OCR A | Year 12 chemistry

Atomic structure

Complete notes

Clear explanations, precise definitions and worked examples for the whole topic. Use the contents or PDF bookmarks to find a section. TEST IT references point to the matching questions in the separate topic Questions & answers pack.

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Atoms & ions

1. How evidence changed the atomic model

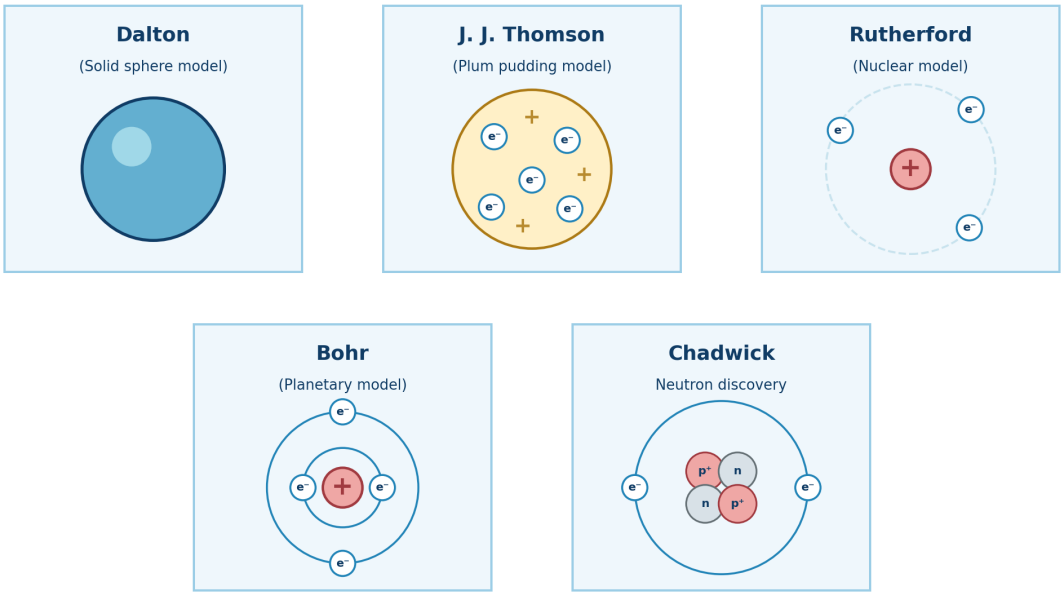
SPEC 2.1.1(b) · HSW1/7

CRACK IT

Scientists do not keep a model just because it is familiar. When new evidence does not fit, the model needs to change. For each model below, connect **what scientists observed** with **what that tells us about the atom**.

For example, most alpha particles passing through the foil suggests that most of the atom is empty space. The few large deflections suggest that the positive charge is concentrated in a very small region. Those are two different observations supporting two different conclusions.

The atomic model changed when new evidence appeared



Model	Evidence and interpretation
Dalton (solid sphere model)	Atoms pictured as tiny, solid, indivisible spheres.
J. J. Thomson (plum pudding model)	Discovery of the electron showed atoms were divisible; electrons were placed within diffuse positive charge.
Rutherford (nuclear model)	Alpha scattering showed a tiny, dense, positively charged nucleus and an atom that is mostly empty space.
Bohr (planetary model)	Electrons occupy fixed energy levels, helping explain periodic properties.
Chadwick	Discovery of the neutron completed the nuclear model and helped explain isotope masses.

WORKED EXAMPLE

Observation → inference

Most alpha particles pass through thin foil; some undergo large deflections and a few rebound.

Explain what these observations tell you about the structure of the atom.

Worked answer

• Most pass through: most of the atom is empty space.

• Rare large deflections: positive charge and most mass are concentrated in a tiny, dense nucleus.

Connect each observation to the conclusion it supports.

EXAM TRAP A list of scientists is not an explanation. Link the evidence to the change in the model.

TEST IT

Try question 1 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can explain how evidence led from a solid-sphere model to a nuclear atom with energy levels.

2. Fundamental particles

SPEC 2.1.1(b)

CRACK IT

An atom has a tiny central nucleus containing protons and neutrons. Electrons occupy regions outside the nucleus. The table gives the relative masses and charges you need to know.

Protons and neutrons are much heavier than electrons, so almost all the atom's mass is in its nucleus. An electron's mass is very small, but it is not zero.

In a neutral atom, each positive proton is balanced by one negative electron. That is why a neutral atom has equal numbers of protons and electrons.

Particle	Relative charge	Relative mass	Location
Proton	+1	1	Nucleus
Neutron	0	1	Nucleus
Electron	−1	Approximately 1/1840	Orbitals around the nucleus

EXAM TRAP Electron mass is very small, not zero.

TEST IT

Try question 2 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can reproduce the particle table and describe the nuclear atom.

3. Particle numbers in atoms and ions

SPEC 2.1.1(b)

CRACK IT

The atomic number tells you which element you have: it is the number of protons. The mass number counts protons **and** neutrons, so subtract the atomic number to find the neutrons. Both numbers are whole numbers with no units.

1. Find the neutral atom first. Its proton number and electron number both equal the atomic number.

2. For a positive ion, remove electrons. A 2+ charge means two electrons have been lost.

3. For a negative ion, add electrons. A 1- charge means one electron has been gained.

4. Leave the proton and neutron numbers alone. Making an ion changes the electrons, not the nucleus.

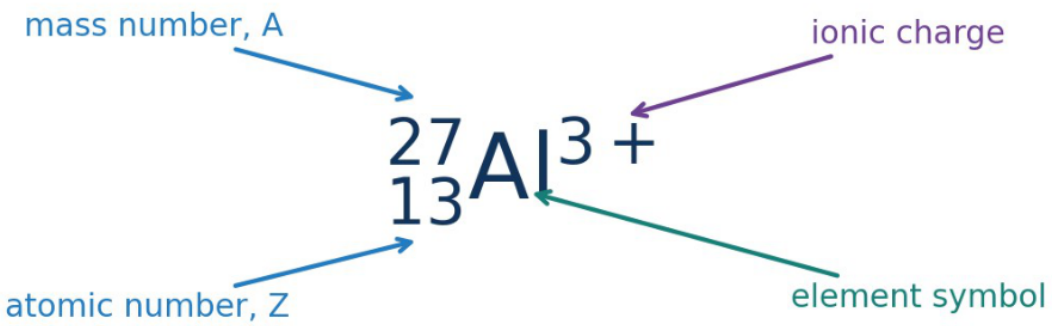
DEFINITIONS & KEY TERMS

Atomic number, Z

The number of protons in the nucleus. It identifies the element.

Mass number, A

The total number of protons and neutrons in one atom of an isotope.



Protons = Z; neutrons = A − Z

A mass number: total number of protons and neutrons; no unit; **Z** atomic number: number of protons; no unit.

WORKED EXAMPLE

Count an ion’s particles

State the numbers of protons, neutrons and electrons in a $^{59}Co^{2+}$ ion. Cobalt has atomic number 27.

Worked answer

1. Protons = 27.

2. Neutrons = 59 − 27 = 32.

3. Electrons = 27 − 2 = 25.

27 protons, 32 neutrons and 25 electrons.

EXAM TRAP Apply the sign of the charge correctly: positive means fewer electrons.

TEST IT

Try questions 3, 4, 5 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can move between nuclide notation and particle counts in both directions.

Isotopes & relative masses

4. Isotopes and their properties

SPEC 2.1.1(a)

CRACK IT

Isotopes are atoms of the same element with the same number of protons but different numbers of neutrons. The proton number keeps the element the same; the extra neutrons change its mass.

Neutral atoms of the isotopes have the same electron configuration. Since chemical reactions depend on electrons, the isotopes have the same chemical properties.

Their masses are different, so physical properties that depend on mass can differ. Keep mass number, which describes one isotope, separate from the element's weighted mean relative atomic mass.

DEFINITIONS & KEY TERMS

Isotopes

Atoms of the same element with the same number of protons but different numbers of neutrons and different masses.

WORKED EXAMPLE

Compare ^{35}Cl and ^{37}Cl

For neutral atoms of ^{35}Cl and ^{37}Cl, state the numbers of protons, neutrons and electrons. Explain why they have the same chemical properties but different masses. Chlorine has atomic number 17.

Worked answer

Isotope	Protons	Neutrons	Electrons
^{35}Cl	17	18	17
^{37}Cl	17	20	17

Same electron configuration; different neutron numbers and masses.

EXAM TRAP Ion charge does not change which isotope a species belongs to. Use proton and neutron numbers.

TEST IT

Try questions 6, 7 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can define isotopes precisely and identify every valid isotope pair from particle data.

5. The carbon-12 relative-mass scale

SPEC 2.1.1(c)

CRACK IT

A relative mass compares a particle's mass with a common reference: **one-twelfth of the mass of one carbon-12 atom**. It is a ratio of two masses, so it has no unit.

Read the particle named in the definition. Relative isotopic mass refers to one isotope. Relative atomic mass is a weighted mean that allows for an element's isotope abundances.

Relative molecular mass refers to molecules. For a substance without separate molecules, such as an ionic compound, use relative formula mass. Molar mass is a different quantity: the mass of one mole, usually in g mol^{-1}.

DEFINITIONS & KEY TERMS

Relative isotopic mass

The mass of an atom of one isotope compared with one-twelfth of the mass of a carbon-12 atom.

Relative atomic mass, A_r

The weighted mean mass of an atom of an element compared with one-twelfth of the mass of a carbon-12 atom.

Quantity	Meaning
Mass number	Whole-number count of protons plus neutrons in one atom.
Relative isotopic mass	Measured relative mass of one isotope; close to, but not necessarily exactly equal to, mass number.
Relative atomic mass	Weighted mean across the isotopes present; often not a whole number.

EXAM TRAP Include “weighted mean”, “atom of an element” and the one-twelfth carbon-12 comparison in A_r.

TEST IT

Try questions 8, 9 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can give the required definitions and distinguish a particle count from a relative mass.

6. Relative molecular and formula masses

SPEC 2.1.1(e)

CRACK IT

The formula tells you how many atoms to include. Add their A_r contributions to find the relative molecular mass or relative formula mass.

Use relative molecular mass for substances made of separate molecules. Use relative formula mass when the formula describes a ratio in a giant structure, such as NaCl. Both relative masses have no units.

Use these terms and calculate the values; formal definitions of these two terms are not required here.

Structure	Term	Examples
Discrete molecules	Relative molecular mass, M_r	CO_2, H_2O, NH_3
Giant ionic or covalent structure	Relative formula mass	NaCl, $MgCl_2$, SiO_2

Relative mass = Σ(A_r × number of each atom in the formula)

A_r relative atomic mass; no unit; **Σ** sum of all the indicated contributions.

WORKED EXAMPLE

Choose the term and calculate

Use C = 12.0, O = 16.0, Mg = 24.3 and Cl = 35.5 to calculate relative masses for CO_2 and $MgCl_2$.

Worked answer

1. CO_2: 12.0 + 2(16.0) = 44.0. It contains molecules.

2. $MgCl_2$: 24.3 + 2(35.5) = 95.3. It has a giant ionic lattice.

$M_r(CO_2)$ = 44.0; relative formula mass($MgCl_2$) = 95.3.

EXAM TRAP Molar mass in g mol^{-1} is different from a unitless relative mass.

TEST IT

Try questions 10, 11 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can select molecular or formula mass from structure and calculate it without units.

Mass spectra & calculations

7. Reading elemental mass spectra

SPEC 2.1.1(d)(i)

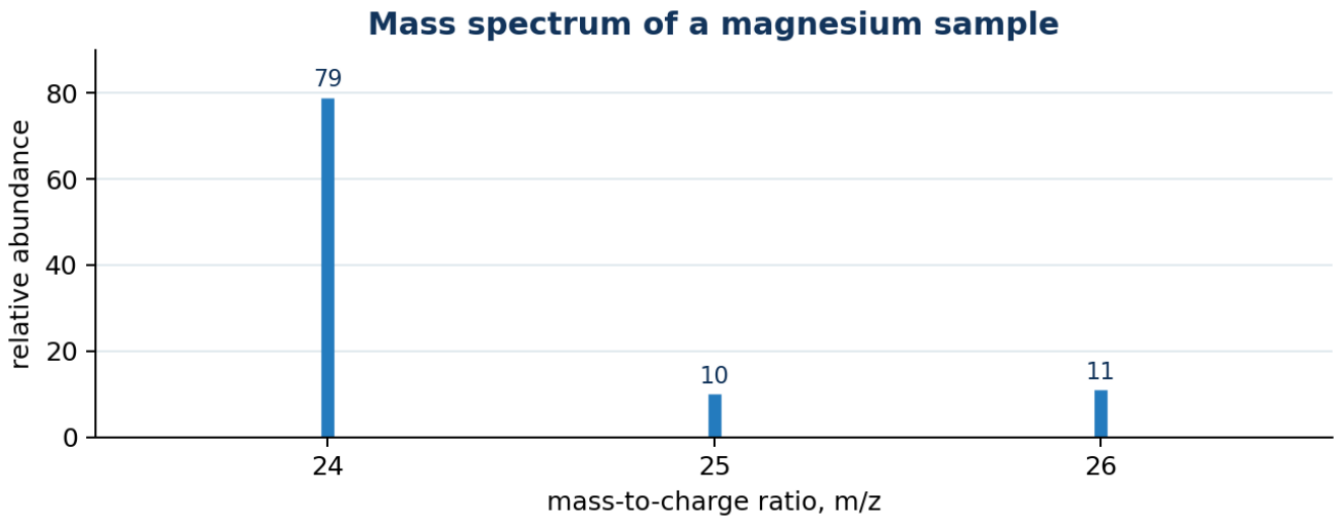
CRACK IT

Use the information on the spectrum. You do not need TOF instrument stages or kinetic-energy calculations here.

• **Peak position:** read m/z from the x-axis. For a singly charged monatomic ion, this is numerically equal to its relative isotopic mass.

• **Peak height:** read relative abundance or intensity from the y-axis. The tallest isotope peak represents the most abundant isotope.

• Check whether abundances are percentages, ratios or raw intensities before calculating the weighted mean.



EXAM TRAP Relative intensities need not add to 100. Only percentages must total 100%.

TEST IT

Try questions 12, 13 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can extract isotope masses and abundances without describing the instrument.

8. Calculating relative atomic mass

SPEC 2.1.1(d)(ii) · M0.2/M1.2

CRACK IT

Relative atomic mass is an average, but the isotopes do not all contribute equally. A common isotope must count more than a rare one. That is what **weighted mean** means.

1. Multiply each isotope's relative mass by its abundance.

2. Add those contributions.

3. Divide by the total abundance. Use 100 for percentages, but add the values yourself for a ratio or raw intensities.

Your answer must lie between the lightest and heaviest isotope masses. It should be closer to the more abundant isotope. Relative atomic mass has no unit.

$$A_r = \Sigma(\text{relative isotopic mass} \times \text{abundance}) / \Sigma(\text{abundances})$$

A_r relative atomic mass; no unit; Σ sum of all the indicated contributions.

WORKED EXAMPLE

All masses and abundances known

Masses 28, 29 and 30 have abundances 92%, 5% and 3%.

Calculate the relative atomic mass of the element.

Worked answer

A_r = Σ(isotopic mass × abundance)/Σ(abundance)
A_r = [28(92) + 29(5) + 30(3)]/100 = 2811/100.

A_r = 28.11.

WORKED EXAMPLE

An unknown isotope mass

Mass 63 has abundance 70.0%. The other isotope has abundance 30.0%. A_r = 63.60.

Calculate the relative isotopic mass of the second isotope.

Worked answer

1. 63.60 = [63(70) + 30x]/100.

2. 6360 = 4410 + 30x.

3. x = (6360 − 4410)/30.

The other relative isotopic mass is 65.0.

WORKED EXAMPLE

Two unknown abundances

Isotope masses are 50, 52 and 54. Mass 50 has abundance 20.0%, and A_r = 52.20.

Calculate the percentage abundances of isotopes 52 and 54.

Worked answer

1. Let mass 52 have abundance x%. Mass 54 has (80 − x)%.

2. 52.20 = [50(20) + 52x + 54(80 − x)]/100.

3. 5220 = 5320 − 2x, so x = 50.0.

Mass 52: 50.0%; mass 54: 30.0%.

EXAM TRAP For three isotopes, the final abundance is 100 − known abundance − x. Keep unrounded intermediate values.

TEST IT

Try questions 14, 15, 16, 17, 18, 19, 20 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can handle percentages, ratios, unnormalised intensities and missing information.

9. Molecular ions: analytical crossover

SPEC 4.2.4(f) · 2.1.3(b–c) crossover

CRACK IT

This is an analytical-chemistry crossover, included to support the molecular-ion questions in your practice pack. It connects this topic to the later organic-analysis content.

A molecular ion is the intact molecule after losing an electron. For a singly charged molecular ion, its m/z gives the molecule's relative molecular mass.

The molecular-ion peak is **usually the peak furthest to the right**. A small M+1 isotope peak can appear just beyond it.

A molecule can also break into smaller ions called fragments. The tallest peak is the base peak; it need not be the molecular-ion peak. Identify the peak the question tells you to use.

DEFINITIONS & KEY TERMS

Molecular ion, M^+

The intact molecule after removal of one electron. For the identified singly charged molecular ion, m/z gives its relative mass.

Base peak

The most intense peak, conventionally scaled to 100. It may represent a fragment ion.

M_r = m/z of the identified singly charged molecular ion

M_r relative molecular or formula mass; no unit; **m/z** mass-to-charge ratio: m represents the ion's relative mass and z its charge number.

Molecular-formula multiplier = M_r / empirical-formula mass

M_r relative molecular or formula mass; no unit.

WORKED EXAMPLE

Use the identified ion

A spectrum has an identified singly charged molecular ion at m/z 72 and a base peak at m/z 43.

Determine the relative molecular mass of the compound and explain which peak you use.

Worked answer

Use the intact molecular ion, not the most intense fragment.

M_r = 72.

EXAM TRAP Do not automatically select the tallest or highest-m/z peak. Isotopic peaks and fragmentation require interpretation.

TEST IT

Try questions 21, 22 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can use an identified molecular ion and distinguish molecular mass from fragment mass.

Shells & orbitals

10. The first four shells

SPEC 2.2.1(a)

CRACK IT

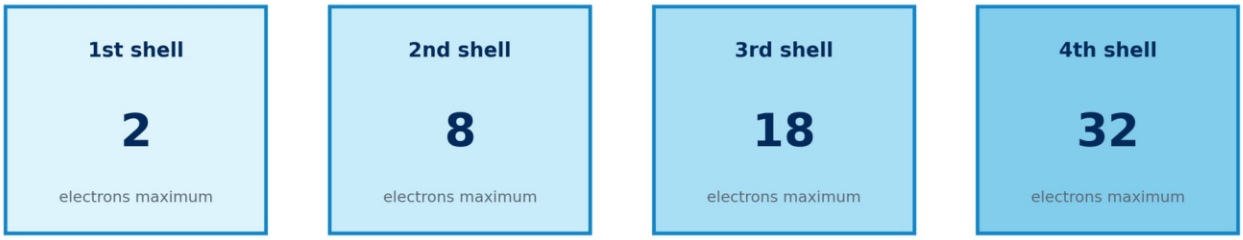
KEY DEFINITION

A shell is a principal energy level. We number the shells n = 1, 2, 3 and 4, starting nearest the nucleus. Each shell contains subshells, which contain orbitals.

The expression $2n^2$ gives the maximum capacity of a shell: 2, 8, 18 and 32 electrons for the first four shells. It does **not** tell you the order in which all the subshells fill.

That distinction matters when you reach 4s and 3d. Use shell capacities for maximum numbers, and the filling-order diagram for actual configurations.

Maximum number of electrons in the first four shells



Maximum shell capacity = $2n^2$

n the principal energy level (electron shell).

WORKED EXAMPLE

Third-shell capacity

Calculate the maximum number of electrons that can occupy the third shell, using $2n^2$.

Worked answer

n = 3, so $2 \times 3^2 = 18$.

The third shell can hold 18 electrons.

EXAM TRAP Capacity is not filling order. Potassium starts 4s before its third shell reaches maximum capacity.

TEST IT

Try question 23 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can recall 2, 8, 18, 32 and use $2n^2$ without confusing capacity and filling.

11. Atomic orbitals and shapes

SPEC 2.2.1(b)(i–ii)

CRACK IT

An orbital describes a region with a high probability of finding an electron. It is not a little circular track followed by the electron.

An s orbital is spherical. A p orbital has two lobes, often called a dumb-bell shape. The nucleus is at the centre.

A p subshell has three orbitals of the same energy. They point in three mutually perpendicular directions. Each orbital can hold up to two electrons, with opposite spins.

When showing where electrons go in a diagram, orbitals are usually drawn as **boxes**. One box represents one orbital; one arrow represents one electron.

DEFINITIONS & KEY TERMS

Atomic orbital

A region around the nucleus that can hold up to two electrons with opposite spins.

One s orbital and the three p orbitals



EXAM TRAP A p orbital is a three-dimensional region, not a figure-of-eight path.

TEST IT

Try question 24 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can give the definition and draw or recognise the required orbital shapes.

12. Subshells, orbitals and capacities

SPEC 2.2.1(b)(iii)

CRACK IT

Count the orbitals first, then double the number to find the maximum electrons. Each orbital holds up to two electrons.

- An s subshell has one orbital, so it holds up to 2 electrons.
- A p subshell has three orbitals, so it holds up to 6 electrons.
- A d subshell has five orbitals, so it holds up to 10 electrons.

An orbital and a subshell are different levels of organisation. Only the s subshell happens to contain a single orbital.

Subshell	Orbitals	Electrons per orbital	Maximum electrons
s	1	2	2
p	3	2	6
d	5	2	10

WORKED EXAMPLE

Why does d hold ten?

Explain the capacity of a d subshell.

Worked answer

1. There are five d orbitals.

2. Each holds at most two electrons with opposite spins.

3. 5 × 2 = 10.

A d subshell holds up to ten electrons.

EXAM TRAP One p orbital holds two electrons; the whole p subshell holds six.

TEST IT

Try question 25 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can move between subshell, orbital count and electron capacity.

13. Electrons-in-box diagrams

SPEC 2.2.1(c)(ii)

CRACK IT

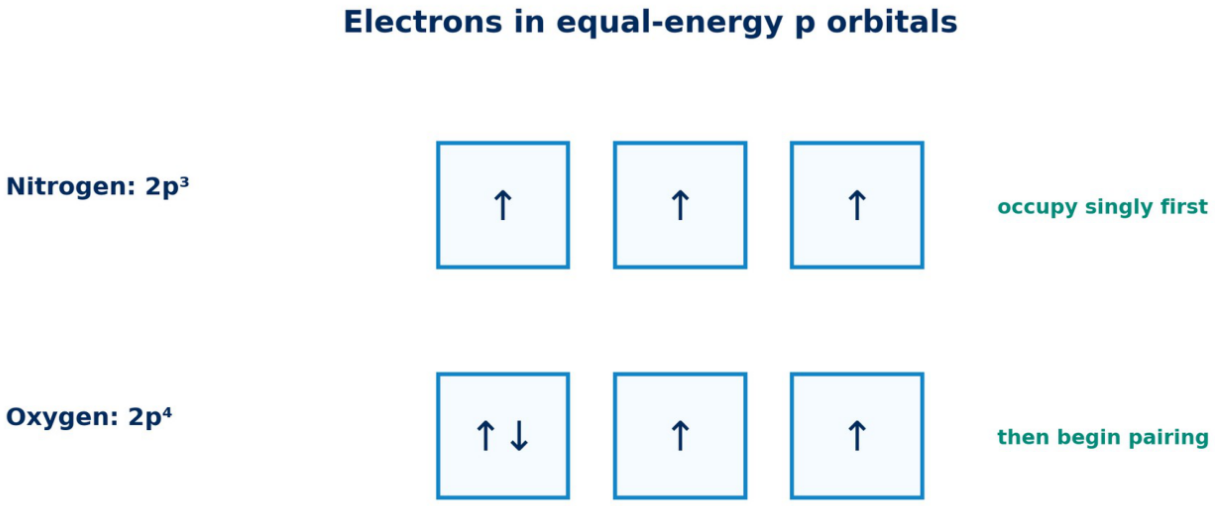
In an electrons-in-boxes diagram, each box is one orbital and each arrow is one electron. The arrow direction represents spin.

1. For equal-energy orbitals, place one electron in each box before adding a second electron to any box.

2. Draw the singly occupied orbitals with parallel spins in these ground-state arrangements.

3. When two electrons share a box, draw opposite arrows. One orbital holds no more than two electrons.

A p subshell therefore uses three boxes; a d subshell uses five. Check both the total electron count and the way they are distributed.



EXAM TRAP For p^2, use two different orbitals. Do not pair while an equal-energy orbital is empty.

TEST IT

Try questions 26, 27, 28 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can construct and diagnose box diagrams using occupancy and spin rules.

Electron configurations

14. Filling order and electron configurations

SPEC 2.2.1(c)(i), 2.2.1(d)(i)

CRACK IT

Start by counting the electrons. A neutral atom has one electron for every proton, so its total equals its atomic number.

1. Follow the filling order shown in the diagram.

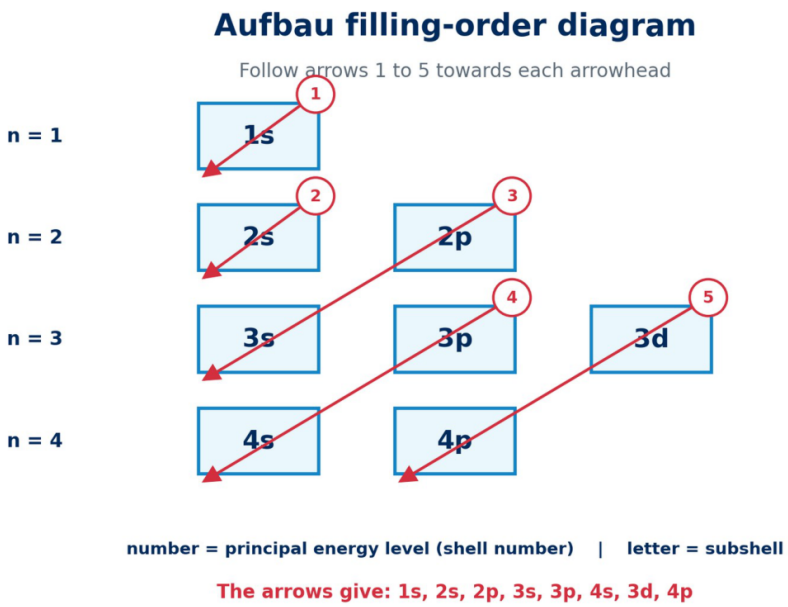
2. Use the capacities s^2, p^6 and d^{10} as you fill each subshell.

3. Stop when all the atom's electrons have been placed.

4. Add the superscripts as a final check: their total must equal Z.

In a configuration, the number names the shell, the letter names the subshell and the superscript counts its electrons. [Ar] is shorthand for the complete 18-electron argon core.

The 4s and 3d energies are close and depend on occupancy. Use the stated filling order without assuming one fixed energy ordering applies to every atom and ion.



1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p

WORKED EXAMPLE

Titanium, Z = 22

Write the full electron configuration and the noble-gas shorthand configuration of a neutral titanium atom. Titanium has atomic number 22.

Worked answer

1. A neutral Ti atom has 22 electrons.

2. Fill 18 core electrons, then $4s^2$ and $3d^2$.

3. Check: 18 + 2 + 2 = 22.

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^2$; shorthand $[Ar]\ 3d^2\ 4s^2$.

EXAM TRAP Writing 3d before 4s is a common convention. It does not mean 3d filled first.

TEST IT

Try questions 29, 30, 31, 32 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can write, translate and check any required neutral-atom configuration through krypton.

15. The chromium and copper exceptions

SPEC 2.2.1(d)(i)

CRACK IT

EXCEPTIONS · CHROMIUM & COPPER

Chromium and copper are the two exceptions to remember when using the simple filling order. Their measured configurations contain **4s¹**, rather than the 4s² you might first predict.

Chromium has a half-filled 3d⁵ subshell; copper has a filled 3d¹⁰ subshell. The 3d and 4s energies are close, and these observed arrangements have lower total energy than the simple predictions.

Use Cr, Z = 24, and Cu, Z = 29, to check the total electrons. Learn their observed configurations without turning the half-filled/full-filled explanation into a rule for every element.

Atom	Simple prediction	Observed configuration
Cr	[Ar] 3d⁴ 4s²	[Ar] 3d⁵ 4s¹
Cu	[Ar] 3d⁹ 4s²	[Ar] 3d¹⁰ 4s¹

EXAM TRAP These are neutral-atom exceptions. The ion configurations in this topic are limited to s- and p-block elements.

TEST IT

Try questions 33, 34 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can state both exceptions exactly and check their electron totals.

16. Electron configurations of s- and p-block ions

SPEC 2.2.1(d)(ii)

CRACK IT

Required scope: s- and p-block ions of elements up to Z = 36. Transition-metal ion configurations are outside this requirement.

1. Write the neutral atom's electron configuration.

2. Use the charge to work out how many electrons it has lost or gained.

3. For a positive ion, remove electrons from the highest occupied principal shell, taking p before s within that shell.

4. For a negative ion, add electrons to the available outer subshell.

5. Check the final electron total.

For Ga^{3+}, remove the 4p electron and both 4s electrons, leaving [Ar] 3d¹⁰. Do not treat the ion as a new neutral atom and blindly refill its electrons.

Ion	Neutral atom configuration	Ion configuration	Electron count
O^{2-} (Z = 8)	O: $1s^2\ 2s^2\ 2p^4$	[Ne]	10
Na^+ (Z = 11)	Na: [Ne] $3s^1$	[Ne]	10
Ca^{2+} (Z = 20)	Ca: [Ar] $4s^2$	[Ar]	18
Br^- (Z = 35)	Br: [Ar] $3d^{10}\ 4s^2\ 4p^5$	[Kr]	36

WORKED EXAMPLE

A p-block ion with an occupied d subshell

A neutral gallium atom has electron configuration [Ar] $3d^{10}\ 4s^2\ 4p^1$ and atomic number 31. Write the electron configuration of Ga^+ and explain which electron is removed.

Worked answer

1. Ga^+ has 31 − 1 = 30 electrons.

2. Remove the outer 4p electron.

3. Keep $3d^{10}$ and $4s^2$; check 18 + 10 + 2 = 30.

Ga^+: [Ar] $3d^{10}\ 4s^2$.

EXAM TRAP A positive charge means fewer electrons; a negative charge means more.

TEST IT

Try questions 35, 36, 37, 38, 39 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can build and check the permitted ion configurations, including p-block cations with filled 3d.

17. Putting electron structure together

SPEC 2.2.1(a–d)

CRACK IT

These questions connect several electron-structure skills. Keep returning to the electron count so you do not lose track of the atom or ion.

1. Use atomic number to count electrons in a neutral atom.

2. If an ion is given, use its charge to relate its electron count to the neutral atom.

3. Use the supplied atomic numbers to identify the element.

4. Write the configuration, then translate it into orbital boxes if asked. Paired electrons need opposite spins.

Show each step. A correct total alone does not prove the electrons occupy the correct subshells.

Identify representation → count electrons → apply rules → check charge and total

EXAM TRAP Do not answer a request for a full configuration with only a noble-gas core.

TEST IT

Try questions 40, 41, 42 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can choose and combine the required rules without being told the route.

Ionisation energies

18. First ionisation energy and attraction

SPEC 3.1.1(c), 3.1.1(c)(i)

CRACK IT

Periodicity connection: ionisation energies are included here to show how electron structure explains experimental evidence.

First ionisation energy is the energy needed to remove one electron from each atom in one mole of gaseous atoms, forming one mole of gaseous 1+ ions. Keep all those details in an exam definition.

Energy is needed to overcome the electron's attraction to the nucleus, so ionisation is endothermic. The unit is kJ mol^{-1}. A second ionisation starts from gaseous 1+ ions; later ionisations start from increasingly positive ions.

DEFINITIONS & KEY TERMS

First ionisation energy

The energy required to remove one electron from each atom in one mole of gaseous atoms to form one mole of gaseous 1+ ions.

$$X(g) \rightarrow X^{+}(g) + e^{-}$$

X an atom of the element in the gas state; X^{+} a gaseous ion of the element with charge +1; e^{-} an electron; **(g)** gas.

Factor	Consequence
More protons	Greater nuclear charge usually strengthens attraction.
Greater atomic radius	The removed electron is further from the nucleus, weakening attraction.
More inner-electron shielding	Weaker attraction to the electron being removed.
Higher-energy subshell	Less additional energy may be needed to remove its electron.
Paired electrons in an orbital	Electron repulsion can make one easier to remove.

Structural change → attraction changes → energy required changes

EXAM TRAP Finish your explanation with attraction and the energy needed; do not stop at “bigger atom”.

TEST IT

Try question 43 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can define first IE precisely and connect structure to removal energy.

19. Ionisation-energy trends and exceptions

SPEC 3.1.1(c)(i)

CRACK IT

Periodicity connection: explain each trend through the attraction between the nucleus and the electron being removed.

Across a period: nuclear charge increases while electrons enter the same main shell. Inner-shell shielding changes little, the radius decreases and attraction strengthens. First ionisation energy generally increases.

Down a group: the outer electron is further away and more shielded. These effects outweigh the increased nuclear charge, so attraction weakens and first ionisation energy generally decreases.

For exceptions, check the subshell and electron pairing. Removing a higher-energy p electron, or an electron repelled by its partner in a p orbital, can require less energy than the simple trend suggests.

EXCEPTIONS TO THE TREND

Decrease	Configurations	Explanation
Be → B	Be $1s^2\ 2s^2$; B $1s^2\ 2s^2\ 2p^1$	B loses a higher-energy, more shielded 2p electron rather than 2s.
N → O	N ends $2p^3$; O ends $2p^4$	O has one paired p orbital. Pair repulsion makes an electron easier to remove.
Mg → Al	Mg [Ne] $3s^2$; Al [Ne] $3s^2\ 3p^1$	Al loses a higher-energy, more shielded 3p electron rather than 3s.
P → S	P ends $3p^3$; S ends $3p^4$	S has a paired p orbital; pair repulsion lowers the energy needed.

EXAM TRAP The s → p decrease and the pairing decrease have different explanations. Name the relevant subshell or orbital.

TEST IT

Try question 44 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can explain the general trends and both types of small decrease.

20. Using successive ionisation energies

SPEC 3.1.1(c)(ii)

CRACK IT

Periodicity connection: a sequence of ionisation energies can reveal the atom's shell structure.

The energies rise as electrons are removed from an increasingly positive ion. A much larger jump marks the start of removal from an inner shell, where electrons are closer to the nucleus and less shielded.

1. Find the first large jump.
2. Count the electrons removed before that jump. This is the outer-shell electron count.
3. For a main-group element, link that number to the group.
4. Use any further large jumps to deduce the populations of inner shells.

Outer-shell electrons	Group
1 or 2	Group 1 or 2
3, 4, 5, 6, 7, 8	Groups 3, 4, 5, 6, 7, 0 respectively

WORKED EXAMPLE

A large jump after three removals

Al has successive IEs 578, 1817, 2745 and 11 578 kJ mol^{-1}.

Identify where the largest jump occurs and explain what it shows about the number of outer-shell electrons and the group of the element.

Worked answer

1. The large jump is between IE_3 and IE_4.
2. Three outer electrons have been removed before the jump.
3. The fourth electron comes from an inner shell.

Three outer electrons: Group 3.

WORKED EXAMPLE

Read more than one shell

All 13 successive ionisations of an atom show large jumps after removals 3 and 11.

Deduce the electron arrangement by shells and identify the element. Explain how the jumps support your answer.

Worked answer

1. First 3 removals: outer shell contains 3 electrons.
2. Next 8 removals: second shell contains 8 electrons.
3. Last 2 removals: innermost shell contains 2 electrons.

Shell arrangement 2, 8, 3: aluminium.

Second IE: $X^+(g) \rightarrow X^{2+}(g) + e^-$

Third IE: $X^{2+}(g) \rightarrow X^{3+}(g) + e^-$

EXAM TRAP If the jump is between IE_n and IE_{n+1}, the outer shell had n electrons, not n + 1. Use the period or further data when identifying the exact element.

TEST IT

Try question 45 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can deduce outer-shell and inner-shell counts from jumps and write the corresponding ionisation equations.