9701 CHEMISTRY · TOPIC 1 · AS LEVEL

Atomic Structure

01 · SUBATOMIC PARTICLES

Particle	Charge	Rel. mass
proton	+1	1
neutron	0	1
electron	−1	1/1836

Notation $^{A}_{Z}X$ — Z = protons (= atomic number), A = mass number = p + n, so **n = A − Z**. Nucleus holds nearly all the mass; charge = protons − electrons.

02 · ISOTOPES

Same element, same Z, different number of neutrons.

Same chemical properties (same electron configuration). **Different** physical properties — mass, density, rate of diffusion, boiling point, radioactivity.

Uses: C-14 dating, Co-60 radiotherapy, I-131 thyroid imaging.

03 · RELATIVE ATOMIC MASS

$$A_r = \Sigma(\text{abundance} \times \text{mass}) \div 100$$

Mass spectrum: x-axis = m/z, y-axis = relative abundance. Weighted mean, so A_r sits nearer the more abundant isotope.

> **Worked example.** Cl-35 (75.8 %), Cl-37 (24.2 %):
> (35 × 75.8 + 37 × 24.2) ÷ 100 = **35.48**
> 2 d.p., no units — A_r is a ratio.

04 · ELECTRON CONFIGURATION

Shell n holds max **$2n^2$**. Subshell capacity: s 2, p 6, d 10, f 14.

Fill order
1s 2s 2p 3s 3p **4s 3d** 4p 5s 4d 5p 6s 4f 5d 6p

Aufbau lowest energy first · **Pauli** max 2 e^- per orbital, opposite spins · **Hund** singly fill degenerate orbitals before pairing.

Condensed: Fe = [Ar] $4s^2$ $3d^6$. Exceptions: Cr = [Ar] $3d^5$ $4s^1$, Cu = [Ar] $3d^{10}$ $4s^1$.

Ions: remove the outermost (highest n) electrons first — Fe^{3+} = [Ar] $3d^5$, not $3d^3 4s^2$.

05 · ORBITALS A2

An orbital is a region of high probability of finding an electron; it holds up to 2 e^-.

s spherical, one per shell. **p** two-lobed, three per shell along x, y, z, equal in energy. Draw orbital diagrams as boxes with arrows, applying Hund.

06 · IONISATION ENERGY

1st IE: $X(g) \rightarrow X^+(g) + e^-$
Always endothermic; species must be **gaseous**.

Across a period ↑ — greater nuclear charge, same shell, similar shielding. **Down a group** ↓ — outer electron further out and more shielded.

Dips: Be→B (electron enters a higher-energy 2p) and N→O (paired-electron repulsion in one 2p orbital). These dips are the evidence for sub-shells.

Successive IEs always rise; a large jump marks the start of a new inner shell, so the number of electrons removed before the jump gives the group.

07 · EVIDENCE FOR SHELLS AND SUB-SHELLS

Plot log(IE) against the number of the electron removed. The **large jumps** mark the start of each new inner shell, and the number of electrons removed before the first jump gives the group.

Within a shell the smaller steps mark sub-shells: for Al the 3p electron leaves first, then the two 3s electrons cost noticeably more.

Successive ionisation energies always rise — each electron is pulled from an increasingly positive ion.

08 · PERIODICITY

Property	→ period	↓ group
Atomic radius	↓	↑
Ionisation energy	↑	↓
Electronegativity	↑	↓
Electron affinity	more −ve	less −ve
Metallic character	↓	↑

Ionic radius: cations smaller than the atom, anions larger. Across an isoelectronic series (N^{3-} → Al^{3+}) radius falls as charge rises.

Oxides across period 3: basic (Na_2O, MgO) → amphoteric (Al_2O_3) → acidic (P_4O_{10}, SO_3). Melting point peaks at Si (giant covalent) and collapses at the noble gas.

09 · WORKED EXAMPLE — SUCCESSIVE IONISATION ENERGIES

An element has first five ionisation energies of 578, 1817, 2745, 11 578 and 14 831 kJ mol^{-1}. Which group is it in?

The big jump comes between the 3rd and 4th values, so three electrons are removed easily. → **Group 13**, and with these values the element is aluminium.

Always quote the position of the jump, not just its size.

DEFINITIONS TO QUOTE EXACTLY

First ionisation energy — the energy needed to remove one mole of electrons from one mole of gaseous atoms.

Electronegativity — the ability of an atom to attract a shared pair of electrons in a covalent bond.

Isotopes — atoms of the same element with the same number of protons but different numbers of neutrons.

Relative atomic mass — the weighted mean mass of an atom relative to carbon-12 taken as exactly 12.

MARKS LOST HERE

— Omitting **(g)** or the electron in an ionisation equation.

— Writing 3d before 4s when 4s fills first, or removing 3d electrons before 4s when forming ions.

— Saying "shielding increases" across a period; it stays roughly constant — nuclear charge is doing the work.

— Explaining a trend by "more shells" when the ions are isoelectronic.

9701 CHEMISTRY · TOPIC 3 · AS + A LEVEL

Chemical Bonding

10 · WHICH BOND TYPE?

Δ electronegativity	Bond
< 0.4	non-polar covalent
0.4 – 1.8	polar covalent
> 1.8	ionic

Metal + non-metal → ionic · non-metal + non-metal → covalent · metal + metal → metallic. Bonding is a **continuum**, so treat the cut-offs as guides and use the bonding triangle when asked.

11 · IONIC BONDING

Electrostatic attraction between oppositely charged ions in a **giant lattice**. Formula is empirical — the ratio, not a molecule.

Properties: high melting point, brittle, conducts when molten or aqueous but not solid (ions fixed), generally soluble in polar solvents.

Lattice enthalpy ↑ with larger ionic charges and smaller ionic radii — MgO ≫ NaCl.

12 · COVALENT BONDING

A shared pair of electrons attracted by both nuclei. As **bond order rises, length falls and strength rises**: C–C > C=C > C≡C in length, reversed in enthalpy.

Coordinate (dative) bond: both electrons from one atom — NH_4^+, H_3O^+, Al_2Cl_6. Identical to a normal covalent bond once formed.

13 · LEWIS STRUCTURES

1 · Count valence electrons (add for negative charge, subtract for positive). 2 · Least electronegative atom central. 3 · Single bonds, complete octets, then multiple-bond the leftovers. 4 · Show **all** lone pairs and the charge in brackets.

Formal charge = valence – (lone-pair e^- + ½ bonding e^-). The best structure keeps formal charges nearest zero, negative on the most electronegative atom.

Resonance (O_3, NO_3^-, CO_3^{2-}, benzene): delocalised electrons, all bonds equal and intermediate in length and strength.

A2 Period-3 atoms can exceed an octet: PCl_5, SF_6, ClF_3, XeF_4.

14 · VSEPR — SHAPES & ANGLES

Dom.	lp	Shape	Angle	Ex.
2	0	linear	180°	CO_2
3	0	trigonal planar	120°	BF_3
3	1	bent	<120°	SO_2
4	0	tetrahedral	109.5°	CH_4
4	1	trigonal pyramidal	107°	NH_3
4	2	bent	104.5°	H_2O
5	0	trigonal bipyramidal	90 / 120°	PCl_5
5	1	see-saw	<90 / <120°	SF_4
5	2	T-shaped	<90°	ClF_3
5	3	linear	180°	XeF_2
6	0	octahedral	90°	SF_6
6	1	square pyramidal	<90°	BrF_5
6	2	square planar	90°	XeF_4

Rows with 5 or 6 domains are A2. Repulsion **lp–lp > lp–bp > bp–bp**; each lone pair closes the angle by ~2.5°. Count domains, not atoms — a double bond is one domain.

15 · POLARITY

A bond is polar if $\Delta\chi > 0$ → dipole $\delta+ \rightarrow \delta-$. A **molecule** is polar only if the bond dipoles do not cancel.

Non-polar despite polar bonds (symmetrical): CO_2, CCl_4, BF_3, CH_4, SF_6. **Polar:** H_2O, NH_3, $CHCl_3$, SO_2.

Symmetry beats bond count — check the shape first, then add the vectors.

16 · INTERMOLECULAR FORCES

Weakest → strongest:

1 London (dispersion) — in everything; stronger with more electrons (higher M_r) and greater surface contact, so pentane boils above 2,2-dimethylpropane.

2 Dipole–dipole — between permanent dipoles in polar molecules.

3 Hydrogen bonding — H bonded directly to N, O or F, plus a lone pair to accept. Explains the anomalous boiling points of H_2O, NH_3 and HF, and ice being less dense than water.

Melting and boiling points break **intermolecular** forces, never covalent bonds. "Like dissolves like" for solubility.

17 · METALLIC & GIANT COVALENT

Metallic: lattice of cations in a sea of delocalised electrons. Strength ↑ with ionic charge and ↓ with radius (Na < Mg < Al). Conducts, malleable, high melting point; alloys are harder because different sizes disrupt the layers.

Giant covalent: diamond — tetrahedral, 4 bonds, very hard, non-conductor. Graphite — hexagonal layers, 3 bonds + 1 delocalised e^-, conducts along layers, soft lubricant. SiO_2 resembles diamond; C_{60} is molecular, not giant.

18 · HYBRIDISATION, Σ & Π A2

Hybrid	Domains	Geometry	Ex.
sp^3	4	tetrahedral 109.5°	CH_4
sp^2	3	trigonal planar 120°	C_2H_4
sp	2	linear 180°	C_2H_2

σ = head-on overlap along the internuclear axis. **π** = side-on overlap of parallel p orbitals. Double bond = 1σ + 1π; triple = 1σ + 2π. π bonds block rotation, giving cis/trans isomers.

Delocalisation: in benzene the six p orbitals overlap sideways into one π system above and below the ring, so all six carbon–carbon bonds are identical and intermediate between a single and a double bond.

19 · WORKED EXAMPLE — DEDUCE THE SHAPE

Predict the shape and bond angle of SF_4.

S has 6 valence electrons; four bond to F, leaving one lone pair.
5 electron domains → trigonal bipyramidal arrangement
The lone pair takes an equatorial position → **see-saw**
Angles slightly under 90° and 120°.

DATA BOOKLET & MARKS LOST

Look up, never memorise: electronegativity values, ionic and covalent radii, bond enthalpies and lengths, first ionisation energies, the electromagnetic spectrum, and the periodic table itself.

— Confusing electron domain geometry with molecular shape: NH_3 is tetrahedral in domains, **trigonal pyramidal** in shape.

— Calling a molecule with polar bonds polar without checking symmetry.

— Saying covalent bonds break on boiling a simple molecular substance.

— Drawing Lewis structures without lone pairs or the ion's charge bracket.