


Figure 3.21: Neon has more protons in the nucleus, but the amount of shielding from inner electrons (highlighted in blue) is roughly the same as that in lithium.

As you go across the period, the number of protons increases, but the amount of shielding remains roughly the same.

> Exceptions in the first ionisation energy across Period 2

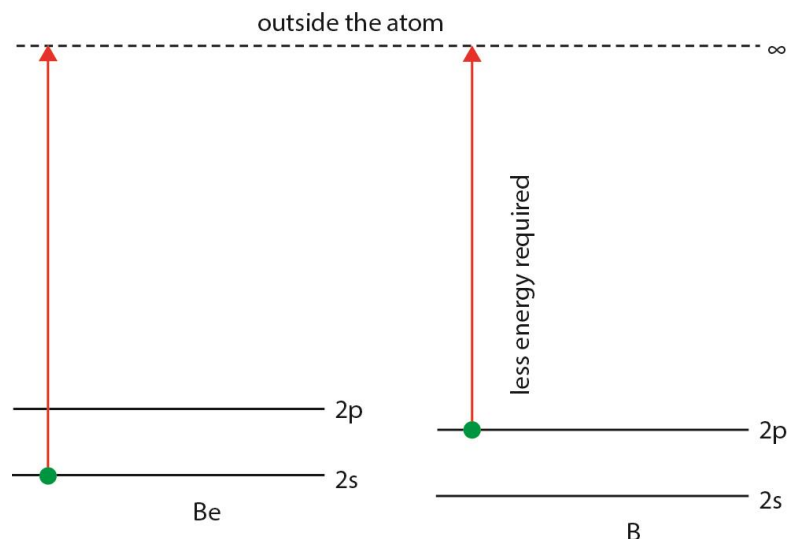


Figure 3.22: The 2p sub-shell in boron is higher in energy than the 2s sub-shell in beryllium.

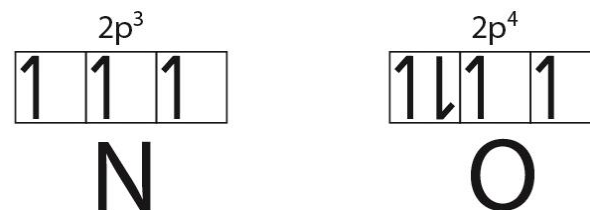


Figure 3.23: Electrons in the 2p sub-levels of nitrogen and oxygen.