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 $c = 3.00 \times 10^8$ 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 $h = 6.63 \times 10^{-34}$ 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.

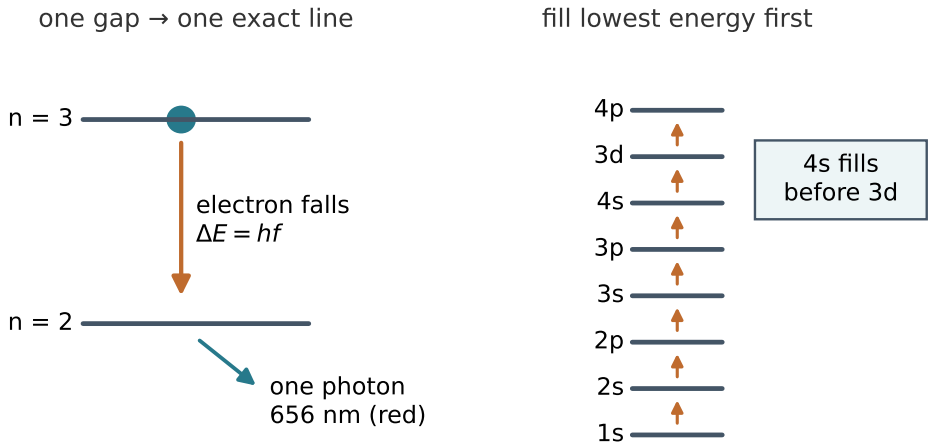
Where the lines come from

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: $f = \dfrac{c}{\lambda} = \dfrac{3.00 \times 10^{8}}{656 \times 10^{-9}} = 4.57 \times 10^{14}$ 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** $n = 1, 2, 3, \ldots$ 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.

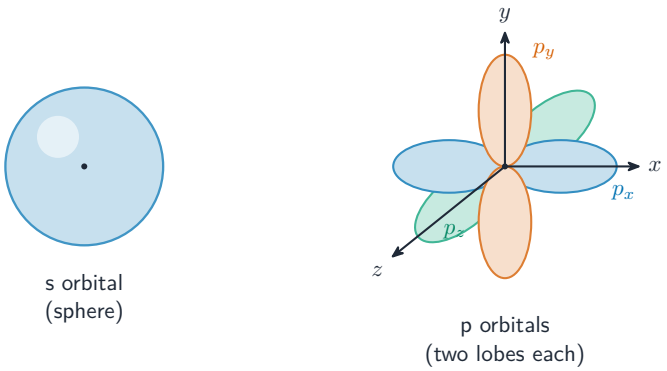
Sublevel	Orbitals	Maximum electrons
s	1	2
p	3	6
d	5	10
f	7	14

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:

$$1s \to 2s \to 2p \to 3s \to 3p \to 4s \to 3d \to 4p$$

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, $Z = 26$: $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^6$

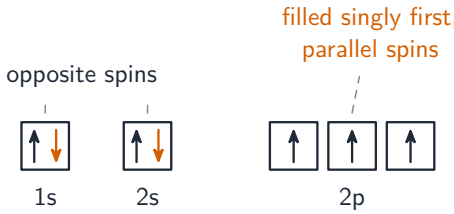
A **condensed configuration** replaces the inner electrons with the symbol of the noble gas before the element, in square brackets:

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

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 $[\mathrm{Ar}]\,4s^2\,3d^6$. 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, $Z = 24$: $[\mathrm{Ar}]\,4s^1\,3d^5$, not $4s^2\,3d^4$
- copper, $Z = 29$: $[\mathrm{Ar}]\,4s^1\,3d^{10}$, 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	$[\mathrm{Ar}]\,4s^2\,3d^6$
Fe^{2+}	$[\mathrm{Ar}]\,3d^6$
Fe^{3+}	$[\mathrm{Ar}]\,3d^5$
Cu^+	$[\mathrm{Ar}]\,3d^{10}$

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

Practice

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

Answers.

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

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.