AQA | 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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Mass spectra & relative masses page 12

Shells, sub-shells & orbitals page 17

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Atoms, ions & isotopes

1. How the atomic model changed

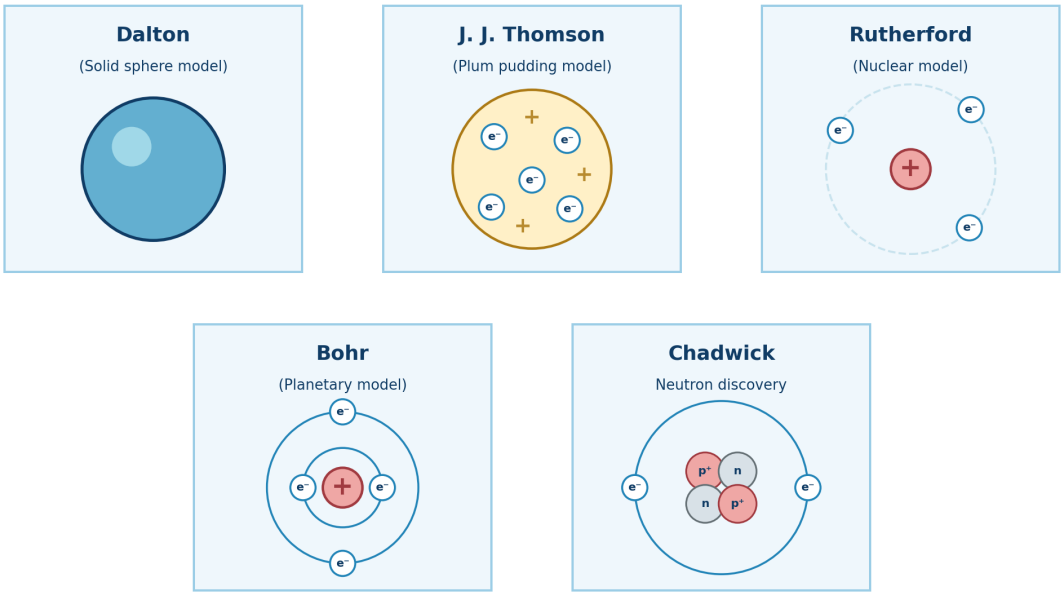
SPEC 3.1.1.1

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



DEFINITIONS & KEY TERMS

Dalton (solid sphere model)

Atoms pictured as tiny, solid, indivisible spheres.

J. J. Thomson (plum pudding model)

The discovery of electrons showed atoms were divisible. Electrons were placed within diffuse positive charge.

Rutherford (nuclear model)

Alpha scattering supported a tiny, dense, positive nucleus, with most of the atom empty space.

Bohr (planetary model)

Electrons placed in fixed energy levels.

Chadwick

The neutron completed the nuclear model and helped explain isotope masses.

WORKED EXAMPLE

Alpha scattering: observation → inference

Most alpha particles passed through; some were deflected through large angles; very few rebounded.

Explain what each observation tells you about the structure of the atom.

Worked answer

1. Most pass through → most of the atom is empty space.

2. Rare large deflections or rebounds → positive charge and most mass are concentrated in a tiny, dense nucleus.

Use the evidence in your explanation.

EXAM TRAP Do not merely list the models. State the evidence, then the conclusion.

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 observations led to changes in the atomic model.

2. Fundamental particles and the atom

SPEC 3.1.1.1

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
Proton	+1	1
Neutron	0	1
Electron	−1	≈ 1/1840

MEMORY HOOK Protons are positive. Neutrons are neutral. Electrons are negative and have negligible relative mass.

TEST IT

Try questions 2, 3 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 structure of an atom.

3. Mass number, atomic number and ions

SPEC 3.1.1.2

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.

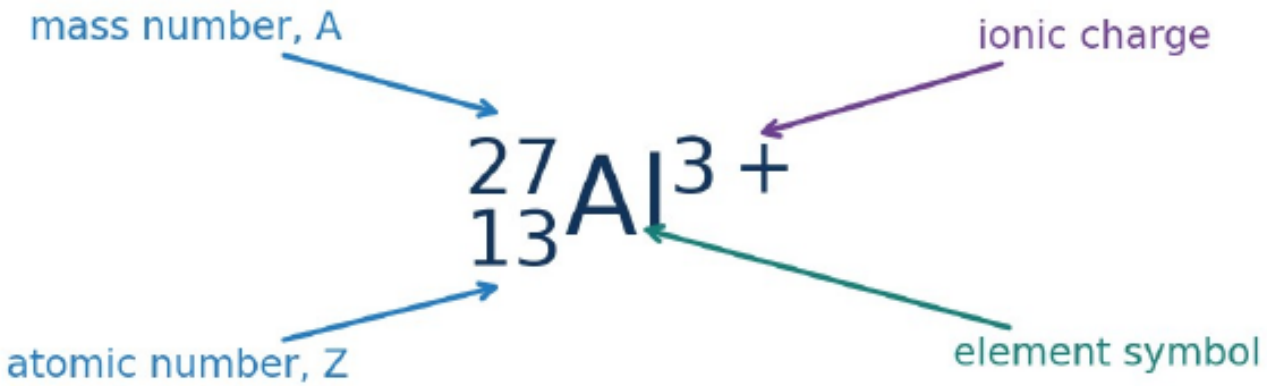
DEFINITIONS & KEY TERMS

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 a particular isotope. It is a whole number.



A = Z + number of neutrons

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

WORKED EXAMPLE

Finding particle numbers in an ion

State the number of protons, neutrons and electrons in $^{56}Fe^{2+}$. The atomic number of iron is 26.

Worked answer

1. Iron has Z = 26, so it contains **26 protons**.

2. Neutrons = 56 − 26 = **30**.

3. Start with 26 electrons, then subtract 2 because the ion is 2+.

26 protons, 30 neutrons and 24 electrons.

EXAM TRAP Work out the neutral atom first. Then subtract electrons for a positive ion or add electrons for a negative ion. This is easy to reverse under pressure.

TEST IT

Try questions 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 ion notation and particle numbers in both directions.

4. Isotopes

SPEC 3.1.1.2

CRACK IT

KEY DEFINITION

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.

WORKED EXAMPLE

Comparing isotopes

Compare neutral atoms of ^{35}Cl and ^{37}Cl. State their numbers of protons, neutrons and electrons, then explain why they have the same chemical properties but different masses. The atomic number of chlorine is 17.

Worked answer

1. ^{35}Cl and ^{37}Cl both contain **17 protons**.

2. ^{35}Cl contains **18 neutrons**; ^{37}Cl contains **20 neutrons**.

3. Both neutral atoms contain **17 electrons** and have the same electron configuration, so they react in the same way.

Their identical electron configurations make them react in the same way, while their different neutron numbers give them different masses.

DO NOT MIX THESE UP Mass number describes one isotope and is a whole number. Relative atomic mass is a weighted mean for the element and is often not a whole number.

TEST IT

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

DONE WHEN You can define isotopes and explain their similarities and differences.

How mass spectrometry works

5. The simple TOF mass spectrometer

SPEC 3.1.1.2

CRACK IT

A time-of-flight mass spectrometer identifies ions by timing their journey to a detector. Follow what happens to the particles at each stage, rather than learning five names without their meanings.

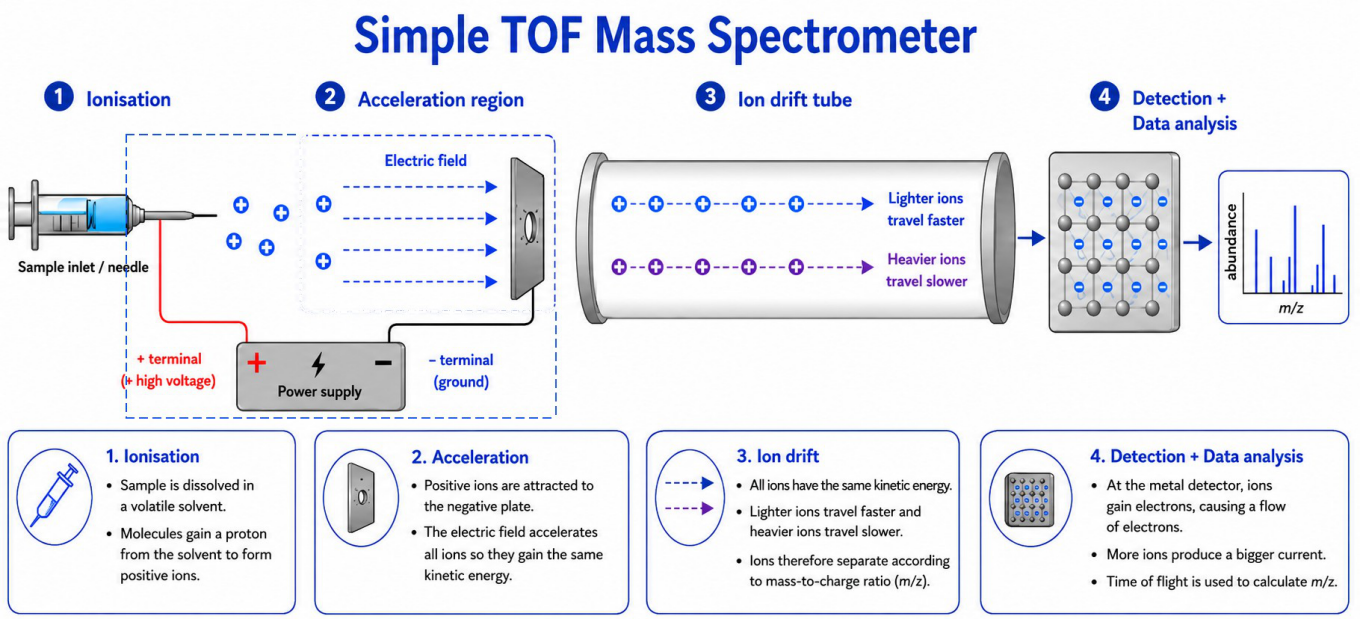
1. **Ionise:** make positive ions using **electrospray ionisation** or **electron impact**, as described below.

2. **Accelerate:** an **electric field** accelerates the positive ions. Ions with the same charge gain the same kinetic energy when accelerated through the same potential difference.

3. **Drift:** the ions travel through an evacuated, field-free tube, keeping the **same kinetic energy** they gained during acceleration. For ions of the same charge, this means equal kinetic energies but different speeds. The vacuum prevents collisions with gas particles.

4. **Detect:** positive ions gain electrons at the detector. This electron movement produces a current. More arriving ions produce a larger current.

5. **Analyse:** flight time is used to find m/z, while current gives relative abundance.



EXAM TRAP Acceleration uses an electric field. The detector current tells you abundance; it does not directly measure mass.

Ionisation context

DEFINITIONS & KEY TERMS

Electrospray ionisation

The sample is dissolved in a volatile solvent and passed through a fine needle at high voltage to form charged droplets. The solvent evaporates and molecules gain a proton, forming $[MH]^+$ ions. Useful for large or thermally unstable molecules; generally causes little fragmentation.

$$M(g) + H^+(g) \rightarrow [MH]^+(g)$$

M the original neutral molecule; **$[MH]^+$** the protonated molecule: M with an extra H^+ attached; **H^+** a proton; **(g)** gas.

DEFINITIONS & KEY TERMS

Electron impact

The sample is vaporised and bombarded with high-energy electrons. A collision knocks an electron from a gaseous atom or molecule, forming a positive ion. Commonly used for small volatile molecules; molecular ions may fragment.

$$M(g) + e^- \rightarrow M^+(g) + 2e^-$$

M a gaseous atom or molecule of the sample; M^+ the singly charged positive ion formed by electron loss; e^- an electron; **(g)** gas.

TEST IT

Try questions 7, 8, 9, 10 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can explain all five stages and connect flight time and current to the spectrum.

6. Why lower-m/z ions arrive first

SPEC 3.1.1.2

CRACK IT

For ions with the same charge, acceleration through the same potential difference gives equal kinetic energy. Equal kinetic energy does not mean equal speed: a heavier ion moves more slowly than a lighter ion.

1. Using the kinetic-energy equation, KE = ½mv²: if mass is larger while KE stays the same, speed must be smaller.

2. Both ions travel the same distance. The slower, heavier ion therefore reaches the detector later.

For ions with the same charge, lower mass means lower m/z, so lower-m/z ions arrive first.

$$KE = \tfrac{1}{2}mv^2$$

KE kinetic energy of one ion, in J; **m** mass of one ion, in kg; **v** speed of the ion, in m s^{-1}.

EXAM TRAP State the equal-charge or equal-KE condition before using the mass comparison.

TEST IT

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

DONE WHEN You can explain the arrival order, including the assumptions behind the comparison.

TOF calculations

7. TOF calculations: the calculation toolkit

SPEC 3.1.1.2 · MS 1.1

CRACK IT

A TOF calculation is a chain of linked equations. You do not have to guess the whole chain at once. Start with the quantity the question asks for and find the next missing piece.

1. Write an equation containing your target, then rearrange it. For time, start with t = d/v.

2. Put in the quantities you know. If speed is still unknown, use the kinetic-energy equation to find it.

3. Keep going until every quantity needed for the calculation is known.

4. Convert to kg, m and s before substituting: mass of one ion in kg, distance in m and time in s. In particular, convert microseconds to seconds.

5. Keep the calculator's full values during the working. Round only your final answer.

The equations below are your toolkit. Relative isotopic mass has no units; it is not the mass of one ion in kg. For a singly charged mononuclear ion, its numerical value equals m/z.

$$v = d/t \quad t = d/v \quad d = vt$$

d distance travelled by the ion, in m; **t** flight time of the ion, in s; **v** speed of the ion, in m s^{-1}.

$$KE = \tfrac{1}{2}mv^2 \quad m = 2KE/v^2 \quad v = \sqrt{(2KE/m)}$$

KE kinetic energy of one ion, in J; **m** mass of one ion, in kg; **v** speed of the ion, in m s^{-1}.

$$\text{Mass of one ion (kg)} = \text{relative mass} \times 10^{-3} / L$$

L Avogadro constant, 6.022 × 10^{23} mol^{-1}.

$$\text{Relative mass} = m \times L \times 1000$$

L Avogadro constant, 6.022 × 10^{23} mol^{-1}; **m** mass of one ion, in kg.

WORKED EXAMPLE

Forward: relative mass → flight time

A singly charged $^{40}Ar^{+}$ ion has relative mass 40.0 and KE 6.00×10^{-16} J. It travels 1.50 m. Use $L = 6.022 \times 10^{23}$ mol^{-1}.

Calculate the time of flight of the ion, giving your answer in seconds and microseconds.

Worked answer

1. Target t: $t = d/v$. Speed is unknown, so use $v = \sqrt{(2KE/m)}$.

2. Mass is still unknown: $m = (\text{relative isotopic mass} \times 10^{-3})/L$.
$m = (40.0 \times 10^{-3})/(6.022 \times 10^{23}) = 6.642 \times 10^{-26}$ kg.

3. $v = \sqrt{(2KE/m)}$
$v = \sqrt{[(2 \times 6.00 \times 10^{-16})/(6.642 \times 10^{-26})]} = 1.34 \times 10^{5}$ m s^{-1}.

4. $t = d/v$.
$t = 1.50/(1.344098... \times 10^{5}) = 1.12 \times 10^{-5}$ s.

t = 11.2 µs

WORKED EXAMPLE

Reverse: flight time → m/z

A singly charged ion has KE 5.00×10^{-16} J and travels 1.60 m in 13.0 µs.

Calculate the mass of one ion in kg and its mass-to-charge ratio, m/z. Use $L = 6.022 \times 10^{23}$ mol^{-1}.

Worked answer

1. Target relative mass: relative mass = $m \times L \times 1000$.

2. Find m from $m = 2KE/v^2$. Speed is unknown, so use $v = d/t$.

3. $t = 13.0 \times 10^{-6}$ s.
$v = d/t$.
$v = 1.60/(13.0 \times 10^{-6}) = 1.230769... \times 10^{5}$ m s^{-1}.

4. $m = 2KE/v^2$.
$m = (2 \times 5.00 \times 10^{-16})/(1.230769... \times 10^{5})^2 = 6.6015625 \times 10^{-26}$ kg $= 6.60 \times 10^{-26}$ kg (3 s.f.).

5. Relative mass = $m \times L \times 1000$.
Relative mass = $(6.6015625 \times 10^{-26}) \times (6.022 \times 10^{23}) \times 1000 = 39.754609... = 39.8$.

$m = 6.60 \times 10^{-26}$ kg; m/z = 39.8

WORKED EXAMPLE

Two ions: what cancels?

Two ions of masses m_1 and m_2 have equal kinetic energies and travel equal distances in times t_1 and t_2. Derive an expression for t_2/t_1 in terms of m_1 and m_2.

Worked answer

1. $\frac{1}{2}m_1v_1^2 = \frac{1}{2}m_2v_2^2$. Multiply by 2.

2. Substitute $v = d/t$: $m_1(d/t_1)^2 = m_2(d/t_2)^2$.

3. Only the identical d^2 cancels: $m_1/t_1^2 = m_2/t_2^2$.

4. Rearrange: $t_2^2/t_1^2 = m_2/m_1$, then take the positive square root.

$t_2/t_1 = \sqrt{(m_2/m_1)}$

WORKED EXAMPLE

Comparing $^{24}Mg^+$ and $^{26}Mg^+$

$^{24}Mg^+$ and $^{26}Mg^+$ ions have the same kinetic energy and travel the same flight distance. State which ion arrives first and calculate the ratio $t(^{26}Mg^+)/t(^{24}Mg^+)$.

Worked answer

$t_2/t_1 = \sqrt{(m_2/m_1)}$
$t_2/t_1 = \sqrt{(26/24)} = 1.0408$.

$^{24}Mg^+$ arrives first. The heavier ion takes about 4.1% longer.

EXAM TRAP Use the ratio shortcut only for equal KE and equal distance. For a direct m/z comparison, charges must also be equal. Do not cancel different masses, speeds or times.

TEST IT

Try questions 12, 13, 14, 15 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can build the route from the requested unknown, use SI units and justify what cancels.

Mass spectra & relative masses

8. Reading elemental mass spectra

SPEC 3.1.1.2

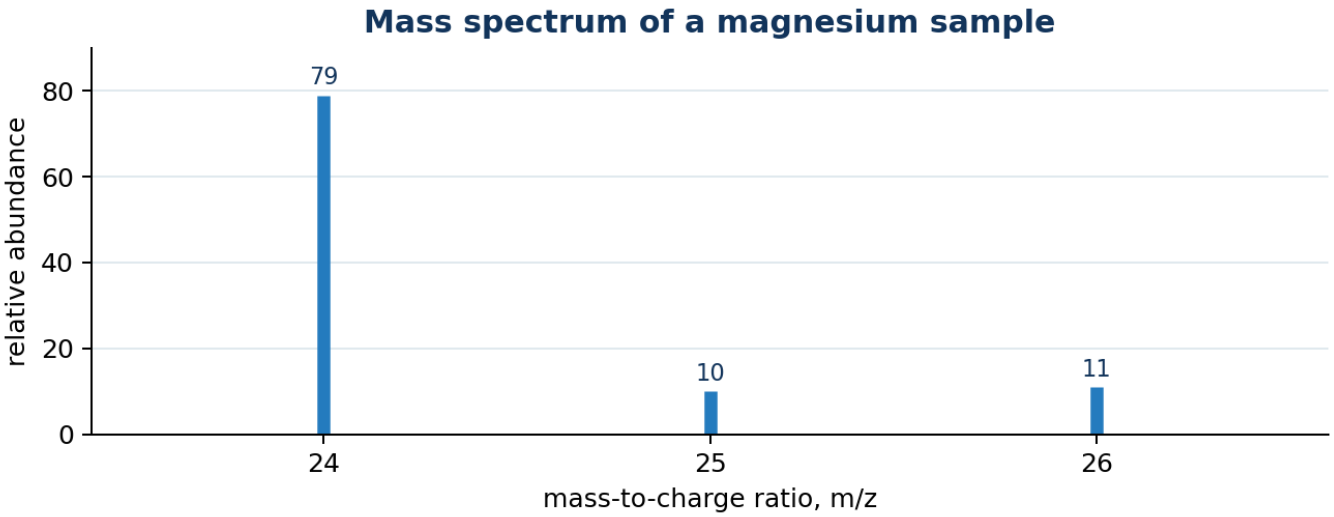
CRACK IT

Read a mass spectrum using its axes. The **x-axis** shows m/z; the **y-axis** shows the relative abundance of each ion.

• The x-axis is mass-to-charge ratio, m/z. For singly charged mononuclear ions, it is numerically equal to relative isotopic mass.

• The y-axis is relative abundance or intensity. A taller peak means more ions of that isotope.

• Use the isotope pattern and calculated weighted mean to identify the element. Check against its Periodic Table value.



EXAM TRAP Peak heights are relative quantities. They need not add to 100 unless they are given as percentages.

TEST IT

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

DONE WHEN You can interpret both axes, identify an element and distinguish abundance from flight time.

9. Calculating relative atomic mass

SPEC 3.1.1.2 · MS 1.2

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 = Σ(isotopic mass × abundance) / Σ(abundances)

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

WORKED EXAMPLE

Type 1: all masses and abundances known

Isotopes 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.

A_r = 28.11

WORKED EXAMPLE

Type 2: one mass unknown

An element has A_r = 63.62. Isotope 63 has abundance 69%; the other isotope has abundance 31%.

Calculate the relative isotopic mass of the second isotope.

Worked answer

1. 63.62 = [63(69) + 31x] / 100.

2. 6362 = 4347 + 31x.

3. x = (6362 − 4347) / 31 = 65.

The second mass number is 65.

WORKED EXAMPLE

Type 3: two abundances unknown

Isotopes 24, 25 and 26 give A_r = 24.32. Isotope 24 has abundance 79.0%.

Calculate the percentage abundances of isotopes 25 and 26.

Worked answer

1. Let isotope 25 have abundance x%. Isotope 26 then has abundance (21 − x)%.

2. 24.32 = [24(79) + 25x + 26(21 − x)] / 100.

3. 2432 = 2442 − x, so x = 10.

Isotope 25: 10%; isotope 26: 11%.

EXAM TRAP For three isotopes, the last abundance is 100 − known abundance − x.

TEST IT

Try questions 19, 20, 21 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can solve all three weighted-mean question types and check the result.

10. Relative molecular mass from mass spectra

SPEC 3.1.1.2

CRACK IT

First identify **which ion** the question describes. A molecular ion formed by electron impact has lost one electron; its mass is effectively the mass of the original molecule.

The molecular-ion peak is **usually the peak furthest to the right**, because the intact molecule is heavier than its fragments. Isotope peaks, such as a small M+1 peak, can appear just beyond it.

For a singly charged molecular ion, use its m/z as M_r. An electrospray $[MH]^+$ ion includes an extra proton, so subtract 1 from its m/z to find M_r of M.

The base peak is simply the most intense peak. It may be a fragment, so it does not automatically give the mass of the intact molecule. These shortcuts assume singly charged ions; check the charge and ion label first.

DEFINITIONS & KEY TERMS

Molecular-ion peak, M^+

The intact molecule after one electron is removed. For a singly charged molecular ion, its m/z gives the relative mass of that molecular ion.

Base peak

The tallest peak, representing the most abundant ion. It is not automatically the molecular ion.

Electron impact: M_r = m/z of the identified M^+ ion

M^+ the singly charged molecular ion; **M** a neutral molecule; M^+ is its positive molecular ion and $[MH]^+$ is its protonated 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.

Electrospray: M_r = m/z of $[MH]^+ - 1$

$[MH]^+$ the protonated molecule: M with an extra H^+ attached; **M** a neutral molecule; M^+ is its positive molecular ion and $[MH]^+$ is its protonated 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.

WORKED EXAMPLE

Read the right peak

A $[MH]^+$ ion appears at 151. In another spectrum, the base peak is 43 and the identified M^+ peak is 72.

Determine the relative molecular mass of the compound in each spectrum.

Worked answer

For the protonated ion, subtract 1. For the identified molecular ion, use its m/z.

M_r = 150 and 72 respectively.

EXAM TRAP Do not automatically choose the tallest or the highest-m/z peak. Identify the intact molecular ion and account for charge/protonation.

TEST IT

Try questions 22, 23 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can extract M_r from the identified M^+ or $[MH]^+$ peak.

11. Relative masses: definitions and language

SPEC 3.1.2.1

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.

Relative molecular mass, M_r

The mean mass of a molecule compared with one-twelfth of the mass of a carbon-12 atom.

Relative formula mass

The sum of A_r values in one formula unit. Use this term for ionic compounds.

$$M_r \text{ or relative formula mass} = \Sigma(A_r \times \text{number of each atom})$$

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

WORKED EXAMPLE

Molecules or ionic compounds?

Calculate the relative molecular mass of CO_2 and the relative formula mass of NaCl. Use A_r values: C = 12.0, O = 16.0, Na = 23.0 and Cl = 35.5.

Worked answer

1. CO_2 is molecular: M_r = sum of the A_r values of all atoms in the formula
$M_r = 12.0 + 2(16.0) = 44.0$.

2. NaCl is ionic: relative formula mass = 23.0 + 35.5 = 58.5.

44.0 and 58.5; neither has units.

EXAM TRAP Include “weighted mean” in A_r and the one-twelfth carbon-12 reference in both definitions.

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 precise definitions and choose the correct term without adding units.

Shells, sub-shells & orbitals

12. Shells, sub-shells and orbitals

SPEC 3.1.1.3

CRACK IT

Think of electron structure as three levels of organisation: **shells contain subshells, and subshells contain orbitals**. These names describe different things, so do not use them interchangeably.

An orbital can hold up to two electrons. An s subshell contains one orbital, a p subshell three and a d subshell five. That gives capacities of 2, 6 and 10 electrons respectively. The definitions and diagram below show how the levels fit together.

When drawing where electrons go, orbitals are usually represented by **boxes**. Each box is one orbital and each arrow is one electron; a pair of electrons in one box has opposite spins.

DEFINITIONS & KEY TERMS

Principal energy level (shell)

The number n. In 3p, the 3 identifies the principal energy level.

Sub-shell

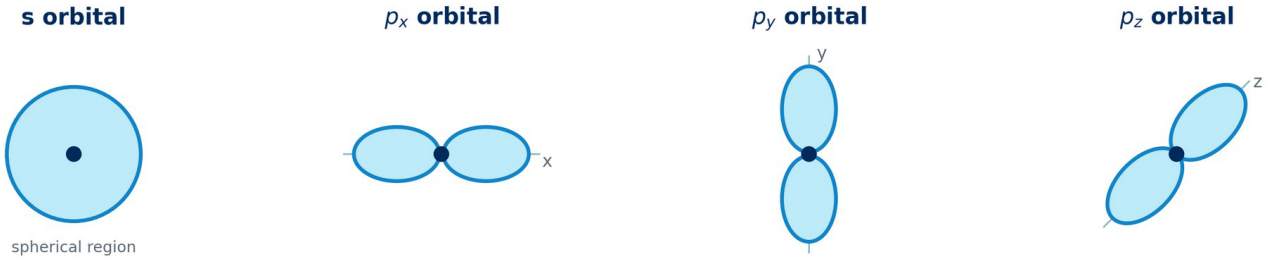
The letter, such as s, p or d. In 3p, p is a sub-shell within level 3.

Orbital

A region of space occupied by up to two electrons with opposite spins.

Sub-shell	Orbitals	Maximum electrons
s	1	2
p	3	6
d	5	10

One s orbital and the three p orbitals



EXAM TRAP A p sub-shell contains three orbitals and up to six electrons. One p orbital holds only two.

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 connect the three levels and recall the capacities 2, 6 and 10.

Electron configurations

13. Filling sub-shells and writing configurations

SPEC 3.1.1.3

CRACK IT

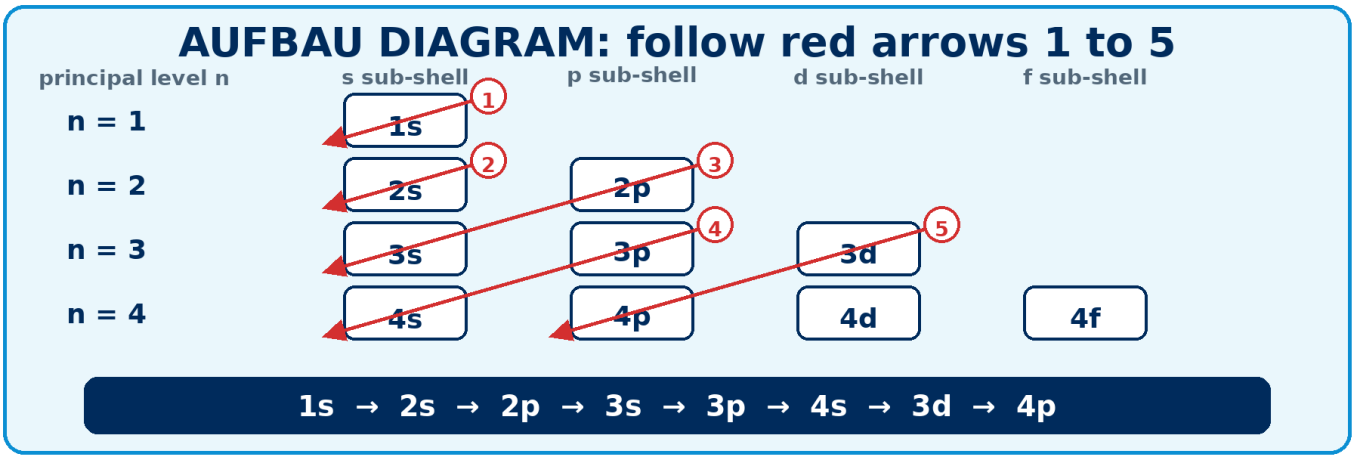
KEY DEFINITION

An electron configuration is a record of where an atom's electrons go. Put electrons into the available subshells in increasing energy, following the arrows in the diagram.

• In $2p^4$, the 2 tells you the shell, p tells you the subshell and 4 tells you how many electrons are in it.

• Use the s, p and d capacities of 2, 6 and 10. Check that the superscripts add to the atom's total electron number.

• Within a set of equal-energy orbitals, put one electron in each orbital before pairing. Two electrons in one orbital must have opposite spins.



1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p

WORKED EXAMPLE

Bromine, Z = 35

Write the full electron configuration and the noble-gas shorthand configuration of a neutral bromine atom. Bromine has atomic number 35.

Worked answer

1. A neutral atom has 35 electrons.

2. Fill in order, respecting s^2, p^6 and d^{10} capacities.

3. The first 18 electrons are the [Ar] core.

4. Check: 18 + 10 + 2 + 5 = 35.

Full: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$.
Shorthand: [Ar] $3d^{10}\ 4s^2\ 4p^5$.

EXAM TRAP Add the superscripts. For an atom they must equal Z; for an ion apply the charge first.

TEST IT

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

DONE WHEN You can build, check and abbreviate configurations up to krypton.

14. The chromium and copper exceptions

SPEC 3.1.1.3

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 $4s^2$ you might first predict.

Chromium has a half-filled $3d^5$ subshell; copper has a filled $3d^{10}$ 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.

Cr: [Ar] $3d^5$ $4s^1$

Cu: [Ar] $3d^{10}$ $4s^1$

EXAM TRAP Do not write Cr as [Ar] $3d^4$ $4s^2$ or Cu as [Ar] $3d^9$ $4s^2$.

TEST IT

Try question 28 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can recall Cr and Cu correctly and describe their 3d occupancies.

15. Electron configurations of ions

SPEC 3.1.1.3

CRACK IT

Start with the neutral atom's configuration. The charge then tells you how many electrons to remove or add. A positive ion has lost electrons; a negative ion has gained them.

When removing electrons, start with the highest occupied principal shell. For transition-metal ions, remove the 4s electrons before the 3d electrons. For example, losing two electrons from $4s^2$ leaves 4s empty.

Check the final electron total against atomic number and charge. Counting is a useful check, but remember that removing electrons from an atom is not the same as refilling a new neutral atom from scratch.

Transition-metal ions: remove 4s before 3d

Ion	Neutral atom configuration	Ion configuration	Electrons removed or added
O^{2-}	O: $1s^2\ 2s^2\ 2p^4$	$1s^2\ 2s^2\ 2p^6$	Gain 2 electrons
Ca^{2+}	Ca: [Ar] $4s^2$	[Ar]	Remove $4s^2$
Fe^{2+}	Fe: [Ar] $3d^6\ 4s^2$	[Ar] $3d^6$	Remove both 4s electrons
Fe^{3+}	Fe: [Ar] $3d^6\ 4s^2$	[Ar] $3d^5$	Remove both 4s electrons and one 3d electron

WORKED EXAMPLE

Work backwards from an ion

X^{2+} has configuration [Ar] $3d^7$. Identify X and reconstruct its neutral configuration. Atomic numbers: Fe = 26, Co = 27, Ni = 28.

Worked answer

1. X^{2+} has 18 + 7 = 25 electrons.

2. The neutral atom has 27 electrons, so Z = 27: cobalt.

3. Reverse ion formation by returning two electrons to 4s.

X is Co: [Ar] $3d^7\ 4s^2$.

EXAM TRAP 4s fills before 3d in the simple building-up order, but 4s electrons are removed first from these ions.

TEST IT

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

DONE WHEN You can count electrons, apply charge and reconstruct atoms and ions.

16. Electron configuration and the Periodic Table

SPEC 3.2.1.1

CRACK IT

The Periodic Table helps you predict electron structure. An element's block tells you the type of subshell being filled across that part of the table.

Look for the **differentiating electron**: the electron that distinguishes this element's configuration from the preceding element's. Do not simply choose the subshell written last on the page.

In the table below, n means the outer-shell principal energy level. Electron configurations up to Z = 36 use s, p and d subshells. You should also recognise where the f block sits.

Block	Position	Typical ending
s	Groups 1 and 2, plus helium	ns^1 or ns^2
p	Groups 3–7 and 0, except helium	np^1 to np^6
d	Central block	$(n-1)d^1$ to $(n-1)d^{10}$
f	Two rows below the main table	$(n-2)f^1$ to $(n-2)f^{14}$

WORKED EXAMPLE

Identify the block

An atom has configuration [Ar] $3d^5$ $4s^2$. State its block.

Worked answer

The differentiating electron enters 3d, even though $4s^2$ may be written last.

d block.

TEST IT

Try question 32 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can connect sub-shell occupancy to block position, including helium as s block.

Ionisation energies

17. First and successive ionisation energies

SPEC 3.1.1.3

CRACK IT

Ionisation energy measures how much energy is needed to remove electrons. First ionisation energy removes one electron from each gaseous atom. The precise definition below includes the amount, gaseous state and ions formed.

Removing a negative electron from the attraction of a positive nucleus needs energy, so ionisation is endothermic. The unit is kJ mol^{-1}.

The second ionisation energy starts with gaseous 1+ ions, not neutral atoms. Each successive ionisation removes another electron from an increasingly positive ion.

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.

Step	Equation
First	$Mg(g) \rightarrow Mg^{+}(g) + e^{-}$
Second	$Mg^{+}(g) \rightarrow Mg^{2+}(g) + e^{-}$
Third	$Mg^{2+}(g) \rightarrow Mg^{3+}(g) + e^{-}$

EXAM TRAP For the nth ionisation, begin with charge (n − 1)+ and finish with n+. Include (g) for the atom or ion on both sides.

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 give the precise definition and write each ionisation equation correctly.

18. What controls ionisation energy?

SPEC 3.1.1.3

CRACK IT

Ask one central question: **how strongly is the electron being removed attracted to the nucleus?** Stronger attraction means more energy is needed to remove it.

• More protons give a greater nuclear charge and tend to strengthen attraction.

• An electron further from the nucleus is less strongly attracted.

• Inner electrons shield an outer electron from some of the nuclear attraction.

• Subshell energy and repulsion between paired electrons can explain exceptions to a simple trend.

Compare the relevant factors together. Saying only that an atom has more protons is not enough if the electron is also further away and more shielded.

Factor	Effect
More protons	Greater nuclear charge strengthens attraction.
Greater distance	Weaker attraction to the electron.
More inner-shell shielding	Weaker attraction to the electron being removed.
Higher-energy sub-shell	Less additional energy needed to remove the electron.
Electron pairing	Repulsion within an orbital can make one electron easier to remove.

Structural change → attraction changes → energy changes

EXAM TRAP “The atom is bigger” or “more shielding” is incomplete. Finish the chain with attraction and the energy required.

TEST IT

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

DONE WHEN You can choose the relevant factor and finish a cause-and-effect explanation.

19. First ionisation energy across Period 3

SPEC 3.1.1.3 · 3.2.1.2

CRACK IT

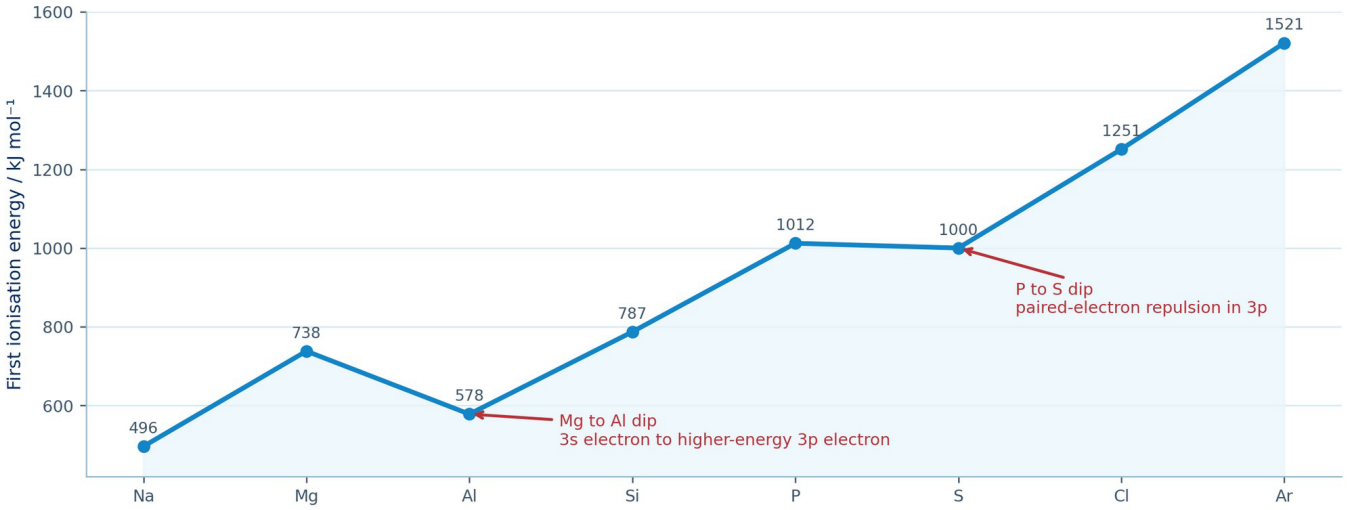
Across Period 3, first ionisation energy generally rises. The nucleus gains protons, while the added electrons enter the same main shell. Inner-shell shielding stays broadly similar.

The outer electron is attracted more strongly and the atomic radius decreases. More energy is therefore needed to remove that electron.

EXCEPTIONS · THE TWO DIPS

From Mg to Al, the removed electron is in the higher-energy 3p subshell. From P to S, the removed 3p electron is paired, so electron-electron repulsion makes removal easier. Use these specific explanations for the exceptions.

First ionisation energies across Period 3



EXCEPTIONS TO THE TREND

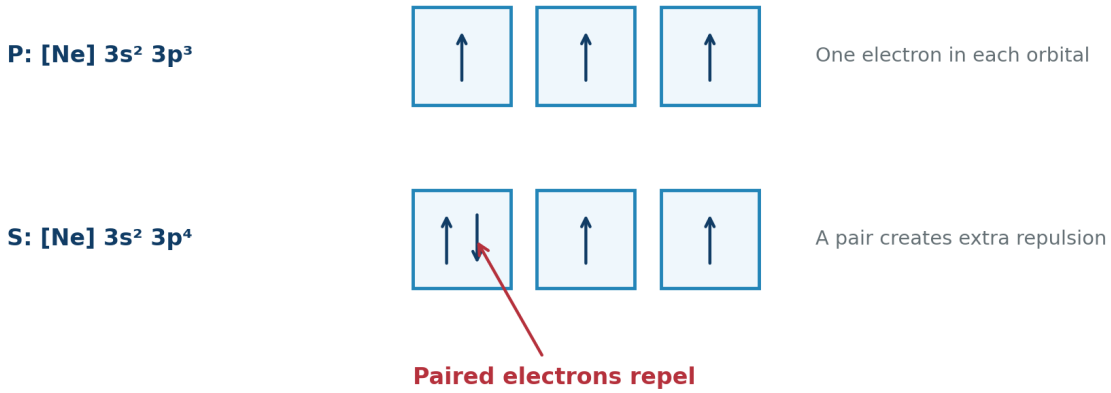
Mg → Al

Mg: [Ne] $3s^2$. Al: [Ne] $3s^2$ $3p^1$. The electron removed from Al is in a higher-energy, slightly more shielded 3p sub-shell, so is easier to remove.

P → S

P: [Ne] $3s^2$ $3p^3$. S: [Ne] $3s^2$ $3p^4$. Sulfur has a pair in one 3p orbital. Repulsion in that pair makes an electron easier to remove.

The P to S dip: what changes inside 3p?



EXAM TRAP Use sub-shell energy for Mg → Al and paired-electron repulsion for P → S. They are different explanations.

TEST IT

Try questions 37, 38, 39, 40 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can explain the overall trend and both anomalies with the correct mechanism.

20. First ionisation energy down Group 2

SPEC 3.1.1.3 · 3.2.2

CRACK IT

Down Group 2, first ionisation energy falls even though the nucleus contains more protons. The electron being removed is now in a shell further from the nucleus.

1. There are more occupied shells.

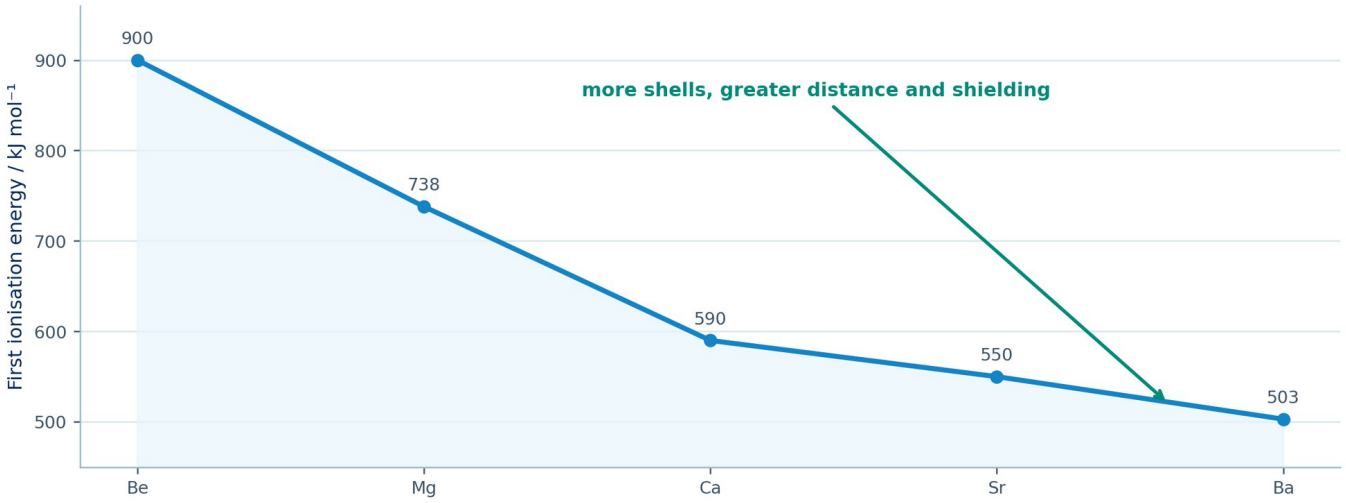
2. The outer electron is further away and more shielded by inner electrons.

3. These effects outweigh the larger nuclear charge, so the attraction is weaker.

4. Less energy is needed to remove the outer electron.

The repeated drop when a new outer shell begins to fill is evidence for the shell model.

First ionisation energy down Group 2



EXAM TRAP Do not stop at “larger atoms”. State greater distance and shielding, then weaker attraction and lower IE.

TEST IT

Try question 41 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can explain why first IE decreases despite increasing nuclear charge.

21. Successive ionisation energies and shell structure

SPEC 3.1.1.3

CRACK IT

Each successive ionisation removes an electron from an ion that is already positive, so the energy rises. A **particularly large jump** tells you that the next electron comes from an inner shell.

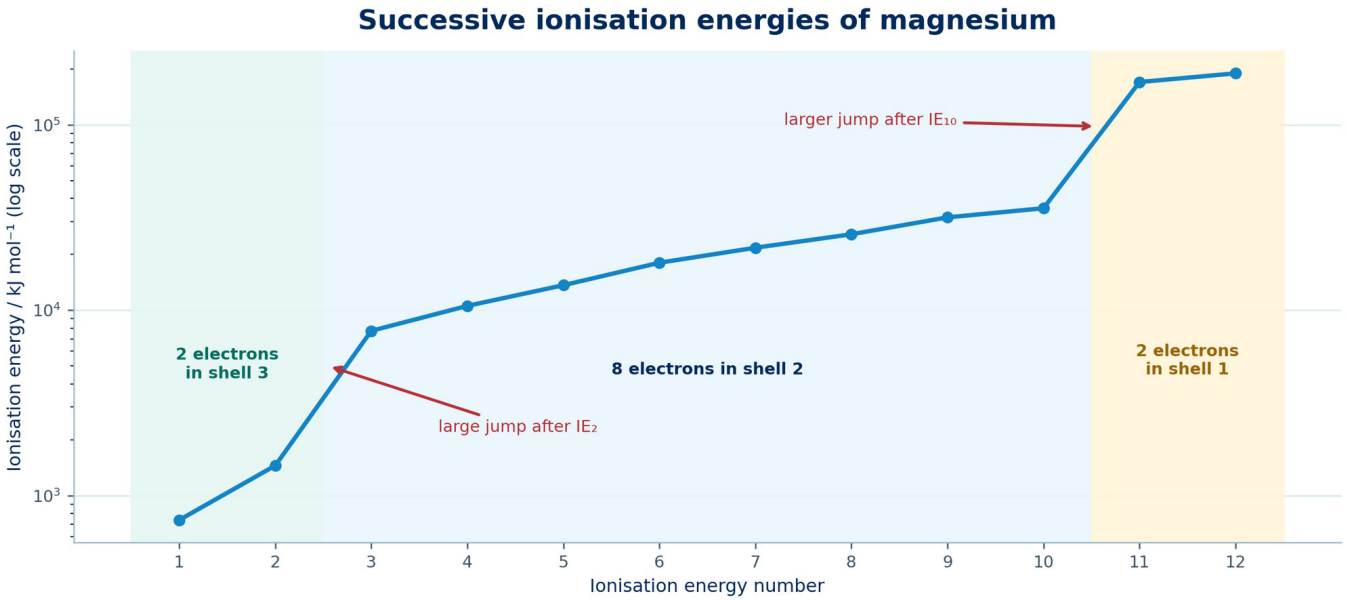
Inner-shell electrons are closer to the nucleus and less shielded. They are much more strongly attracted than the outer electrons just removed.

1. Locate the first large jump.

2. Count the electrons removed **before** it. That is the number in the outer shell.

3. For a main-group element, connect this count to the group: three outer electrons means Group 3; six means Group 6.

4. If more large jumps are shown, use them to work out further shell populations.



Period 3 element	First major jump after
Na	IE_1
Mg	IE_2
Al	IE_3
Si	IE_4
P	IE_5
S	IE_6
Cl	IE_7
Ar	IE_8

WORKED EXAMPLE

Identify a Period 3 element

Successive IEs: 578, 1817, 2745 and 11 578 kJ mol^{-1}.

These are the first four successive ionisation energies of a Period 3 element. Identify the element and explain your reasoning. Write its full electron configuration.

Worked answer

1. Large jump between IE_3 and IE_4.

2. Three outer-shell electrons, then an inner-shell electron is removed.

3. The element is in Group 3. In Period 3, this is aluminium.

Al: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$.

EXAM TRAP A jump after the third electron means three outer electrons, not four.

TEST IT

Try questions 42, 43, 44, 45, 46 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN You can use the data to infer outer-electron number, group, element and shell structure.