



2022 JC1 H2 CHEMISTRY (9729)
CORE IDEA 1 – MATTER
Topic 1: ATOMIC STRUCTURE

Name: _____

Civics Group: _____

LEARNING OUTCOMES

Students should be able to:

[From the topic of **Atomic Structure**]

- (a) Identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses
- (b) Deduce the behaviour of beams of protons, neutrons and electrons in an electric field
- (c) Describe the distribution of mass and charges within an atom
- (d) Deduce the numbers of protons, neutrons and electrons present in both atoms and ions given proton and nucleon numbers (and charge)
- (e) (i) Describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number
(ii) Distinguish between isotopes on the basis of different numbers of neutrons present
- (f) Describe the number and relative energies of the s, p and d orbitals for the principal quantum numbers 1, 2 and 3 and also the 4s and 4p orbitals
- (g) Describe the shapes of s, p and d orbitals [knowledge of wave functions is not required]
- (h) State the electronic configuration of atoms and ions given the proton number (and charge)
- (i) Explain the factors influencing the ionisation energies of elements (see the Data Booklet)
- (j) Deduce the electronic configurations of elements from successive ionisation energy data
- (k) Interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table

[From the topic of **The Periodic Table**]

- (l) Recognise variation in the electronic configurations across a Period and down a Group
- (m) Describe and explain qualitatively the trends and variations in atomic radius, ionic radius, first ionisation energy and electronegativity:
 - (i) Across a Period in terms of shielding and nuclear charge
 - (ii) Down a Group in terms of increasing number of electronic shells and nuclear charge

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REFERENCES

1.	Chemistry (for CIE AS & A Level) by Peter Cann & Peter Hughes	540 CAN
2.	Chemistry: The Molecular Nature of Matter & Change by Martin S. Silberberg	540 SIL
3.	Calculations in A Level Chemistry (4th Edition) by E.N. Ramsden	540 RAM
4.	Calculations for AS/A Level Chemistry by Jim Clark	540 CLA

1 The Atom and the Subatomic Particles

1.1 Subatomic Particles

Learning Outcome:

- (a) Identify and describe protons, neutrons and electrons in terms of their relative charges and relative masses
- (c) Describe the distribution of mass and charges within an atom

An **atom** is the smallest particle found in an element that can take part in a chemical reaction. Particles that are smaller than the atom are called **subatomic particles**. The three main **subatomic particles** that form an atom are **protons**, **neutrons**, and **electrons**. Protons and neutrons are collectively known as **nucleons**. The centre of the atom is called the **nucleus**.

Particles	Symbol	Position in atom	Relative Charge	Mass / amu*	Actual mass / kg
Protons	p	Nucleus	+1	1	1.67×10^{-27}
Neutrons	n	Nucleus	0	1	1.67×10^{-27}
Electrons	e	Orbitals	-1	$\frac{1}{1840}$	9.11×10^{-31}

* Atomic mass units, or amu. It is defined as $\frac{1}{12}$ the mass of one atom of carbon-12.

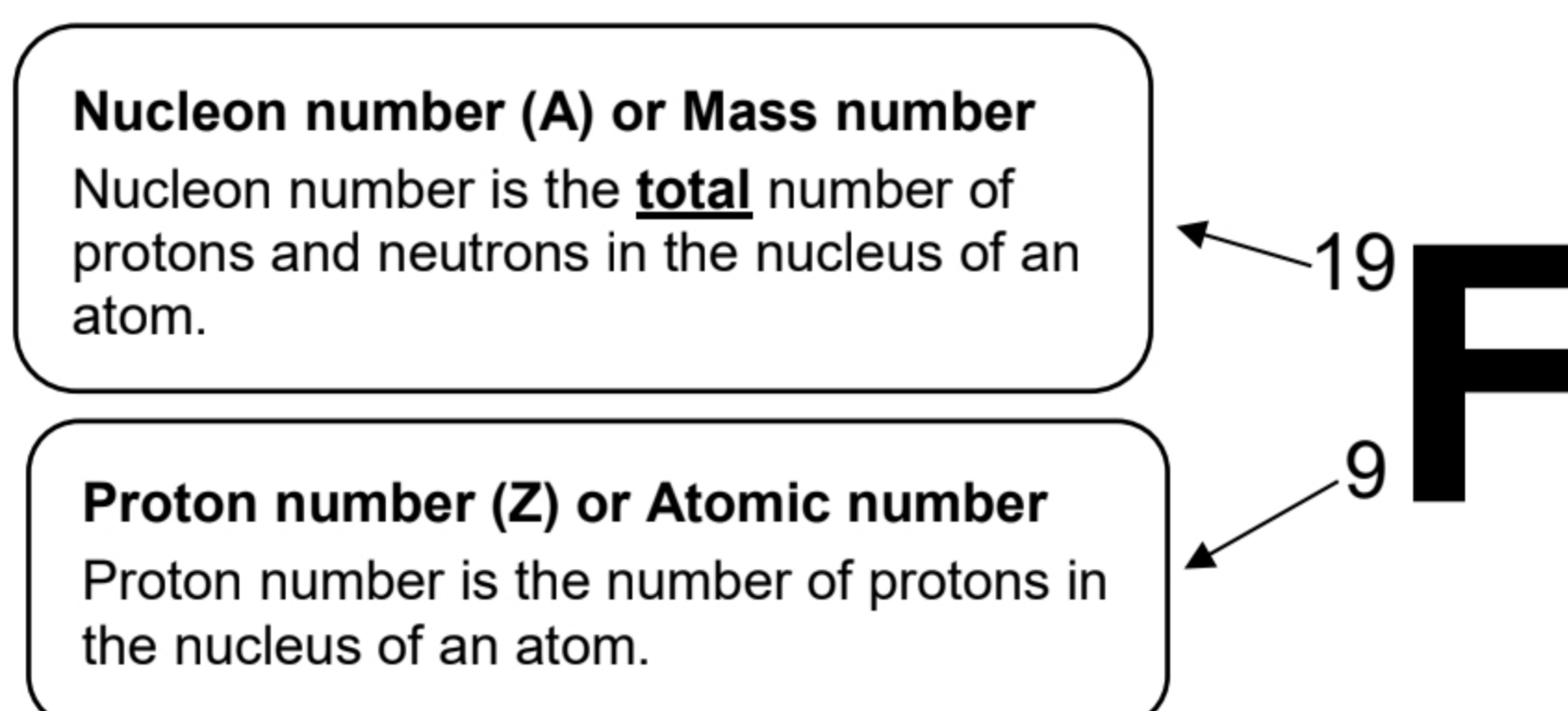
Almost the whole mass of the atom is concentrated in the nucleus, which takes up an extremely small space relative to the size of the whole atom. The size of an atom is easily more than 10,000 times that of the nucleus.

1.2 Nuclides and Isotopes

Learning Outcome:

- (d) Deduce the numbers of protons, neutrons and electrons present in both atoms and ions given protons and nucleon numbers (and charge)
- (e) (i) Describe the contribution of protons and neutrons to atomic nuclei in terms of proton number and nucleon number
- (ii) Distinguish between isotopes on the basis of different numbers of neutrons present

A nuclide is an atomic species whose proton and nucleon number are specified. It is usually represented in the manner below, using fluorine, F as an example:



1.3 Behaviour of Subatomic Particles in an Electric Field

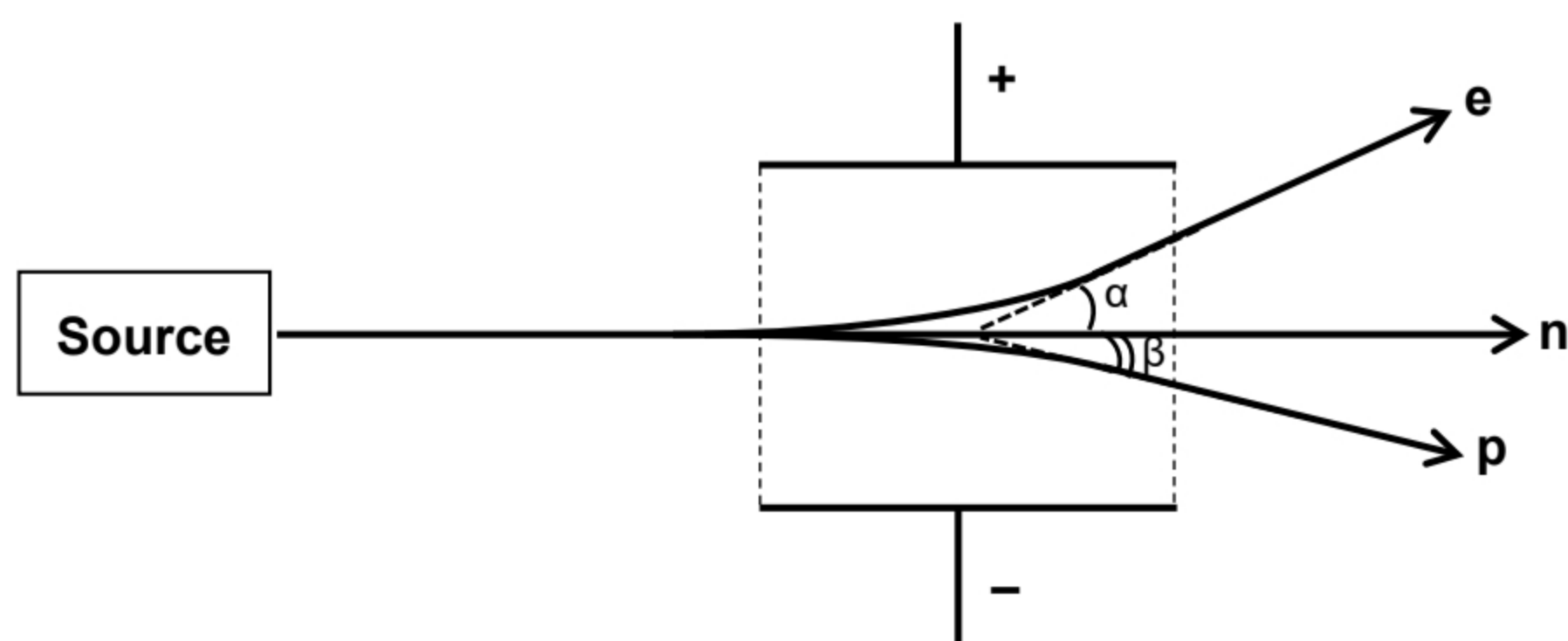
Learning Outcome:

(b) Deduce the behaviour of beams of protons, neutrons and electrons in an electric field

Protons, electrons and neutrons behave differently in an electric field due to differences in their **charges** and **relative masses**.

When beams of the three types of subatomic particles with the **same speed** are all travelling through an electric field of constant strength, each beam differs in their path travelled based on:

- **Direction** of deflection
- **Angle** of deflection



Subatomic particles	Direction of deflection	Angle of deflection
Proton, p (positive charge)	curve path towards the negative plate	β
Electron, e (negative charge)	curve path towards the positive plate	α
Neutron, n (uncharged)	undeflected	zero

Deflection of a beam of charged particles **only starts when the beam enters the electric field**. Since an attractive force continuously acts on the charged particles in the beam, the beam travels in a **curve path** as it undergoes acceleration.

Once **out of the electric field**, no attractive force acts on the charged particles in the beam. Hence, the beam continues its path in a **straight line**.

Although electrons and protons have the same magnitude of charge, **electrons are lighter**, and are hence **deflected to a greater extent** (i.e. $\alpha > \beta$).

In general,

- **Direction** of deflection is dependent on charge of a particle
- **Angle** of deflection is dependent on the charge to mass ratio of a particle

$$\text{angle of deflection} \propto \left| \frac{q}{m} \right|$$

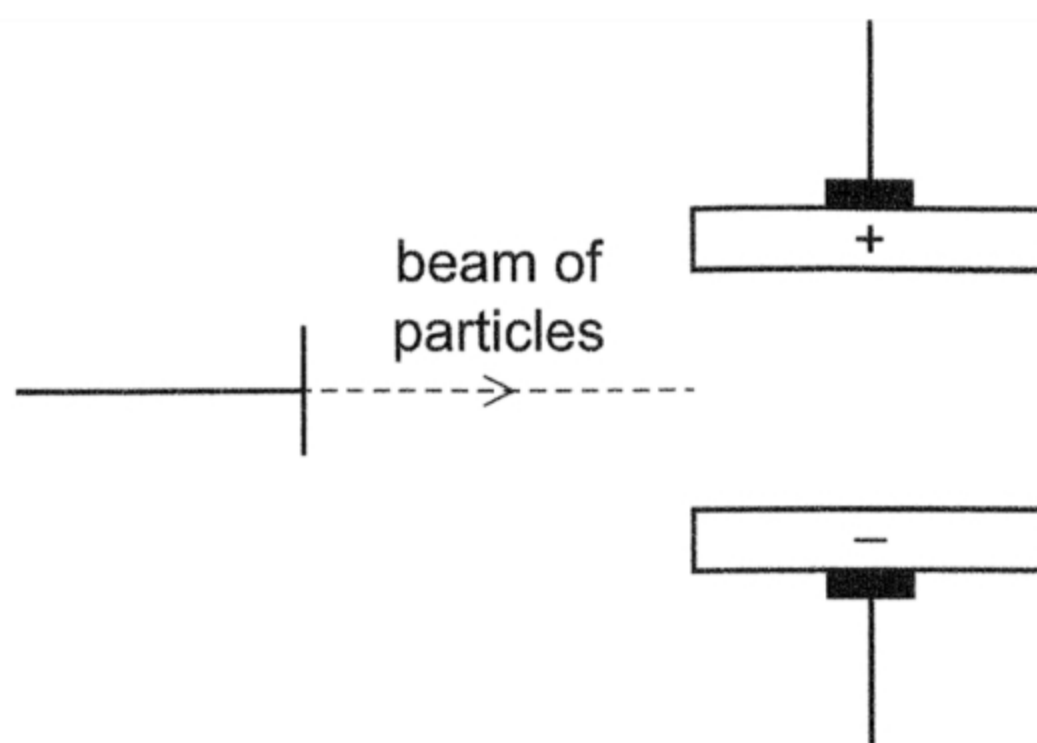
where q is the charge of the particle, m is the mass of the particle

Hence, particles with **smaller mass** and/or **higher charge** will be **deflected more** in the electric field.

Example 1B

A Levels/2021/P1/Q1

In two separate experiments a beam of protons and a beam of electrons, travelling at the same velocity, pass through an electric field as shown.



Which statements are correct?

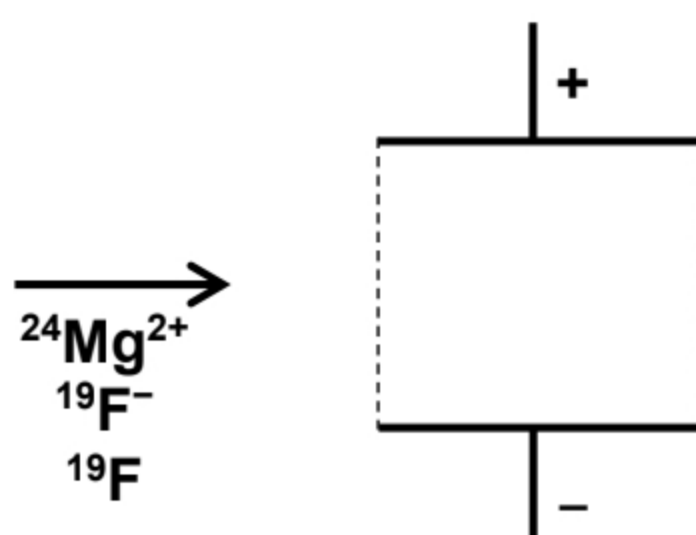
- 1 The electrons are deflected to a larger extent than the protons.
- 2 The electron beam is deflected in the opposite direction to the proton beam.
- 3 The proton beam travels in a straight path towards the negatively charged plate.

A 1, 2 and 3 **B** 1 and 2 only **C** 2 and 3 only **D** 3 only

Example 1C

Sketch the path which a $^{24}\text{Mg}^{2+}$ ion, a $^{19}\text{F}^-$ ion and a ^{19}F atom will take in an electric field.

Particle	Charge	Relative Mass	Deflection	$\left \frac{q}{m}\right $
$^{24}\text{Mg}^{2+}$ ion	+2	24.0		
$^{19}\text{F}^-$ ion	-1	19.0		
^{19}F atom	0	19.0		

**Note:**

- Deflection only occurs when beam passes into electric field
- Particles take a straight path again once out of the electric field

_____ deflects at a larger angle as compared to _____ as it has a **larger** $\frac{q}{m}$ value.

Self Check 1A

Beams of charged particles are deflected by an electric field.

In an experiment, protons are deflected by an angle of $+15^\circ$. In another experiment, under identical conditions, particle **X** is deflected by an angle of -5° .

What could be the composition of particle **X**?

	protons	neutrons	electrons
A	1	2	2
B	2	3	3
C	3	3	4
D	4	5	1

2 The Arrangement of Electrons

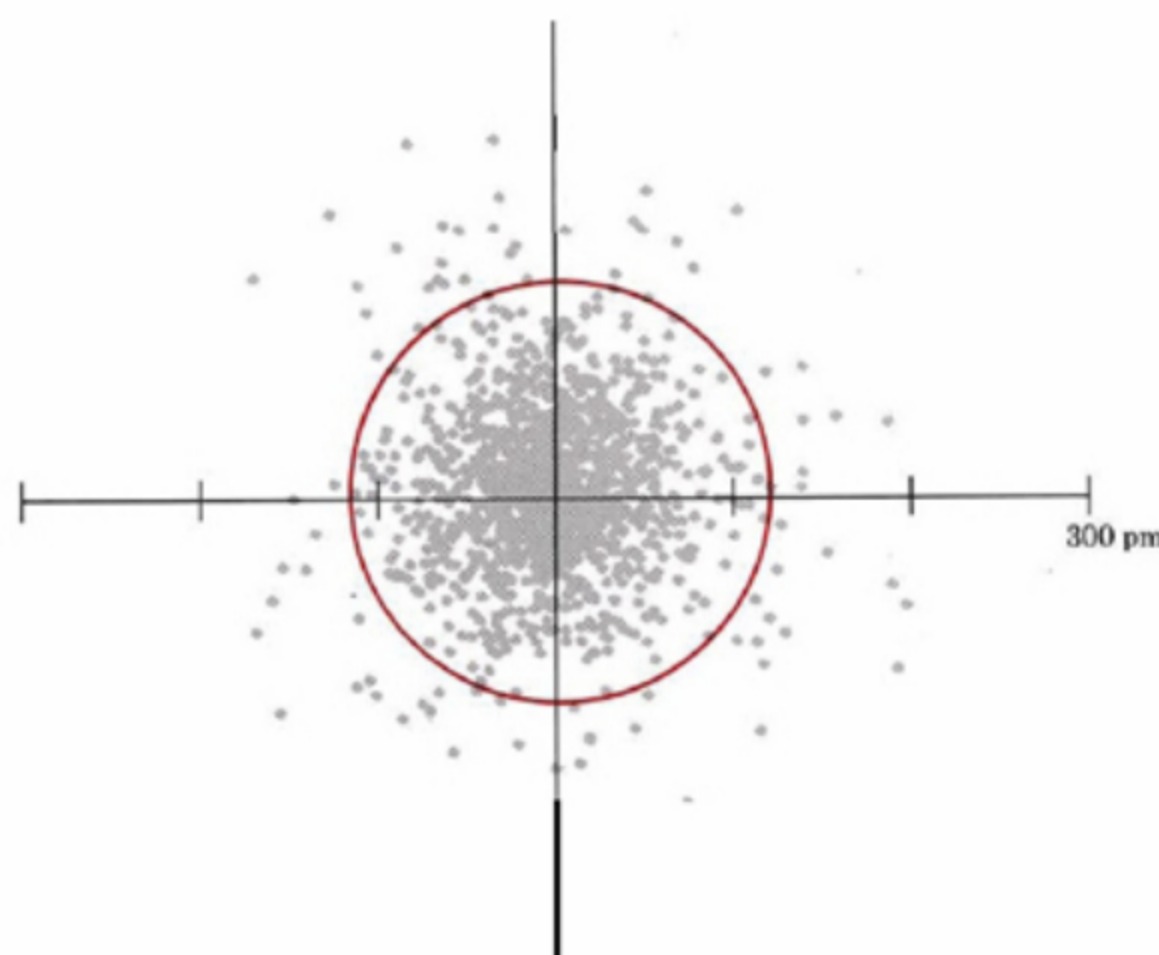
Electrons are not randomly distributed within an atom. Rather, they occupy specific volume regions, which have specific energies associated with them.

2.1 Atomic Orbitals

Learning Outcome:

(g) Describe the shapes of s, p and d orbitals. [knowledge of wave functions is not required]

Knowing that electrons move around the nucleus, if we plot the position of a particular electron in a hydrogen atom every ten seconds over a period of time, we will see that the electron can be found anywhere within a spherical space around the nucleus, as shown in the diagram below.

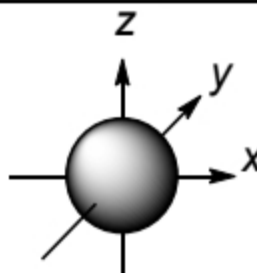
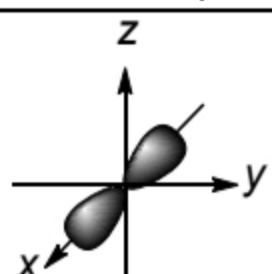
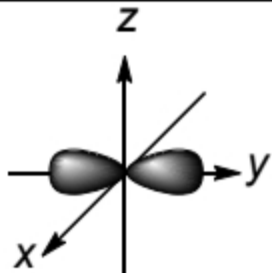
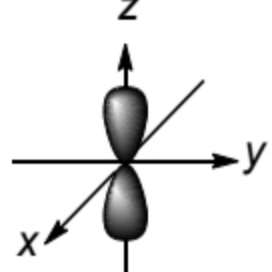
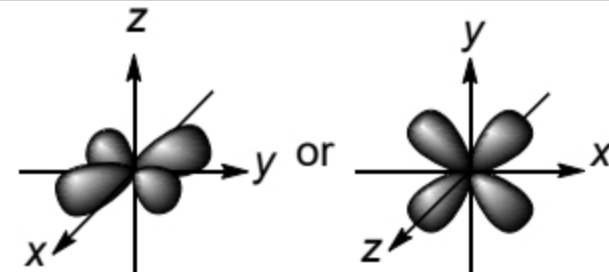
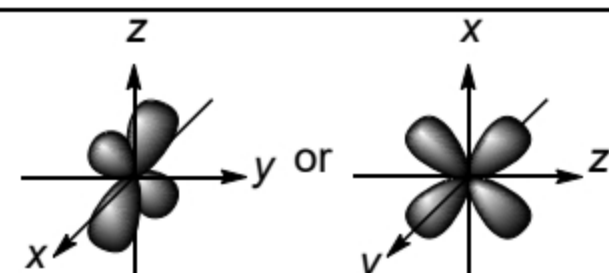
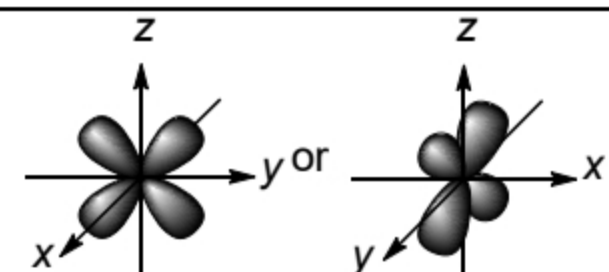
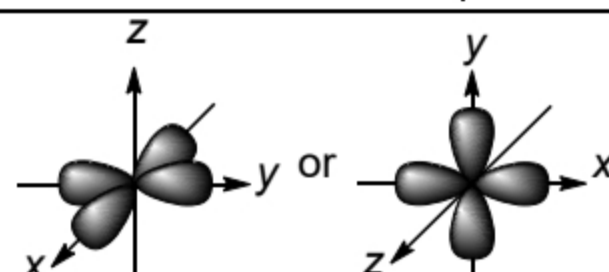
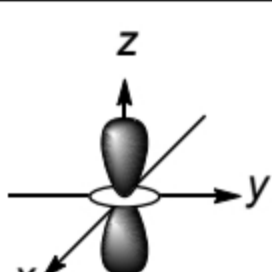


The circle in the diagram demarcates the region of space in which you will be able to find the electron **95% of the time**. This region of **three dimensional space** is called an **orbital**.

In other words, an **orbital** is a region of space in which there is a high probability (95%) of finding an electron. Each orbital contains a maximum of 2 electrons. The energy of an orbital is the energy of the electrons occupying it.

Atomic Structure

There are different types of orbitals with different shapes and energies (further elaborated on in Section 2.2).

type	shape	description	
s orbital		<ul style="list-style-type: none"> s orbitals are spherical. There is only one s orbital in any subshell. 	
p orbital		p_x	<ul style="list-style-type: none"> p orbitals are dumbbell shaped. Each orbital has two lobes of equal size. There are a total of three p orbitals in any subshell. The three p orbitals have different orientations in space. Each orbital is aligned along the axis corresponding to its subscript, e.g. the p_x orbital is aligned along the x-axis. All p orbitals are mutually perpendicular to one another. The three p orbitals have the same energy i.e. they are degenerate. Putting all the three p orbitals together, we get a sphere. Hence, a p orbital is 1/3 the volume of a sphere.
		p_y	
		p_z	
d orbital		d_{xy}	Lobes point between axes <ul style="list-style-type: none"> There are a total of five d orbitals in any subshell. The five d orbitals have different orientations in space. The five d orbitals have the same energy i.e. they are degenerate. Putting all the five d orbitals together, we get a sphere. Hence, a d orbital is 1/5 the volume of a sphere.
		d_{xz}	
		d_{yz}	
		$d_{x^2-y^2}$	Lobes point along axes
		d_{z^2}	

Self Check 2A

A Levels/2020/P1/Q1

The shape of each p-orbital is represented as two lobes.
How many 3d orbitals have four lobes?

A 2 **B** 3 **C** 4 **D** 5



Visualising the shapes of orbitals

2.2 Relationship between Principal Quantum Shells, Subshells and Orbitals

Learning Outcome:

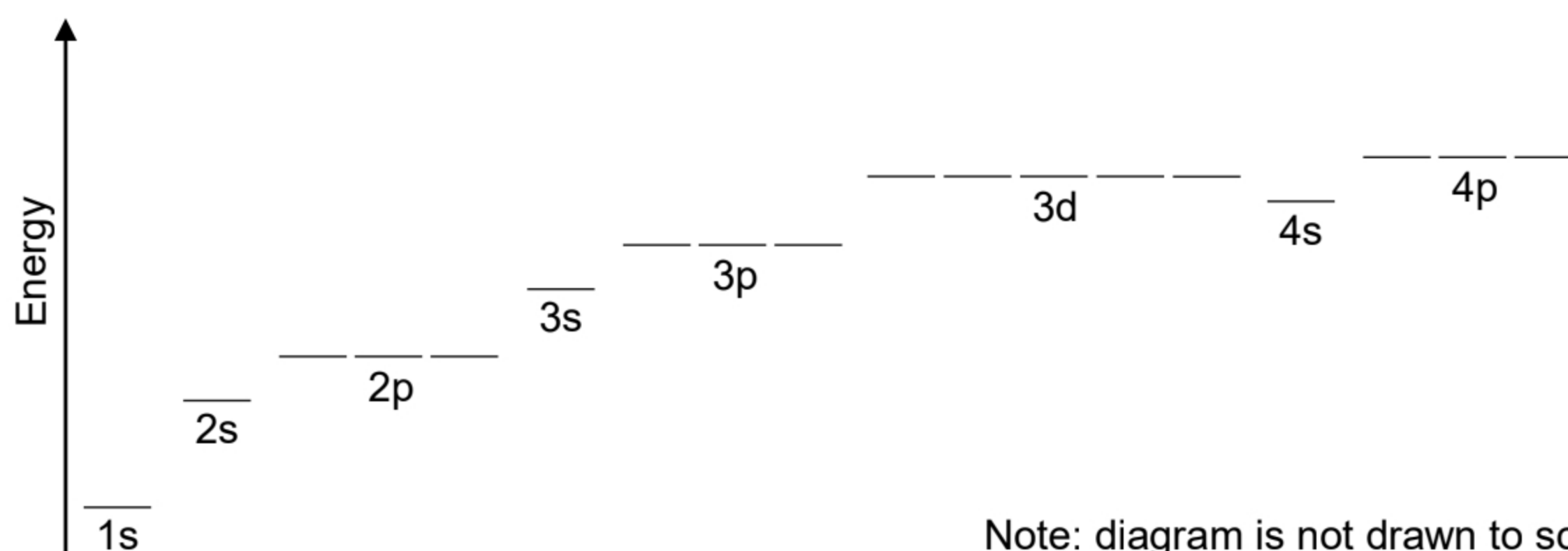
- (f) Describe the number and relative energies of the s, p and d orbitals for the principal quantum numbers 1, 2 and 3 and also the 4s and 4p orbitals.

Electrons are arranged in the following manner:

		Principal Quantum Shells (Electronic Shells)											
Orbitals	Subshells	<ul style="list-style-type: none">Each shell consists of a certain number of subshells, depending on the principal quantum number, n, where $n = 1, 2, 3, \dots$ (numbered outwards from the nucleus). <table><tr><th>n</th><th>Type of subshell(s)</th></tr><tr><td>1</td><td>s subshell</td></tr><tr><td>2</td><td>s subshell, p subshell</td></tr><tr><td>3</td><td>s subshell, p subshell, d subshell</td></tr><tr><td>4</td><td>s subshell, p subshell, d subshell, f subshell</td></tr></table> <ul style="list-style-type: none">The higher the value of n,<ul style="list-style-type: none">➤ the further the electron is from the nucleus;➤ the higher the energy level of the electron;➤ the less strongly the electron is attracted to the nucleus;➤ the larger and more diffused (i.e. lower electron probability density) the orbitals in the shell.	n	Type of subshell(s)	1	s subshell	2	s subshell, p subshell	3	s subshell, p subshell, d subshell	4	s subshell, p subshell, d subshell, f subshell	
n	Type of subshell(s)												
1	s subshell												
2	s subshell, p subshell												
3	s subshell, p subshell, d subshell												
4	s subshell, p subshell, d subshell, f subshell												
	<ul style="list-style-type: none">Each subshell consists of a certain number of orbitals, depending on the type of subshell. <table><tr><th>Type of subshell</th><th>Type and number of orbital(s)</th></tr><tr><td>s</td><td>one s orbital</td></tr><tr><td>p</td><td>three p orbitals</td></tr><tr><td>d</td><td>five d orbitals</td></tr><tr><td>f</td><td>seven f orbitals</td></tr></table> <ul style="list-style-type: none">Orbitals in the same subshell have the same energy i.e. they are degenerate but they have different orientation in space.The relative energies of the subshells are in the order of $s < p < d < f$ for the same principal quantum number.	Type of subshell	Type and number of orbital(s)	s	one s orbital	p	three p orbitals	d	five d orbitals	f	seven f orbitals		
Type of subshell	Type and number of orbital(s)												
s	one s orbital												
p	three p orbitals												
d	five d orbitals												
f	seven f orbitals												

Putting everything together,

Principal quantum number, n	Type of subshell(s)	Number of orbital(s)	Max number of electrons	
			in each subshell	in each quantum shell (max no. of electrons = $2n^2$)
1	s	1	2	2
2	s	1	2	8
	p	3	6	
3	s	1	2	18
	p	3	6	
	d	5	10	
4	s	1	2	32
	p	3	6	
	d	5	10	
	f	7	14	



Note: diagram is not drawn to scale

3 Electronic Configuration

Learning Outcome:

(h) State the electronic configuration of atoms and ions given the proton number (and charge)

The **electronic configuration** of an element refers to the arrangement of electrons in the principal quantum shells, subshells and orbitals.

Knowing the electronic configuration enables us to identify the electron(s) to be removed in a chemical reaction. We will be able to know which orbital the electron to be removed resides in, and consequently the amount of energy required to remove it.

3.1 Rules for Arranging Electrons

Rule 1: Pauli's Exclusion Principle

Two electrons in the **same orbital** must have **opposite spins**.

11

 Same spins
WRONG!

1↓

 Opposite spins
RIGHT!

Electrons are often described with a special property known as spin. This does not relate to the physical movement of the particles, but rather, their tendency to be deflected in a magnetic field. There are two possible orientations for electron spin, represented by arrows pointing in opposite directions.

Electron spin gives rise to the formation of magnetic fields. If two electrons in the same orbital have the same spin, the magnetic field created will be repulsive, causing the energy level of these two electrons to be higher, and thus being less stable as compared to a pair of electrons with opposite spins.



What exactly is the 'spin' of subatomic particles such as electrons and protons?

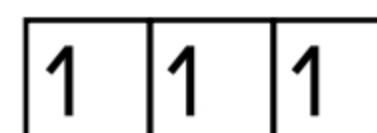
Rule 2: Hund's Rule

Orbitals of a subshell must be **singly occupied first with parallel spins before pairing occurs**.

For example, when filling **six** electrons into the **p subshell**,

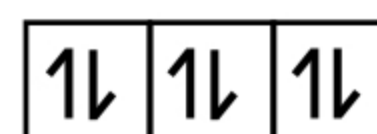
After filling the first three electrons:

- Orbitals are singly occupied, electrons have parallel spins



After filling all six electrons:

- Orbitals contain paired electrons with opposite spins



This happens as electrons repel one another electrostatically. Hence, they will want to remain as far apart as possible from one another by occupying different orbitals (i.e. different regions of space) first.

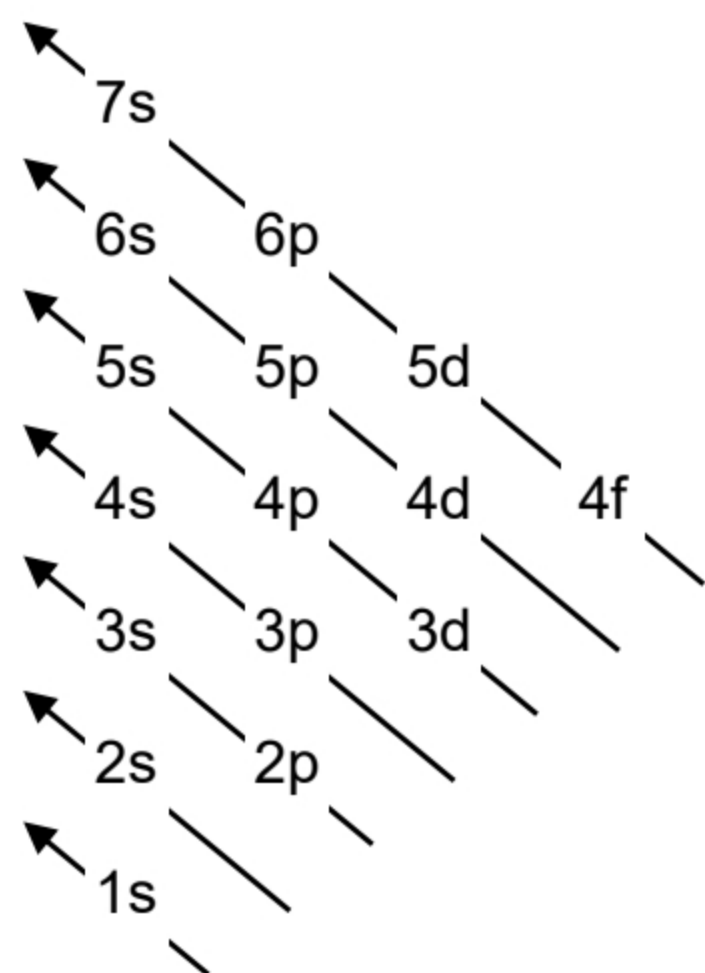
Rule 3: The Aufbau Principle

Place electrons into orbitals, **starting with those of the lowest energy** (nearest to the nucleus) **and then working upwards**.

Electrons in their lowest energy states is known as the **ground state** (i.e. when they are not excited). Energy can be supplied to move an electron from a lower energy state to a higher energy state (i.e. the excited state).

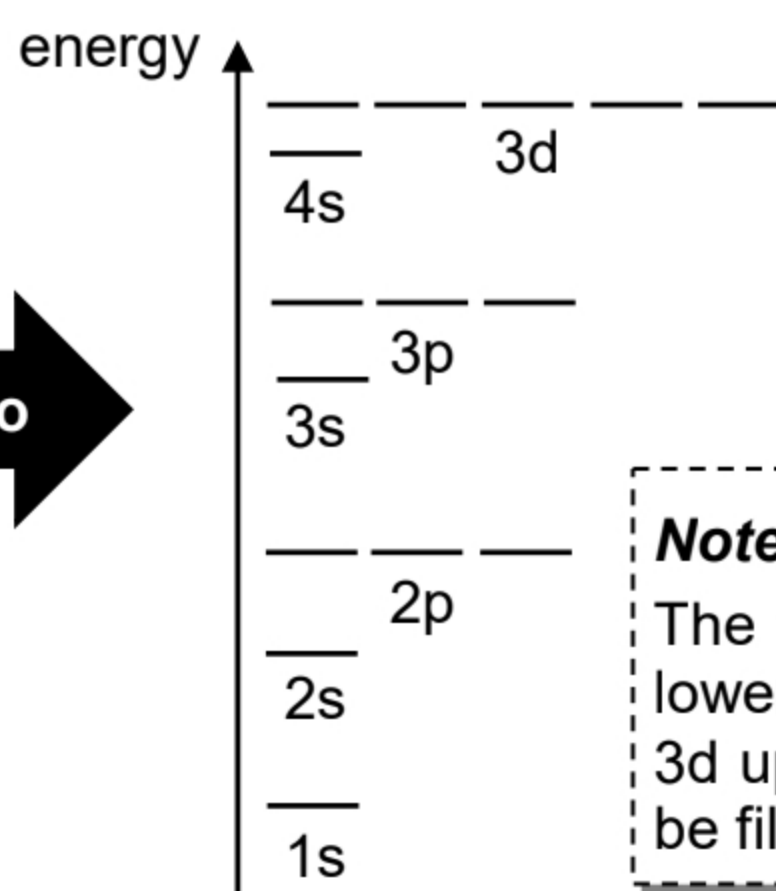
The following diagram is a convenient way to remember the sequence of orbitals from the lowest to highest in energy level.

highest energy



lowest energy

translates to

**Note:**

The 4s subshell is at a lower energy level than 3d up till Ca, hence will be filled first.

3.2 Electronic Configuration of an Atom

Steps for working out electronic configuration of an atom

1. Determine the **total number of electrons** in the atom.
2. Fill the orbitals **from the lowest energy upwards**, making sure that there are a **maximum of two electrons** in each orbital.
3. For subshells with more than one orbital i.e. p, d and f subshells, **fill all the orbitals with one electron each before putting in the second electron**.
4. If an orbital contains two electrons, the electrons must have **opposite spins**.

Example 3A

Represent the electronic configuration of the **potassium atom** in the ways stated in the table below.

Potassium atom has **19** electrons.

Drawing electronic configuration	$ \begin{array}{ccccccc} \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow\downarrow & \uparrow \\ \hline 1s & 2s & & 2p & & 3s & & 3p & & 4s \end{array} $
Writing/stating full electronic configuration	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
Writing/stating short form notation of electronic configuration	$[\text{Ar}] 4s^1$
Drawing energy level diagram	<p>The diagram shows a vertical axis labeled 'Energy' with an upward arrow. Six horizontal lines represent energy levels, labeled from bottom to top: 1s, 2s, 2p, 3s, 3p, and 4s. The 1s, 2s, and 3s levels each contain one orbital with a pair of electrons (up and down arrows). The 2p level contains three orbitals, each with a pair of electrons. The 3p level contains three orbitals, each with a pair of electrons. The 4s level contains one orbital with a single electron.</p>

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Note:

For atoms of d-block elements,

- **Fill** 4s orbital before 3d orbitals
- **Write/draw** 3d subshell before 4s subshell



How do all the orbitals come together in the Sc atom? View the visualisation [here](#).

3.3 Electronic Configuration of Atoms and the Periodic Table

Learning Outcome:

(l) Recognise variation in the electronic configurations across a Period and down a Group

The Periodic Table is compartmentalised into blocks, namely the s block, p block, d block and f block. The **name of the block** indicates the **last occupied subshell** of the atom.

1	2											13	14	15	16	17	18			
		<div>1s</div>																<div>1s</div>		
<div>2s</div>																		<div>2p</div>		
<div>3s</div>	3	4	5	6	7	8	9	10	11	12						<div>3p</div>				
<div>4s</div>						<div>3d</div>										<div>4p</div>				
<div>5s</div>						<div>4d</div>										<div>5p</div>				
<div>6s</div>	57–71 lanthanoids					<div>5d</div>										<div>6p</div>				
<div>7s</div>	89–103 actinoids					<div>6d</div>										<div>7p</div>				
lanthanoids									<div>4f</div>											
actinoids									<div>5f</div>											

The **period number** indicates the **principal quantum number, n**, of the **valence (outermost) shell**. Elements in the same period have the same number of shells occupied with electrons.

The **group numbers** of the s and p block elements indicate the **number of electrons in the valence shell**. Elements in the same group have the same number of valence electrons and hence, same valence shell electronic configuration.

	Group 1	Group 2	Group 13	Group 14	Group 15	Group 16	Group 17	Group 18
valence shell electronic configuration	ns^1	ns^2	$ns^2 np^1$	$ns^2 np^2$	$ns^2 np^3$	$ns^2 np^4$	$ns^2 np^5$	$ns^2 np^6$ (except He)
	s block		p block					

Example 3C

An ion X^+ has the electronic configuration $[\text{Ne}] 3s^2 3p^1$. Which group does X belong to?

A 1

B 2

C 13

D 14

3.4 Electronic Configuration of an Ion

Steps for working out electronic configuration of an ion

1. Work out the electronic configuration of the **atom**.
2. For an **anion**, **add** the number of electrons equal to the negative charge **to the outermost shell**.
For a **cation**, **remove** the number of electrons equal to the positive charge **from the outermost shell**.

Example 3D

Represent the electronic configuration of the **sulfur ion, S^{2-}** in the ways stated in the table below.

The S atom has **16** electrons. The S^{2-} ion has **18** electrons.

Drawing electronic configuration	$\uparrow\downarrow$ 1s $\uparrow\downarrow$ 2s $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ 2p $\uparrow\downarrow$ 3s _____ 3p
Writing/stating electronic configuration	
Drawing energy level diagram	<div style="text-align: center;"> Energy \uparrow _____ 3p $\uparrow\downarrow$ _____ 3s $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ _____ 2p $\uparrow\downarrow$ _____ 2s $\uparrow\downarrow$ _____ 1s </div>

Example 3E

Represent the electronic configuration of the **iron(III) ion, Fe^{3+}** in the ways stated in the table below.

Fe is a **d-block element**. The Fe atom has **26** electrons. The Fe^{3+} ion has **23** electrons.

Drawing electronic configuration	$\uparrow\downarrow$ 1s $\uparrow\downarrow$ 2s $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ 2p $\uparrow\downarrow$ 3s $\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$ 3p \uparrow \uparrow \uparrow \uparrow \uparrow 3d	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$
Writing/stating electronic configuration		
Drawing energy level diagram	<p style="text-align: center;"><i>(working)</i></p> <p><u>Fe atom:</u></p>	<p><u>Fe³⁺ ion:</u></p>

3.5 Anomalous Electronic Configurations

For the Period 4 d-block elements i.e. Sc through Zn, the electronic configurations of the atoms generally take the form $[\text{Ar}] 3d^n 4s^2$, where $n = 1$ for scandium and $n = 10$ for zinc. However, there are two exceptions:

1. Cr: **[Ar] 3d⁵ 4s¹** instead of [Ar]3d⁴4s²
2. Cu: **[Ar] 3d¹⁰ 4s¹** instead of [Ar]3d⁹4s²

The **$3d^5$ (half-filled subshell)** and **$3d^{10}$ (fully-filled subshell)** are **energetically preferred** configurations due to the **symmetrical 3d electron cloud around the nucleus**. This allows for charges to be spread out evenly and as far apart as possible, leading to greater stability.

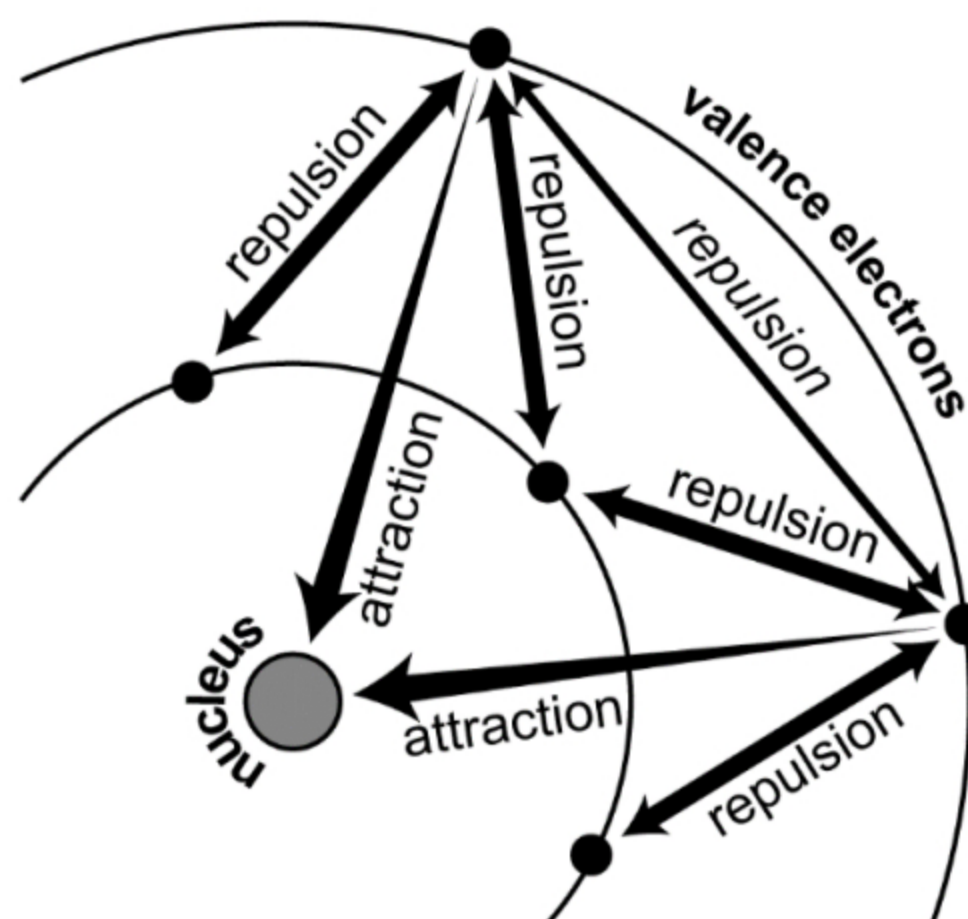
Note that at the 'A' Levels, we will consider the anomalous electronic configuration only for the Cr and Cu elements. For Fe atom which has an electronic configuration of $[\text{Ar}]3d^64s^2$, Fe^{2+} will have the electronic configuration of $[\text{Ar}]3d^6$, and not $[\text{Ar}]3d^54s^1$.

4 Factors Affecting Atomic Properties and Periodic Trends

The elements in the periodic table are arranged in order of increasing atomic number. All of these elements display similar trends in:

- Ionisation Energy
- Atomic and Ionic Radius
- Electronegativity

The following factors affect the **electrostatic forces of attraction between the valence electrons and the nucleus**, giving rise to the various trends.



1a. Charge of nucleus (nuclear charge)

- More protons in nucleus, larger positive charge of nucleus
- Stronger electrostatic forces of attraction between the nucleus and the valence electrons

1b. Number of electrons between valence electrons and nucleus (shielding or screening effect)

Shielding or screening effect refers to the inter-electronic repulsion between the valence (outermost) electrons and inner shell electrons.

- Inner shell electrons confer the most significant shielding. Shielding by electrons within the same shell is generally more insignificant in comparison.
- Fewer electrons in the inner shells which leads to weaker shielding effect
- Stronger electrostatic forces of attraction between the nucleus and the valence electrons

Bringing together the effects of nuclear charge and shielding effect: **Effective Nuclear Charge**

The **effective nuclear charge** is the strength of the **net** electrostatic forces of **attraction** felt by the valence electrons after taking into account the shielding effect of the inner shell electrons.

$$\text{Effective nuclear charge} = \text{nuclear charge} - \text{shielding effect}$$

(det by no. of protons) (det by no. of inner shell electrons)

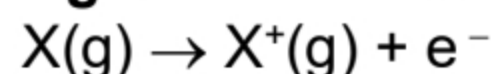
2. Distance of electron from nucleus

- Smaller distance between nucleus and valence electron
- Stronger electrostatic forces of attraction between the nucleus and the valence electron

5 Trends in Ionisation Energies

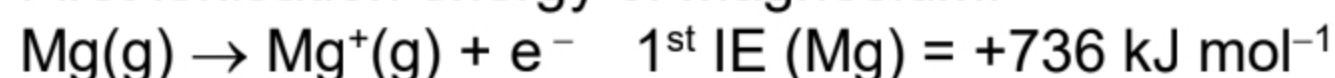
5.1 Ionisation Energy (I.E.)

The **first** ionisation energy is the **energy required** to remove **1 mole of electrons** from **1 mole of gaseous atoms** to form **1 mole of singly charged gaseous cations**.

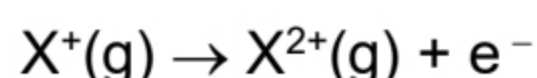


E.g.

First ionisation energy of magnesium:

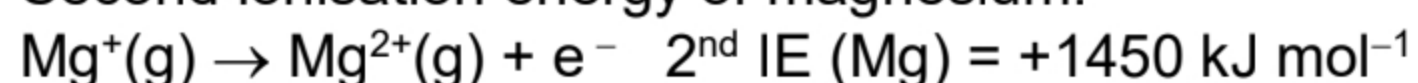


The **second** ionisation energy is the **energy required** to remove **1 mole of electrons** from **1 mole of singly charged gaseous cations** to form **1 mole of doubly charged gaseous cations**.



E.g.

Second ionisation energy of magnesium:



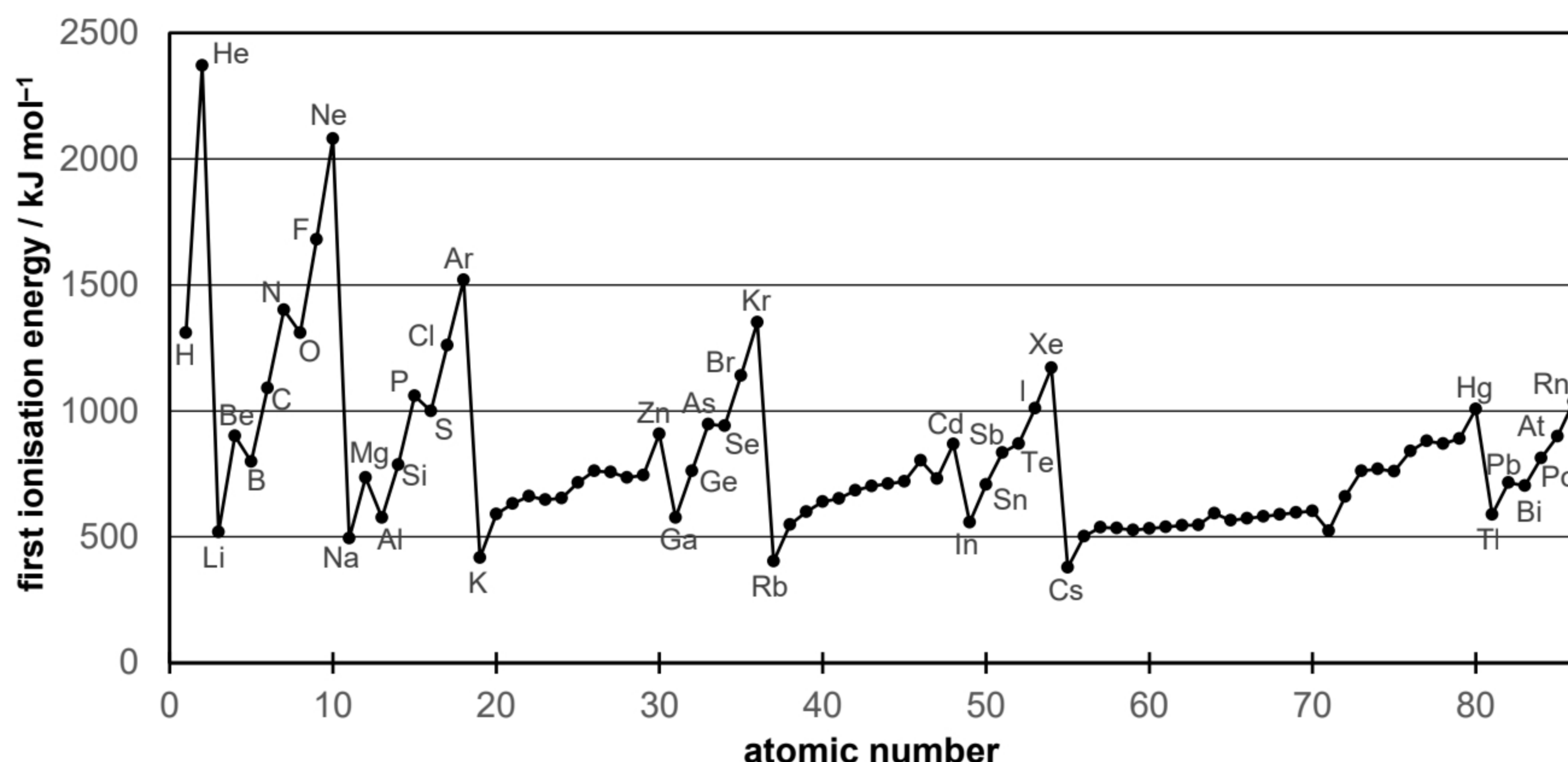
Ionisation energy is always a **positive** value (i.e. **endothermic**) because energy is **required** to overcome the electrostatic forces of attraction between the nucleus and valence electrons.

5.2 Trends of 1st I.E.

Learning Outcome:

- (i) Explain the factors influencing the ionisation energies of elements (*see the Data Booklet*).
- (m) Describe and explain qualitatively the trends and variations in first ionisation energy:
 - (i) Across a Period in terms of shielding and nuclear charge
 - (ii) Down a Group in terms of increasing number of electronic shells and nuclear charge

The following chart shows the 1st ionisation energies of elements with atomic numbers from 1 to 86.



5.2.1 Across the Period (e.g. Li, Be, B, C, O, N, F, Ne)

General increase in 1st I.E. across the period

- Number of protons in the nucleus of the atom increases, thus **nuclear charge increases**
- Same number of inner shell electrons, thus **shielding effect is approximately constant**
- **Increase in effective nuclear charge**
- **Increase in electrostatic forces of attraction** between the nucleus and valence electron
- **More** energy needed to remove the valence electron
- **Increase** in 1st I.E. across the period

Exception 1: Decrease in 1st I.E. from Group 2 to Group 13 (e.g. Be to B)

- Valence shell: Group 2: ns^2 Group 13: $ns^2 np^1$
- **np electron is of a higher energy level than the ns electron**
- **Less** energy is required to remove the valence np electron from a Group 13 element

Exception 2: Decrease in 1st I.E. from Group 15 to 16 (e.g. N to O)

- Valence shell Group 15: $\begin{array}{|c|c|c|} \hline \uparrow\downarrow & 1 & 1 & 1 \\ \hline ns^2 & np^3 & & \end{array}$ Group 16: $\begin{array}{|c|c|c|c|} \hline \uparrow\downarrow & \uparrow\downarrow & 1 & 1 \\ \hline ns^2 & np^4 & & \end{array}$
- There is **inter-electronic repulsion between the paired electrons in the same orbital** for a Group 16 element
- **Less** energy is required to remove the np electron from Group 16 than Group 15

5.2.2 Down the Group (e.g. He, Ne, Ar, Kr, Xe, Rn)

Decrease in 1st I.E. down the group

- **Both nuclear charge and shielding effect increase.**
- However, valence electrons are located in a shell with a larger principal quantum number, n , and are **further away from the nucleus**
- **Decrease in electrostatic forces of attraction** between the nucleus and the valence electron
- **Less** energy needed to remove the valence electron
- **Decrease** in 1st I.E. down the group

5.3 Successive I.E. of an Atom

Learning Outcome:

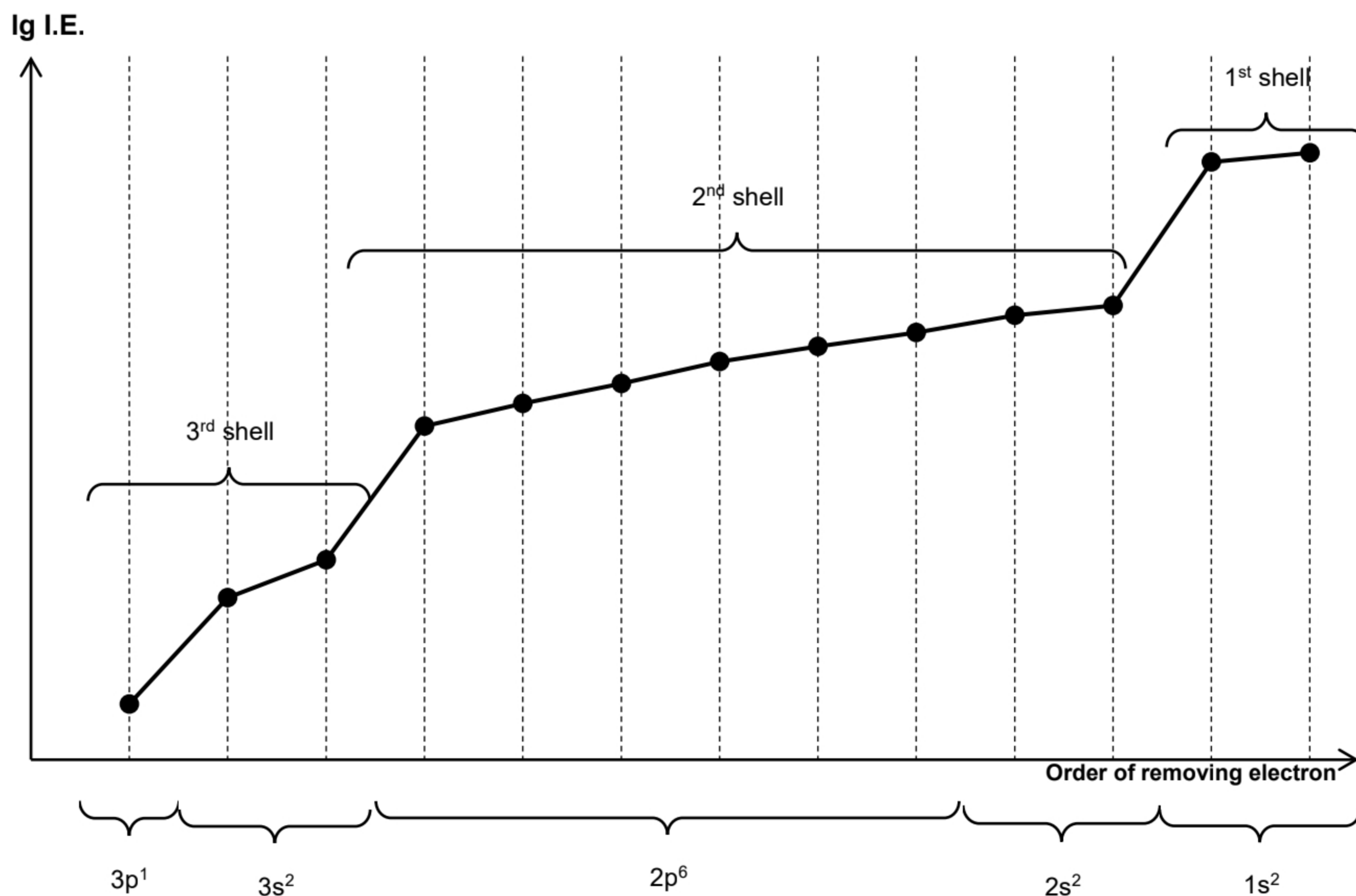
- (j) Deduce the electronic configurations of elements from successive ionisation energy data
 (k) Interpret successive ionisation energy data of an element in terms of the position of that element within the Periodic Table

General Trend:

- **Decrease** in **inter-electronic repulsion** and hence **shielding effect decreases** as electrons are removed
- **Nuclear charge remains the same**, hence **effective nuclear charge increases**
- Resulting in **increase in electrostatic forces of attraction** between the nucleus and the **remaining** electrons
- **More** energy needed for subsequent removal of electrons
- Successive I.E. of an atom **always increases**

5.3.1 Deducing Electronic Configuration Using Successive I.E.

The following graph and table show the successive ionisation energies of an **aluminium** atom (Al: $1s^2 2s^2 2p^6 3s^2 3p^1$).



Order of removal	1 st	2 nd	3 rd	4 th	5 th	6 th	7 th	8 th	9 th	10 th	11 th	12 th	13 th
I.E. / kJ mol^{-1}	577	1820	2740	11600	14800	18400	23300	27500	31900	38500	42600	201000	222000

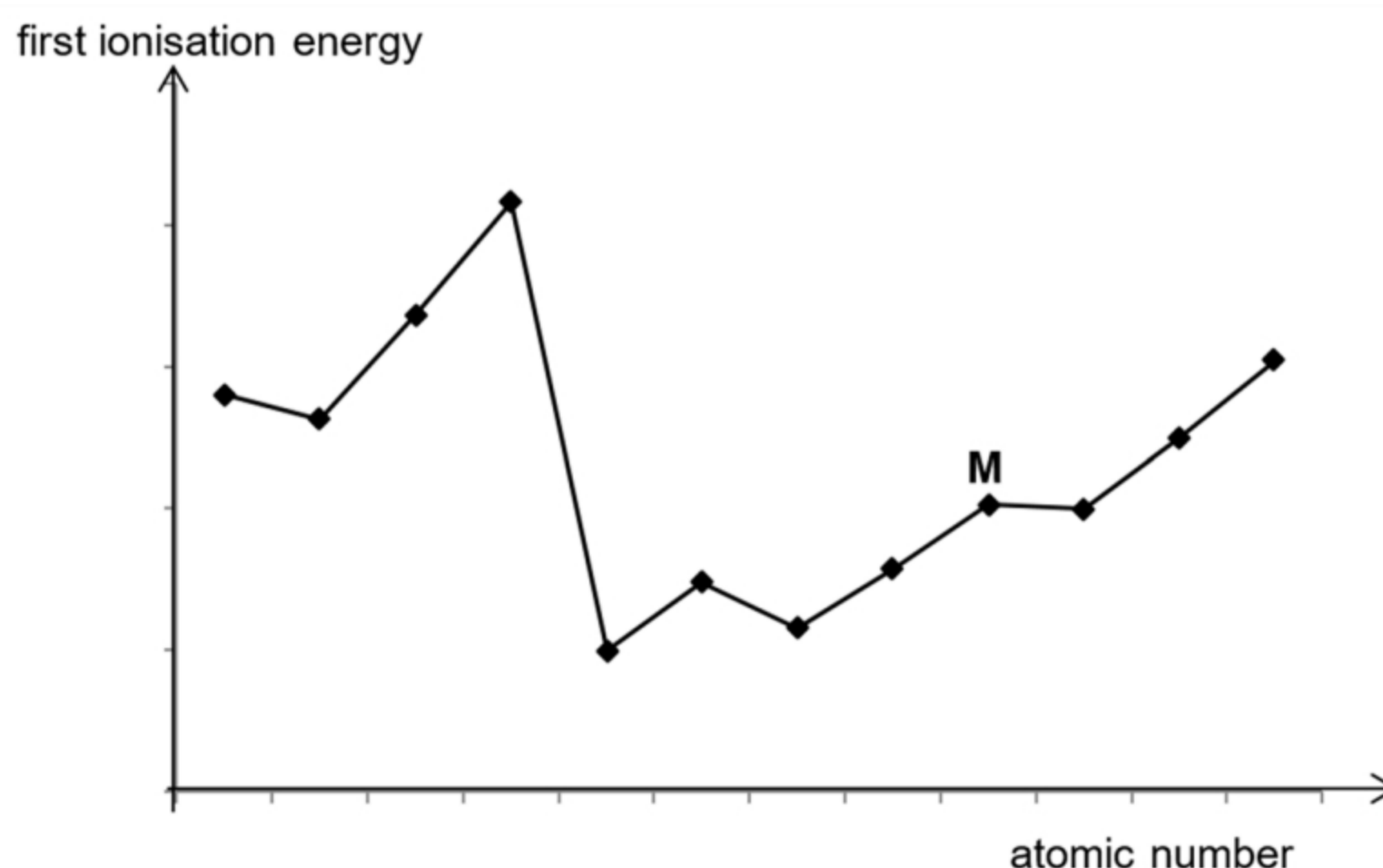
Difference btw successive I.E.:	1243	920	8860	3200	3600	4900	4200	4400	6600	4100	158400	21000
	3 rd shell			2 nd shell						1 st shell		

- A **large increase** in I.E. represents a **change in principal quantum shell**.
 - Electron is removed from an inner principal quantum shell which is **closer to the nucleus**, and hence experiences **stronger** electrostatic forces of attraction.
- The **number of electrons that are removed** before the **first large increase** in I.E. indicates the **number of valence electrons** in the atom, and hence the **group** the element is in.
- Using these pieces of information, the **valence shell electronic configuration of the atom** can be deduced.

Example 5A

NJC/2015/P1/Q3 (modified)

The diagram below shows the first ionisation energy of some elements with atomic numbers less than 20.



Which is the most likely formula of the chloride of **M**?

- A** MCl **B** MCl_2 **C** MCl_3 **D** MCl_4

Example 5B

HCI/2014/P1/Q3

The successive ionisation energies of two elements, **P** and **Q**, are given below.

Ionisation energies / kJ mol^{-1}	1 st	2 nd	3 rd	4 th	5 th	6 th	7 th	8 th
P	740	1450	7720	10540	13630	18020	21700	25660
Q	1011	1907	2910	4960	6270	21270	25431	29872

What is the formula of the compound formed when **P** reacts with **Q**?

- A** P_2Q_3 **B** P_3Q_2
C P_2Q_5 **D** P_5Q_2

6 Trends in Atomic Radius, Ionic Radius, and Electronegativity

Learning Outcome:

- (m) Describe and explain qualitatively the trends and variations in atomic radius, ionic radius and electronegativity:
- Across a Period in terms of shielding and nuclear charge
 - Down a Group in terms of increasing number of electronic shells and nuclear charge

Apart from ionisation energies, electronic configuration can help us to understand **atomic radius**, **ionic radius**, and **electronegativity**. This is because these properties are also **dependent on the strength of attraction between the nucleus and the valence electrons or the shared electrons in a covalent bond**.

Atomic radius is defined as *half the distance* between the centres of two adjacent atoms found in the structure of the element.

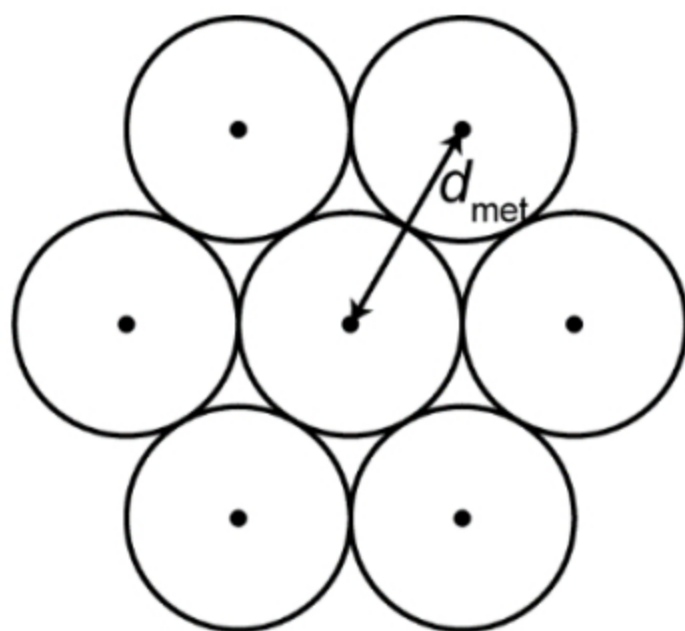
Due to differences in inter-atomic bonding in different elements, the way atomic radius is measured for each element may be different:

metallic radius

- The metallic radius of an atom is half the distance between the **centres of two adjacent atoms in the metal**.

$$r_{\text{met}} = \frac{d_{\text{met}}}{2}$$

- Metallic radius is obviously restricted to those elements that form **metallic lattices**.

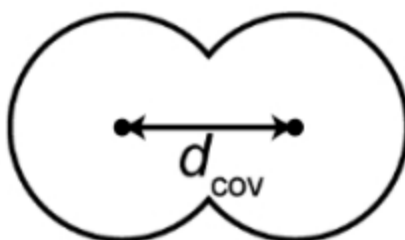


covalent radius

- The covalent radius of an atom is half the distance between the **centres of two adjacent atoms that are covalently bonded**.

$$r_{\text{cov}} = \frac{d_{\text{cov}}}{2}$$

- Covalent radius may be measured for **most non-metal elements**.

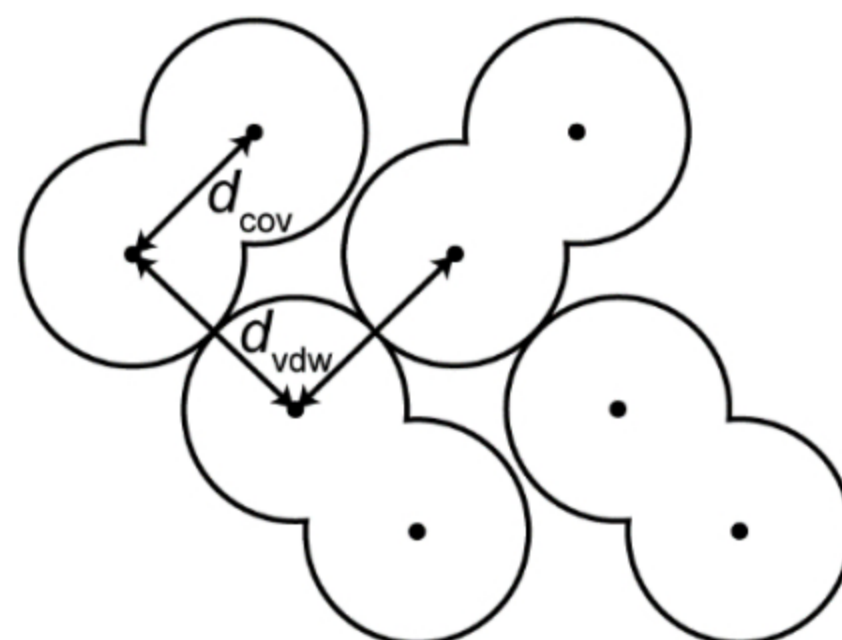


van der Waals radius

- The van der Waals' radius of an atom is half the distance between the **centres of two adjacent atoms which are not chemically bonded**.

$$r_{\text{vdw}} = \frac{d_{\text{vdw}}}{2}$$

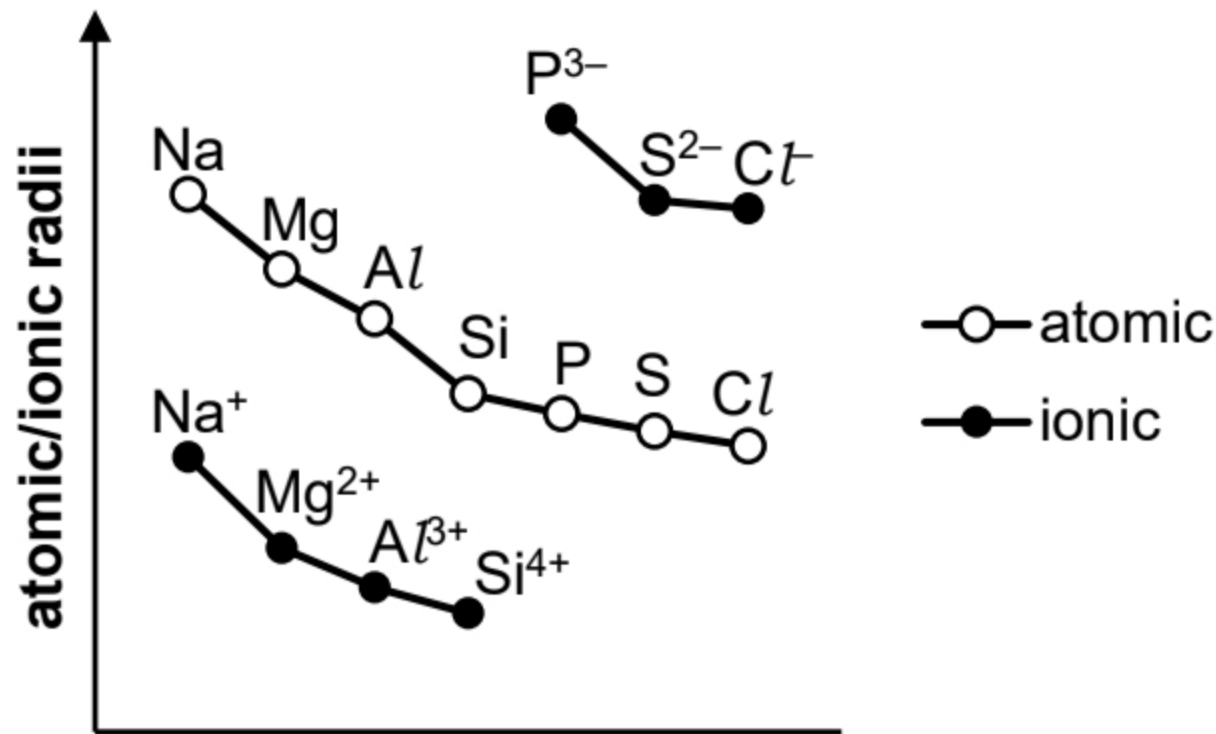
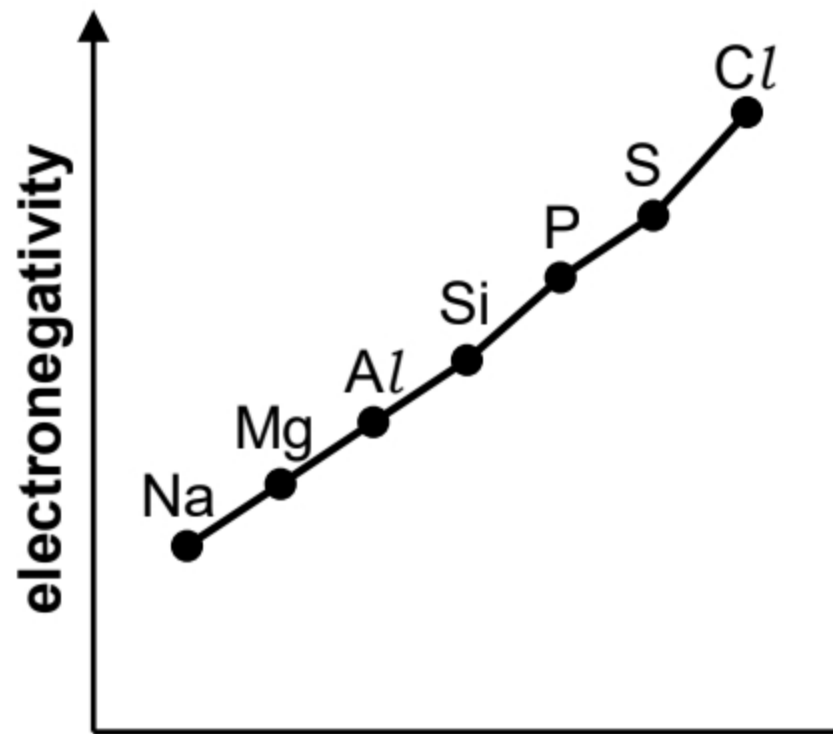
- van der Waal's radius is most easily determined for **non-metals**, and is particularly useful for the **noble gases**.



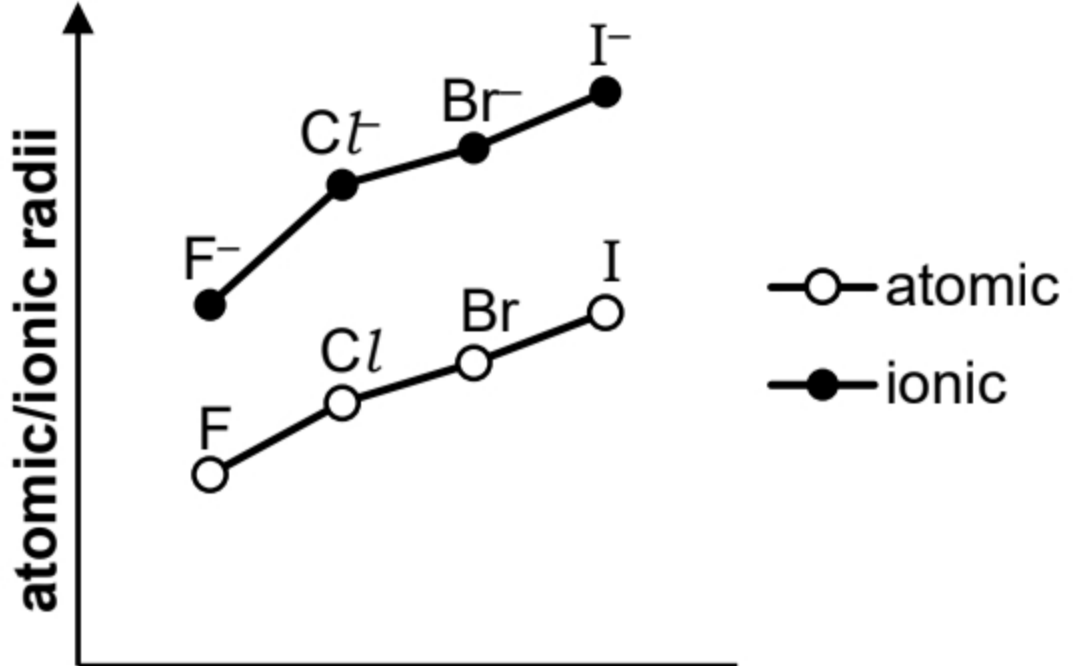
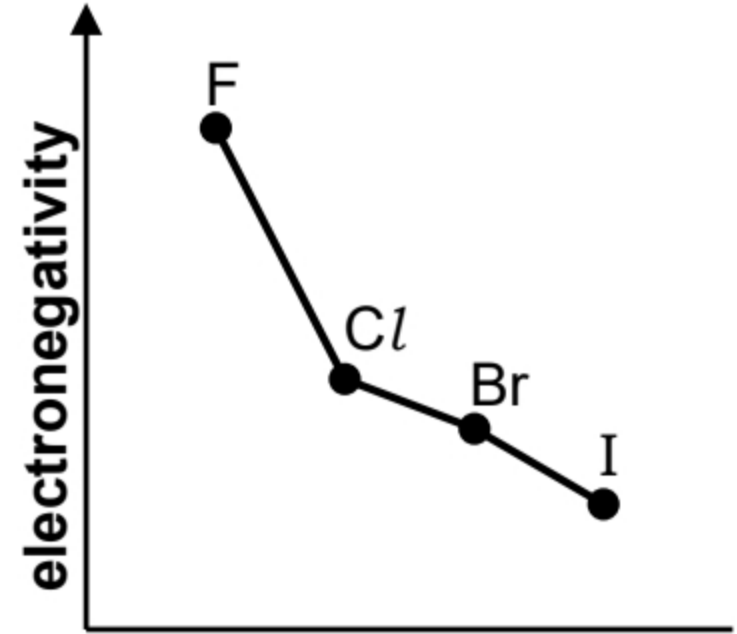
Ionic radius is defined as the average distance between the nuclei of two adjacent ions of the same element.

Electronegativity refers to the ability of an atom to attract the shared pair(s) of electrons in a covalent bond.

6.1 Trends Across the Period

atomic and ionic radii	electronegativity
	
<p><u>Atomic radius decreases across the period</u></p> <ul style="list-style-type: none"> • Number of protons in the nucleus of the atom increases, thus <u>nuclear charge increases</u> • Same number of inner shell electrons, thus <u>shielding effect is approximately constant</u> • <u>Increase in effective nuclear charge</u> • <u>Increase in electrostatic forces of attraction</u> between the nucleus and valence electron <p><u>Cationic radii decreases from Na⁺ to Si⁴⁺</u></p> <ul style="list-style-type: none"> • Nuclear charge increases • Same inter-electronic repulsion since the cations are isoelectronic (same number of electrons) • Stronger electrostatic forces of attraction between the nucleus and the valence electrons <p><u>Anion radii decreases from P³⁻ to Cl⁻</u></p> <ul style="list-style-type: none"> • Nuclear charge increases • Same inter-electronic repulsion since the anions are isoelectronic (same number of electrons) • Stronger electrostatic forces of attraction between the nucleus and the valence electrons 	<p><u>Electronegativity increases across the period</u></p> <ul style="list-style-type: none"> • Number of protons in the nucleus of the atom increases, thus <u>nuclear charge increases</u> • Same number of inner shell electrons, thus <u>shielding effect is approximately constant</u> • <u>Increase in effective nuclear charge</u> • <u>Increase in electrostatic forces of attraction</u> between the nucleus and valence electron

6.2 Trends Down the Group

atomic and ionic radii	electronegativity
	
<p>Atomic and ionic radii increase down the group</p> <ul style="list-style-type: none"> Both nuclear charge and shielding effect increase However, valence electrons are located in a shell with a larger principal quantum number, n, and are further away from the nucleus Decrease in electrostatic forces of attraction between the nucleus and the valence electron 	<p>Electronegativity decreases down the group</p> <ul style="list-style-type: none"> Both nuclear charge and shielding effect increase However, valence electrons are located in a shell with a larger principal quantum number, n, and are further away from the nucleus Decrease in electrostatic forces of attraction between the nucleus and the valence electron

6.3 More Observations About Ionic Radii

Cations are smaller than their corresponding atoms

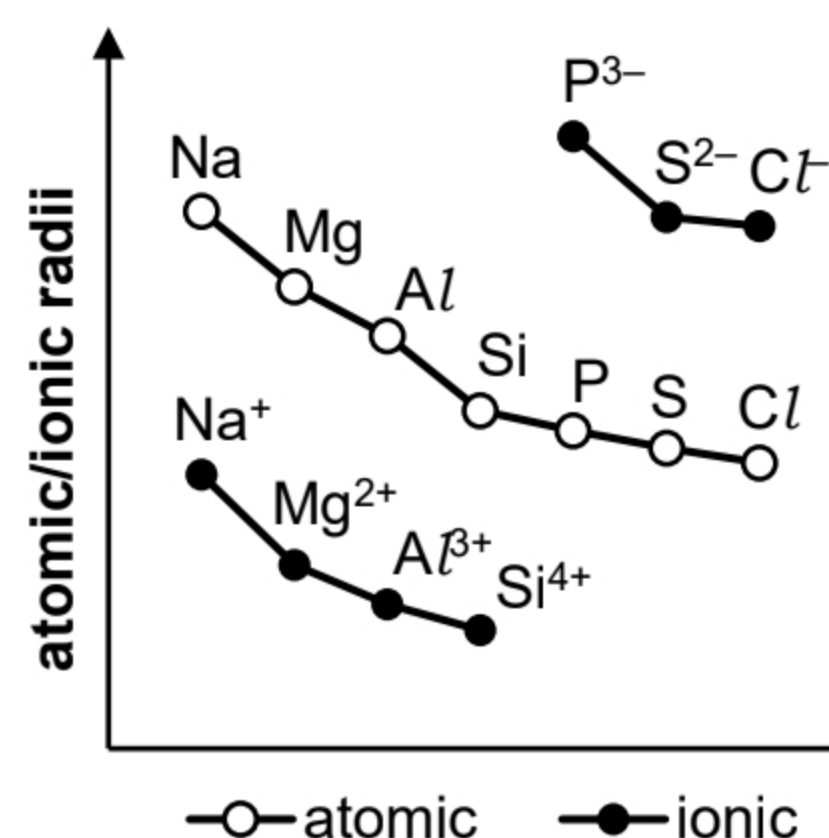
E.g. Electronic configurations of Na: $1s^2 2s^2 2p^6 3s^1$
 Electronic configurations of Na^+ : $1s^2 2s^2 2p^6$

- Nuclear charge **remains the same**
- Cation has less electrons than the atom
- Inter-electronic repulsion **weaker**
- Increase** in the electrostatic forces of attraction between the nucleus and the valence electrons in cation

Anions are larger than their corresponding atoms

E.g. Electronic configurations of Cl: $1s^2 2s^2 2p^6 3s^2 3p^5$
 Electronic configurations of Cl^- : $1s^2 2s^2 2p^6 3s^2 3p^6$

- Nuclear charge **remains the same**
- Anion has more electrons than the atom
- Inter-electronic repulsion **stronger**
- Decrease** in the electrostatic forces of attraction between the nucleus and the valence electrons in anion

**The anions (P^{3-} , S^{2-} and Cl^-) are larger than the cations (Na^+ , Mg^{2+} , Al^{3+} , Si^{4+})**

E.g. Electronic configurations of Na^+ , Mg^{2+} , Al^{3+} , Si^{4+} : $1s^2 2s^2 2p^6$
 Electronic configurations of P^{3-} , S^{2-} and Cl^- : $1s^2 2s^2 2p^6 3s^2 3p^6$

- Anions have **one more filled principal quantum shell** compared to cations
- Valence electrons in anions are **further** from the nucleus than those in cations
- Weaker** electrostatic forces of attraction between the nucleus and valence electrons in anions than in cations

KEY IDEAS

The Atom and the Subatomic Particles

What are the relative charges and relative masses of protons, neutrons and electrons?

Where are these subatomic particles found in an atom? What is the definition of nucleon number and proton number?

How do these subatomic particles behave in an electric field?

Can you deduce the number of protons, neutrons and electrons in atoms and ions given proton and nucleon number (and charge)?

The Arrangement of Electrons

What is a principal quantum shell, subshell and orbital?

Can you draw the energy level diagram of the orbitals from $n=1$ to $n=4$?

Can you draw and describe the shape of s, p and d orbitals correctly?

Electronic Configuration

How does electronic configuration change across a period and down a group?

Can you write/draw the electronic configuration and energy level diagram of an atom and ions?

How do you deduce electron configuration given successive ionisation energy data?

Trends in Ionisation Energies, Atomic and Ionic Radii, and Electronegativity

Can you define ionisation energy, atomic radius, ionic radius and electronegativity?

What are the factors that affect atomic properties (ionisation energy, atomic radius, ionic radius and electronegativity)?



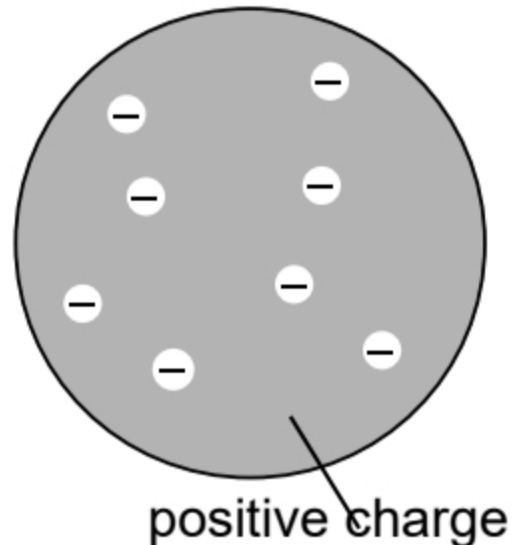

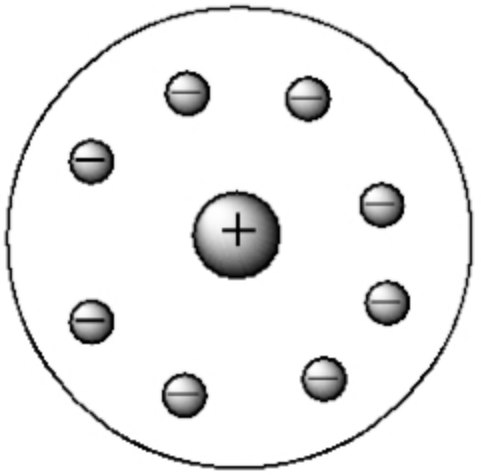
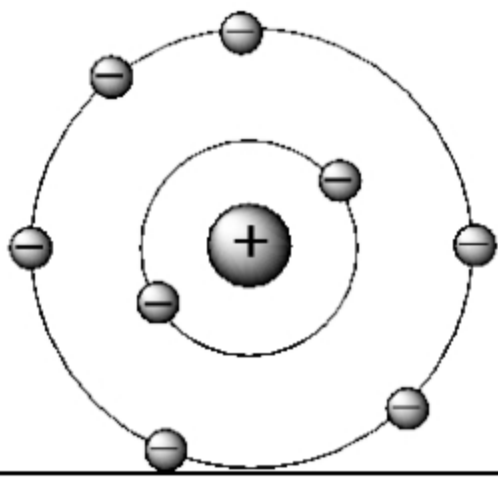

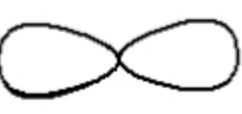
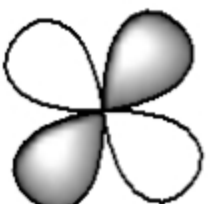
How do these factors change across the period and down a group?

How do these atomic properties change across the period and down a group? Draw the graphs for these trends.

What are the anomalies in the trend of 1st IE across a period?

Can you compare between the radii of corresponding atoms and ions?

ANNEX 1 HISTORICAL PERSPECTIVE OF ATOMIC STRUCTURE

When?	Who?	What?	Diagram
500BC	Democritus	<ul style="list-style-type: none"> Postulated Particle theory of matter: Matter composed of small, indivisible particles called atoms. 	—
1803	John Dalton	Postulated Atomic theory of matter. <ul style="list-style-type: none"> All matter is composed of atoms. Atoms cannot be made or destroyed. All atoms of the same element are identical. Different elements have different types of atoms. 	—
1897	JJ Thomson	<ul style="list-style-type: none"> Discovered electrons. Proposed a 'Plum Pudding' model of the atom: electrons embedded in a cloud of positive charge. Discovery of electrons: <div style="display: flex; justify-content: space-around; align-items: center;">   </div> <div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">Cathode Ray Tube Experiment</div> <div style="text-align: center;">Millikan's Oil Drop Experiment</div> </div>	
1911	Ernest Rutherford	<ul style="list-style-type: none"> Discovered protons. Proposed that most of the mass of the atom is concentrated in a very small volume known as nucleus. Rutherford's model of an atom depicts a nucleus at the centre of the atom, with electrons moving around the nucleus, like planets orbiting around a sun. Discovery of protons: <div style="text-align: center;">  </div> <div style="text-align: center;">Rutherford's Gold Foil Experiment</div>	
1913	Niels Bohr	<ul style="list-style-type: none"> Modifying Rutherford's model, Bohr stated that electrons are confined to well-defined circular orbits, each having discrete energy level. **(This is the model described at 'O' Level.)	
1927	Erwin Schrodinger	<ul style="list-style-type: none"> Using Louis de Broglie's 1924 proposal that electrons behave as waves in an atom, Schrodinger wrote out a wave equation for the electrons in an atom. Solutions of the Schrodinger equation describe the energy level of each electron and the region an electron is likely to be found (called orbitals) around the nucleus. **(For 'A' Level, students need to know the shapes and relative energies of these orbitals.)	<div style="display: flex; justify-content: space-around; align-items: center;"> <div style="text-align: center;">  <p>s-orbital</p> </div> <div style="text-align: center;">  <p>p-orbital</p> </div> </div> <div style="text-align: center; margin-top: 20px;">  <p>d-orbital</p> <p>one of the d-orbitals</p> </div>
1932	James Chadwick	<ul style="list-style-type: none"> Discovered neutrons. Neutrons are electrically neutral particles found in the nucleus of an atom, having the same mass as protons. 	—

ANNEX 2 ELECTRONIC CONFIGURATIONS OF D-BLOCK ELEMENTS

Up till Ca, the 4s orbital is lower in energy compared to the 3d orbitals. However, **from Sc onwards**, there is a crossover between the energies of the 3d and 4s orbitals (see Figure A below), and the **4s** becomes the **outermost (highest energy) orbital**, while the **3d** orbital is **penultimate** (2nd from the last). Hence, **when representing the electronic configuration** in writing, **3d is written before 4s**.

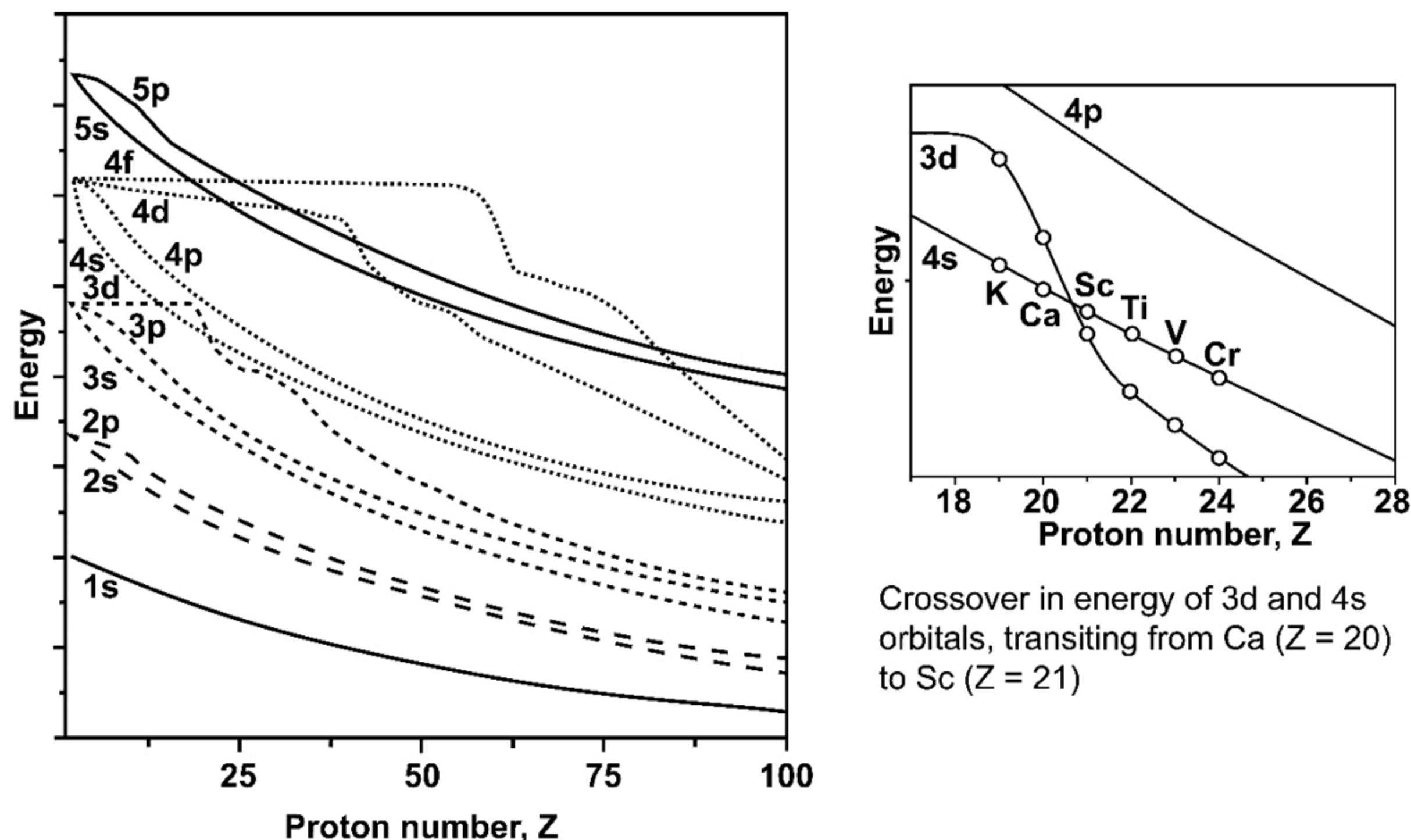


Figure A Crossover between energy of 3d and 4s orbitals between Ca and Sc

However, **when filling up the orbitals of an atom of a d-block element**, the **4s orbital is filled before the 3d**. For example, spectroscopic results show that Sc has the electronic configuration [Ar] 3d¹ 4s², instead of [Ar] 3d³ or [Ar] 3d² 4s¹. This is due to the **3d subshell being more compact than the diffuse 4s orbital**. The most probable distance of a 3d electron from the nucleus is less than that of a 4s electron i.e. the 3d electrons are more likely to be found closer to the nucleus (see Figure B), so two 3d electrons repel each other more strongly than two 4s electrons. Hence, **the more electrons occupying the 3d subshell, the larger the electron repulsion**.

For Sc, electronic configuration [Ar] 3d¹ 4s² is more favourable as it minimises the strong electron-electron repulsions in the 3d orbitals. Even though energy is required to have electrons populate the higher energy 4s orbital, the total energy of the atom is the least.

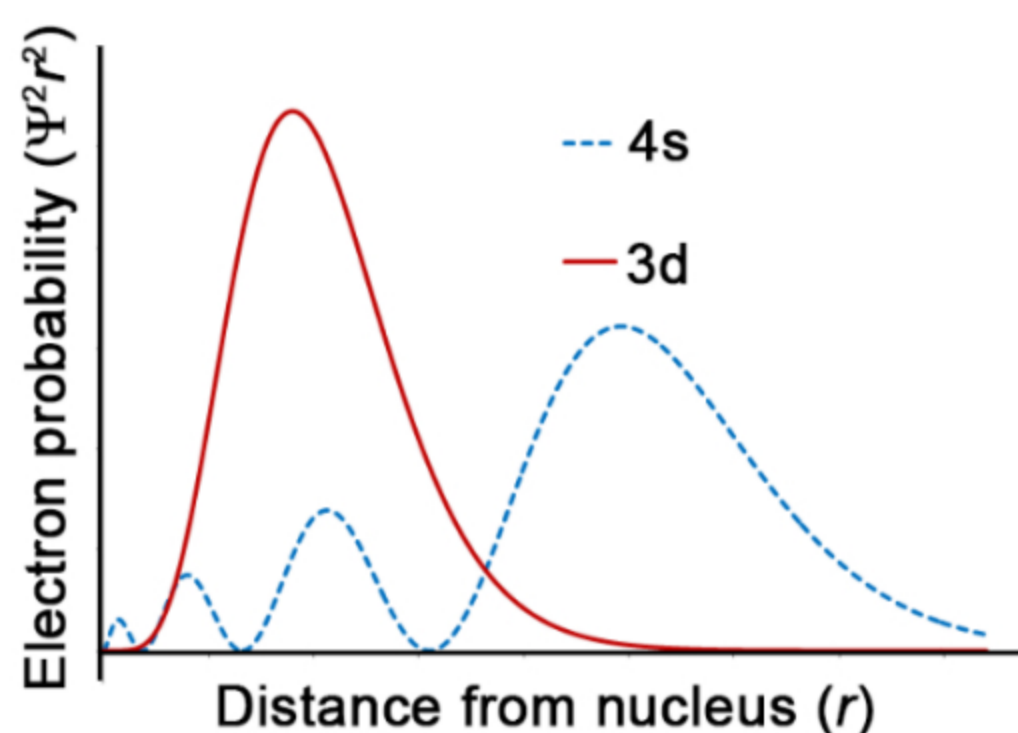


Figure B

Probability of finding an electron at different distances from the nucleus