

Structure 1.3 · Electron configurations

International Baccalaureate · IB Diploma · Chemistry · SL

Scope and prerequisites

This handout teaches Structure 1.3, Electron configurations, for the course first assessed in 2025.

Prerequisites: protons, neutrons and electrons from Structure 1.2, the atomic number Z , and arithmetic with powers of ten. You will use three relations from the data booklet: $c = f\lambda$, $E = hf$ and the Avogadro constant N_A .

Light, energy and emission spectra

■ Why do atoms give out coloured light?

Put a little sodium salt in a flame and the flame turns orange-yellow. Pass a high voltage through hydrogen gas in a tube and it glows pink. Each element gives its own colours. The colours tell us how the electrons in the atom are arranged.

■ Light carries energy in packets

Light is part of the **electromagnetic spectrum**. All of it travels at the same speed $c = 3.00 \times 10^8 \text{ m s}^{-1}$, and its frequency f and wavelength λ are linked by

$$c = f\lambda$$

Light is given out and taken in as packets of energy called **photons**. The energy of one photon depends only on its frequency:

$$E = hf$$

Here $h = 6.63 \times 10^{-34} \text{ J s}$ is the Planck constant. So **higher frequency means higher energy and shorter wavelength**.

Region	Wavelength	Frequency and photon energy
infrared	longer than about 700 nm	lowest of the three
visible: red → violet	about 700 nm → 400 nm	rising
ultraviolet	shorter than about 400 nm	highest of the three

In the visible region, red light has the longest wavelength and the lowest energy; violet light has the shortest wavelength and the highest energy.

■ Continuous and line spectra

White light from a hot solid, such as a lamp filament, contains every visible wavelength. A prism spreads it into a **continuous spectrum** : a smooth band of colour with no gaps.

Light from excited gas atoms is different. A prism spreads it into a few sharp coloured lines on a dark background. This is a **line emission spectrum** . Every element has its own pattern of lines, so the spectrum works like a fingerprint for the element.

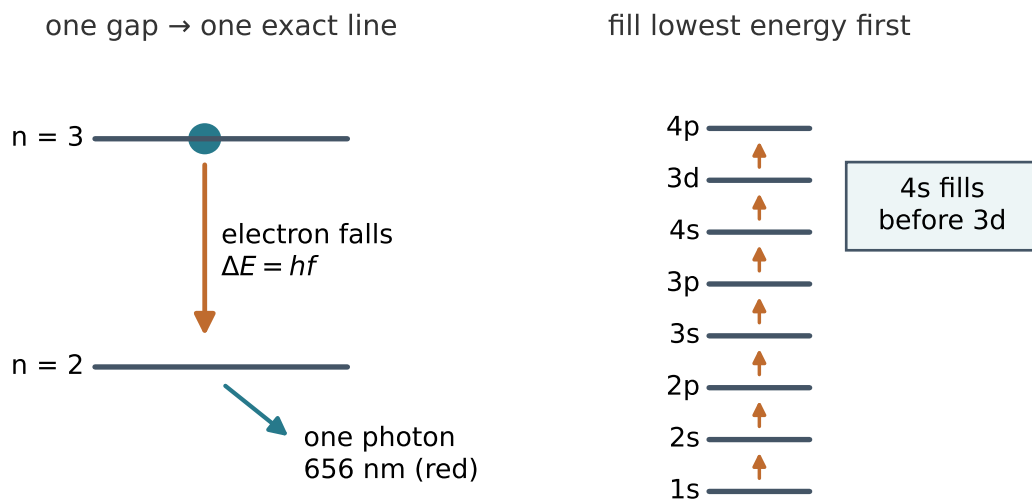
■ Where the lines come from

An electron in an atom can only have certain fixed energies, called **energy levels** . When the atom absorbs energy (from a flame or an electric current), an electron moves up to a higher level. The atom is now in an **excited state** .

The electron then falls back to a lower level. It gives out the energy difference as **one photon**:

$$\Delta E = E_{\text{upper}} - E_{\text{lower}} = hf$$

Only certain gaps exist, so only certain photon energies, and therefore only certain frequencies, appear. That is why we see separate lines and not a continuous band.



One fixed energy gap gives one line; on the right, sublevels fill lowest energy first, 4s before 3d

■ The hydrogen spectrum is evidence for energy levels

Hydrogen has one electron, so its spectrum is the simplest. Two features matter:

- **The lines are separate.** If the electron could have any energy, hydrogen would give a continuous spectrum. The separate lines show that the energy of the electron is **quantized** : it can only take fixed values.
- **The lines get closer together at higher frequency.** The levels themselves get closer together as n increases, so the lines **converge** . Above the **convergence limit** there are no more lines.

Which line appears depends on the level the electron falls to. Falls to $n = 1$ give the largest gaps, so those photons are ultraviolet. Falls to $n = 2$ give visible light, such as the red line at 656 nm. Falls to $n = 3$ give infrared.

Worked example. The red line of hydrogen has $\lambda = 656$ nm. Find the energy gap it comes from.

1. Convert the wavelength: $\lambda = 656 \times 10^{-9}$ m.
2. Find the frequency: $f = \frac{c}{\lambda} = \frac{3.00 \times 10^8}{656 \times 10^{-9}} = 4.57 \times 10^{14}$ Hz.
3. Find the energy: $E = hf = 6.63 \times 10^{-34} \times 4.57 \times 10^{14} = 3.03 \times 10^{-19}$ J.

This is the energy gap between $n = 3$ and $n = 2$ for **one** atom.

Energy levels, sublevels and orbitals

■ Main energy levels

The main energy levels are numbered by the **principal quantum number** $n = 1, 2, 3, \dots$ Level n can hold at most $2n^2$ electrons.

n	Maximum electrons $2n^2$	Sublevels
1	2	1s
2	8	2s, 2p
3	18	3s, 3p, 3d
4	32	4s, 4p, 4d, 4f

■ Sublevels and orbitals

Each main level is split into **sublevels** called s, p, d and f. Each sublevel is made of **atomic orbitals** . An orbital is a region around the nucleus where there is a high chance of finding an electron. One orbital holds at most two electrons.

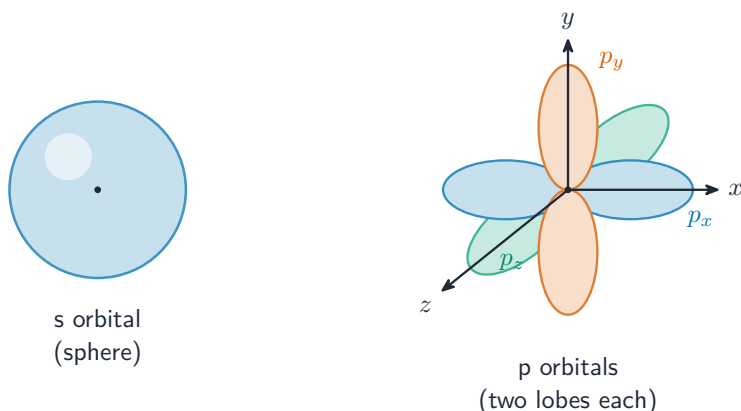
Sublevel	Orbitals	Maximum electrons
s	1	2
p	3	6
d	5	10
f	7	14

Check: level $n = 3$ has $3s + 3p + 3d = 2 + 6 + 10 = 18$ electrons, which matches $2n^2 = 18$.

■ Shapes of s and p orbitals

You need to recognise two shapes:

- An **s orbital** is a sphere centred on the nucleus. A 2s orbital is larger than a 1s orbital.
- A **p orbital** has two lobes on opposite sides of the nucleus, like a dumbbell. The three p orbitals of one level point along the x , y and z axes, at right angles to each other. They are named p_x , p_y and p_z .



An s orbital is a sphere; the three p orbitals are dumbbells along x , y and z

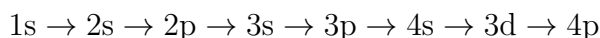
The three p orbitals of one sublevel have the same energy. Orbitals with equal energy are called **degenerate**.

Writing electron configurations

■ Three rules for filling orbitals

1. **Aufbau principle** : electrons go into the lowest-energy orbital available first.
2. **Pauli exclusion principle** : an orbital holds at most two electrons, and they must have **opposite spins**.
3. **Hund's rule** : in a set of degenerate orbitals, electrons go in singly with parallel spins before any orbital gets a second electron. Single electrons in separate orbitals repel each other less.

For atoms up to $Z = 36$, the order of filling is:



Notice that 4s fills **before** 3d. In a neutral atom up to calcium, 4s is lower in energy than 3d.

■ Full and condensed configurations

A **full electron configuration**

lists every sublevel with its number of

electrons as a superscript:

- sulfur, $Z = 16$: $1s^2 2s^2 2p^6 3s^2 3p^4$
- iron, $Z = 26$: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$

A **condensed configuration**

replaces the inner electrons with the

symbol of the noble gas before the element, in square brackets:

- sulfur: $[\text{Ne}] 3s^2 3p^4$
- iron: $[\text{Ar}] 4s^2 3d^6$

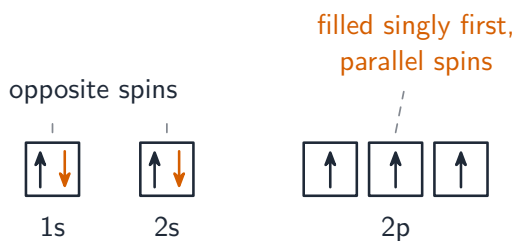
Always check that the superscripts add up to the number of electrons.

■ Orbital diagrams

An **orbital diagram**

draws each orbital as a box and each electron as

a half-arrow. Two arrows in one box point in opposite directions (Pauli). Within a sublevel, fill every box with one arrow, all pointing the same way, before you add a second arrow to any box (Hund).



Nitrogen, $1s^2 2s^2 2p^3$: paired spins in $1s$ and $2s$; the three $2p$ electrons sit singly with parallel spins

Nitrogen therefore has **three unpaired electrons**. Oxygen, $2p^4$, has one pair and two unpaired electrons in its $2p$ sublevel.

| **Worked example.** Draw the orbital diagram of the $3d$ and $4s$ sublevels of iron.

Iron is $[\text{Ar}] 4s^2 3d^6$. The $4s$ box holds two opposite arrows. Six electrons go into five $3d$ boxes: one up-arrow in each of the five boxes, then the sixth pairs up in the first box. Iron has **four** unpaired electrons.

■ Two exceptions: chromium and copper

Two atoms in the first row of the d-block do not follow the simple order:

- chromium, $Z = 24$: $[\text{Ar}] 4s^1 3d^5$, not $4s^2 3d^4$
- copper, $Z = 29$: $[\text{Ar}] 4s^1 3d^{10}$, not $4s^2 3d^9$

In both, one electron moves from 4s into 3d to give a half-full or full 3d sublevel, which gives a lower total energy for these atoms. Learn these two as facts.

■ Configurations of ions

- For a **negative ion**, add electrons to the next available orbital. Oxide, O^{2-} : $1s^2 2s^2 2p^6$, the same as neon.
- For a **positive ion** of a main-group element, remove electrons from the outermost level. Na^+ : $1s^2 2s^2 2p^6$.
- For a positive ion of a **transition element**, remove the **4s electrons first**, then 3d electrons. Once 3d is occupied, 4s is no longer the lower level.

Species	Configuration
Fe	$[\text{Ar}] 4s^2 3d^6$
Fe^{2+}	$[\text{Ar}] 3d^6$
Fe^{3+}	$[\text{Ar}] 3d^5$
Cu^+	$[\text{Ar}] 3d^{10}$

A common error is to write Fe^{2+} as $[\text{Ar}] 4s^2 3d^4$. Remember: **4s fills first and empties first**.

Practice

- A line in the emission spectrum of an element has $\lambda = 589 \text{ nm}$. Calculate the energy of one photon of this light.
- State the maximum number of electrons in the $n = 4$ level, and name its sublevels.
- Write the full configuration of chlorine and the condensed configuration of Cr^{3+} .
- How many unpaired electrons does a phosphorus atom have? Draw its 3s and 3p orbital diagram.
- Explain why the emission spectrum of hydrogen is a line spectrum and not a continuous spectrum.

Answers.

- $f = \frac{3.00 \times 10^8}{589 \times 10^{-9}} = 5.09 \times 10^{14} \text{ Hz}$; $E = 6.63 \times 10^{-34} \times 5.09 \times 10^{14} = 3.38 \times 10^{-19} \text{ J}$.
- $2n^2 = 32$; the sublevels are 4s, 4p, 4d and 4f.
- Cl: $1s^2 2s^2 2p^6 3s^2 3p^5$. Cr is $[\text{Ar}] 4s^1 3d^5$; removing the 4s electron and then two 3d electrons gives Cr^{3+} : $[\text{Ar}] 3d^3$.

4. Three: 3s holds one pair, and each of the three 3p orbitals holds one electron with parallel spins.
5. The electron can only have fixed energies (energy levels). A photon is given out when the electron falls between two levels, so only certain energy gaps, and therefore only certain frequencies, are possible.

Exam tips

- Link **frequency, energy and wavelength** in one sentence: higher frequency means higher photon energy and shorter wavelength.
- To explain a line spectrum, mention **both** ideas: electrons occupy fixed energy levels, and a photon is emitted when an electron **falls** to a lower level.
- The lines **converge** at higher frequency because the energy levels get closer together.
- Write 4s before 3d when filling, but **remove 4s first** when forming a transition-metal ion.
- Learn Cr ($4s^1 3d^5$) and Cu ($4s^1 3d^{10}$) as exceptions.