MEGA LECTURE

IB DP CHEMISTRY

Structure 1: Models of the Particulate Nature of Matter

Structure 1.3 Electron Configurations

Revision Notes · Standard and Higher Level

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What the syllabus requires

Structure 1.3 explains how electrons are arranged inside atoms and how that arrangement is deduced from experimental evidence. Use this checklist to confirm you can do each item before an exam.

Understanding	You should be able to...
Emission spectra	Describe how line spectra provide evidence for discrete (quantised) energy levels in atoms.
Main energy levels	Relate the principal quantum number n to shells and use the $2n^2$ rule for maximum electrons.
Sub-levels and orbitals	State the number of orbitals in the s, p, d and f sub-levels and the maximum electrons each holds.
Filling rules	Apply the Aufbau principle, the Pauli exclusion principle and Hund's rule to build configurations.
Writing configurations	Give full and condensed configurations for atoms and ions from Z = 1 to 36.
Anomalies (HL)	Explain the configurations of chromium and copper in terms of stable half-filled and full sub-levels.
Ionization energy (HL)	Interpret first and successive ionization energies as evidence for shells and sub-levels.

> **Exam note:** The core of Structure 1.3 (energy levels, orbitals, filling rules and configurations to Z = 36) is common to SL and HL. Orbital diagrams, the Cr and Cu anomalies and the ionization-energy evidence are examined at **HL** and are flagged (HL) throughout these notes.

1. From the Bohr model to energy levels

An atom's electrons are not free to have any energy. They are restricted to a set of allowed values called **main energy levels** or **shells**, each labelled by a whole number called the **principal quantum number**, *n* = 1, 2, 3, 4, ... The shell with n = 1 lies closest to the nucleus and is lowest in energy; energy rises as n increases, and the levels crowd closer together (converge) at high n.

Evidence: emission line spectra

When hydrogen gas is given energy (for example in a discharge tube) its electrons are promoted to higher levels. As each electron falls back to a lower level it emits a photon whose energy equals the gap between the two levels: $E = hf$. Because only certain gaps exist, only certain photon energies (and therefore only certain frequencies and colours) appear. The result is a **line spectrum** – a set of sharp coloured lines on a dark background – rather than a continuous rainbow.

Two conclusions follow directly from the spectrum, and both are common exam marks:

- Electron energy is **quantised** (only discrete values are allowed), because a continuous range of energies would give a continuous spectrum.
- The lines **converge** at higher frequency, showing that the energy levels themselves get closer together as n increases; convergence marks the ionization limit, where the electron escapes the atom.

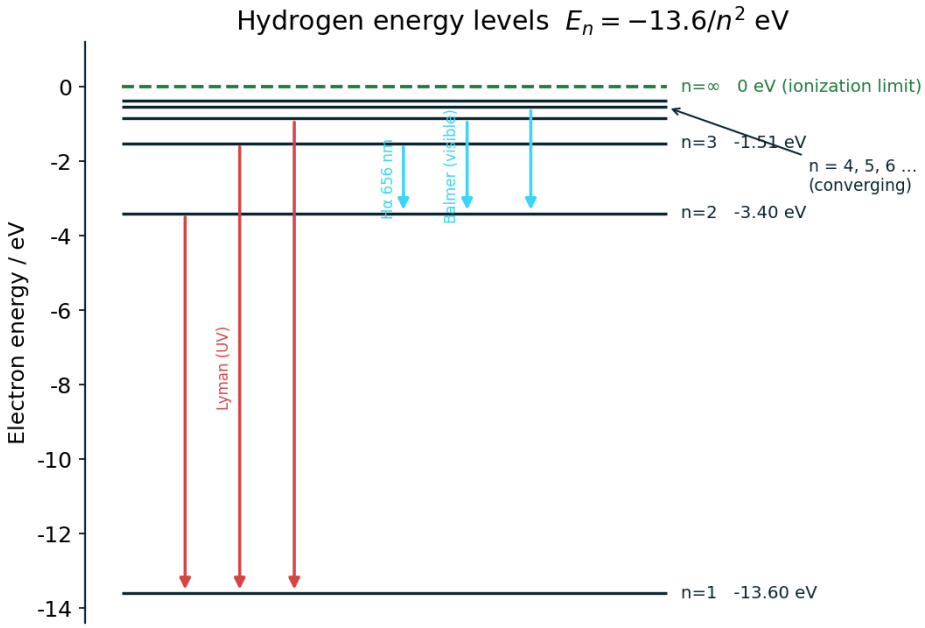

Figure 1. Hydrogen energy levels $E_n = -13.6/n^2$ eV. Levels converge toward the ionization limit (n = ∞, 0 eV). A falling electron emits a photon of energy equal to the level gap; the Balmer Hα line (n = 3 → 2) gives ≈ 656 nm.

Maximum electrons in a shell

The greatest number of electrons a main energy level can hold is given by:

$$\textbf{maximum electrons} = 2n^2$$

Shell (n)	Sub-levels present	Max electrons ($2n^2$)
1	1s	2
2	2s, 2p	8
3	3s, 3p, 3d	18
4	4s, 4p, 4d, 4f	32

> **Careful:** $2n^2$ is the theoretical *capacity* of a shell. It is not the same as the number of electrons that actually occupy the outer shell of an atom, nor the same as the period pattern (2, 8, 8, 18...) you met for the first 20 elements, which reflects the order sub-levels fill.

2. Sub-levels and orbitals

Each main energy level is divided into **sub-levels** (sub-shells) of slightly different energy, labelled s, p, d and f. A sub-level is made up of one or more **orbitals**. An orbital is a region of space around the nucleus in which there is a high probability of finding an electron, and **each orbital holds a maximum of two electrons** (which must have opposite spins).

Sub-level	Number of orbitals	Max electrons	Shells in which it appears
s	1	2	every shell (n ≥ 1)
p	3	6	n ≥ 2

Sub-level	Number of orbitals	Max electrons	Shells in which it appears
d	5	10	$n \geq 3$
f	7	14	$n \geq 4$

Shapes of the orbitals

- An **s orbital** is spherical, centred on the nucleus. A 2s orbital is a larger sphere than a 1s orbital.
- A **p orbital** is dumb-bell (two-lobed) shaped, with the two lobes on opposite sides of the nucleus. The three p orbitals in a sub-level point along mutually perpendicular axes and are labelled p_x, p_y and p_z.
- The five **d orbitals** have more complex shapes (four have four lobes; one has two lobes with a ring). You are not required to reproduce these, only to know that there are five d orbitals holding up to ten electrons.

Relative energies of sub-levels

Within one shell the energy order is s < p < d < f. Between shells the sub-levels overlap: the 4s sub-level lies slightly **below** 3d in energy, so 4s fills before 3d. This single overlap is responsible for much of the behaviour of the first transition series and is examined repeatedly.

3. The three filling rules

Electron configurations are built by placing electrons into orbitals using three rules together.

(a) The Aufbau principle

Electrons fill the **lowest-energy** orbital available first. The usual filling order (aufbau means 'building up' in German) is:

1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p → 5s → 4d → 5p

Note the key crossover: **4s fills before 3d** because 4s is lower in energy when the sub-levels are empty. A useful memory aid is the diagonal rule, in which sub-levels are listed in rows (1s; 2s 2p; 3s 3p 3d; 4s 4p 4d 4f...) and read along successive diagonals from top-right to bottom-left.

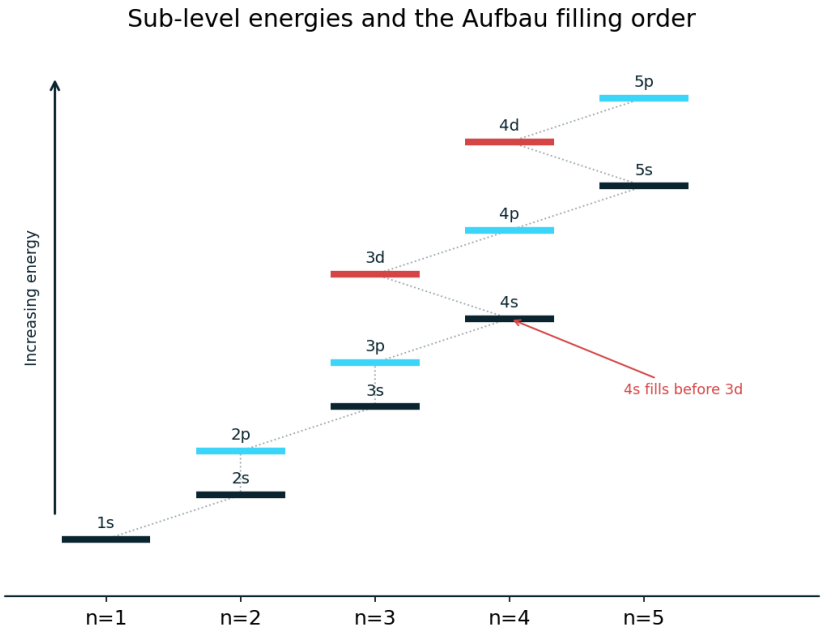

Figure 3. Sub-level energies and the Aufbau filling order (1s → 2s → 2p → 3s → 3p → 4s → 3d ...). The 4s sub-level lies below 3d, so it fills first.

(b) The Pauli exclusion principle

An orbital holds at most two electrons, and if it holds two they must have **opposite spins**. In an orbital diagram this is drawn as one arrow up and one arrow down in the same box: [↑ ↓]. No two electrons in an atom can have the same set of four quantum numbers.

(c) Hund's rule of maximum multiplicity

When electrons enter a set of orbitals of **equal energy** (for example the three 2p orbitals), they occupy them **singly with parallel spins** first, and only pair up once every orbital in the sub-level already has one electron. Singly filled orbitals minimise electron-electron repulsion and give a lower-energy, more stable arrangement.

Orbital diagrams for the 2p filling of carbon, nitrogen and oxygen show Hund's rule in action (2s is filled first in each):

```
N  (2p³):   2s [↑↓]   2p [↑] [↑] [↑]
O  (2p■):   2s [↑↓]   2p [↑↓] [↑] [↑]
```

Nitrogen has three parallel, unpaired 2p electrons; oxygen is forced to pair the fourth 2p electron, which is why the first ionization energy of oxygen is slightly lower than that of nitrogen (see section 6).

> **Exam tip:** Draw boxes left to right, put one up-arrow in each box before adding any down-arrows, and keep all the single arrows pointing the same way. Losing a mark for pairing too early is one of the most common orbital-diagram errors.

4. Writing electron configurations

A configuration lists each occupied sub-level with the number of electrons it holds written as a superscript. The superscripts must add up to the total number of electrons (equal to the atomic number Z for a neutral

atom).

Full configuration writes every sub-level from 1s upward. For example, sulfur (Z = 16):

$$\text{S: } 1s^2 2s^2 2p^6 3s^2 3p^4$$

Condensed (noble-gas core) configuration replaces the inner electrons with the symbol of the previous noble gas in square brackets, then lists only the outer electrons:

$$\text{S: } [Ne]3s^2 3p^4$$

Selected configurations, Z = 1 to 36

Order the sub-levels by energy when filling, but it is conventional to write them grouped by shell (so 3d is written after 3p and before 4s in the final answer, even though 4s filled first). Both orderings are accepted in exams provided the superscripts are correct.

Z	Element	Full configuration	Condensed
1	H	$1s^1$	$1s^1$
6	C	$1s^2 2s^2 2p^2$	$[He]2s^2 2p^2$
10	Ne	$1s^2 2s^2 2p^6$	$[He]2s^2 2p^6$
11	Na	$1s^2 2s^2 2p^6 3s^1$	$[Ne]3s^1$
17	Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	$[Ne]3s^2 3p^5$
18	Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$	$[Ne]3s^2 3p^6$
19	K	$...3p^6 4s^1$	$[Ar]4s^1$
20	Ca	$...3p^6 4s^2$	$[Ar]4s^2$
21	Sc	$...4s^2 3d^1$	$[Ar]3d^1 4s^2$
26	Fe	$...4s^2 3d^6$	$[Ar]3d^6 4s^2$
30	Zn	$...4s^2 3d^{10}$	$[Ar]3d^{10} 4s^2$
35	Br	$...3d^{10} 4s^2 4p^5$	$[Ar]3d^{10} 4s^2 4p^5$
36	Kr	$...3d^{10} 4s^2 4p^6$	$[Ar]3d^{10} 4s^2 4p^6$

Configurations of ions

- **Positive ions (cations)** form by removing the highest-energy (outermost) electrons. For main-group metals remove the outer s and p electrons: Na → Na^+ is [Ne]; Mg → Mg^{2+} is [Ne]; Al → Al^{3+} is [Ne].
- **Negative ions (anions)** form by adding electrons into the next available orbitals: Cl + e^- → Cl^- is [Ar]; O + $2e^-$ → O^{2-} is [Ne].
- **Transition-metal cations** follow a crucial rule: **the 4s electrons are removed before the 3d electrons**, even though 4s filled first. This is because once 3d is occupied it drops below 4s in energy.

Species	Configuration	Comment
Fe	$[Ar]3d^6 4s^2$	neutral atom, 26 electrons

Species	Configuration	Comment
Fe^{2+}	$[Ar]3d^6$	remove both 4s electrons first
Fe^{3+}	$[Ar]3d^5$	then one 3d; stable half-filled d^5
Cu	$[Ar]3d^{10}4s^1$	anomalous atom (section 5)
Cu^{2+}	$[Ar]3d^9$	remove 4s then one 3d
Zn^{2+}	$[Ar]3d^{10}$	remove both 4s electrons

> **Most common mistake:** Writing Fe^{2+} as $[Ar]3d^4 4s^2$ by taking electrons from 3d. Always take the 4s electrons out first for a d-block ion.

5. (HL) Orbital diagrams and the Cr and Cu anomalies

At HL you should be able to draw full orbital (arrow-in-box) diagrams and to explain two configurations that break the simple Aufbau pattern.

Full orbital diagram of iron (HL)

Fe = $[Ar]3d^6 4s^2$. The valence part is:

```
3d [↑↓] [↑] [↑] [↑] [↑]    4s [↑↓]
```

Note the four unpaired 3d electrons, which is why iron and its compounds are paramagnetic and coloured.

Chromium: $[Ar]3d^5 4s^1$ (HL)

The expected configuration would be $[Ar]3d^4 4s^2$, but the actual configuration is $[Ar]3d^5 4s^1$. One 4s electron shifts into 3d so that **both the 3d and 4s sub-levels are exactly half-filled**:

```
Cr  3d [↑] [↑] [↑] [↑] [↑]    4s [↑]
```

Chromium: $[Ar]3d^4 4s^2 \rightarrow [Ar]3d^5 4s^1$. A half-filled d sub-level (d^5) has one electron in each of the five orbitals with parallel spins, giving a symmetrical distribution and an extra stability associated with reduced repulsion and favourable exchange energy.

Copper: $[Ar]3d^{10}4s^1$ (HL)

The expected $[Ar]3d^9 4s^2$ is replaced by $[Ar]3d^{10}4s^1$, because a **completely full** d sub-level (d^{10}) is more stable than an almost-full one:

```
Cu  3d [↑↓] [↑↓] [↑↓] [↑↓] [↑↓]    4s [↑]
```

> **How to phrase it:** In an exam, state that a **half-filled (d^5) or fully filled (d^{10}) d sub-level has extra stability**, and that promoting one 4s electron into 3d achieves this arrangement. Do not just assert 'it is more stable' without naming the half- or fully-filled d sub-level.

6. (HL) Ionization energy as evidence

The **first ionization energy** (IE_1) is the energy needed to remove one mole of electrons from one mole of gaseous atoms:

$$X(g) \rightarrow X^{+}(g) + e^{-} \quad \Delta H = IE_1$$

It is always endothermic (positive) because energy is required to overcome the attraction between the nucleus and the electron. Ionization energy is direct experimental evidence for the shell-and-sub-level model.

First IE across a period

Across a period IE_1 **increases** overall: nuclear charge rises, electrons enter the same shell, so shielding is roughly constant and the atomic radius falls, holding the outer electron more tightly. Two dips interrupt the trend in period 3 and are themselves evidence for sub-levels:

- **Al is lower than Mg:** aluminium's outer electron is in a 3p orbital, higher in energy and better shielded than magnesium's 3s electron, so it is easier to remove. This shows the 3s and 3p sub-levels differ in energy.
- **S is lower than P:** sulfur's fourth 3p electron is paired in one orbital ($3p^4$), and the extra electron-electron repulsion between the paired electrons makes it easier to remove than phosphorus's half-filled $3p^3$ set. This shows the effect of electron pairing predicted by Hund's rule.

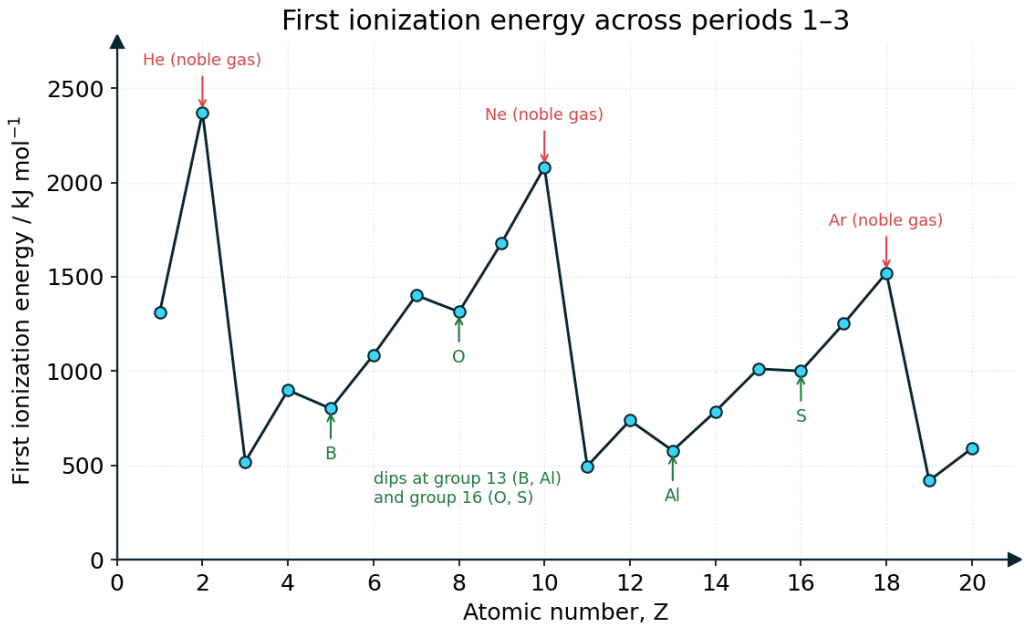

Figure 2. First ionization energy across periods 1–3. Peaks fall on the noble gases (He, Ne, Ar); dips at group 13 (B, Al) and group 16 (O, S) are direct evidence for the s and p sub-levels and for electron pairing.

First IE down a group

Down a group IE_1 **decreases**: each successive element has an extra full shell, so the outer electron is further from the nucleus and better shielded by inner electrons; the increased nuclear charge is outweighed by distance and shielding, so the electron is easier to remove.

Successive ionization energies

Removing electrons one after another from the same atom gives the **successive ionization energies** (IE_1, IE_2, IE_3 ...). They always increase, because each electron is pulled from an increasingly positive ion. Crucially, there are **large jumps** whenever the next electron must come from a shell closer to the nucleus.

A graph of log(IE) against the number of electrons removed shows these jumps as sharp steps. Counting the electrons removed **before** the first big jump gives the number of electrons in the outer shell, which

equals the **group number** and identifies the element's group.

Electron removed	IE / kJ mol^{-1}	Comment (example: sodium, group 1)
1st	496	outer 3s electron – easy to remove
2nd	4560	big jump: now removing from the full n = 2 shell
3rd	6910	steady rise within n = 2
...	...	...
9th	141 000	another big jump: removing from n = 1 (1s)

Sodium shows one electron removed before the first large jump, confirming one outer electron and placement in group 1, with its electrons arranged 2, 8, 1.

> **Reading a log-IE graph:** Count electrons in each 'plateau' between jumps: the plateaus give the shell populations from the outside in. A 2, 8, 8, 2 pattern (jumps after the 2nd, 10th and 18th electrons) identifies calcium.

7. Worked examples

Worked example 1 – full and condensed configuration

Write the full and condensed electron configurations of a vanadium atom (Z = 23).

Fill in energy order to 23 electrons: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^3$. Check: 2+2+6+2+6+2+3 = 23. →

Full: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^3 4s^2$

Condensed: $[Ar]3d^3 4s^2$

Worked example 2 – a transition-metal ion

Write the electron configuration of the Mn^{2+} ion (Mn is Z = 25).

Neutral Mn: $[Ar]3d^5 4s^2$. To form Mn^{2+} remove two electrons, and for a d-block ion **remove the 4s electrons first**.

Remove both 4s electrons → **Mn^{2+}: $[Ar]3d^5$**, a stable half-filled d sub-level.

Pitfall check: it is *not* $[Ar]3d^3 4s^2$.

Worked example 3 — identify the element from IE data

Successive ionization energies of an element (kJ mol^{-1}) are: 738, 1451, 7733, 10 540, 13 630. Deduce the group.

Look for the first large jump: 1451 → 7733 is roughly a fivefold rise, far bigger than the step before it.

Two electrons are removed easily before the jump, so there are **two electrons in the outer shell**. The element is in **group 2** (this data is for magnesium).

Worked example 4 — explain an anomaly (HL)

Explain why copper has the configuration $[Ar]3d^{10}4s^{1}$ rather than the expected $[Ar]3d^{9}4s^{2}$.

Promoting one 4s electron into 3d gives a **completely filled 3d** sub-level (d^{10}). A fully filled d sub-level is more stable (lower in energy) than the d^{9} arrangement, so the $d^{10}4s^{1}$ configuration is adopted.

Worked example 5 — orbital diagram and unpaired electrons (HL)

Draw the orbital diagram of the valence electrons of oxygen (Z = 8) and state the number of unpaired electrons.

O = $1s^{2}2s^{2}2p^{4}$. Valence:

```
2s [↑↓]    2p [↑↓] [↑] [↑]
```

By Hund's rule the 2p electrons singly occupy two orbitals before pairing, leaving **two unpaired electrons**.

8. Common pitfalls

- Forgetting that 4s fills before 3d when building an atom's configuration.
- Removing 3d electrons before 4s when forming a transition-metal cation — always remove 4s first.
- Pairing electrons in p or d orbitals too early, breaking Hund's rule in orbital diagrams.
- Writing $3d^{4}4s^{2}$ for chromium or $3d^{9}4s^{2}$ for copper instead of the anomalous d^{5} and d^{10} forms (HL).
- Confusing $2n^{2}$ (a shell's capacity) with the 2, 8, 8, 18 period pattern of electron arrangement.
- Saying ionization is exothermic — it is always endothermic, because energy is absorbed to pull the electron away.

9. Quick reference

Idea	Statement
Max electrons in shell n	$2n^{2}$ (2, 8, 18, 32 for n = 1, 2, 3, 4)
Orbitals per sub-level	s = 1, p = 3, d = 5, f = 7 (each holds 2 electrons)

Idea	Statement
Max electrons per sub-level	s = 2, p = 6, d = 10, f = 14
Filling order	1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p (4s before 3d)
Aufbau / Pauli / Hund	lowest energy first / max 2 per orbital, opposite spins / singly fill degenerate orbitals
Ion rule (d-block)	remove 4s electrons before 3d
Anomalies (HL)	Cr = [Ar]$3d^5 4s^1$; Cu = [Ar]$3d^{10} 4s^1$
First IE trends	increases across a period, decreases down a group
Successive IE (HL)	big jump = electron removed from an inner shell; count before jump = group number

10. Test yourself

Attempt these without notes; full worked answers follow.

1. Write the full electron configuration of a phosphorus atom (Z = 15).

2. Write the condensed configuration of a nickel atom (Z = 28) and of the Ni^{2+} ion.

3. Explain, in terms of energy levels, why the emission spectrum of hydrogen consists of discrete lines that converge at high frequency.

4. (HL) Draw the orbital diagram for the valence electrons of nitrogen and state the number of unpaired electrons.

5. (HL) Explain why the first ionization energy of sulfur is lower than that of phosphorus.

6. (HL) Explain why chromium is [Ar]$3d^5 4s^1$ and not [Ar]$3d^4 4s^2$.

7. The first six successive IEs of an element are 578, 1817, 2745, 11 580, 14 840, 18 380 kJ mol^{-1}. Deduce its group.

8. Write the electron configuration of the O^{2-} ion and name a neutral atom with the same configuration.

Answers

1. P (15 electrons): $1s^2 2s^2 2p^6 3s^2 3p^3$ (check 2+2+6+2+3 = 15).

2. Ni: [Ar]$3d^8 4s^2$. For Ni^{2+} remove the two 4s electrons first → [Ar]$3d^8$.

3. Electrons occupy discrete (quantised) energy levels. When an excited electron falls to a lower level it emits a photon of energy equal to the gap (E = hf), so only certain frequencies appear as lines. The levels converge in energy as n increases, so the gaps − and the emitted frequencies − converge at high frequency, ending at the ionization limit.

4. N = $1s^2 2s^2 2p^3$. 2s [↑ ↓] 2p [↑] [↑] [↑]. **Three unpaired electrons.**

5. Sulfur's outer configuration is $3p^4$: its fourth 3p electron is paired in one orbital, and the repulsion between the two electrons sharing that orbital makes it easier to remove. Phosphorus has a stable half-filled $3p^3$ set with no such pairing, so its IE_1 is higher.

6. Moving one 4s electron into 3d gives a half-filled $3d^5$ sub-level (one electron in each of the five d orbitals, parallel spins) together with a half-filled $4s^1$. This symmetrical, half-filled arrangement is lower in energy (more stable) than $3d^4 4s^2$.

7. The first large jump is between the 3rd (2745) and 4th (11 580) ionization energies, so three electrons are removed easily. The element has three outer electrons and is in **group 13** (the data is for aluminium).

8. O gains two electrons: O^{2-} = $1s^2 2s^2 2p^6$ = [Ne]. It is isoelectronic with a neon atom (also Na^+, Mg^{2+}, F^-).