01 Atomic Structure

1 Sub-atomic Particles

1.1 Protons, neutrons and electrons

Particle	Relative charge	Relative mass
proton	+1	1
neutron	_____	1
electron	−1	_____

- Protons and neutrons reside together in the **nucleus**, which holds almost all the mass and all the positive charge.
- Electrons are found in regions of space around the nucleus, and are **attracted electrostatically** by the protons.

1.2 Proton number and nucleon number

DEFINITION **Nucleon number**: total number of _____ in the nucleus of an atom.

DEFINITION **Proton number**: number of _____ in the nucleus of an atom. It determines the _____ of the element.

DEFINITION **Nuclide**: a specific combination of protons and neutrons in a nucleus.

$^{35}_{17}Cl$ — **35** nucleon number (mass number) = p + n; **17** proton number (atomic number) = p

Atom	Cation	Anion
no. of p = no. of e^-	loses e^-: p > e^-	gains e^-: e^- > p

1.3 Isotopes

DEFINITION **Isotopes** are atoms of the same element with the same number of _____ but different numbers of _____.

^{35}Cl	17 p, 18 n
^{37}Cl	17 p, 20 n

Same electronic configuration
Same _____

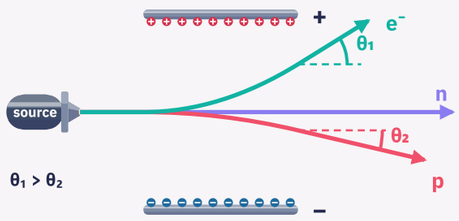
Different masses
Different _____

Name an isotope with its nucleon number, e.g. ^{2}H. In every stable isotope except ^{1}H and ^{3}He, neutrons ≥ protons.

1.4 Beams of p, n and e^- in an electric field

angle of deflection ∝ $\frac{\square}{\square}$

- **Protons** are deflected towards the negatively charged plate.
- **Electrons** are deflected towards the positively charged plate. They are much lighter than protons, so are deflected to a **larger extent**.
- **Neutrons** have no charge and are undeflected.



WORKED EXAMPLE A beam of $^{241}Am^+$ ions is deflected by +2°. Under the same conditions, find the angle of deflection of $^{32}S^-$ ions.

$\theta = k \times \frac{charge}{mass}$ Am^+: $+2 = k \times \frac{+1}{241} \rightarrow k = 482$ S^-: $\theta = 482 \times \frac{-1}{32} = \mathbf{-15.1°}$

2 Relative Masses of Atoms

2.1 Relative isotopic mass

DEFINITION **Relative isotopic mass**: the mass of one mole of atoms of an _____ relative to 1/12 the mass of one mole of ^{12}C atoms.

2.2 Relative abundance

Relative abundance: the _____ of atoms of each isotope in a naturally occurring sample of the element.

e.g. chlorine: 75% ^{35}Cl, 25% ^{37}Cl

2.3 Relative atomic mass, A_r

DEFINITION **Relative atomic mass**: the _____ mass of one mole of atoms of an element relative to 1/12 the mass of one mole of ^{12}C atoms.

$A_r = \frac{\Sigma \text{ (relative isotopic mass} \times \text{relative abundance)}}{\text{total abundance (100)}}$ Cl: $\frac{(35 \times 75) + (37 \times 25)}{100} =$ _____

3 Shells, Subshells and Orbitals

3.1 Principal quantum shells, subshells and orbitals

DEFINITION **Orbital**: the region of space where there is a _____ _____ (95%) of finding an electron. Each orbital can accommodate _____ electrons.

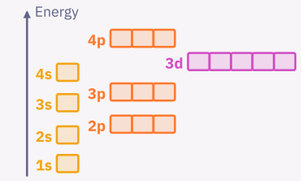
Atom → **principal quantum shells (n)** → **subshells (s, p, d, f)** → **orbitals** → **max. 2 e^- each**

A larger n gives a larger, more diffused orbital further from the nucleus, and hence a higher energy.

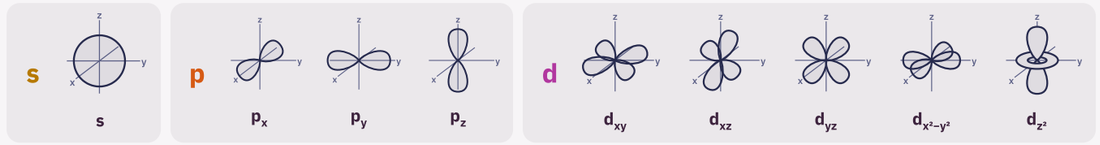
n	Subshell	No. of orbitals	Types of orbitals	Total (n^2)	Max e^- ($2n^2$)
1	1s	1	1s	1	2
2	2s	1	2s	4	8
	2p	3	$2p_x$, $2p_y$, $2p_z$		
3	3s	1	3s	9	18
	3p	3	$3p_x$, $3p_y$, $3p_z$		
	3d	5	$3d_{xy}$, $3d_{xz}$, $3d_{yz}$, $3d_{x^2-y^2}$, $3d_{z^2}$		
4	4s 4p 4d (4f)	1, 3, 5	4f not in syllabus	16	32

3.2 Relative energies of the orbitals

- Within a shell: **s < p < d < f**, as an s electron is more likely to be near the nucleus than a p, and a p than a d.
- Levels get closer as n increases. First overlap: _____ and _____ (4s fills first).



3.3 Shapes of orbitals



- **s** spherical, **p** dumb-bell. Orbitals within a subshell have the same energy: **degenerate**.
- $d_{x^2-y^2}$, d_{z^2}: along the axes. d_{xy}, d_{xz}, d_{yz}: between the axes.

4 Electronic Configuration

4.1 Rules for filling orbitals

1. Aufbau principle

Electrons fill the orbitals of _____ first.
After 3p, **4s** is filled before 3d.

2. Pauli exclusion principle

An orbital holds a maximum of two electrons, of _____.

3. Hund's rule

Orbitals of a subshell are filled **singly** first, with parallel spins, before pairing.
This gives less _____.

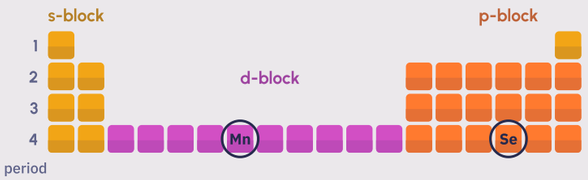


Electrons-in-boxes: label the boxes with the subshell only (2p, not $2p^6$). **Ground state**: all e^- in the lowest energy levels.
Excited state: an e^- promoted, e.g. O: $1s^2\ 2s^2\ 2p^3\ 3s^1$.

4.2 Writing configurations of atoms

From the Periodic Table

1. **Period** = n of the valence shell. A new period starts when e^- enter a new principal quantum shell
2. **Block**: the subshell filled last. The d-block is one shell behind: 3d in Period 4
3. **Position in the block**: the number of e^- in that subshell



e.g. **Mn**: Period 4, 5th in the d-block → [Ar] $3d^5\ 4s^2$

e.g. **Se**: Period 4, 4th in the p-block → [Ar] $3d^{10}\ 4s^2\ 4p^4$

Elements in the same Group have similar valence shell configurations.

Noble gas configuration

Inner electrons shown as the previous noble gas:
Li: [He] $2s^1$.

EXAM TIP Write the **full** configuration in order of increasing n: **...$3d^6\ 4s^2$**.

Anomalies: Cr and Cu

Cr [Ar] **$3d^5\ 4s^1$** ~~$3d^4\ 4s^2$~~

Cu [Ar] **$3d^{10}\ 4s^1$** ~~$3d^9\ 4s^2$~~

A half-filled (d^5) or fully-filled (d^{10}) 3d subshell is more stable.

4.3 Configurations of ions

- Write the configuration of the atom first.
- **Cation**: electrons are removed from the outermost shell of the ground state configuration (_____ before 3d).
- **Anion**: electrons are added to the empty or partially-filled valence orbitals.

S^{2-}	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6$
Na^+	$1s^2\ 2s^2\ 2p^6$
Fe^{2+}	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^6$

5 Ionisation Energy

DEFINITION **Ionisation energy**: the energy required to remove 1 mole of _____ from 1 mole of _____ atoms or ions.

DEFINITION **2nd IE**: the enthalpy change when 1 mole of electrons is removed from 1 mole of gaseous, singly charged cations.

$X(g) \rightarrow X^+(g) + e^-$ ΔH = 1st IE of X

$X^+(g) \rightarrow X^{2+}(g) + e^-$ ΔH = 2nd IE of X

$X^{(n-1)+}(g) \rightarrow X^{n+}(g) + e^-$ ΔH = n^{th} IE of X

All IEs are **endothermic**. Always show (g) in the equation.

5 Ionisation Energy (continued)

5.1 Trends in first IE Z_{eff} = Z – shielding constant

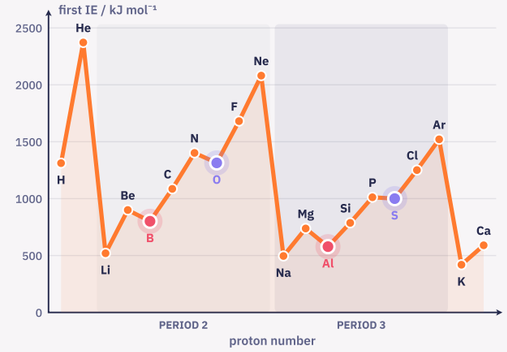
Across periods 2 and 3, 1st IE generally ↑

1. Nuclear charge ↑, while there is a _____ ↑ in inner shell _____, as e^- are added to the same shell
2. → effective nuclear charge _____, atomic radius _____
3. → valence e^- _____ by the nucleus → _____ required to remove them

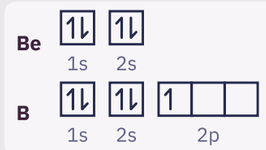
Down a group, 1st IE ↓

1. Atomic radius _____
2. No. of principal quantum shells ↑ → _____ _____ ↑, which _____ the ↑ in nuclear charge
3. → valence e^- _____ by the nucleus → _____ required to remove them

First IE of elements 1 to 20 / kJ mol⁻¹

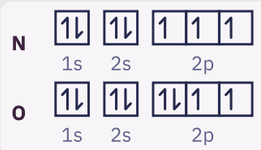


Dip: Be → B also Mg → Al



The 2p e^- removed from B is _____ than the 2s e^- removed from Be → _____ required to remove it → 1st IE of B < Be

Dip: N → O also P → S



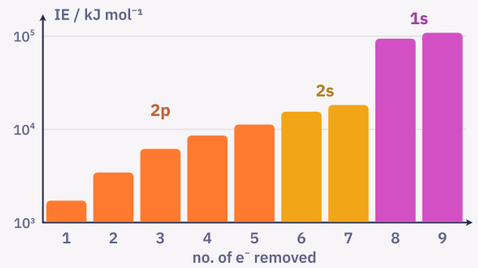
_____ between the _____ 2p e^- in O → easier to remove one of them than an unpaired 2p e^- from N → _____ required → 1st IE of O < N

5.2 Successive ionisation energies

ANSWER STRUCTURE **Reading a successive IE graph**

1. **General trend**: successive IEs ↑ as each e^- is removed from an ion of _____
2. **Gradual increase** (1st to 7th IE): removal of e^- from the _____
3. **Sharp increase** from 7th to 8th IE: 8th e^- removed from an _____, nearer to the nucleus, with less shielding

F: $1s^2\ 2s^2\ 2p^5$ · log IE



Note: the small jump from 5th to 6th IE is an e^- from a _____ (2s after 2p) of the same shell.

WORKED EXAMPLE The successive IEs of element X are shown below. Predict the Group of X.

IE / kJ mol⁻¹	870	1800	3000	3600	5800	7000	13000

1. Successive IEs ↑ as each e^- is removed from an ion of _____
2. 1st to 6th IE ↑ gradually: removal of the _____ e^- only
3. Sharp ↑ from 6th to 7th IE: 7th e^- removed from an _____, nearer to the nucleus, with _____
4. ∴ 6 e^- in the outermost shell ($ns^2\ np^4$) → X is in Group _____. Big jumps + 1 = occupied shells.