Electron configurations

Structure 1.3 · SL and AHL

What coloured light tells us about atoms

> The light an element gives out is a record of how its electrons are arranged.

- Sodium turns a flame orange-yellow; hydrogen in a discharge tube glows pink.
- Each element gives its own colours, because its electrons sit in fixed energy levels.
- This unit: spectra $\rightarrow$ energy levels $\rightarrow$ orbitals $\rightarrow$ configurations; AHL adds ionization energies.

Light carries energy in packets

- In vacuum, electromagnetic radiation travels at c $=3.00\times10^{8}$ m s^{-1}.
- Light comes in packets called **photons**; the energy of one **photon** depends only on its frequency.
- Higher frequency means higher energy and shorter wavelength.

$$c = f\lambda \qquad E = hf$$

$$h = 6.63 \times 10^{-34} \text{ J s (Planck constant)}$$

Visible light: red (about 700 nm, lowest energy) to violet (about 400 nm, highest energy).

Continuous spectrum or line spectrum?

Continuous spectrum

White light from a lamp filament.

A smooth band of colour with no gaps.

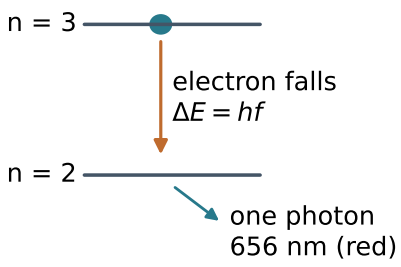
Line emission spectrum

Light from excited gas atoms.

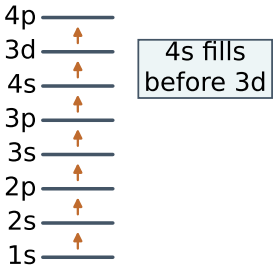
A few sharp coloured lines on a dark background, different for each element.

Where each line comes from

one gap → one exact line



schematic filling order



A fixed model energy gap gives a **photon**: $\Delta E = hf$.

Hydrogen's spectrum is evidence for energy levels

Use the stated initial and final levels when identifying a spectral series.

- Separate lines support discrete allowed energies.
- Within one series, lines crowd towards a finite limit.
- The n=2 series includes visible lines and higher ultraviolet members.

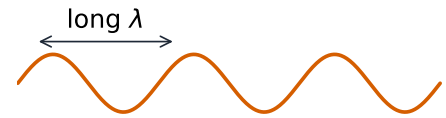
Worked example: the red line at 656 nm

1. **Convert.** $\lambda = 656 \times 10^{-9}$ m
2. **Frequency.** $f = \dfrac{3.00 \times 10^{8}}{656 \times 10^{-9}} = 4.57317\ldots \times 10^{14}$ Hz
3. **Energy.** Use unrounded f: E =3.032012…$\times 10^{-19}$ J, reported 3.03$\times 10^{-19}$ J

Decision

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

Wavelength and photon energy



red light: low frequency
less energy per photon

violet / UV: high frequency
more energy per photon

$E = hf = hc/\lambda$

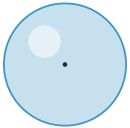
Main levels hold $2n^2$ electrons

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

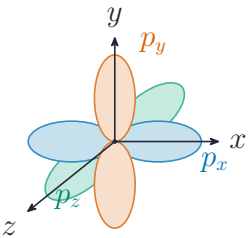
Use the evidence

Check $n = 3$: $2 + 6 + 10 = 18 = 2n^2$.

Shapes of s and p orbitals



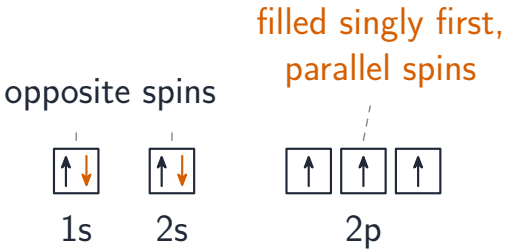
s orbital
(sphere)



p orbitals
(two lobes each)

Probability-region surfaces are not hard boundaries or electron paths.

Three rules for filling orbitals



Pauli limits one box; Hund sets the lowest-energy occupancy of equal-energy boxes.

Order to $Z = 36$: 1s 2s 2p 3s 3p 4s 3d 4p.

Full and condensed configurations

Atom	Full	Condensed
S	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$	[Ne] $3s^2\ 3p^4$
Fe	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$	[Ar] $4s^2\ 3d^6$
Cr	exception	[Ar] $4s^1\ 3d^5$
Cu	exception	[Ar] $4s^1\ 3d^{10}$

Use the evidence

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

Ions: 4s fills first and empties first

Species	Configuration
O^{2-}	$1s^2\,2s^2\,2p^6$ (like neon)
Fe	[Ar] $4s^2\,3d^6$
Fe^{2+}	[Ar] $3d^6$
Fe^{3+}	[Ar] $3d^5$

Use the evidence

Fe^{2+} is not [Ar] $4s^2\,3d^4$.

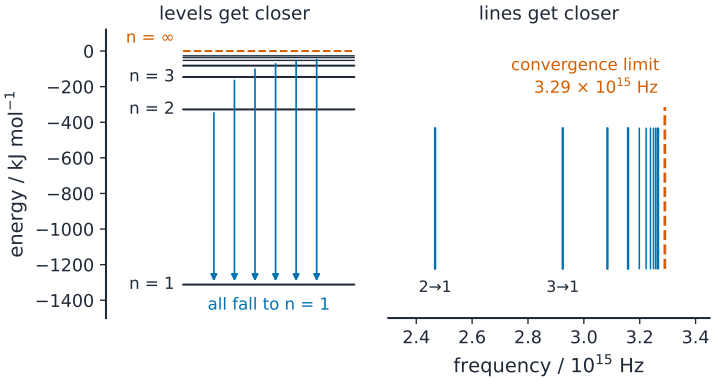
Check: the configuration of Cr^{3+}

Your turn

Which is the configuration of Cr^{3+}?

A. $[\mathrm{Ar}]\,4\mathrm{s}^2\,3\mathrm{d}^1$
B. $[\mathrm{Ar}]\,4\mathrm{s}^1\,3\mathrm{d}^2$
C. $[\mathrm{Ar}]\,3\mathrm{d}^3$
D. $[\mathrm{Ar}]\,3\mathrm{d}^5$

AHL: the convergence limit is ionization



Use the series that ends at n = 1; its limit, 3.29×10^{15} Hz, gives 1312 kJ/mol.

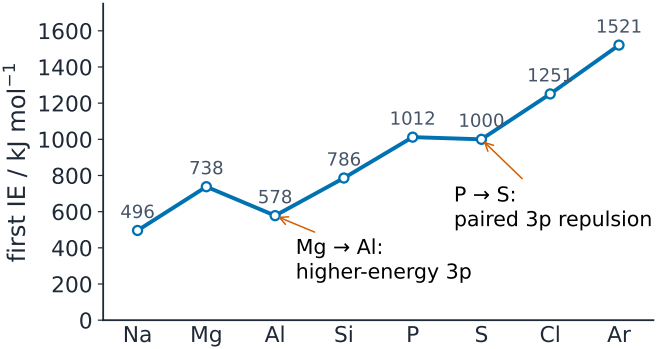
AHL worked example: ionization energy of hydrogen

1. **Frequency.** $f = \dfrac{3.00 \times 10^{8}}{91.2 \times 10^{-9}} = 3.28947\ldots \times 10^{15}$ Hz
2. **One atom.** E $= 2.180921\ldots \times 10^{-18}$ J from the unrounded frequency
3. **One mole.** Multiply unrounded E by N_A: $1.312914\ldots \times 10^{6}$ J mol^{-1}
4. **Convert.** 1.31×10^{3} kJ mol^{-1} to three significant figures

Decision

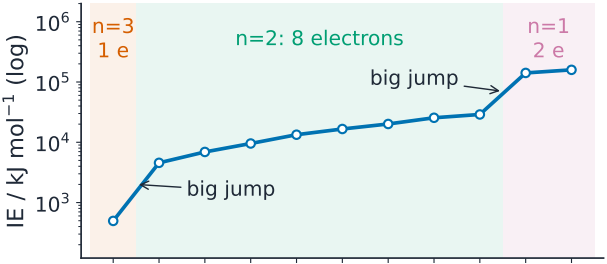
Keep guard digits; distinguish energy per **photon** from energy per mole.

AHL: two dips across Period 3



Mg→Al changes **sublevel**; P→S introduces a paired 3p electron.

AHL: big jumps show the main levels



Big jump: next electron from an inner shell

Use main-group cases; helium is a Group 18 exception.

AHL: which group?

1. **Data.** 578, 1817, 2745, 11 577, 14 842 kJ mol^{-1}
2. **Jump.** 2745 $\rightarrow$ 11 577 more than quadruples
3. **Count.** three electrons before the jump $\rightarrow$ three outer electrons

Decision

Group 13 for this supplied rounded main-group pattern.

Orbital capacity is not filling order

1. **n=3.** 3s +3p +3d: 1+3+5 =9 orbitals
2. **Capacity.** 9×2 =18 electrons =$2n^2$
3. **Order.** 4s can be occupied before 3d is full

Decision

Keep orbital, **sublevel** and main level distinct.

Pauli and Hund answer different questions

Pauli

At most two electrons in one orbital.

A pair with **opposite spins** can satisfy this rule.

Hund

Fill **degenerate** orbitals singly with parallel spins first.

Pair+single+empty is not nitrogen's lowest-energy $2p^3$ arrangement.

Copper ions: remove from the actual configuration

1. **Cu^{+}.** Remove 4s: [Ar]$3d^{10}$, 28 electrons
2. **Cu^{2+}.** Then remove 3d: [Ar]$3d^{9}$, 27 electrons

Decision

A filling mnemonic is not a universal order of ionization.

AHL: an excited-series limit

1. **Given.** Supplied H series ends at $n = 2$: $\lambda = 364.8$ nm. Use $h = 6.63 \times 10^{-34}$ J s, $c = 3.00 \times 10^{8}$ m/s and $N_A = 6.02 \times 10^{23}$/mol.
2. **Photon.** E $=$hc$/\lambda$ $=$5.4523026…$\times 10^{-19}$ J
3. **Mole.** E $\times$ N_A $\div$ 1000 $=$ 328.2286… kJ mol^{-1}
4. **Meaning.** Ionization from excited n=2, not first ionization from n=1

Decision

The series endpoint determines the ionization reference.

Exam tips

> State the level, occupancy and reference conditions behind the conclusion.

- Line spectrum: fixed energy levels **and** a **photon** given out when an electron falls.
- Lines **converge** because the levels get closer together.
- 4s fills before 3d, but 4s empties first; learn Cr and Cu.
- AHL: multiply by N_A and convert to kJ; count electrons before the first big jump.

Check yourself

Try these

A line has $\lambda = 589$ nm. Find the energy of one photon.

Write the full configuration of Cl and the condensed configuration of Cr^{3+}.

How many unpaired electrons does phosphorus have?

AHL: the sodium convergence limit is at 241 nm. Find the first IE in kJ mol^{-1}.