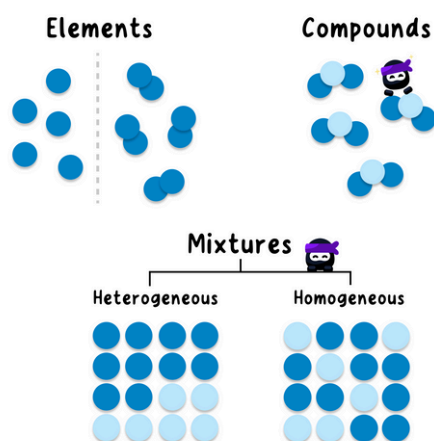


IB CHEMISTRY S1.1 INTRODUCTION TO THE PARTICULATE NATURE OF MATTER



Properties of elements, compounds, and mixtures

- **Element:** pure substance made of **one type** of atom; cannot be chemically broken down
- **Compound:** pure substance of **two or more** elements chemically bonded in a **fixed, simple whole-number ratio**; properties differ from constituent elements
- **Mixture:** physical combination of **two or more** substances (elements and/or compounds) in **no fixed ratio**; components retain their properties and can be separated by physical means
 - **Homogeneous mixture:** uniform composition throughout (e.g., air, salt solution); single visible phase
 - **Heterogeneous mixture:** non-uniform composition (e.g., oil+water, granite); two or more visible phases



Kinetic molecular theory

- Particles are in constant random motion: $E_k \propto T$
- Collisions are elastic (on average energy conserved)
- Intermolecular forces determine proximity and order

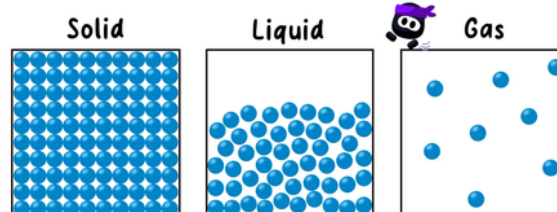


Exam Tip!

If a question says "explain using KMT", mention particle spacing, motion, intermolecular forces, and how these account for observed property.

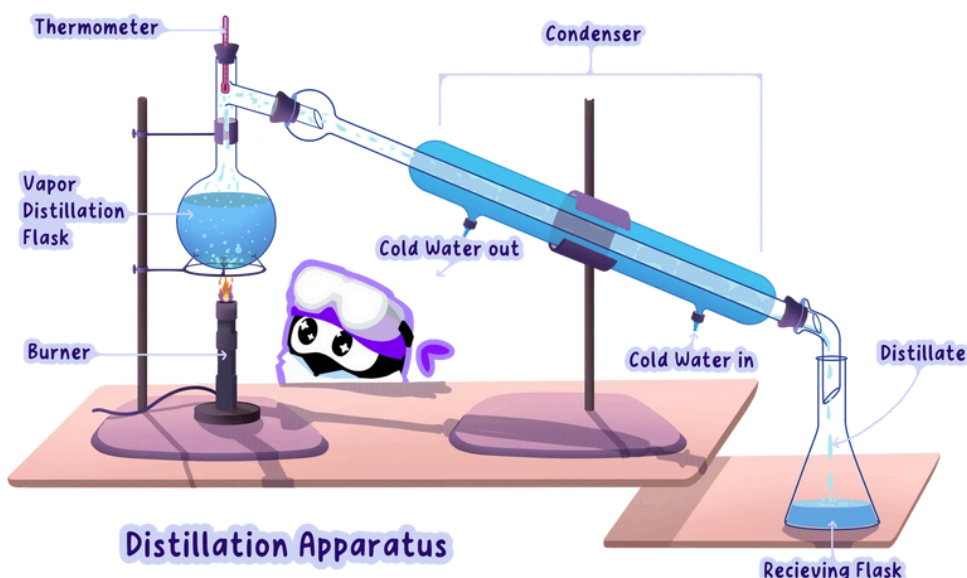
State of matter and state symbols

- **Solid (s):** particles closely packed in fixed positions (vibrate only); strong forces; fixed shape & volume; **lowest E_k**
- **Liquid (l):** particles close but able to slide past; moderate forces; fixed volume, variable shape; **medium E_k**
- **Gas (g):** particles far apart, negligible forces (ideal model); variable volume & shape; **highest E_k**
- **Aqueous (aq):** dissolved in water (not a state of matter!)



Separation techniques you must know

- **Solvation (dissolving):** solute particles become surrounded by solvent particles; used to prepare solutions.
- **Filtration:** separates insoluble solid from liquid using a porous barrier (e.g., sand from water)
- **Recrystallization:** purifies a solid by dissolving hot then crystallizing on cooling; impurities remain in mother liquor
- **Evaporation:** removes solvent to obtain dissolved solid; gentle heating increases rate
- **Distillation:** separates miscible liquids by different boiling points; simple (distill solvent from solute) vs fractional (separate close b.p. liquids)
- **Paper chromatography:** separates mixture based on different affinities between mobile phase (solvent) and stationary phase (paper).



Example:



You can separate ethanol (boiling point $\sim 78^\circ\text{C}$) from water (boiling point $\sim 100^\circ\text{C}$) using a distillation apparatus.

Changes of state

- **Melting:** solid → liquid (endothermic)
- **Freezing:** liquid → solid (exothermic)
- **Vaporization:** liquid → gas (endothermic); includes:
 - **Evaporation:** only at the **surface of the liquid**, at any temperature, when particles near the surface absorb enough energy to escape
 - **Boiling:** throughout the **entire liquid** at a specific temperature where particles throughout the liquid gain enough energy to break free
- **Condensation:** gas → liquid (exothermic)
- **Sublimation:** solid → gas (endothermic)
- **Deposition:** gas → solid (exothermic)



Common Question

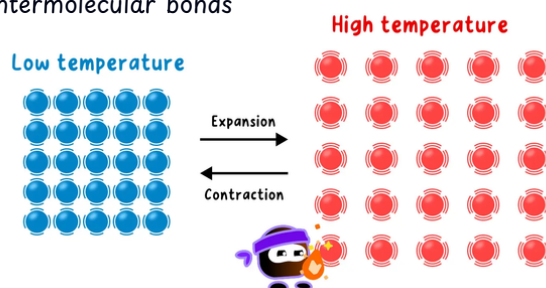


What is the change of state for a solid to a gas?

- Vaporization
- Deposition
- Condensation
- Sublimation

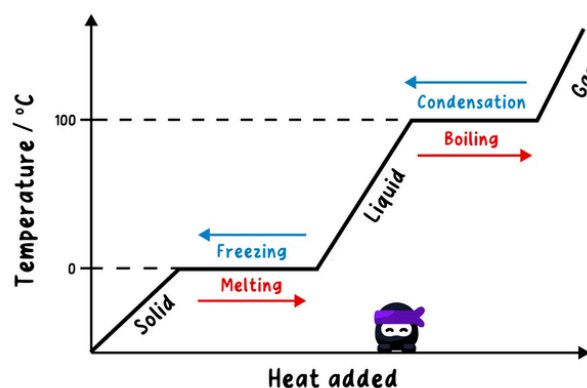
Interpreting changes with temperatures and during phase changes

- Temperature **rises** → particles gain kinetic energy → move more vigorously thus occupy more space → expansion
- Temperature **falls** → particles lose kinetic energy → slow down thus take up less space → contraction
- **Phase change** = **no** temperature change = transferred energy is used to break or form intermolecular bonds



Heating curve

- **Flat regions** = phase changes where temperature remains constant while energy is used to break or form bonds.
- **Sloped regions** = temperature changes as kinetic energy increases or decreases.



Exam Tip!

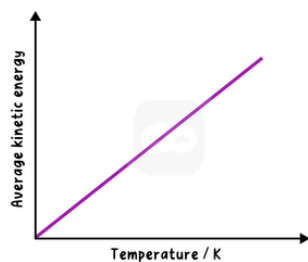


If asked why temperature is constant during melting/boiling, explicitly state:

- energy input changes potential energy to overcome intermolecular forces, not kinetic energy,
- hence temperature remains constant.

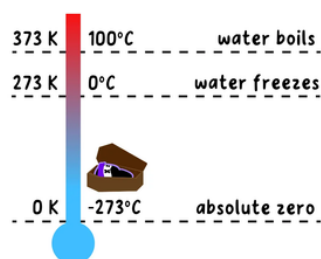
Temperature and kinetic energy

- Absolute temperature $T(K)$ is **directly proportional** to average kinetic energy E_k of particles: $E_k \propto T$
- At the same T , all gases have the same average E_k (regardless of identity); **lighter** molecules move **faster** on average



Kelvin vs Celsius

- Kelvin is SI base unit
- Increment size identical to $^{\circ}C$, but different zero points
- Conversion formulas you must use exactly
 - $T(K) = T(^{\circ}C) + 273.15$
 - $T(^{\circ}C) = T(K) - 273.15$



Example:



- $25^{\circ}C \rightarrow K: T = 25 + 273.15 = 298.15 K (\approx 298 K)$
- $-10^{\circ}C \rightarrow K: T = -10 + 273.15 = 263.15 K$
- $310K \rightarrow ^{\circ}C: T = 310 - 273.15 = 36.85^{\circ}C$

IB CHEMISTRY S1.2

THE NUCLEAR ATOM



Atomic structure, nuclear symbol, subatomic particles

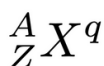
Atoms consist of:

- **Protons:** positive charge (+1), relative mass = 1
- **Neutrons:** no charge (0), relative mass = 1
- **Electrons:** negative charge (-1), relative mass ≈ 0 (negligible compared to nucleons)

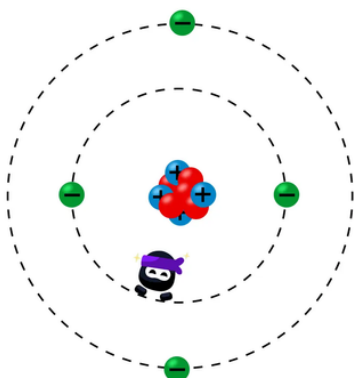
In the **nuclear model** of an atom:

- **Nucleus:** dense, contains nearly all the mass; positively charged because of protons
- **Electrons:** occupy surrounding space, organized into energy levels

Nuclear symbol format:



- **X** = element symbol
- **A** = mass number = protons + neutrons
- **Z** = atomic number = number of protons
- **q** = charge on ion (omitted if neutral)



Isotopes and calculations with relative atomic masses

- **Isotopes** = atoms of the same element (same Z, different A) \rightarrow **same** # protons and electrons, **different** # neutrons
- **Chemical properties:** identical (because determined by electron configuration)
- **Physical properties:** may differ (density, mass, rate of diffusion, melting/boiling points slightly)
- **Relative atomic mass (A_r)** = weighted average of isotopes compared to 1/12 of mass of carbon-12 atom

$$A_r = \frac{\sum(\% \text{ abundance} \times \text{isotopic mass})}{100}$$

Example:



For **magnesium** isotopes: 79% Mg-24, 10% Mg-25 and 11% Mg-26:

$$A_r = (24 \times 79 + 25 \times 10 + 26 \times 11) / 100 = 24.32$$

Common Question



What is the relative atomic mass of a sample of bromine containing 55% of the Br-79 isotope and 45% of the Br-81 isotope?

- A. 79.8
- B. 79.9
- C. 80.0
- D. 80.2

Mass spectrometry and isotopic composition (HL)

- **Mass spectrometry:** technique to separate isotopes by mass-to-charge ratio (m/z)
- **Steps** (not assessed in detail): ionization, acceleration, deflection, detection
- **Key output:** mass spectrum = peaks showing isotopes of an element

Interpreting spectra:

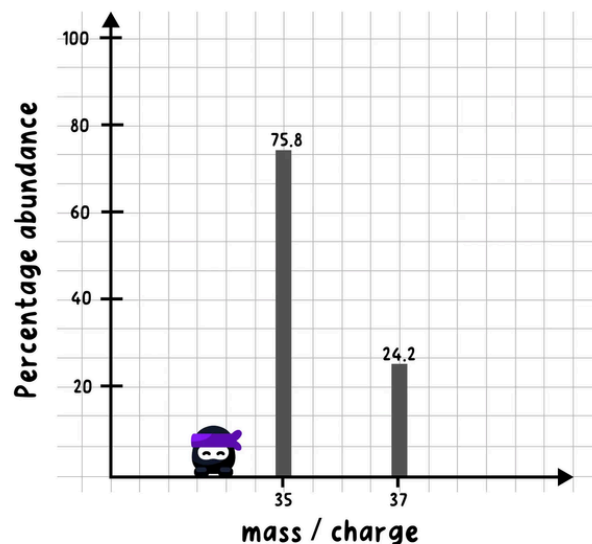
- **x-axis** = m/z (\approx mass number A for singly charged ions)
- **y-axis** = relative abundance (%)
- **Multiple peaks** = multiple isotopes present
- **Relative atomic mass** calculated using weighted average of isotopes from the spectrum

Exam Tip!



If given mass spectrum, explicitly multiply mass \times relative abundance, sum, then divide by total abundance.

Example:



In the graph above:

- **Two** main peaks: $m/z = 35$ and $m/z = 37$ \leftarrow represent naturally occurring isotopes
 - **Cl-35:** higher peak = greater abundance
 - **Cl-37:** lower peak = lesser abundance
- $$A_r = (75.8 \times 35 + 24.2 \times 37) / 100 = 35.45$$

IB CHEMISTRY S1.3

ELECTRON CONFIGURATIONS



Atomic structure, nuclear symbol, subatomic particles

- Emission spectrum** forms when excited electrons drop to lower energy levels and emit photons with energy $E = hf = hc / \lambda$
- Qualitatively:
 - shorter $\lambda \rightarrow$ higher $f \rightarrow$ higher E
 - longer $\lambda \rightarrow$ lower $f \rightarrow$ lower E



- Continuous spectrum:** all λ present with no gaps (e.g., white light through prism)



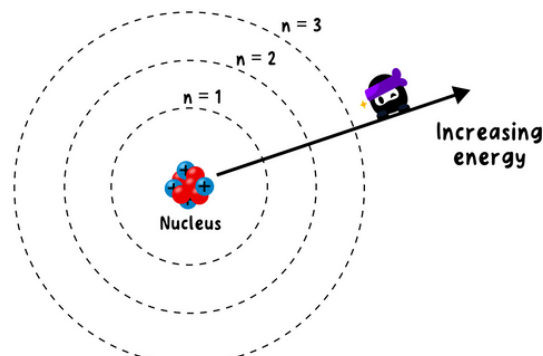
- Absorption spectrum:** discrete dark lines at specific λ only against a continuous background.



Atomic structure, nuclear symbol, subatomic particles

Main energy level n can hold max $2n^2$ electrons:

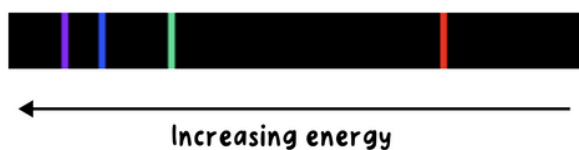
$$n = 1 \rightarrow 2 \quad n = 2 \rightarrow 8 \quad n = 3 \rightarrow 18 \quad n = 4 \rightarrow 32$$



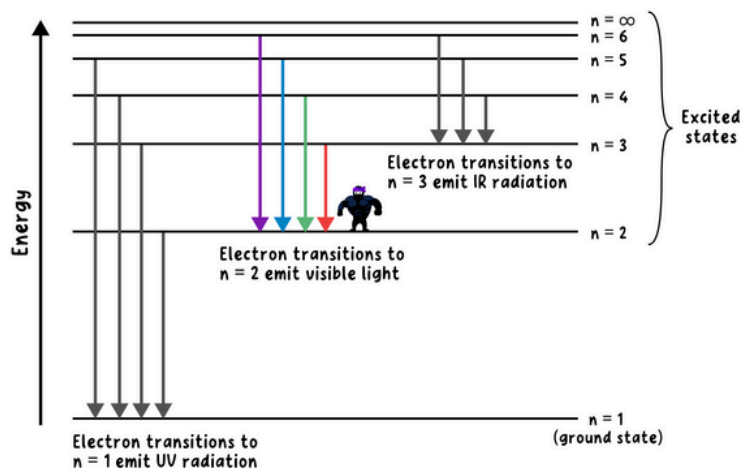
Within a real atom, sublevel energies cause the observed filling order; $2n^2$ is a capacity, not a filling sequence

Hydrogen line spectrum & discrete energy levels

- Hydrogen in emission** shows distinct lines because electrons move between quantized energy levels; lines get closer (**converge**) at **higher energies**

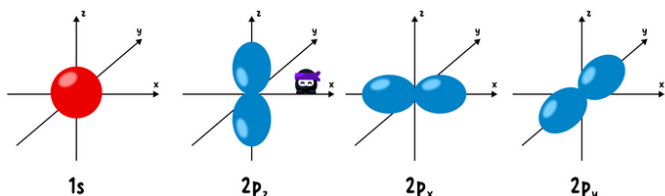


- Transitions:**
 - ending at $n = 1$ produce high-energy UV lines;
 - ending at $n = 2$ produce visible lines;
 - ending at $n = 3$ produce IR lines.
- Convergence** means levels get closer together as n increases \rightarrow approaches the **ionization limit**



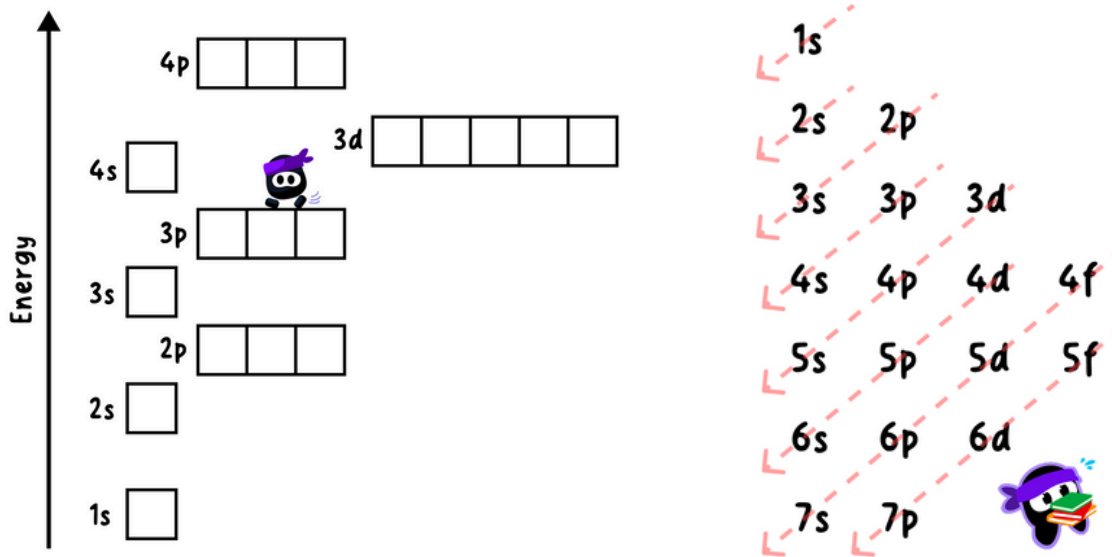
Sublevels and orbital shapes

- Main level splits into **sublevels** of increasing energy: $s < p < d < f$
- Orbitals are regions of **high electron probability**; **each** orbital holds **max 2** electrons
- Counts **per sublevel**: 1 s orbital ($2e^-$); 3 p orbitals ($6e^-$); 5 d orbitals ($10e^-$); 7 f orbitals ($14e^-$)
- Recognize **shapes**:
 - s orbital**: spherical, centered on nucleus
 - p orbitals**: three dumbbells oriented along x, y, z (denoted p_x, p_y, p_z)
 - d and f orbitals**: beyond IB scope



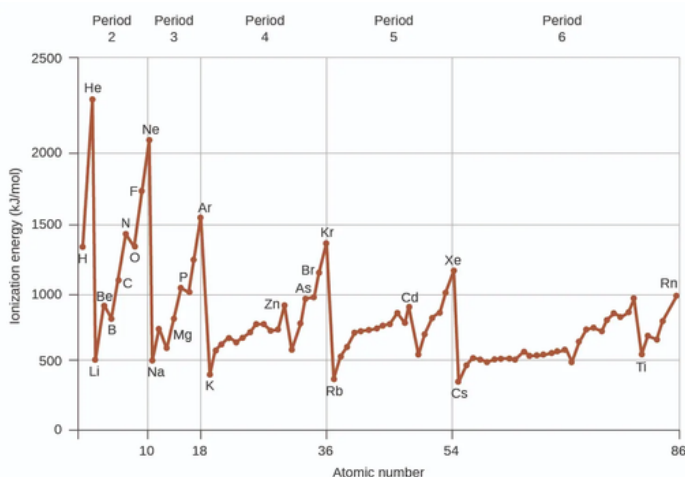
Aufbau, Hund, Pauli; configurations up to $Z = 36$, Cr & Cu exceptions

- Filling order (Aufbau)**: $1s \ 2s \ 2p \ 3s \ 3p \ 4s \ 3d \ 4p \ 5s \ 4d \ 5p \ 6s \dots$ (use diagonal/energy ordering)
- Hund's rule**: within a sublevel, place $1e^-$ per orbital with parallel spins before pairing
- Pauli exclusion**: an orbital holds max $2e^-$ with opposite spins ($\uparrow \downarrow$)
- Orbital diagrams:
 - boxes** = orbitals
 - arrows** = electrons with spin
 - fill per Hund then pair
- Canonical **exceptions**:
 - Cr: $[\text{Ar}]3d^5 4s^1$ (not $[\text{Ar}]3d^4 4s^2$) \rightarrow **stabilized half-filled d**
 - Cu: $[\text{Ar}]3d^{10} 4s^1$ (not $[\text{Ar}]3d^9 4s^2$) \rightarrow **stabilized filled d**
- For **ions**, adjust from the outermost shells first:
 - Cations** of transition metals lose **4s before 3d**:
 $\text{Fe } [\text{Ar}]3d^6 4s^2 \rightarrow \text{Fe}^{2+} [\text{Ar}]3d^6$; $\text{Fe}^{3+} \rightarrow [\text{Ar}]3d^5$
 - Anions** add to p sublevel until noble gas: $\text{Cl}^- \rightarrow [\text{Ar}]$



Covergence limit, first IE trends & calculations (HL)

- **Convergence limit:** highest-frequency line as levels converge corresponds to removing e^- from ground state to $n = \infty$ (ionization)
- **First ionization energy (IE_1):** $X(g) \rightarrow X^+(g) + e^-$; energy required per mole
- **Trends across a period:** IE generally increases (\uparrow effective nuclear charge, \downarrow atomic radius)
- **Discontinuities:**
 - **Group 2 \rightarrow 13** (Be \rightarrow B, Mg \rightarrow Al): drop because the e^- removed is from higher-energy p vs s sublevel
 - **Group 15 \rightarrow 16** (N \rightarrow O, P \rightarrow S): drop due to electron repulsion when pairing in a p orbital (half-filled p^3 is relatively stable)
- **Trend down a group:** IE decreases ($\uparrow n$, \uparrow shielding, \uparrow radius) despite higher nuclear charge
- Calculate IE from convergence limit:
 - **Per atom:** $\Delta E = hf = hc/\lambda$
 - **Per mole:** $IE = NA \cdot hc/\lambda$ (or $NA \cdot h \cdot f$); give in $J \text{ mol}^{-1}$ or $kJ \text{ mol}^{-1}$



Source: <https://pressbooks.online.ucf.edu/chemistryfundamentals/chapter/8-8-electron-affinities-and-metallic-character-chemistry-libretexts/>



Common Mistake

- Don't mistakenly assume that ionization energy always increases across a period.
- Always consider **sublevel stability** and **electron repulsion effects** for discontinuities.

Successive IEs & deducing group (HL)

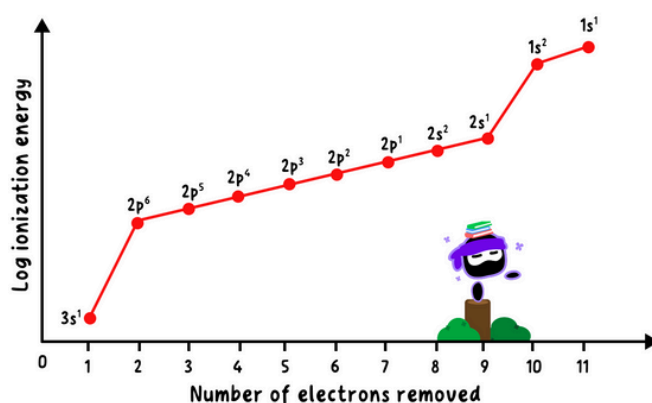
- **Successive IE data show large "jump"** after all valence e^- are removed; **position of jump** \rightarrow number of valence electrons \rightarrow **group**

Example:



Consider the following dataset ($kJ \text{ mol}^{-1}$):

- Element X:
 - $IE_1 = 738$,
 - $IE_2 = 1451$,
 - $IE_3 = 7733$,
 - $IE_4 = 10500 \dots$
- Big jump between IE_2 and IE_3 \rightarrow **two** valence e^- \rightarrow **Group 2**



This graph shows successive ionization energies of **sodium**, starting for the **3rd** energy level.

IB CHEMISTRY S1.4 COUNTING PARTICLES BY MASS: THE MOLE



The mole and Avogadro's constant; counting entities

- n (mol) = **amount of substance**
- **1 mol** contains N_A elementary entities exactly
- **Elementary entity** can be atom/molecule/ion/electron/other specified group
- **Relationships:** $N = n \cdot N_A$ and $n = N/N_A$
- **Units:** N_A in mol^{-1} ; n in mol; N is a pure count (no units)
- Use the **booklet** value for N_A in calculations

Exam Tip!



If the question asks for "number of oxygen atoms in x mol of CO_2 ", first find molecules (N), then multiply by 2.

Relative atomic and formula masses

- **Ar** is average mass of an atom on scale where $\text{Ar}({}^{12}\text{C}) = 12$ exactly
- **Mr** is sum of Ar of all atoms in a formula unit
- Ar and Mr have **no units**
- Use Ar from the **data booklet** (to 2 d.p.) for all calculations
- For **molecules** (covalent) use "relative **molecular mass**"; for ionic/formula units use "relative **formula mass**"

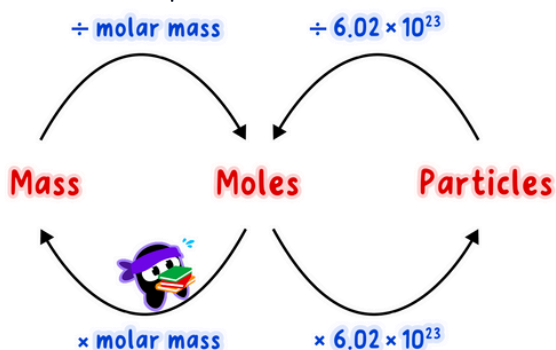
Example:



$$\text{Mr}((\text{NH}_4)_2\text{SO}_4) = 2(14.01 + 4 \cdot 1.01) + 32.07 + 4 \cdot 16.00 = 132.13$$

Molar mass

- **Molar mass M** is in g mol^{-1} and is numerically \approx Mr for a substance
- **Core equations:**
 - $n = m/M \rightarrow$ moles
 - $m = n \cdot M \rightarrow$ mass
 - $N = n \cdot N_A \rightarrow$ particles



Empirical vs molecular formula; % composition

- **Empirical formula (EF)** = simplest whole-number ratio
- **Molecular formula (MF)** = actual numbers in a molecule
- **% to EF steps:**
 - Assume 100 g
 - Convert % to g
 - Convert g to mol
 - Divide by smallest
 - Scale to whole numbers
- **MF from EF:**
 - Find $n = M(\text{MF})/M(\text{EF})$
 - Multiply EF subscripts by n
 - If ratio close to $\times 0.50$, multiply all by 2; for $\times 0.33/\times 0.66$ multiply by 3, etc.

Example:



For 40.00% C, 6.71% H, 53.29% O:

- Moles: C = 3.33, H = 6.66, O = 3.33
- Ratio: 3.33:6.66:3.33 = 1:2:1
- EF = CH_2O
- If $M = 180 \text{ g mol}^{-1}$ then $n = 180/30 = 6$
 $\rightarrow \text{MF} = \text{C}_6\text{H}_{12}\text{O}_6$

Molar concentration and solutions calculations

- **Concentration** notation: $[X] = c$ in mol dm^{-3} ; also use g dm^{-3} when required
- Key relations:
 - $n = C \cdot V$ (with V in dm^3)
 - $C = n/V$
 - C (g dm^{-3}) = m/V
 - Link mass via $m = C \cdot V \cdot M$
- **Unit** facts: $1 \text{ dm}^3 = 1 \text{ L}$; $1 \text{ cm}^3 = 1 \text{ mL} = 10^{-3} \text{ dm}^3$

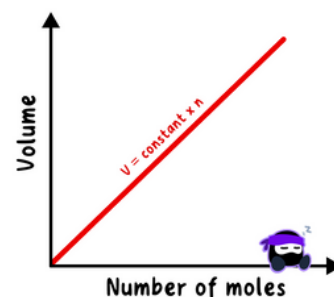
Exam Tip!



If a **dilution** is involved, use $C_1V_1 = C_2V_2$ (same solute moles before = after) and then convert to requested units

Avogadro's law and gas volumes

- **Avogadro's law:** at same T and p , equal volumes of gases contain equal numbers of molecules $\rightarrow V \propto n$
- The **molar volume** you should know by heart: STP (273 K, $1.00 \times 10^5 \text{ Pa}$) $\approx 22.7 \text{ dm}^3 \text{ mol}^{-1}$ (the value can be also found in the **data booklet**)
- In gas **stoichiometry** under **same conditions**, volume ratios = mole ratios



IB CHEMISTRY

S1.5 IDEAL GASES



Ideal gas model & assumptions

- **Ideal gas** =
 - point particles in **constant random** motion
 - **negligible** particle volume
 - **no** intermolecular forces
 - **perfectly elastic** collisions
 - **continuous, random** straight-line motion between collisions
- **Temperature** relates to average kinetic energy; collision duration \ll time between collisions
- **Pressure** arises from particle collisions with container walls; time-averaged, isotropic
- **Internal energy** depends only on temperature (not on volume or pressure)

Common Mistake



Don't say that gas has "negligible mass"; it's negligible **volume of particles**, not mass.

Common Question



Suggest why ammonia vapour (NH_3) deviates significantly from ideal behaviour when the gas is cooled, whereas neon (Ne) does not. [2 marks]

Real gases & limitations

- **Real gases deviate** notably at **low T** (IMFs become significant \rightarrow condensation) and **high p** (finite molecular volume matters)
- **Deviation sources:**
 - attractive forces (lower p than ideal)
 - repulsive/finite size (raises p vs ideal at very high p)
 - possible association (e.g., H-bonding) and non-sphericity
- Conditions **closest to ideal**: high T, low p, small/nonpolar molecules (He , Ne , H_2 , N_2)

Note!



No van der Waals math required here: just the **qualitative reasons** (IMFs and finite size).

Ideal gas equation & combined gas law

- **Core equations** (SI units only):
 - $PV = nRT$
 - $P_1V_1/T_1 = P_2V_2/T_2$
- **Units:** P in Pa (N m^{-2}), V in m^3 , T in K, n in mol, $R = 8.31 \text{ J mol}^{-1} \text{ K}^{-1}$
- **Conversions:** $1 \text{ atm} = 1.01325 \times 10^5 \text{ Pa}$; $1 \text{ dm}^3 = 1 \text{ L} = 1 \times 10^{-3} \text{ m}^3$; $1 \text{ cm}^3 = 1 \text{ mL} = 1 \times 10^{-6} \text{ m}^3$

Molar volume & T-p-V relationships, given fixed amount of gas

- **Molar volume V_m** is **constant** at a specified T and p (data booklet): at STP (273 K, $1.00 \times 10^5 \text{ Pa}$) $V_m \approx 22.7 \text{ dm}^3 \text{ mol}^{-1}$

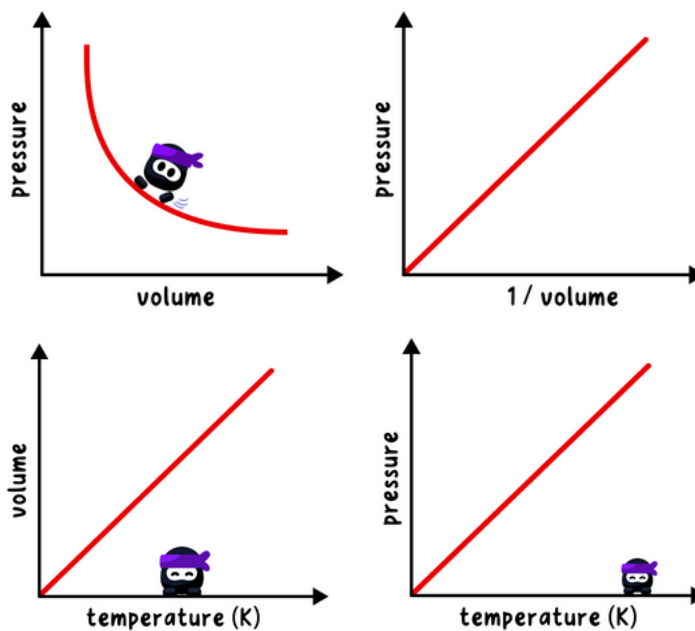
For **fixed n**:

- **P-V** (at **constant T**):
 - inverse relationship
 - graph is a rectangular hyperbola
 - $P \cdot V = \text{constant}$
- **V-T** (at **constant p**):
 - directly proportional
 - straight line through origin when T in K
- **P-T** (at **constant V**):
 - directly proportional
 - straight line through origin when T in K

Common Mistake



Plotting versus $^{\circ}\text{C}$ gives incorrect lines (not through origin). Please don't forget to always convert to K, especially in calculations.



IB CHEMISTRY S2.1

THE IONIC MODEL



Cations, anions & predicting ionic charge

- **Ion formation:**
 - metals **lose** e^- → **cations** (positive)
 - non-metals **gain** e^- → **anions** (negative)
- Predicting charge from electron configuration: atoms tend to achieve **nearest noble-gas configuration** (minimize energy)
- Main-group shortcuts:
 - Group 1 → +1
 - Group 2 → +2
 - Group 13 → +3
 - Group 15 → -3
 - Group 16 → -2
 - Group 17 → -1
 - Group 18 → 0
- Use configurations:
 - Na $[\text{Ne}]3s^1 \rightarrow \text{Na}^+ [\text{Ne}]$
 - Mg $[\text{Ne}]3s^2 \rightarrow \text{Mg}^{2+} [\text{Ne}]$
 - O $[\text{He}]2s^2 2p^4 \rightarrow \text{O}^{2-} [\text{Ne}]$
 - N $[\text{He}]2s^2 2p^3 \rightarrow \text{N}^{3-} [\text{Ne}]$
- **Transition metals:**
 - **Variable charges** because 3d and 4s sublevels are close in energy
 - Remove **4s before 3d** when ionizing
e.g., $\text{Fe}[\text{Ar}]3d^6 4s^2 \rightarrow \text{Fe}^{2+}[\text{Ar}]3d^6; \text{Fe}^{3+}[\text{Ar}]3d^5$

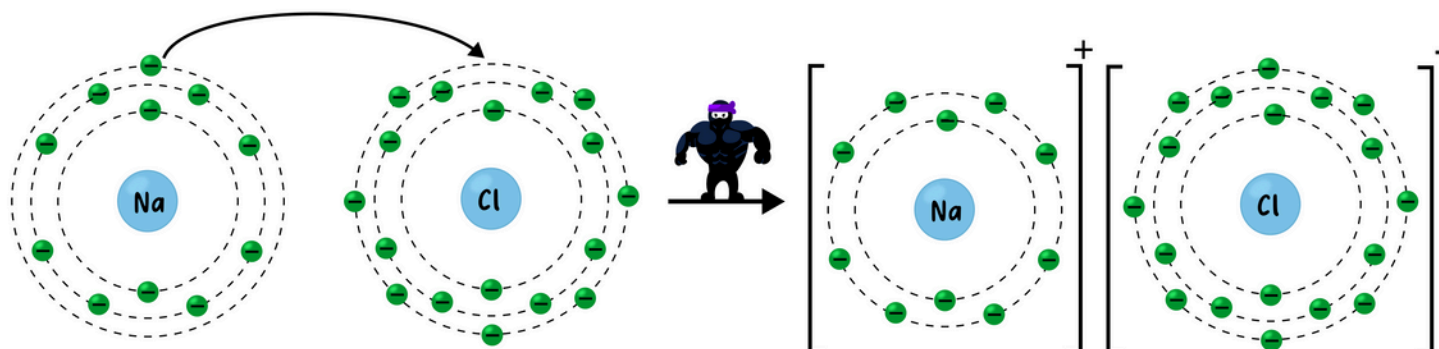
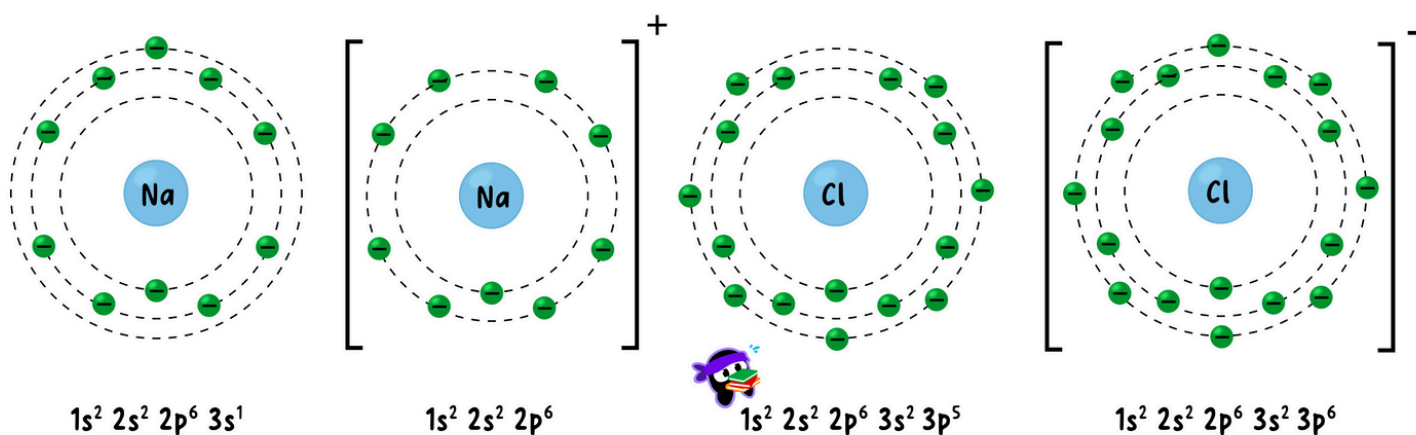
Ionic bonding: formulas & names

- **Ionic bond:**
 - Electrostatic attraction between oppositely charged ions
 - Strength **increases** with **higher charge** and **smaller ionic radii**
- **Binary ionic naming:** cation name first, then anion with “-ide” (e.g., sodium chloride, calcium oxide); transition-metal charge in Roman numerals (e.g., copper(II) oxide)
- **Charge balance:** total positive charge = total negative charge in the empirical formula
- **Polyatomic ions** to know:
 - ammonium NH_4^+
 - hydroxide OH^-
 - nitrate NO_3^-
 - hydrogencarbonate HCO_3^-
 - carbonate CO_3^{2-}
 - sulfate SO_4^{2-}
 - phosphate PO_4^{3-}



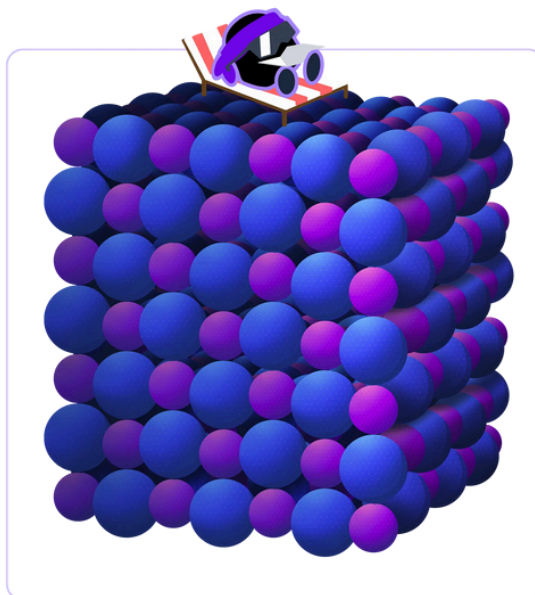
Exam Tip!

When converting **name to formula** for a transition metal, deduce the cation charge from the Roman numeral before balancing.



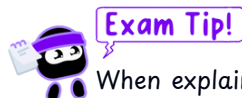
Ionic lattices, lattice enthalpy & properties

- **Structure:** Ionic compounds form **giant 3D lattices** of alternating cations/anions; formulas are empirical (minimum whole-number ratio)
- **Lattice enthalpy** (qualitative):
 - Energy change when 1 mol of an ionic solid forms from its gaseous ions (measure of ionic bond strength)
 - Absolute value of lattice enthalpy **increases** with **higher ionic charge** and **smaller ionic radii**
- **Volatility:** low (bonds strong → high melting/boiling points)
- **Electrical conductivity:**
 - **No** if solid (constrained ions)
 - **Yes** if molten or aqueous (free-moving ions)
- **Solubility:**
 - Often **soluble** in **polar** solvents like water (ion-dipole attractions can overcome lattice forces);
 - Trends depend on balance between lattice enthalpy and hydration enthalpy
- **Brittleness:** shattering when like charges are forced adjacent (slippage aligns same charges → repulsion)



 **Anion**
(negative ion)

 **Cation**
(positive ion)



Exam Tip!

When explaining a property, link directly to **electrostatic attractions** and, where relevant, to **charge/radius** (e.g., “higher charge density → stronger attractions → higher mp”)



Common Question

Explain the decrease in radius from K to K⁺.
[2 marks]

Outline, in terms of their electronic structures, why the ionic radius of the phosphide ion is greater than that of the nitride ion.
[1 mark]

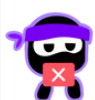
IB CHEMISTRY S2.2

THE COVALENT MODEL



Formation of covalent bonds

- **Covalent bond** = electrostatic attraction between a shared electron pair and two positively charged nuclei.
- **Octet rule**: many main-group atoms tend toward 8 valence electrons (duet for H).
- Some valid molecules have **<8 on the central atom** (e.g., BF_3) or an odd total (e.g., NO).
- **Lewis formulas** show **all valence e⁻** (bonding and lone pairs); use **dots/crosses/dashes**.

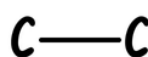


Common Mistake

Don't forget to add/subtract electrons for **charged ions** (e.g., +1 removes one electron).

Single/double/triple bonds: length vs strength

- **Trend** (same atom pair): more shared pairs → shorter and stronger bond.
- **Length**: single > double > triple
- **Strength**: triple > double > single
- **Reason**:
 - more **electron density** between nuclei increases attraction and draws nuclei closer;
 - higher **bond order** → higher bond **energy**.



147 pm

347 kJ mol⁻¹



134 pm

614 kJ mol⁻¹

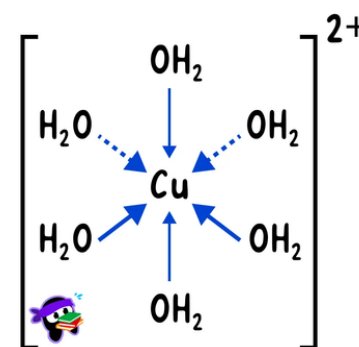


120 pm

839 kJ mol⁻¹

Coordination bonds

- **Coordination bond**: both electrons in the shared pair originate from the same atom (the donor/Lewis base) and are **accepted** by an **electron-deficient** atom/ion (Lewis acid).
- Once formed, it's still a **covalent bond**.
- **Spotting in formulas/structures**: look for a lone-pair donor → to an electron-poor center (H^+ , B, transition metal).
- Often drawn with an **arrow** (e.g., $\text{N} \rightarrow \text{H}$).

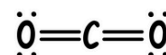


Exam Tip!

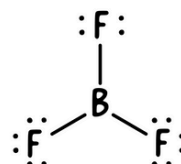
Keep in mind that coordination bonds often create **cations** (e.g., NH_4^+) without changing the octet on the donor.

VSPR theory

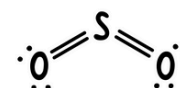
- **Rules**: **electron domains** (bonding pairs - single/multiple count as ONE domain - and lone pairs) repel; **geometry** minimizes repulsion.
- **Lone pairs** repel more than bonding pairs; **multiple bonds** exert slightly more repulsion than single.
- **Electron domain geometry** → **Molecular geometry (central atom)** → **Typical angles**:
 - 2 domains: linear →
 - **linear** (AX_2) → 180°
 - 3 domains: trigonal planar →
 - **trigonal planar** (AX_3 , $\sim 120^\circ$)
 - **bent** (AX_2E , $\sim 120^\circ \rightarrow \sim 117^\circ$)
 - 4 domains: tetrahedral →
 - **tetrahedral** (AX_4 , 109.5°)
 - **trigonal pyramidal** (AX_3E , $\sim 107^\circ$)
 - **bent** (AX_2E_2 , $\sim 104.5^\circ$)



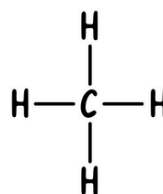
Linear



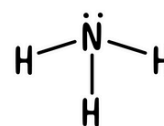
Trigonal planar



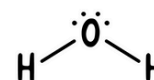
Bent



Tetrahedral



Trigonal pyramidal



Bent

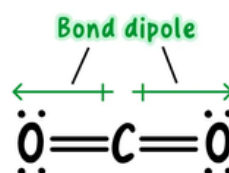
Bond polarity

- **Bond polarity** arises from ΔEN between atoms; higher ΔEN → more polar bond; extremes give ionic bonding.
- **Notation**: $\delta^+ - \delta^-$ (partial charges) and/or dipole vector arrow (→ toward δ^-).

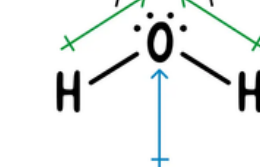


Exam Tip!

Use data booklet EN values **qualitatively**: $\Delta\text{EN} \lesssim 0.4$ (nonpolar), $\sim 0.5 - 1.7$ (polar covalent), larger tends ionic, but boundaries are fuzzy.



Bond dipole



Molecular dipole

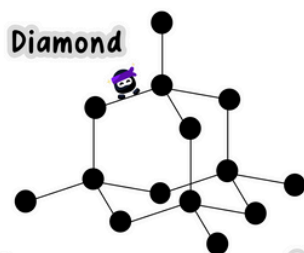
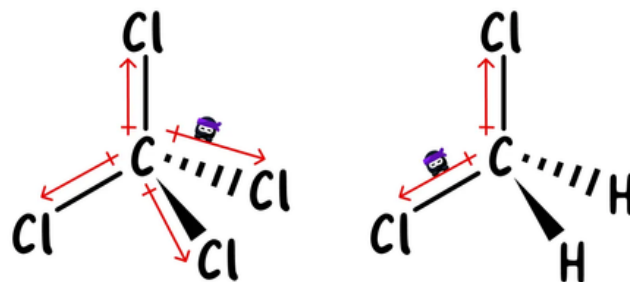
Molecular polarity

- **Rule:** a molecule/ion is polar if its bond dipoles do not cancel (net dipole $\neq 0$). Symmetry often cancels dipoles.
- **Canonical outcomes** (≤ 4 domains):
 - **Linear** AX_2 (CO_2): nonpolar (equal & opposite).
 - **Trigonal planar** AX_3 (BF_3): nonpolar; AX_2E (SO_2): polar.
 - **Tetrahedral** AX_4 (CCl_4): nonpolar; AX_3E (NH_3): polar; AX_2E_2 (H_2O): polar.
 - $CHCl_3$ vs CCl_4 : $CHCl_3$ is polar (vectors don't cancel due to H).

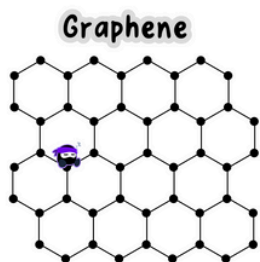
Exam Tip!



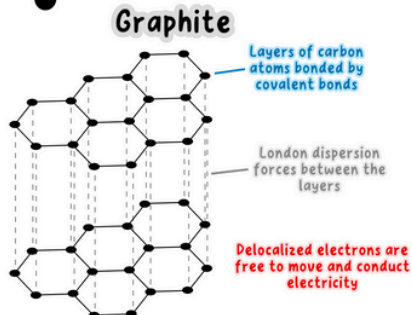
Draw vectors on each bond, then sum; mention symmetry (e.g., "tetrahedral but with one different substituent \rightarrow net dipole")



Diamond



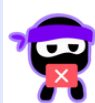
Graphene



Graphite

Covalent networks

- **Diamond** (sp^3): each C tetrahedrally bonded to 4 C; giant 3D network \rightarrow extremely hard, very high mp, electrical insulator, thermally conductive, insoluble.
- **Graphite** (sp^2): layers of hexagonal sheets; within a sheet strong σ + delocalized π ; between sheets weak forces \rightarrow layers slide (lubricant); conducts electricity/heat along planes; opaque, soft.
- **Graphene:** single graphite layer; exceptional electrical/thermal conductivity, very strong yet flexible, high surface area.
- **Fullerenes** (C_{60}): discrete molecular cages; simple molecular solid \rightarrow lower mp, soluble in nonpolar solvents, semiconducting behavior.
- **Silicon** (sp^3 network) & **Silicon dioxide** (SiO_2): giant covalent lattices; high mp/hard; Si is a semiconductor (temperature-dependent conductivity); SiO_2 is an electrical insulator, hard, insoluble; tetrahedral Si-O-Si network.



Common Mistake

Don't say that "graphite is soft because bonds are weak". In reality, **in-plane** bonds are **strong**; softness is due to **weak interlayer forces**.

Intermolecular forces (IMF)

Use "**van der Waals forces**" as an inclusive term for:

- **London (dispersion):** present in all molecules/atoms; strength \uparrow with molar mass & surface area (linear $>$ branched).
- **Dipole-dipole:** between permanent dipoles (polar molecules).
- **Dipole-induced dipole:** polar molecule induces a dipole in a non-polar neighbor.
- **Hydrogen bonding** (H-bonding): a particularly strong dipole-dipole when H is covalently bound to N, O, or F and interacts with a lone pair on N/O/F of a neighboring molecule ($X-H\dots Y$).

Exam Tip!



To deduce IMFs quickly:

1. **Any N-H/O-H/F-H?** \rightarrow H-bonding + dipole-dipole + London.
2. **Polar bonds arranged asymmetrically?** \rightarrow dipole-dipole + London.
3. **Non-polar overall?** \rightarrow London (and possibly dipole-induced dipole with polar neighbors).

IMF strength order & properties

- **General strength** (similar molar mass): London $<$ dipole-dipole $<$ H-bonding (network covalent \gg any IMF).
- **Volatility/boiling point:** stronger IMF \rightarrow lower volatility, higher b.p. (branched isomers boil lower than straight chains).
- **Electrical conductivity:** simple molecular substances do not conduct (no mobile ions/electrons); acids/bases conduct in solution via ions.
- **Solubility** ("like dissolves like"): polar/H-bonding solutes dissolve in polar solvents (e.g., alcohols in water); non-polar solutes dissolve in non-polar solvents (e.g., hexane + iodine).



Common Question

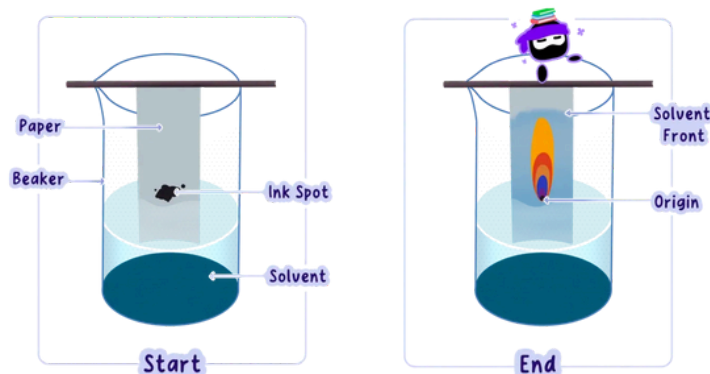
Which molecule is polar?

- A. CO_2
- B. BF_3
- C. CCl_4
- D. SO_2

Chromatography

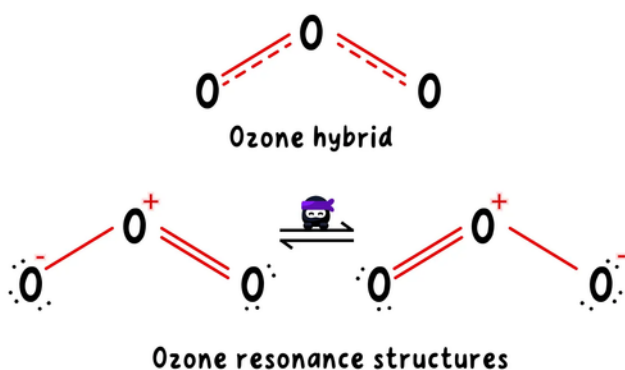
- **Principle:** separation by different attractions (IMFs) to stationary phase vs mobile phase.
- **Interpretation** (silica/alumina = polar stationary phase, non-polar mobile):
 - more polar solute → lower R_f (sticks to plate)
 - less polar → higher R_f .

$$R_f = \frac{\text{distance traveled by solute}}{\text{distance traveled by solvent front}}$$



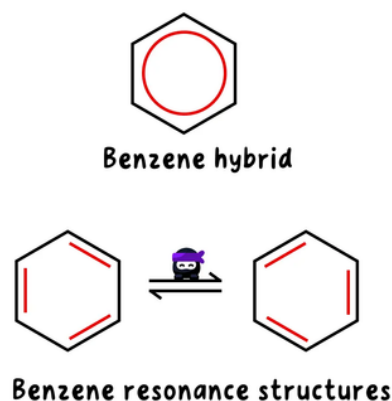
Resonance structures (HL)

- **Resonance structures:** two or more valid Lewis formulas differing only in position of π bonds and/or lone pairs (atom positions unchanged).
- The true structure is a delocalized **resonance hybrid**;
- **Bond order** often **fractional**
- All contributing forms linked by a **double-headed arrow** (\leftrightarrow).
- **Examples:** NO_3^- , NO_2^- , CO_3^{2-} , O_3 , benzene.



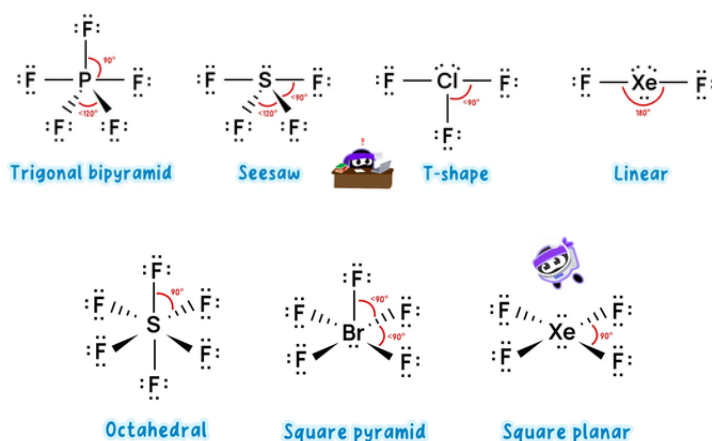
Benzene (HL)

- **Bond lengths:** all C-C bonds identical (~139 pm), intermediate between C-C and C=C.
- **Thermochemistry:** heat of hydrogenation $\ll 3 \times$ (cyclohexene); indicates resonance stabilization.
- **Chemical behavior:** prefers electrophilic substitution over addition (preserves aromatic system).
- **Spectroscopy/shape:** planar hexagon, $\sim 120^\circ$; one ^1H NMR signal (all H equivalent).



Expanded octets & VSEPR (HL)

- Period 3+ centers can **exceed an octet**.
- **Count electron domains** (bonds = 1 domain; lone pair = 1).
- **Five domains** → trigonal bipyramidal ED geometry (axial 180° , equatorial 120° , axial-equatorial 90°):
 - **5 bonding:** PF_5 (TBP).
 - **4 bonding + 1 LP:** SF_4 (see-saw, LP equatorial).
 - **3 bonding + 2 LP:** ClF_3 (T-shaped, both LP equatorial).
 - **2 bonding + 3 LP:** ICl_2^- (linear).
- **Six domains** → octahedral ED geometry (all $90^\circ/180^\circ$):
 - **6 bonding:** SF_6 (octahedral).
 - **5 bonding + 1 LP:** BrF_5 (square pyramidal).
 - **4 bonding + 2 LP:** XeF_4 (square planar; LP trans).

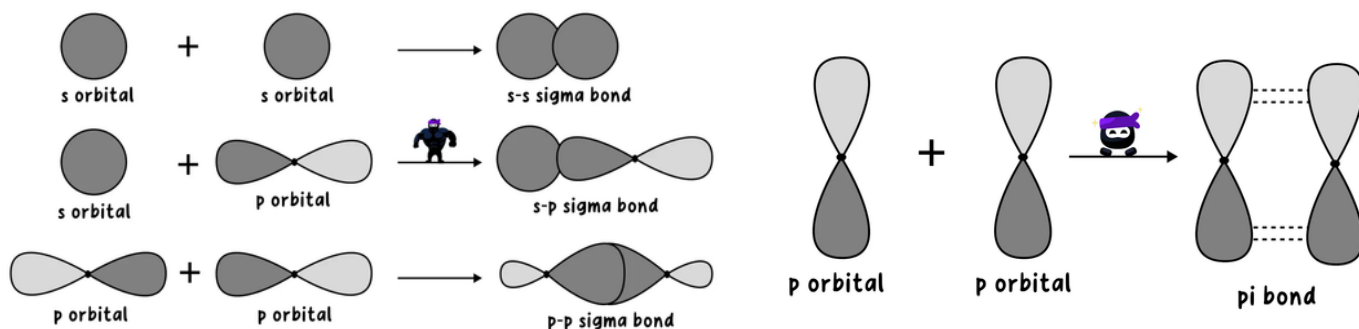


Formal charge (FC) (HL)

- **Formula:** $\text{FC} = \text{valence } e^- - [\text{nonbonding } e^- + \frac{1}{2}(\text{bonding } e^-)]$.
- **Preferred structure** tends to minimize charge, place negative FC on more electronegative atoms, and match the overall charge.

σ and π bonds (HL)

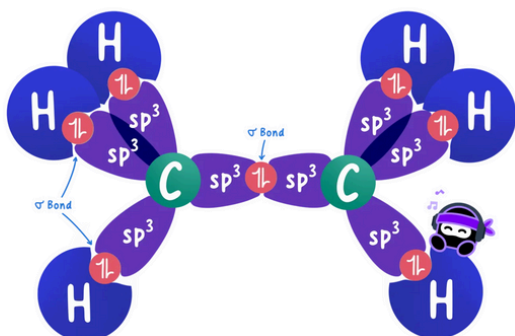
- **σ bond:** head-on overlap along internuclear axis (s-s, s-p, p-p, or hybrid-hybrid).
- **π bond:** side-on overlap of unhybridized p orbitals; electron density above/below bond axis.
- **Rule:** single bond = 1 σ ; double = 1 σ + 1 π ; triple = 1 σ + 2 π .



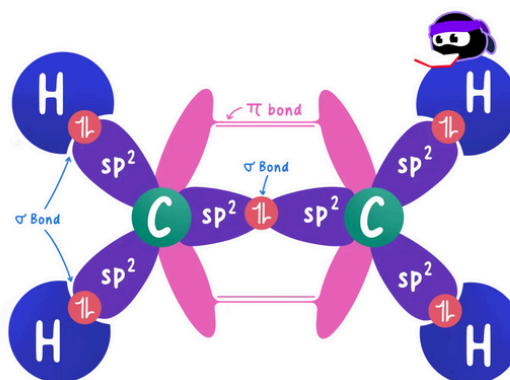
Hybridization (sp , sp^2 , sp^3) (HL)

- Map **central-atom electron domains** to **hybridization & shape**:
 - sp (2 domains):** linear (180°) — e.g., BeCl_2 , $\text{HC}\equiv\text{CH}$ (each C is sp ; two π bonds from two unhybridized p's).
 - sp^2 (3 domains):** trigonal planar (120°) — e.g., BF_3 , $\text{H}_2\text{C}=\text{CH}_2$ (each C sp^2 with one unhybridized p giving the π bond).
 - sp^3 (4 domains):** tetrahedral (109.5°) — e.g., CH_4 (AX_4), NH_3 (AX_3E), H_2O (AX_2E_2).
- Resonance tip:** atoms adjacent to π systems often adopt sp^2 to allow p-p overlap (e.g., amide N is effectively sp^2 , planar).
- Predicting workflow:** Lewis \rightarrow count domains (lone pairs included) \rightarrow assign hybridization \rightarrow predict geometry; or given geometry \rightarrow infer hybridization.

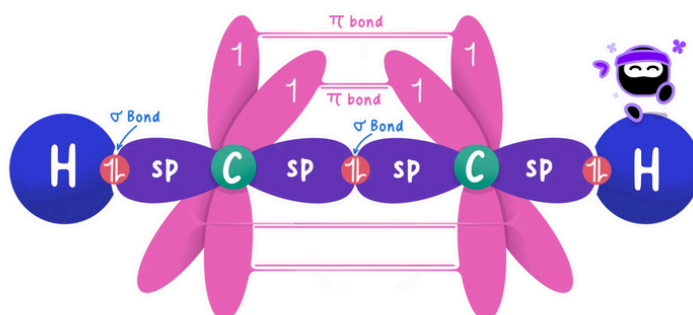
sp^3 hybridization



sp^2 hybridization



sp hybridization



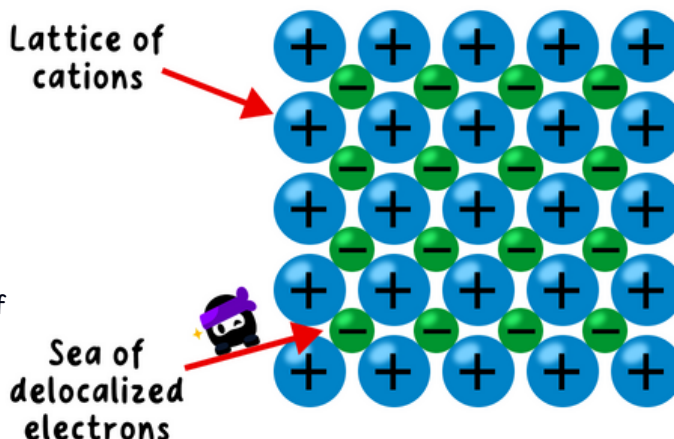
IB CHEMISTRY S2.3

THE METALLIC MODEL



Metallic bonding & key properties

- **Metallic bond** = electrostatic attraction between a regular lattice of metal cations and a "sea" of delocalized valence electrons
- **Electrical conductivity**: delocalized electrons move under an applied potential → metals conduct in solid and liquid states
- **Thermal conductivity**: mobile electrons transfer kinetic energy; vibrations of the lattice (phonons) also carry heat → metals are good heat conductors
- **Malleability/ductility**: non-directional bonding; layers of ions can slide without breaking the overall attraction to the electron sea → metals can be hammered into sheets/drawn into wires
- Uses linked to properties:
 - **Copper** for electrical wiring (high conductivity, ductile);
 - **Aluminum** for heat sinks/foil (light, conductive, malleable);
 - **Gold** for contacts (corrosion-resistant, conductive);
 - **Alloys** for strength/hardness (controlled by disrupting lattice with different-sized atoms)



Exam Tip!

When explaining a **property**, name the micro-cause explicitly: "delocalized electrons" for conductivity, "non-directional attraction to electron sea" for malleability

Factors affecting metallic bond strength & melting point trends

- **Bond strength increases** with **cation charge** (higher positive charge attracts electrons more strongly) and **decreases** with **larger ionic radius** (lower charge density)
- **Electron density**: higher number of delocalized electrons per atom strengthens bonding (e.g., Al has 3 vs Na has 1)
- **Down a group (s-block)**: ionic radius increases, charge unchanged → weaker bonding → melting points generally decrease
 - Group 1: Li > Na > K > Rb > Cs
 - Group 2: Be > Mg > Ca > Sr > Ba
- **Across a period (s → p metals)**: In s/p blocks, increasing charge and electron contribution typically strengthen bonding → melting points tend to rise from Group 1 to Group 13 metal (e.g., Na < Mg < Al in Period 3), before dropping for post-metal p-block elements where metallic bonding weakens



Exam Tip!

Phrase **trend** answers as "greater charge and smaller radius → greater electrostatic attraction between cations and electron sea → higher m.p./hardness"

Transition elements: delocalized d-electrons, high melting point, conductivity (HL)

- **Transition metals** have **partially filled d subshells**; their d electrons contribute to the delocalized electron pool → higher electron density and strong metallic bonding
- **High melting points**: stronger cation-electron attraction from greater charge density and additional d-electron participation (e.g., Fe, Ni, W with very high m.p.)
- **Excellent electrical conductivity**: overlapping s and d bands provide many available states for electrons to move into under a potential difference
- **Mechanical properties**:
 - Generally **hard/tough** due to strong bonding
 - **Amenable to alloying** because d-electrons allow varied metallic radii and bonding types

IB CHEMISTRY S2.4 FROM MODELS TO MATERIALS



Bonding continuum & the bonding triangle

- Bonding lies on a **continuum** between ionic, covalent, and metallic; many solids have **mixed character**
- Bonding triangle** (use data booklet):
 - corners="ideal" ionic/covalent/metallic
 - real materials plot inside based on mixed contributions
- Use **models** → **properties**:
 - ionic** (lattice, strong electrostatics) → high mp, brittle, conducts when molten/aq;
 - covalent** (network/molecular) →
 - network: very hard, very high mp, insulator
 - simple molecular: low mp/soft
 - metallic** → conductive, malleable, variable mp

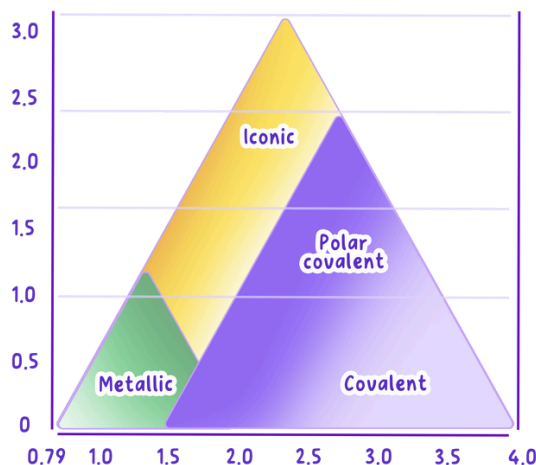
Position in the bonding triangle from electronegativity & predicting properties

- Placement idea:**
 - larger EN difference** (ΔEN) between two elements → more ionic character
 - similar EN** → more covalent
 - presence of **metal atoms** contributing delocalized e^- → metallic character
- How to **place a binary compound quickly**:
 - identify metal/non-metal
 - estimate ΔEN from booklet
 - consider polarizability (size/charge density) to adjust toward covalent if ions are highly polarizing
- Predict properties from position:**
 - more **ionic** → higher mp, brittle, soluble in polar solvents
 - more **covalent (molecular)** → low mp/volatile
 - more **covalent (network)** → very hard/insulating (semiconducting for some)
 - more **metallic** → electrical/thermal conductivity, malleability

Polymers

- Polymers** = macromolecules from repeating monomers; properties arise from chain length, branching, polarity, cross-linking, crystallinity
- Common plastic traits:** low density; soft to tough; electrical insulators
- Microstructure:**
 - more branching** → lower crystallinity → softer, clearer
 - linear/regular chains** → higher crystallinity → stronger, opaque

Electronegativity difference: $\Delta\chi = \chi_a - \chi_b$



% covalent	% ionic
8	92
25	75
50	50
75	25
100	0

Average electronegativity: $\bar{\chi} = \frac{(\chi_a + \chi_b)}{2}$

Alloys

- Alloys** = metal + other metals/non-metals;
- Non-directional metallic bonding** remains, but lattice is disrupted by different-sized atoms → dislocation motion hindered
- Property boosts:**
 - strength/hardness ↑ (dislocation pinning),
 - corrosion resistance ↑ (passivating oxides, Cr_2O_3 in stainless)
 - toughness/tailored conductivity/melting point changes



Common Mistake

Don't think that alloying "breaks" metallic bonding: delocalized electrons still bind the lattice, so we just impede layer motion



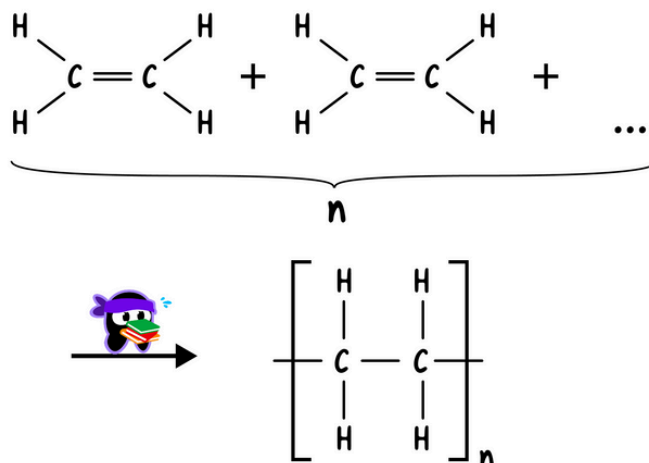
Common Question

Adding carbon atoms into the lattice of iron forms distortions that prevent the layers of iron atoms from sliding easily. Which property of the resulting alloy increases as a result?

- Electrical conductivity
- Ductility
- Hardness
- Malleability

Addition polymers

- **Mechanism idea:**
 - π bond of each alkene **breaks**
 - **new σ bonds** link monomers into a chain
 - no small molecule eliminated
- **Repeating-unit notation:**
 - Draw the two-carbon backbone from the alkene with substituents, put in **brackets with "n" subscript**
 - **Side groups preserved** from monomer

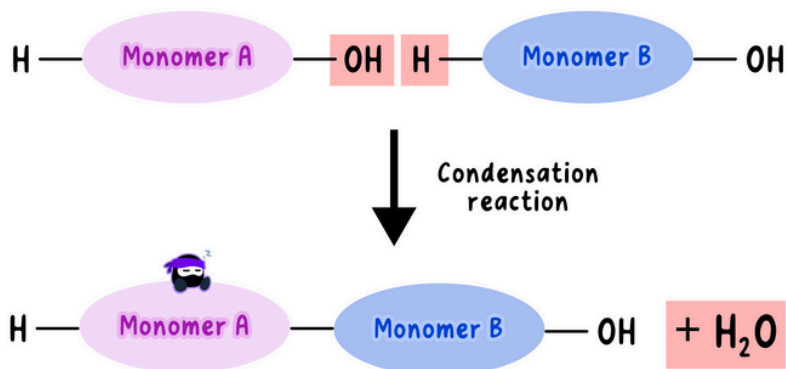


Exam Tip!

Start from the alkene, erase the double bond, extend two new single bonds left/right through brackets to indicate continuation.

Condensation polymers (HL)

- **Condensation polymerization:** functional groups on monomers react to form links while eliminating a small molecule (usually H_2O or HCl)
- **Polyamides** (diamine + diacid chloride/diacid):
 - amide ($-\text{CONH}-$) link
 - e.g., Nylon-6,6 from hexamethylenediamine and adipic acid \rightarrow repeating unit $-\text{NH}-(\text{CH}_2)_6-\text{NH}-\text{CO}-(\text{CH}_2)_4-\text{CO}-$
- **Polyesters** (diol + diacid):
 - ester ($-\text{COO}-$) link
 - e.g., PET from ethane-1,2-diol and terephthalic acid \rightarrow repeating unit $-\text{O}-\text{CH}_2-\text{CH}_2-\text{O}-\text{CO}-\text{C}_6\text{H}_4-\text{CO}-$
- **Repeating-unit notation:**
 - Draw between brackets the **linkage fragment** with end bonds extended;
 - Do not include the eliminated small molecule in the unit



Exam Tip!

- Circle the two atoms that join
- Write the linkage ($-\text{CONH}-$ or $-\text{COO}-$) in the bracket
- Add " $+ n\text{H}_2\text{O}$ " (or HCl) to balance if asked for an equation

IB CHEMISTRY S3.1 THE PERIODIC TABLE: CLASSIFICATION OF ELEMENTS



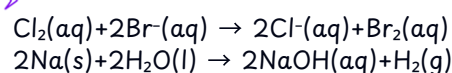
Periods, groups, blocks; metals/metalloids/non-metals

- **Periods** = horizontal rows; **groups** = vertical columns (1-18)
- **Blocks** by last-filled **sublevel**: s-block (G1-2+He), p-block (G13-18), d-block (transition), f-block (lanthanides/actinides)
- **Metals**: left/bottom of staircase
- **Non-metals**: right/top
- **Metalloids** on staircase (B,Si,Ge,As,Sb,Te,Po*)
- **General properties**:
 - **metals** (conductive, malleable, form cations);
 - **non-metals** (insulators, brittle as solids, form anions/share e⁻);
 - **metalloids** = intermediate/semiconducting

Group trends

- **G1 reactivity increases down the group**; reaction with water:
 - $2M(s) + 2H_2O(l) \rightarrow 2M^+(aq) + 2OH^-(aq) + H_2(g)$
 - Li slow \rightarrow K very vigorous
- **G17 (halogens) reactivity decreases down the group**: halogen higher in group oxidizes halide of lower one
 - Cl_2 displaces Br⁻/I⁻
 - Br_2 displaces I⁻

Example:



Period number \rightarrow outer level; group \rightarrow valence

- **Period number** = n of outermost occupied main level; group for s/p elements \rightarrow number of valence e⁻
- **From position to configuration**:
 - Period 3, G14 (Si) $\rightarrow [Ne]3s^23p^2$
 - Period 4, G2 (Ca) $\rightarrow [Ar]4s^2$
 - Period 4, d-block (G8 Fe) $\rightarrow [Ar]3d^64s^2$
- **From configuration to position**: count outer ns/np for s/p groups; last e⁻ in d \rightarrow transition group
- **Known families**: alkali metals(G1), halogens(G17), transition elements(d-block), noble gases(G18)



Note!

You can be assessed on deducing electron configuration of the element up to Z=36.

Periodicity: atomic/ionic radius, IE, EA, EN

- **Across a period (\rightarrow)**:
 - atomic radius \downarrow (Z_{eff} \uparrow pulls e⁻ closer)
 - first IE \uparrow generally
 - EA becomes more negative
 - EN \uparrow
 - metallic character \downarrow
- **Down a group (\downarrow)**:
 - atomic radius \uparrow (more shells)
 - first IE \downarrow
 - EA less exothermic
 - EN \downarrow
 - metallic character \uparrow
- **Ionic radius**:
 - anions > parent atom (coulombic expansion)
 - cations < parent atom (loss of a shell/increased Z_{eff} per e⁻)



Exam Tip!

Link **property** \rightarrow **cause** explicitly, e.g., "IE increases across due to smaller radius and greater Z_{eff}"

Continuum of metallic and non-metallic properties

- **Basic metal oxides** (Group 1 and 2):
 - If M = Group 1:
 - $MO + H_2O \rightarrow M^+(aq) + OH^-(aq)$
 - $M_2O + H_2O \rightarrow 2MOH$
 - If M = Group 2:
 - $MO + H_2O \rightarrow M(OH)_2$
- **Amphoteric oxides** (e.g., Al₂O₃, ZnO): react with acids and bases
- **Acidic non-metal oxides**:
 - $CO_2 + H_2O \rightleftharpoons H_2CO_3(aq)$
 - $SO_2 + H_2O \rightarrow H_2SO_3$
 - $SO_3 + H_2O \rightarrow H_2SO_4$;
 \rightarrow non-metal oxides form acids
- **Environmental**: acid rain from SO₂/SO₃/NO_x; ocean acidification:
 $CO_2(g) \rightleftharpoons CO_2(aq) + H_2O \rightleftharpoons H_2CO_3 \rightleftharpoons H^+ + HCO_3^- (\rightarrow CaCO_3 \text{ dissolution})$

Oxidation states

- **Oxidation state (OS)** charge an atom would have if bonds were ionic
- **Key rules**:
 - elemental forms OS = 0 (e.g., Na(s), O₂(g), P₄(s));
 - monoatomic ion OS = its charge;
 - sum of OS in neutral compound = 0 (in ion = ion charge)
- **Some of the common OS**:
 - Group 1: +1;
 - Group 2: +2;
 - F: -1;
 - H: +1 (except metal hydrides: -1);
 - O: -2 (except peroxides: -1; with F positive)



Common Question

- Which property of elements decreases down a group but increases across a period?
- Metallc character
 - Electronegativity
 - Atomic radius
 - Atomic mass

First-IE discontinuities as evidence for sublevels (HL)

- **General trend across a period:** $IE_1 \uparrow$ as $Z_{\text{eff}} \uparrow$ and atomic radius \downarrow , but two predictable dips each short period arise from orbital energy and e^-e^- repulsion
- **Be \rightarrow B dip:** removed e^- is from higher-energy 2p (B) vs 2s (Be) \rightarrow less energy required $\rightarrow IE_1(\text{B}) < IE_1(\text{Be})$
- **N \rightarrow O dip:** in O the fourth 2p electron pairs with an existing one in a 2p orbital \rightarrow intra-orbital repulsion raises its energy \rightarrow easier to remove $\rightarrow IE_1(\text{O}) < IE_1(\text{N})$
- **Period 3 parallels:** Mg \rightarrow Al and P \rightarrow S show the same reasons (3s \rightarrow 3p energy step; first pairing in 3p)
- Therefore, the pattern demands **sublevels** (s and p) of **different energies** and the concept of e^- pairing within degenerate orbitals



Common Mistake

Don't explain the **discontinuities** with "half-filled is especially stable" alone; IB expects an **energy-of-removed-electron** argument: higher sublevel energy and pairing repulsion.

Transition elements (HL)

- **Transition elements** are d-block elements Sc \rightarrow Zn with an **incomplete d sublevel** in the element or common ions
- **Variable oxidation states:** successive removal of similar-energy 4s/3d electrons allows multiple OS (e.g., Fe²⁺/Fe³⁺, Mn(II)–Mn(VII))
- **High melting points:** strong metallic bonding with d-electron participation \rightarrow high charge density, many mobile electrons
- **Magnetic properties** (knowledge of types is not assessed):
 - **unpaired d electrons** \rightarrow paramagnetism (common)
 - **paired** \rightarrow diamagnetism
- **Catalytic properties:** variable OS and partially filled d orbitals facilitate **adsorption, bond weakening, and electron transfer** at surfaces/complexes
- **Coloured compounds:** ligand fields **split d-levels**; d-d or charge-transfer absorptions give colors
- **Complex ion formation:** metal centers accept **lone pairs** from ligands to form coordinate bonds (e.g., $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$)



Exam Tip!

When asked "why **colored**/why **catalytic**," name "split d-sublevels/variable OS & adsorption" explicitly.

Variable oxidation states in transition elements (HL)

- **Reason for variable oxidation states in transition elements:** successive IEs for removing 4s and then 3d electrons are close in value \rightarrow several oxidation states are accessible depending on conditions/ligands



Exam Tip!

To deduce electron configurations of ions, remove 4s before 3d; start from neutral atom (remember Cr, Cu exceptions) then subtract electrons.



Example:

To deduce Fe³⁺ from Fe $[\text{Ar}]3d^64s^2$, remove 4s² then one 3d $\rightarrow [\text{Ar}]3d^5$.

Coloured transition element complexes (HL)

- **Cause of color:**
 - Ligand field **splits the five d orbital**
 - Absorbing a photon **promotes an electron** between split d levels
 - The **absorbed** band's color is **complementary** to the **observed** solution color
- **Complementary pairs** (use a simple wheel):
 - red \leftrightarrow green
 - orange \leftrightarrow blue
 - yellow \leftrightarrow violet
 - blue-green \leftrightarrow red-purple
- **Relating to wavelength λ and frequency f :**
 - $c = \lambda f$ and $E = hf$
 - shorter $\lambda \rightarrow$ higher $f \rightarrow$ higher E
 - **larger d-level splitting** \rightarrow absorption shifts toward higher energy (blue/violet)



Example:

- $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$ appears blue \rightarrow absorbs orange (~600 nm)
- $[\text{Ni}(\text{H}_2\text{O})_6]^{2+}$ appears green \rightarrow absorbs red (~650–700 nm)
- $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$ appears purple \rightarrow absorbs yellow-green (~560 nm)

IB CHEMISTRY S3.2 FUNCTIONAL GROUPS: CLASSIFICATION OF ORGANIC COMPOUNDS



Representation of organic molecules

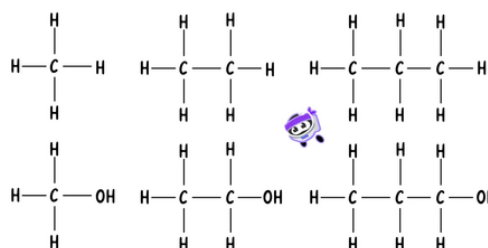
- **Empirical formula:** simplest whole-number ratio (e.g., CH_2O).
- **Molecular formula:** actual atom counts (e.g., $\text{C}_6\text{H}_{12}\text{O}_6$).
- **Structural formulas:**
 - **Full** (show all bonds); condensed (e.g., $\text{CH}_3\text{CH}_2\text{OH}$).
 - **Skeletal** (zig-zag lines for C-C; H on C omitted; heteroatoms & H on heteroatoms shown).
 - **Stereochemical** (when needed): wedge (out), dash (back) around a stereocenter.
- **Inverting:** count carbons & heteroatoms \rightarrow place on a skeletal backbone \rightarrow expand to condensed/full as required.
- **3D models:** build mental/wedge-dash or kit/virtual for tetrahedral (sp^3), trigonal planar (sp^2), linear (sp) centers.

Homologous series

- **Alkanes** $\text{C}_n\text{H}_{2n+2}$
- **Alkenes** C_nH_{2n}
- **Alkynes** $\text{C}_n\text{H}_{2n-2}$
- **Halogenoalkanes** $\text{C}_n\text{H}_{2n+1}\text{X}$
- **Alcohols** $\text{C}_n\text{H}_{2n+2}\text{O}$ (R-OH)
- **Aldehydes** $\text{C}_n\text{H}_{2n}\text{O}$ (R-CHO)
- **Ketones** $\text{C}_n\text{H}_{2n}\text{O}$ (R-CO-R')
- **Carboxylic acids** $\text{C}_n\text{H}_{2n}\text{O}_2$ (R-COOH)
- **Ethers** $\text{C}_n\text{H}_{2n+2}\text{O}$ (R-O-R')
- **Amines** $\text{C}_n\text{H}_{2n+3}\text{N}$ (primary R-NH₂ baseline)
- **Amides** $\text{C}_n\text{H}_{2n}\text{O}$ N (R-CONH₂ baseline)
- **Esters** $\text{C}_n\text{H}_{2n}\text{O}_2$ (R-COOR')

Functional groups

- **Halogeno** (R-X): X = F, Cl, Br, I.
- **Hydroxyl** (-OH): alcohols.
- **Carbonyl** (C=O): aldehyde (-CHO, end of chain), ketone (-CO-, within chain).
- **Carboxyl** (-COOH): carboxylic acids.
- **Alkoxy** (-OR): ethers R-O-R'.
- **Amino** (-NH₂ / -NHR / -NR₂): amines.
- **Amido** (-CONH₂ / -CONHR / -CONR₂): amides.
- **Ester** (-COOR').
- **Phenyl** (-C₆H₅): benzene ring as substituent.
- **Saturated vs unsaturated:** only C-C single bonds vs having C=C/C \equiv C.



Common Mistake



Don't mix **aldehyde** (-CHO) with **alcohol** (-CH₂OH): better check for C=O vs O-H next to carbon.

Physical trends in homologous series

- **Boiling/melting points:** increase with chain length (\uparrow London dispersion: greater surface area & polarizability).
- **Branching:** lowers b.p. (smaller surface area contact).
- **Hydrogen bonding:** raises b.p. (alcohols > alkanes of similar Mr).
- **Solubility:** in water decreases with longer carbon chains (hydrophobic effect) for polar groups; hydrocarbons are insoluble.

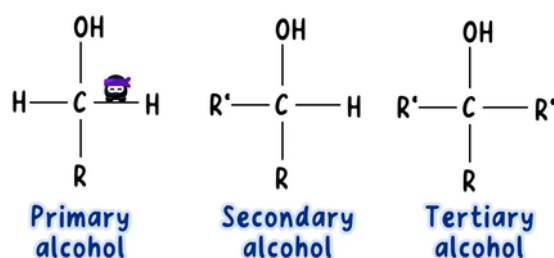
IUPAC nomenclature

Workflow:

- **Longest parent chain** containing the highest-priority functional group / C=C if present ($\leq \text{C}_6$).
- **Number** to give the **lowest locants** (position of a functional group or substituent) to the principal functional group and unsaturation.
- **Name substituents** (methyl, ethyl, fluoro/chloro/bromo/iodo, hydroxy, oxo for =O in aldehyde/ketone contexts).
- **Assemble:** prefix (substituents, alphabetized; di-, tri- ignored for ordering) + parent + infix for unsaturation (-ene) + suffix for main functional group (-ol, -al, -one, -oic acid). Include locants.

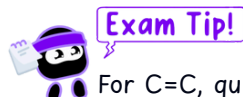
Structural isomerism

- **Chain (skeletal) isomers:** different carbon skeletons (butane vs 2-methylpropane).
- **Position isomers:** same functional group, different position (propan-1-ol vs propan-2-ol; bromo on C-1 vs C-2).
- **Functional-group isomers:** different functional groups ($\text{C}_3\text{H}_6\text{O}$: propanal vs propanone).
- **Primary (1°), secondary (2°), tertiary (3°) classification** (where applicable):
 - **Alcohols & halogenoalkanes:** by the number of carbons attached to the functional carbon (-C-OH or -C-X).
 - **Amines:** by the number of carbon groups on N (RNH₂ 1°, R₂NH 2°, R₃N 3°).



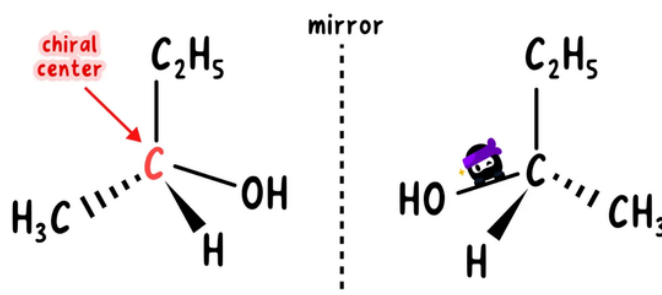
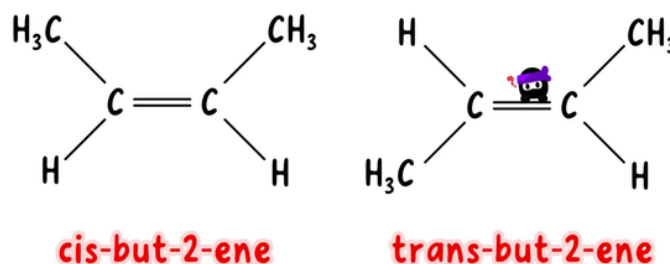
Stereoisomerism: cis-trans and chirality (HL)

- **Stereoisomers:** same connectivity; different 3D arrangement.
- **Cis-trans (geometric) isomerism** requires restricted rotation and each end of the unit having two different substituents:
- **Alkenes:** C=C with each sp^2 C bearing two different groups \rightarrow cis (same side) vs trans (opposite) across the double bond.
- **Cycloalkanes** (C_3, C_4): ring prevents rotation; cis = substituents on same face; trans = opposite faces.
- **Chiral carbon (stereocenter):** sp^3 C bonded to four different groups \rightarrow two enantiomers (non-superimposable mirror images).
- **Draw with wedge-dash** (solid wedge = out of plane; dashed wedge = behind).
- **Optical activity:** enantiomers rotate plane-polarized light in equal and opposite directions; racemic mixtures are optically inactive.
- **Recognition:** superimpose models (real/virtual). If one cannot be rotated to match the other \rightarrow enantiomers.



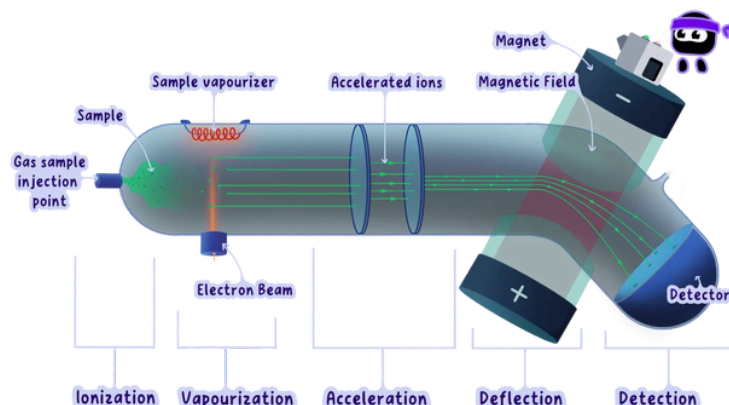
Exam Tip!

For C=C, quickly check "two different groups on each carbon". If not, no cis-trans possible.



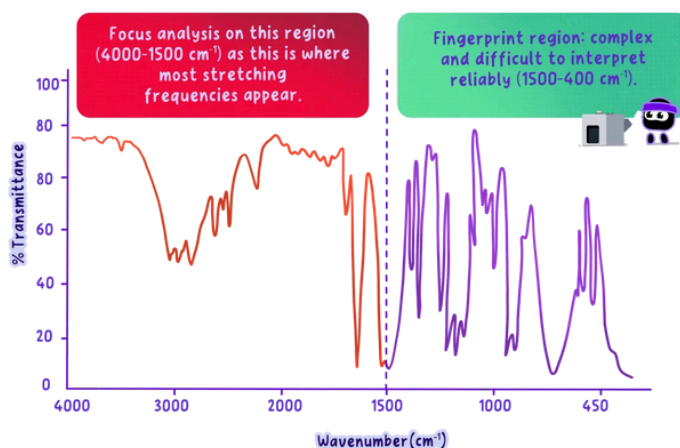
Mass spectrometry (MS) (HL)

- **Molecular ion (M^+):** the highest- m/z isotopic cluster corresponding to the intact molecule (often weak/absent for easy-fragmenting compounds).
- **Base peak:** tallest peak (100% intensity) = most stable/abundant fragment.
- **Data booklet** gives **key m/z**
- **Strategy:** use M^+ for formula clue, isotope pattern for heteroatoms, diagnostic fragments for functional groups.



IR spectroscopy (HL)

- **Functional-group region ($\approx 4000-1500\text{ cm}^{-1}$):**
 - **O-H (alcohol):** broad $3200-3600$; O-H (acid): very broad $2500-3300 + C=O$.
 - **N-H:** $3300-3500$, sharper (1° amine: two bands; 2° : one).
 - **C=O:** strong ~ 1700 (aldehyde/ketone $\sim 1710-1725$; acid ~ 1710 ; ester $\sim 1735-1750$; amide $\sim 1650-1700$).
 - **C \equiv N/C \equiv C:** $\sim 2200-2260$ (sharp; C \equiv N stronger).
 - **C-O:** $1050-1300$ (alcohol/ether/ester).
 - Other important regions are given in the data booklet
- **Fingerprint region ($\leq 1500\text{ cm}^{-1}$):** complex pattern; use to confirm identity with a known spectrum.
- **Greenhouse gases:** absorb IR via vibrations that change dipole moment (e.g., CO_2 asymmetric stretch, H_2O bends/stretch) \rightarrow trap outgoing IR.



¹H NMR: signals, chemical shift, integration (HL)

- **Number of signals:** count distinct H environments (symmetry can merge sites).
- **Chemical shift (δ , ppm):** environment clues (approx.):
- 0.8-1.2 alkyl CH₃; 1.2-1.7 CH₂; ~2-3 next to π /heteroatom (allylic, benzylic, α -to-C=O).
- ~3-4.5 next to O/N/halogen; ~4.5-6.5 vinylic (C=C-H); ~6.5-8 aromatic; ~9-10 aldehyde; ~10-12 acid (broad).
- **Integration:** area under a signal \propto relative number of H in that environment (gives ratios).

¹H NMR splitting (n+1 rule) (HL)

- **Spin-spin coupling:** non-equivalent neighboring protons (usually within 3 bonds) split signals; n neighboring H \rightarrow n+1 peaks.
 - **Singlet (s):** no neighbors (n=0).
 - **Doublet (d):** one neighbor (n=1).
 - **Triplet (t):** two neighbors (n=2).
 - **Quartet (q):** three neighbors (n=3).
- **Classic ethyl pattern:** -CH₃ (t) integrating 3H coupled to -CH₂; -CH₂ (q) integrating 2H coupled to -CH₃.

Combining data to solve structures (HL)

Workflow:

- **MS:** read M⁺ (Mr) and isotopes \rightarrow presence of halogens; note key fragments.
- **IR:** identify functional groups (C=O? O-H? N-H? C \equiv N?).
- **¹H NMR:** number of signals (symmetry), δ ranges (environment), integration (H count), splitting (connectivity).
- **Assemble pieces** to fit the formula/DBE (unsaturation count if needed), cross-check all spectra.

IB CHEMISTRY R1.1 MEASURING ENTHALPY CHANGES



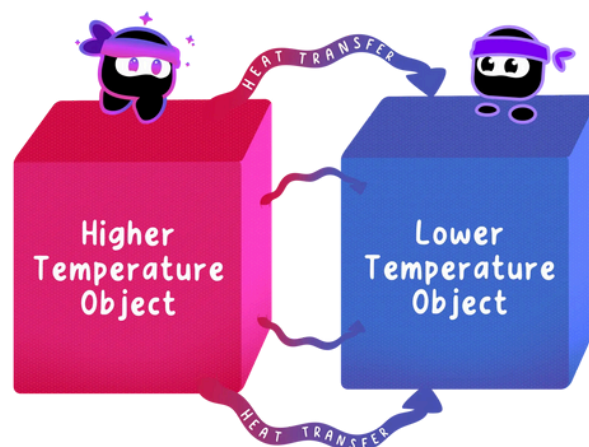
Energy transfer; heat vs temperature

- **Heat (q): energy transfer** due to a **temperature difference**; path-dependent; flows system \rightleftharpoons surroundings
- **Temperature (T):** measure of **average kinetic energy** of particles; state property; determines direction of heat flow
- **System vs surroundings**
 - **System:** the chemicals that react;
 - **Surroundings:** everything else (often the solution, calorimeter, air)
- **Conservation of energy:** $q(\text{system}) + q(\text{surroundings}) = 0$



Note!

Unlike heat, **temperature** is a **state function**, meaning it depends only on the **current state** of the system, not how the system reached that state.



Endothermic vs exothermic; temperature changes

- **Endothermic**
 - System **absorbs** heat: $\Delta H > 0$
 - Temperature of surroundings **decreases**
- **Exothermic**
 - System **releases** heat: $\Delta H < 0$
 - Temperature of surroundings **increases**
- **Thermometer view:** In a simple solution calorimetry, thermometer reads surroundings' temperature change (\approx solution)

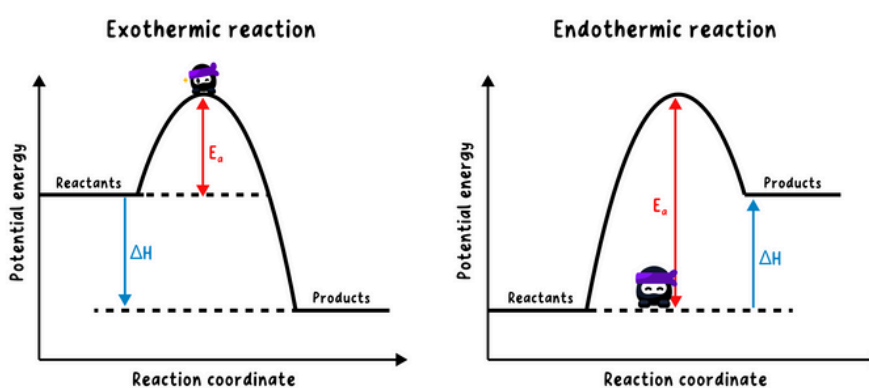


Common Question

- Which describes an endothermic reaction?
- Heat flows from the system to the surroundings, and the enthalpy of reactants is greater than that of products.
 - Heat flows from the surroundings to the system, and the enthalpy of reactants is greater than that of products.
 - Heat flows from the surroundings to the system, and the enthalpy of products is greater than that of reactants.
 - Heat flows from the system to the surroundings, and the enthalpy of products is greater than that of reactants.

Energy profiles; stability vs enthalpy

- **Energy profile axes**
 - x: reaction coordinate (progress)
 - y: potential energy
- **Exothermic profile;**
 - Products **lower** than reactants
 - $\Delta H = E(\text{products}) - E(\text{reactants}) < 0$
- **Endothermic profile;**
 - Products **higher** than reactants
 - $\Delta H = E(\text{products}) - E(\text{reactants}) > 0$
- **Relative stability**
 - **Lower** potential energy = **greater** thermodynamic **stability**
 - **Exothermic** reactions form **more stable** products than reactants



Common Mistake

Don't forget to label **axes** and **ΔH arrow**: direction matters!

Standard enthalpy change ΔH^\ominus ; calorimetry

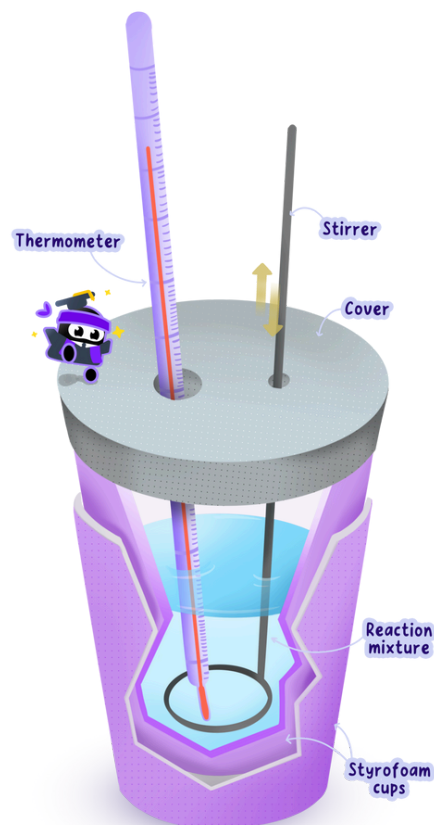
- **ΔH^\ominus : enthalpy change** at constant pressure under standard conditions (usually $1.00 \times 10^5 \text{ Pa}$, 298 K) and standard states
- **Calorimetry equations**
 - $Q = mc\Delta T$ (heat gained/lost by surroundings solution)
 - $\Delta H(\text{reaction}) = -Q(\text{surroundings}) / n(\text{limiting})$
- **Units & constants**
 - $c(\text{water}) \approx 4.18 \text{ J g}^{-1} \text{ K}^{-1}$;
 - use m in grams to match units
 - report ΔH in kJ mol^{-1}
- **Sign convention**
 - If solution warms ($\Delta T > 0$), $Q(\text{surroundings}) > 0 \rightarrow$ reaction released heat $\rightarrow \Delta H < 0$
 - If solution cools, $\Delta H > 0$



Note!

Sources of error in calorimetry:

- **Heat loss to surroundings:** heat escapes from the calorimeter \rightarrow the temperature change measured is less than the actual one
- **Incomplete combustion:** fuel may not burn completely in combustion reactions \rightarrow less heat being released than expected
- **Specific heat capacity assumption:** for the solution, it is assumed that its specific heat capacity is the same as of pure water



IB CHEMISTRY R1.2 ENERGY CYCLES IN REACTIONS



Bond breaking/forming; average bond enthalpies

- **Bond-breaking** absorbs energy(+), **bond-forming** releases energy(-):
 - overall $\Delta H \approx \Sigma E(\text{bonds broken}) - \Sigma E(\text{bonds formed})$
- **Average bond enthalpy** = mean energy to break a bond in the gas phase averaged over many compounds → context-dependent values **may differ from experimental ΔH** for a specific reaction
- **Procedure** (using average bond enthalpies):
 - Write balanced equation
 - Draw or list all bonds broken/formed (gas phase)
 - Sum energies
 - $\Delta H \approx \text{broken} - \text{formed}$ (sign tells if endothermic or exothermic)

Hess's law and multistep routes

- **Hess's law:** ΔH depends only on initial and final states; enthalpy changes are path-independent
- **Method:** manipulate given equations (**flip** → change sign; **multiply** → scale ΔH) so they sum to target equation; then sum ΔH values

Example:



- Target: $\text{C}(\text{graphite}) + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}(\text{g})$
- Given:
 - (1) $\text{C} + \text{O}_2 \rightarrow \text{CO}_2$ ΔH_1
 - (2) $\text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}_2$ ΔH_2
- Reverse (2): $\text{CO}_2 \rightarrow \text{CO} + \frac{1}{2}\text{O}_2$ ($\Delta H = -\Delta H_2$);
- Add to (1): $\text{C} + \text{O}_2 + \text{CO}_2 \rightarrow \text{CO}_2 + \text{CO} + \frac{1}{2}\text{O}_2 \rightarrow \text{C} + \frac{1}{2}\text{O}_2 \rightarrow \text{CO}$
- $\Delta H = \Delta H_1 - \Delta H_2$

ΔH_c^\ominus and ΔH_f^\ominus definitions & use (HL)

- **Standard enthalpy of combustion, ΔH_c^\ominus :** enthalpy change when 1 mol of substance burns completely in O_2 under standard conditions (typically negative)
- **Standard enthalpy of formation, ΔH_f^\ominus :** enthalpy change when 1 mol of compound forms from its elements in their standard states (elements: $\Delta H_f^\ominus = 0$)
- **Use:** build cycles or apply summation formulas to solve for unknown ΔH



Note!

Always check **states** (g, l, s, aq) match the table you're using, because ΔH values are **state-dependent**.

Calculating ΔH^\ominus with ΔH_f^\ominus or ΔH_c^\ominus data (HL)

- From **formations** and **combustion** values:

$$\Delta H^\ominus = \Sigma (\Delta H_f^\ominus \text{ products}) - \Sigma (\Delta H_f^\ominus \text{ reactants})$$

$$\Delta H^\ominus = \Sigma (\Delta H_c^\ominus \text{ reactants}) - \Sigma (\Delta H_c^\ominus \text{ products})$$



Common Mistake

Don't mix ΔH_f^\ominus and ΔH_c^\ominus data in the **same summation**: stick to one type per calculation unless you're explicitly constructing a Hess cycle.

Born-Haber cycles (HL)

- **Purpose:** apply Hess's law to lattice formation; link macroscopic ΔH_f^\ominus to atomic-scale steps
- **Typical steps** for $\text{MX}(\text{s})$ from elements (sign conventions in brackets):
 - **Atomization of metal** $\text{M}(\text{s}) \rightarrow \text{M}(\text{g})$ [endothermic, +]
 - **Atomization/dissociation of non-metal** $\frac{1}{2}\text{X}_2(\text{g}) \rightarrow \text{X}(\text{g})$ (or bond enthalpy/2) [endothermic, +]
 - **Ionization of metal** $\text{M}(\text{g}) \rightarrow \text{M}^+(\text{g}) + \text{e}^-$ (IE_1 ; add IE_2 for M^{2+} etc.) [endothermic, +]
 - **Electron affinity of non-metal** $\text{X}(\text{g}) + \text{e}^- \rightarrow \text{X}^-(\text{g})$ (EA_1 often -; EA_2 for O, S is +) [usually exothermic (EA_1 -)]
 - **Lattice enthalpy:** $\text{M}^+(\text{g}) + \text{X}^-(\text{g}) \rightarrow \text{MX}(\text{s})$ [exothermic, very -] (by IB convention often "formation from gaseous ions")
 - **Cycle sums to standard formation:** $\text{M}(\text{s}) + \frac{1}{2}\text{X}_2(\text{g}) \rightarrow \text{MX}(\text{s})$ with ΔH_f^\ominus (usually -)



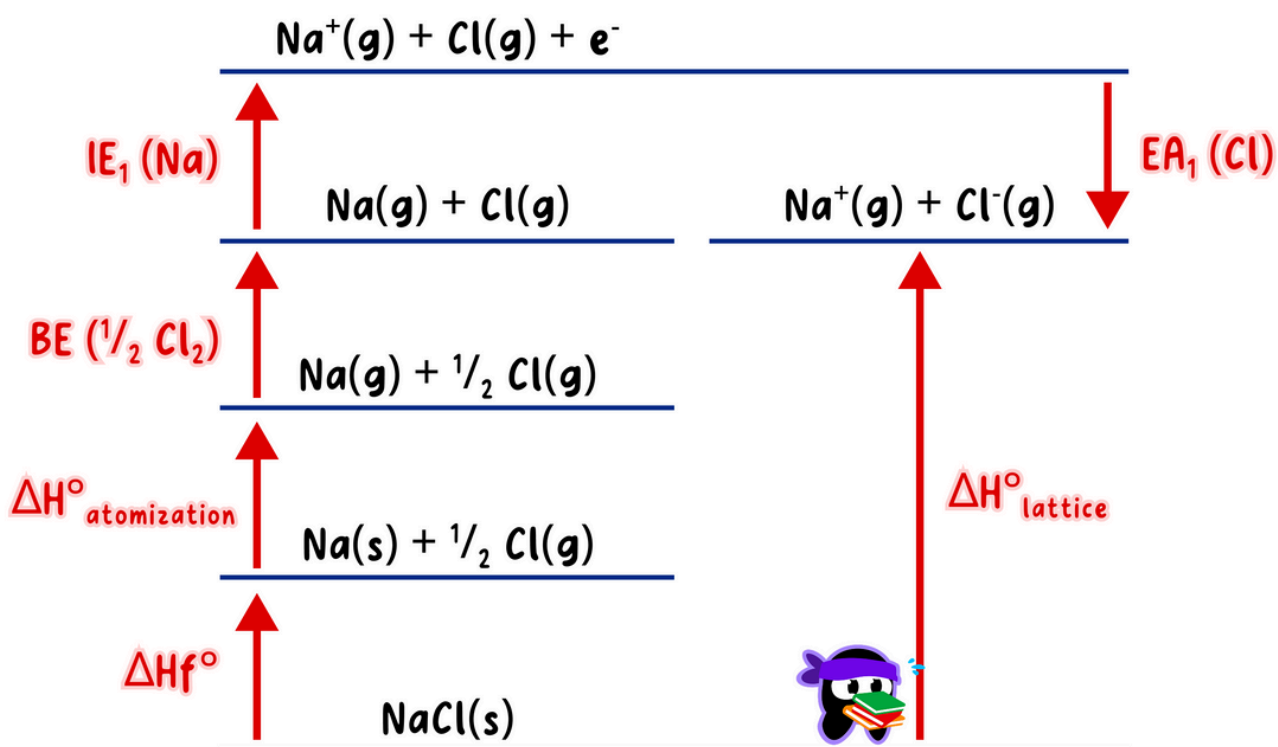
Note!

During IB examination, you will not be asked to construct a complete Born-Haber cycle, but you can be assessed on determining specific enthalpy values involved in the cycle.

Example:



Below you can see the Born-Haber cycle for sodium chloride.



IB CHEMISTRY R1.3 ENERGY FROM FUELS



Combustion of metals, non-metals, hydrocarbons & alcohols

- **Combustion** =
 - redox with O_2 producing oxides;
 - complete combustion of organics yields CO_2 and H_2O ;
 - balance $C \rightarrow H \rightarrow O$ last
- **Metals:**
 - $4Fe(s) + 3O_2(g) \rightarrow 2Fe_2O_3(s)$
 - $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$
- **Non-metals:**
 - $C(s) + O_2(g) \rightarrow CO_2(g)$
 - $S(s) + O_2(g) \rightarrow SO_2(g)$
 - $P_4(s) + 5O_2(g) \rightarrow P_4O_{10}(s)$
- **Hydrocarbons** (general): $C_xH_y + O_2 \rightarrow xCO_2 + (y/2)H_2O$
- **Alcohols** (general): $C_xH_yO + O_2 \rightarrow xCO_2 + ((y/2))H_2O$

Incomplete combustion \rightarrow CO and C

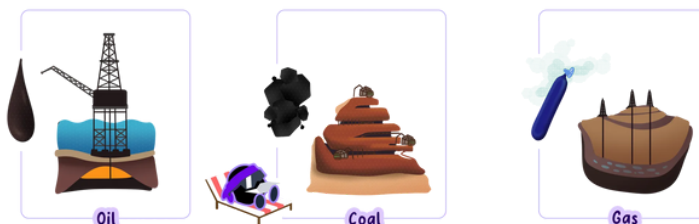
- **Incomplete combustion** occurs under O_2 limitation/poor mixing/low T; products include $CO(g)$ and $C(s)$ with H_2O
- **Hydrocarbons** examples:
 - **CO-rich:**
 - $2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O$
 - $2C_3H_8 + 7O_2 \rightarrow 6CO + 8H_2O$
 - **Soot-rich:** (not unique; many stoichiometries possible)
 - $CH_4 + O_2 \rightarrow C + 2H_2O$
 - $C_3H_8 + 2O_2 \rightarrow 3C + 4H_2O$
- **Alcohols** examples:
 - CO-rich: $2C_2H_5OH + 3O_2 \rightarrow 4CO + 6H_2O$
 - Soot-rich: $C_2H_5OH + O_2 \rightarrow 2C + 3H_2O$

Biofuels, photosynthesis, renewable vs non-renewable

- **Biofuels** include bioethanol, biodiesel (FAME), biogas; "short-cycle" carbon from recent photosynthesis
- **Photosynthesis** (net): $6CO_2 + 6H_2O \rightarrow C_6H_{12}O_6 + 6O_2$ (sunlight, chlorophyll)
- **Renewable vs non-renewable:**
 - Renewable **replenishes** on human timescales (biofuels, solar, wind)
 - Non-renewable **does not** (coal, oil, gas)
- **Advantages of biofuels:** potentially lower net CO_2 over lifecycle, domestic production, biodegradable; some lower PM/CO with proper engines
- **Disadvantages:** land use/deforestation, food vs fuel, variable net GHG when considering fertilizers, processing, transport; lower energy density (ethanol vs gasoline), cold-start issues

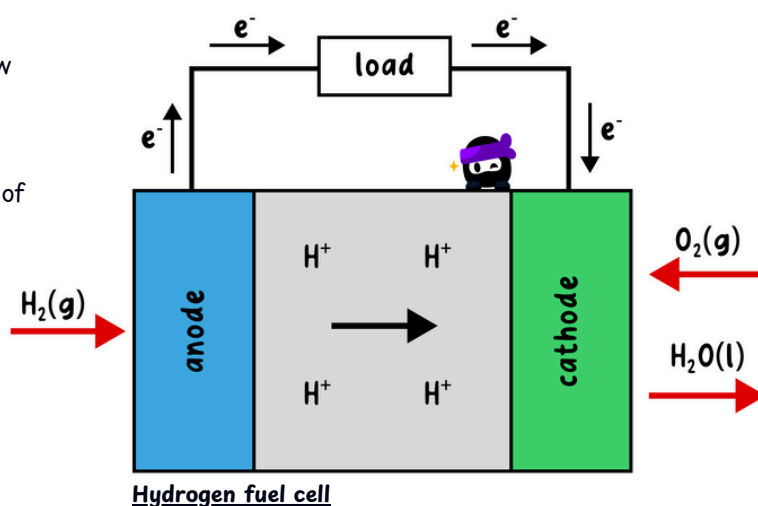
Fossil fuels

- **Fuels & idealized CO_2 per gram** (complete combustion):
 - CH_4 : $16\text{ g} \rightarrow 44\text{ g } CO_2 \rightarrow 2.75\text{ g } CO_2\text{ g}^{-1}$ (high H/C \rightarrow least CO_2 per energy among hydrocarbons)
 - C_8H_{18} : $114\text{ g} \rightarrow 8 \times 44 = 352\text{ g } CO_2 \rightarrow 3.09\text{ g } g^{-1}$
 - Carbon (coal model): $12\text{ g} \rightarrow 44\text{ g } CO_2 \rightarrow 3.67\text{ g } g^{-1}$ (highest $CO_2\text{ g}^{-1}$)
 - Ethanol C_2H_5OH : $46\text{ g} \rightarrow 88\text{ g } CO_2 \rightarrow 1.91\text{ g } g^{-1}$;
 - Methanol CH_3OH : $32\text{ g} \rightarrow 44\text{ g } CO_2 \rightarrow 1.38\text{ g } g^{-1}$
 - H_2 : $0\text{ g } CO_2$ at point of use
- **Incomplete combustion tendency:**
 - Higher with poor O_2 supply, low flame temperature, large droplets/poor atomization, soot-forming aromatics
- **Energy released per mass** (qualitative, typical):
 - $H_2 >$ natural gas (CH_4) $>$ gasoline range (C_5-C_{12}) $>$ diesel/heavier fractions $>$ coal
 - alcohols generally lower than comparable hydrocarbons (O already present reduces ΔH_c)
- **Fossil fuels:**
 - **Natural gas:** low CO_2 per kWh, clean burn, but CH_4 leakage is a potent GHG
 - **Oil/gasoline:** high energy density, infrastructure mature; higher CO_2 per kWh and pollutants without controls
 - **Coal:** abundant, cheap; highest CO_2 per kWh, $SO_2/NO_x/PM$ unless scrubbed
- **Link to greenhouse effect:** CO_2 absorbs IR (vibrational modes) \rightarrow enhanced greenhouse effect; rising atmospheric CO_2 correlates with increased radiative forcing and global warming



Fuel cells (H₂ and methanol)

- **Fuel cells** convert chemical energy directly to electrical via redox at electrodes; continuous fuel/oxidant supply; acidic media equations below
- **Hydrogen fuel cell** (acidic, PEM):
 - Anode(oxidation): $\text{H}_2 \rightarrow 2\text{H}^+ + 2\text{e}^-$
 - Cathode(reduction): $\frac{1}{2}\text{O}_2 + 2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2\text{O}$
 - Overall: $\text{H}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{H}_2\text{O}(\text{l})$ (no CO₂ at point of use)
- **Methanol fuel cell** (acidic, DMFC):
 - Anode: $\text{CH}_3\text{OH} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + 6\text{H}^+ + 6\text{e}^-$
 - Cathode: $(\frac{3}{2})\text{O}_2 + 6\text{H}^+ + 6\text{e}^- \rightarrow 3\text{H}_2\text{O}$
 - Overall: $\text{CH}_3\text{OH} + (\frac{3}{2})\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$
- **Properties/uses:**
 - High efficiency at part load, quiet, modular
 - H₂ FCs suited for vehicles/stationary backup
 - DMFCs for portable/low-power applications



Note!

The concept of redox reactions, which is also relevant to this subtopic, is studied in more detail in **R3.2 Electron transfer reactions**.

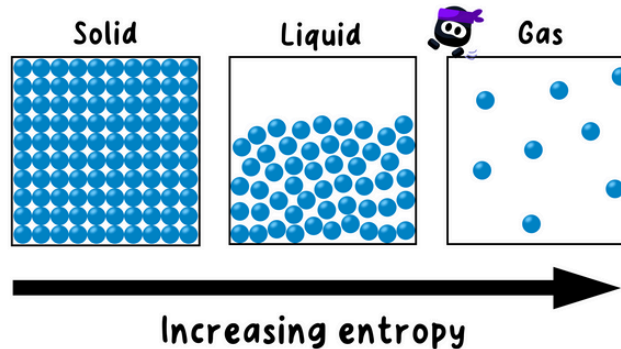
IB CHEMISTRY R1.4 ENTROPY AND SPONTANEITY (HL ONLY)



Entropy S, predicting ΔS , and using S^\ominus tables (HL)

- Entropy idea: microstate count/dispersal of energy and matter; more ways to arrange \rightarrow higher S
- State order at same T, p: gases \gg liquids $>$ solids; more particles and more volume usually \rightarrow higher S
- Qualitative ΔS predictions:**
- Physical changes:** melting(+), vaporization(+), sublimation(+), freezing(-), condensation(-), deposition(-)
- Particle number & gas moles:**
 - if $\Delta n(\text{gas}) > 0$ then ΔS usually > 0
 - if $\Delta n(\text{gas}) < 0$ then ΔS usually < 0
- Mixing/dissolving:**
 - mixing** different gases/solutions typically **increases S**;
 - dissolving** ionic solids in water **often increases S** overall (ions dispersed) but can decrease if strong ordering of solvent dominates (rare at this level)
- Standard entropy calculation:**

$$\Delta S^\ominus = \sum (S^\ominus \text{ products}) - \sum (S^\ominus \text{ reactants})$$



ΔG away from equilibrium; Q and K relations (HL)

- Nonstandard conditions:** $\Delta G = \Delta G^\ominus + RT \ln Q$ where Q is the reaction quotient (activities/approximate with partial pressures or concentrations for ideal cases)
- At equilibrium:** $\Delta G = 0$ and $Q = K \rightarrow \Delta G^\ominus = -RT \ln K$;
 - large K** $\rightarrow \Delta G^\ominus \ll 0$
 - small K** $\rightarrow \Delta G^\ominus \gg 0$
- Constants & units**
 - $R = 8.314 \text{ J K}^{-1} \text{ mol}^{-1}$
 - T in K
 - ΔG in J mol^{-1} from $RT \ln$ terms (convert to kJ if needed)



Note!

Equilibrium constant K and reaction quotient Q are officially covered in **R2.3 How far? The extent of chemical change.**



Common Question

Which change has the greatest decrease in entropy?

- $\text{CO}_2(\text{s}) \rightarrow \text{CO}_2(\text{g})$
- $\text{CO}_2(\text{g}) \rightarrow \text{CO}_2(\text{l})$
- $\text{CO}_2(\text{g}) \rightarrow \text{CO}_2(\text{s})$
- $\text{CO}_2(\text{l}) \rightarrow \text{CO}_2(\text{s})$

Gibbs energy $\Delta G^\ominus = \Delta H^\ominus - T\Delta S^\ominus$ (HL)

- Gibbs energy ΔG** measures maximum non-expansion work obtainable at constant T, p; combines **enthalpy** and **entropy effects**
- Formula use:
 - $\Delta G^\ominus (\text{kJ mol}^{-1}) = \Delta H^\ominus (\text{kJ mol}^{-1}) - T(\text{K}) \cdot \Delta S^\ominus (\text{kJ K}^{-1} \text{ mol}^{-1})$
 - convert ΔS^\ominus from J \rightarrow kJ by $\div 1000$
- Interpreting terms:**
 - $\Delta H^\ominus < 0$ favors spontaneity
 - $\Delta S^\ominus > 0$ favors spontaneity
 - T scales the entropy term



Common Mistake

Don't use $^\circ\text{C}$ instead of K in T and don't mix J and kJ, which leads to $\times 1000$ errors.

Spontaneity, temperature thresholds, and ΔG sign (HL)

- Spontaneity rule:** at constant p, T, the change is:
 - spontaneous** if $\Delta G < 0$
 - non-spontaneous** if $\Delta G > 0$
 - at **boundary** if $\Delta G = 0$
- Temperature of spontaneity:** Set $\Delta G^\ominus = 0 \rightarrow T = \Delta H^\ominus / \Delta S^\ominus$ (ensure consistent units; T in K)
- System vs surroundings**
 - ΔG packs both **system** entropy change ($\Delta S(\text{sys})$) and **surroundings** entropy change via heat flow ($\Delta S(\text{sur}) = -\Delta H/T$);
 - That's why $\Delta G = \Delta H - T\Delta S$ predicts **spontaneity**

ΔH	ΔS	ΔG	Spontaneity
< 0	> 0	Always negative	Always spontaneous
> 0	< 0	Always positive	Always non-spontaneous
< 0	< 0	Negative at low T, positive at high T	Spontaneous at low T
> 0	> 0	Negative at high T, positive at low T	Spontaneous at high T



Common Mistake

Don't use K with nonstandard concentrations! Remember: ΔG^\ominus relates to **K at standard state**; otherwise use Q.

IB CHEMISTRY R2.1 HOW MUCH? THE AMOUNT OF CHEMICAL CHANGE



Writing balanced equations with states

- Chemical equations encode **mole ratios** of reactants → products; **coefficients** are **simplest whole numbers**
- Include **state symbols**: (s), (l), (g), (aq)
- **Balance atoms first**, then charge (if ionic in aqueous), leave O₂/H₂O last when helpful

Example:



- Combustion of ethanol:
$$\text{C}_2\text{H}_5\text{OH}(\text{l}) + 3\text{O}_2(\text{g}) \rightarrow 2\text{CO}_2(\text{g}) + 3\text{H}_2\text{O}(\text{l})$$
- Ionic precipitation:
$$\text{AgNO}_3(\text{aq}) + \text{NaCl}(\text{aq}) \rightarrow \text{AgCl}(\text{s}) + \text{NaNO}_3(\text{aq})$$

Percentage yield

$$\text{Percentage Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100$$

- **Reasons for <100%**:
 - side reactions
 - incomplete reaction
 - loss on transfer/purification
 - impure reagents
- **Reasons for >100%**:
 - wet/impure product
 - solvent trapped
 - calibration errors

Example:



- Assume you are given theoretical NH₃ = 12.2 g
- If 10.0 g collected
→ % yield = (10.0/12.2) × 100 = 82.0%

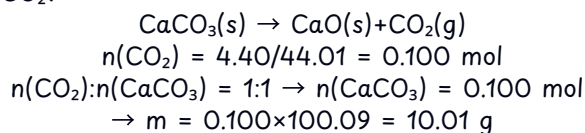
Using mole ratios to get masses, volumes, concentrations

- **Core links**
 - $n = m/M$
 - $n = C \cdot V(\text{dm}^3)$;
 - for gases at same T, p: $V \propto n$
 - at STP $V_m \approx 22.7 \text{ dm}^3 \text{ mol}^{-1}$
- **Procedure**
 - Balance equation
 - Identify known → moles
 - Use mole ratio to find unknown moles
 - Convert to requested unit

Example:



What **mass** of CaCO₃ decomposes to make 4.40 g CO₂?



Atom economy

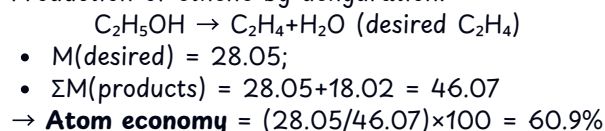
$$\text{Atom Economy} = \frac{\text{Molar Mass of Desired Product}}{\text{Sum of Molar Masses of All Products}} \times 100$$

- **Stoichiometric, theoretical metric**: does not include yield or process energy/solvent impacts
- **Addition/rearrangement reactions** often have high (≈100%), **substitutions/eliminations** - lower

Example:



Production of ethene by dehydration:



Limiting reactant: theoretical yield vs experimental yield

- **Limiting reactant (LR)**: consumed first; fixes maximum amount of product
- **Theoretical yield**: amount of product predicted from LR via stoichiometry
- **Experimental/actual yield**: amount actually obtained in lab

Exam Tip!



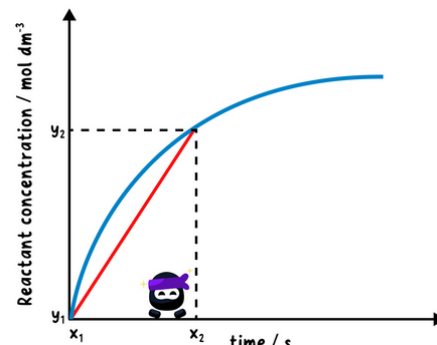
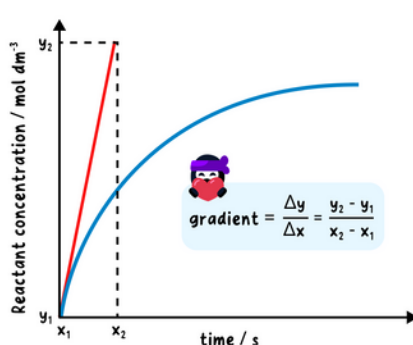
To **identify LR**, convert each reactant amount to moles of the same product: the smaller result indicates the LR.

IB CHEMISTRY R2.2 HOW FAST? THE RATE OF CHEMICAL CHANGE



Defining and determining reaction rate

- **Rate** = $\pm \Delta[\text{species}]/\Delta t$; use product rate positive, reactant rate positive by convention with a minus sign
- **Units:**
 - $\text{mol dm}^{-3} \text{ s}^{-1}$ (or M s^{-1})
 - gas volume data can be converted to moles via molar volume or $PV=nRT$
- **From graphs:**
 - **Instantaneous rate** = slope of tangent to concentration (or volume/mass) vs time curve at a chosen t
 - **Average rate** = secant line connecting two points on the curve



Exam Tip!

To draw tangent lines accurately, use a ruler and ensure the line touches the curve at only one point without crossing it.

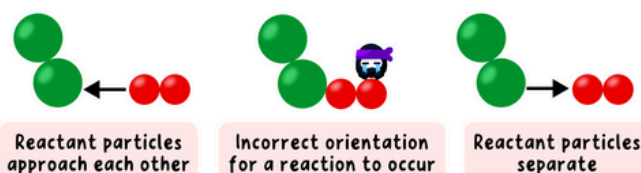
Collision theory

- **Kinetic energy vs temperature:** average $E_k \propto T(\text{K})$
- **Higher T** → particles **move faster on average** and collide more often
- **Sufficient energy:** only collisions with $E \geq E_a$ can react
- **Proper orientation:** reactants must collide with a geometry that allows bonds to break/form (steric factor)
- **Why T matters twice:** higher fraction of molecules above E_a and higher collision frequency

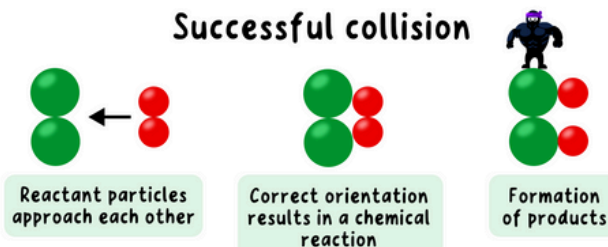
Exam Tip!

When you explain a **rate increase with T**, always mention "fraction of collisions with $E \geq E_a$ increases" and "more frequent collisions" (orientation unchanged)

Unsuccessful collision



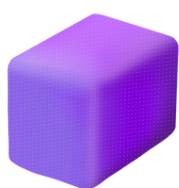
Successful collision



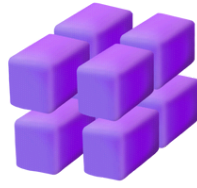
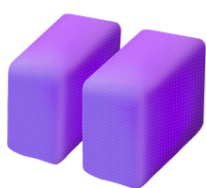
Factors affecting reaction rate

- **Concentration (liquids/solutions)** ↑ → more particles per volume → collision frequency ↑ → **rate** ↑
- **Pressure (gases)** ↑ at constant T → effective concentration ↑ → **rate** ↑
- **Surface area (solid reactant)** ↑ → more exposed sites → collision frequency at surface ↑ → **rate** ↑
- **Temperature** ↑ → fraction with $E \geq E_a$ ↑ and collisions ↑ → **rate** ↑
- **Catalyst** → alternative pathway with lower E_a → greater fraction of effective collisions at same T → **rate** ↑

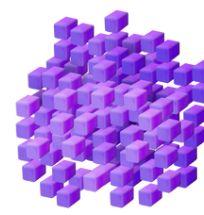
Low surface area



Low rate of reaction



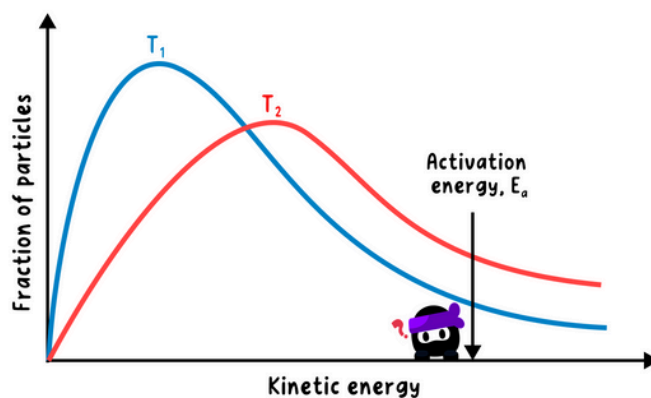
High surface area



High rate of reaction

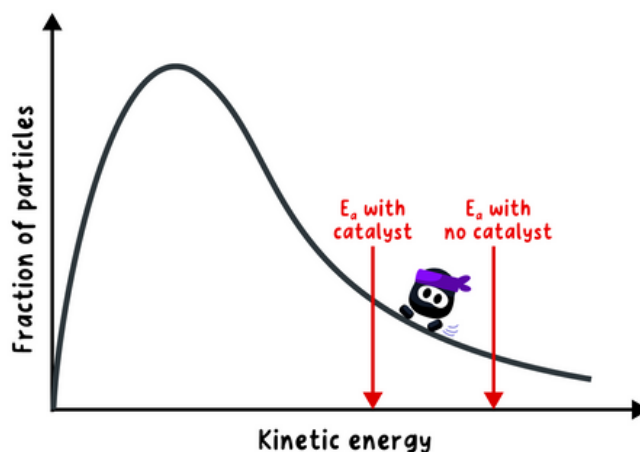
Activation energy & Maxwell-Boltzmann (M-B) distributions

- **M-B curve features:**
 - area under curve = number of particles (constant)
 - peak at most probable energy
 - tail extends to high E
- **Effect of increasing T:**
 - peak **lowers** and **shifts right**
 - **area to the right of E_a** (between the curve and horizontal axis) greatly **increases**



Catalysts: energy profiles and M-B distributions

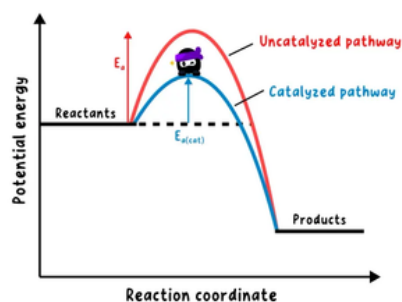
- **Energy profiles (exothermic):**
 - y = potential energy
 - x = reaction coordinate
 - uncatalyzed has higher hump
 - catalyzed path has lower hump(s);
 - ΔH same for both
- **Energy profiles (endothermic):**
 - same idea but products above reactants
 - catalyst reduces E_a (forward and reverse) equally
 - ΔH unchanged
- **M-B with catalyst:**
 - draw one temperature curve and two vertical lines $E_a(\text{uncat})$ and $E_a(\text{cat})$ (left-shifted)
 - shaded "above E_a " region is larger for catalyzed path



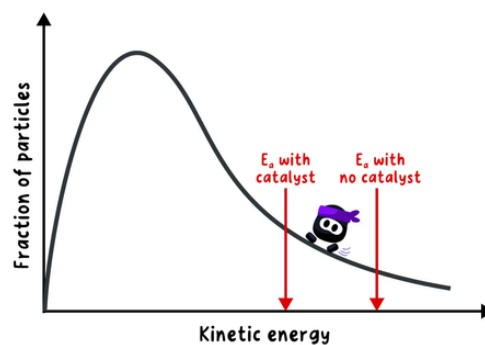
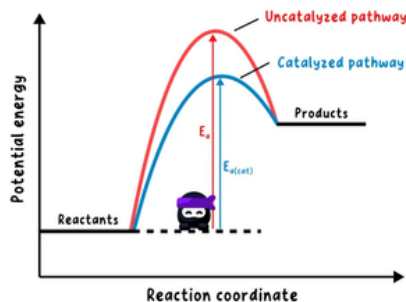
Common Mistake

Don't claim that catalysts "increase the number of collisions"! They primarily **increase the fraction of collisions** that are successful by lowering E_a (though heterogeneous catalysts can also increase effective collision frequency at active sites).

Catalyzed exothermic reaction

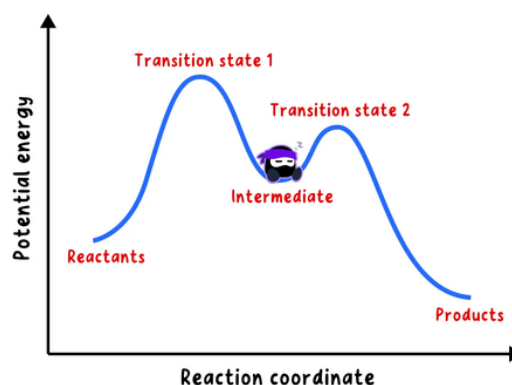


Catalyzed endothermic reaction



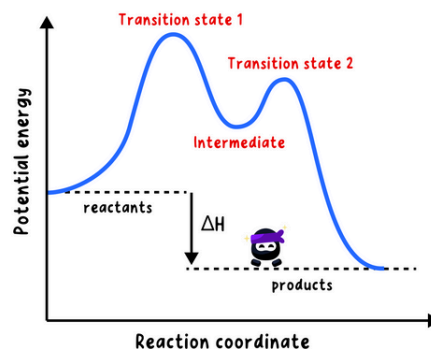
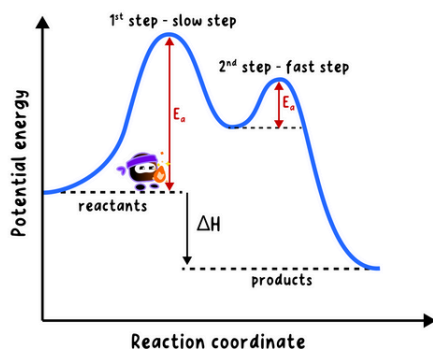
Mechanisms, intermediates, transition states

- **Mechanism** = sequence of elementary steps that sum to overall reaction; must match overall stoichiometry and kinetics
- **Rate-determining step (RDS)** = slowest elementary step; controls the rate law form
- **Intermediate** = species formed then consumed; appears in mechanism steps, not in overall equation; can sometimes be detected/trapped
- **Transition state** = highest-energy configuration along a step; not isolable; shown as peaks on energy profile



Multistep energy profiles & identifying the RDS (HL)

- **Energy profile axes:**
 - x = reaction coordinate
 - y = potential energy
- **Multistep** = multiple peaks(transition states);
- **Valleys** = intermediates
- **RDS** = step with tallest peak(highest E_{act}); its transition state controls the rate
- **How to construct from data:** more steps \rightarrow more distinct kinetic features (e.g., induction period suggests intermediate buildup); catalyst lowers one or more peaks but leaves ΔH unchanged



Common Mistake

Don't call the highest intermediate "transition state":
peaks = transition state, **valleys** = intermediates.

Molecularity of elementary steps (HL)

- **Unimolecular:**
 - one reacting particle in step($A \rightarrow \text{products}$)
 - typical of isomerizations/decompositions
- **Bimolecular:**
 - two particles collide($A+B \rightarrow \dots$ or $A+A \rightarrow \dots$)
 - most common
- **Termolecular:**
 - three particles in one step($A+B+C \rightarrow \dots$)
 - rare(improbable simultaneous collision)

Rate equations (HL)

- **General form:** $\text{rate} = k[A]^m[B]^n \dots$; m, n are orders found experimentally
- **Method (slope or initial rates):** hold all but one concentration constant; vary one and measure initial rate
- **Quick inference rules:**
 - if doubling $[A]$ doubles rate \rightarrow first order in A
 - if rate unchanged \rightarrow zero order
 - if rate quadruples \rightarrow second order

Molecularity of elementary steps (HL)

- **Order wrt a reactant** = exponent in rate law;
- **Overall order** = sum of exponents
- **Connection to mechanism:** for RDS that is elementary, orders match molecularity of that step



Exam Tip!

State axes explicitly; annotate slope/intercept relation to k on the chosen linearized plot

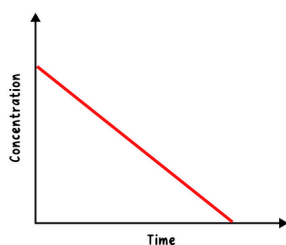
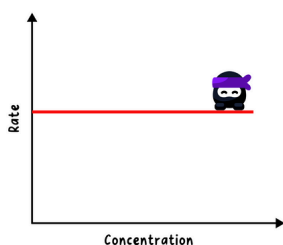
Characteristic concentration-time($[A]$ vs t):

- Zero-order: linear decay (slope = $-k$)
- First-order: exponential decay; straight line in $\ln[A]$ vs t with slope = $-k$
- Second-order (1:1): curved; straight line in $1/[A]$ vs t with slope = $+k$

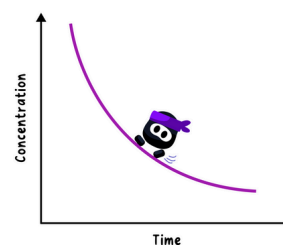
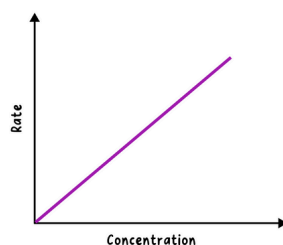
Characteristic rate-concentration(rate vs $[A]$):

- Zero: horizontal line (rate = k)
- First: straight line through origin (slope = k)
- Second: parabola (rate = $k[A]^2$)

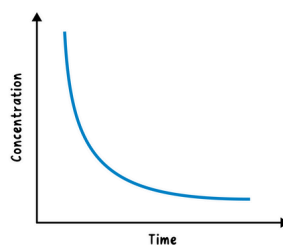
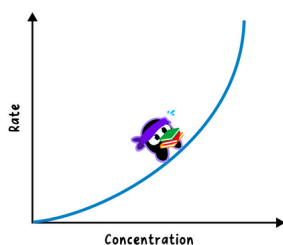
Zero-order reaction



First-order reaction



Second-order reaction



Rate constant (HL)

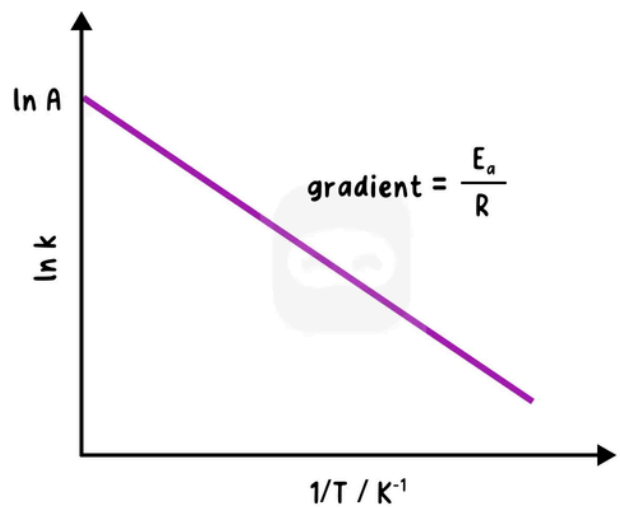
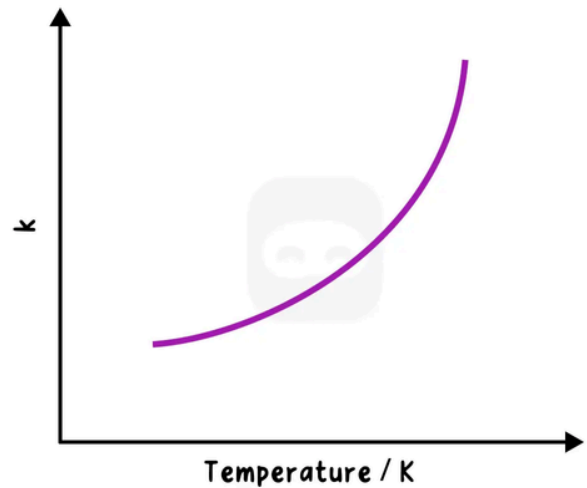
- **Units** depend on **overall order** so that rate ($\text{mol dm}^{-3} \text{s}^{-1}$) = $k \cdot (\text{concentration})^{\text{order}}$
- **Common unit patterns:**
 - Overall **zero** → k : $\text{mol dm}^{-3} \text{s}^{-1}$
 - Overall **first** → k : s^{-1}
 - Overall **second** (1:1) → k : $\text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$
 - Overall **third** → k : $\text{dm}^6 \text{mol}^{-2} \text{s}^{-1}$
- Procedure: solve $k = \text{rate}/([\text{A}]^m[\text{B}]^n\dots)$ with SI-consistent mol dm^{-3} and s

Arrhenius equation (HL)

- **Qualitative link:** as $T \uparrow$, $k \uparrow$ because a larger fraction of molecules have $E \geq E_a$ and A can also be T -dependent slightly
- **Arrhenius forms:**
 - $k = A \cdot e^{(-E_a/RT)}$
 - $\ln k = \ln A - (E_a/R)(1/T) \rightarrow$ straight line: $y = \ln k$, $x = 1/T$, slope = $-E_a/R$, intercept = $\ln A$
- Using two temperatures: $\ln(k_2/k_1) = (E_a/R)(1/T_1 - 1/T_2)$
- Graph reading: plot $\ln k$ vs $1/T$; find slope m ; $E_a = -mR$; $A = e^{(\text{intercept})}$

Arrhenius factor A (HL)

- **Physical meaning of A:**
 - frequency of properly oriented, collision-ready encounters ("pre-exponential")
 - includes steric factor and collision frequency

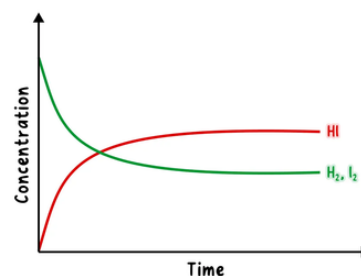
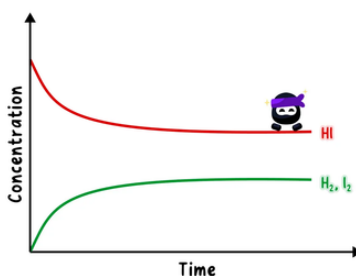
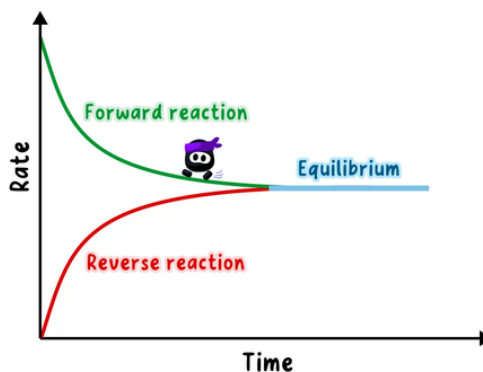


IB CHEMISTRY R2.3 HOW FAR? THE EXTENT OF CHEMICAL CHANGE



Dynamic equilibrium in closed systems

- **Definition:**
 - in a closed system, equilibrium is reached when rate(forward) = rate(backward);
 - macroscopic properties (concentration, pressure, color) are constant in time.
- **Characteristics:**
 - Both reactions continue (dynamic, not static).
 - Concentrations are constant but not necessarily equal.
 - Equilibrium composition depends on T (and total pressure for gaseous systems).
 - Reached from either side (same final composition at given T, total n, V).
- **Physical equilibria:** e.g., $\text{H}_2\text{O}(l) \rightleftharpoons \text{H}_2\text{O}(g)$ in a sealed flask (evaporation = condensation).
- **Chemical equilibria:** e.g., $\text{N}_2\text{O}_4(g) \rightleftharpoons 2 \text{NO}_2(g)$ (colorless \rightleftharpoons brown).



The equilibrium law & constant

- For a homogeneous reaction: $aA + bB \rightleftharpoons cC + dD$

$$K_c = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$
- Use activities \approx concentrations (mol dm^{-3}) for solutions; for gases, a K_p may be used but is not required by IB syllabus.
- **Omit** pure solids and pure liquids (activity ≈ 1).
- Always include **stoichiometric powers**.

Le Châtelier's principle

Predict **qualitative shifts** when a stress is applied to a system at equilibrium:

- **Concentration:**
 - add a reactant \rightarrow shifts right
 - remove it \rightarrow left. K unchanged.
- **Pressure/volume (gases):**
 - decrease V/increase P \rightarrow shifts to fewer moles of gas
 - increase V \rightarrow more moles of gas. K unchanged.
- **Temperature:** treat heat as a reagent.
 - **Exothermic** ($\Delta H < 0$): $\uparrow T$ shifts left and decreases K .
 - **Endothermic** ($\Delta H > 0$): $\uparrow T$ shifts right and increases K .



Common Mistake

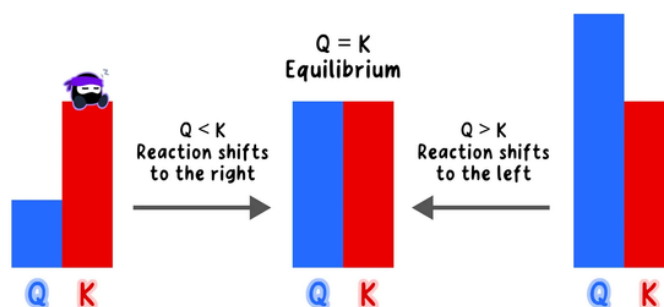
Don't claim that **catalysts** change K . They don't; they change rate to reach equilibrium, not the position.

Magnitude of K & temperature dependence

- **Extent at fixed T:**
 - $K \ll 1$: mostly reactants.
 - $K < 1$: reactants favored.
 - $K = 1$: appreciable amounts of both.
 - $K > 1$: products favored.
 - $K \gg 1$: mostly products.
- **Relationships at the same T:**
 - **Reverse reaction:** $K_{\text{rev}} = 1/K$.
 - **Multiplying coefficients by n:** $K' = K^n$.
 - **Adding reactions:** $K_{\text{sum}} = K_1 \times K_2$ (multiply constants).

Reaction quotient (HL)

- Use the same expression as K but with instantaneous concentrations/pressures:
 - **If $Q < K$:** system has too many reactants \rightarrow shifts right to make products.
 - **If $Q > K$:** system has too many products \rightarrow shifts left to make reactants.
 - **If $Q = K$:** at equilibrium.



Quantifying equilibrium compositions (HL)

Workflow (homogeneous only):

- Write K expression.
- Set up **I-C-E (Initial-Change-Equilibrium)** table in molarity.
- Express equilibrium concentrations in terms of x; substitute into K.
- If K is **very small** or **large**, use the small-x approximation (e.g., $a-x \approx a$) and check after.
- **Approximation cue:** if the computed $x/a < 5\%$, your approximation is fine.

Gibbs free energy and equilibrium (HL)

Relationship (data booklet):

$$\Delta G^\ominus = -RT \ln K$$

At **fixed T**:

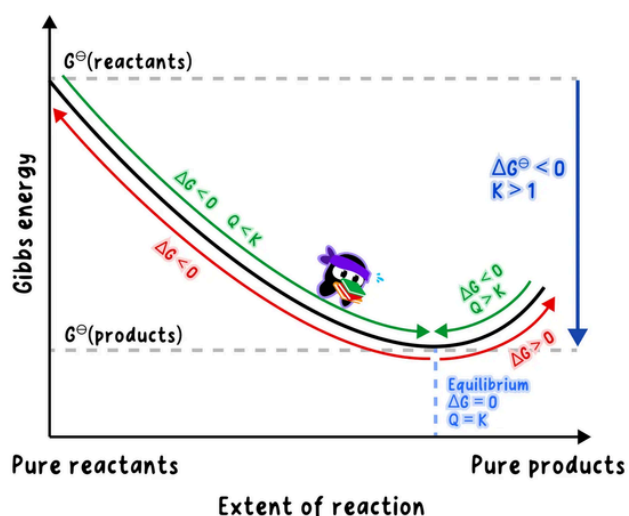
- $K > 1 \Rightarrow \Delta G^\ominus < 0$ (products favored).
- $K = 1 \Rightarrow \Delta G^\ominus = 0$
- $K < 1 \Rightarrow \Delta G^\ominus > 0$ (reactants favored).



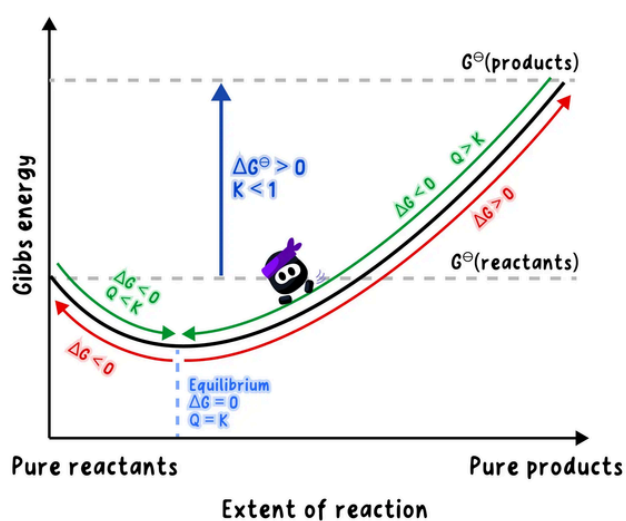
Common Mistake

Don't mix J and kJ! Keep track of that when using R.

Spontaneous reaction



Non-spontaneous reaction



Neutralization

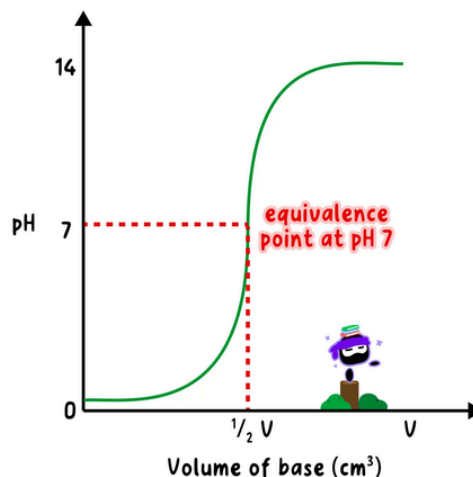
General reactions (don't forget writing states):

- Acid + metal oxide → salt + water
- Acid + metal hydroxide → salt + water
- Acid + carbonate → salt + CO₂ + H₂O
- Acid + hydrogencarbonate → salt + CO₂ + H₂O
- Acid + ammonia/amine → ammonium/alkylammonium salt (no H₂O unless extra base present)



Exam Tip!

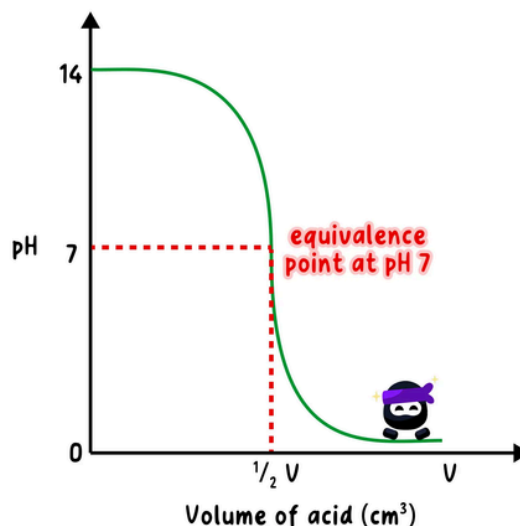
For **carbonates**, always show CO₂(g) + H₂O(l).



pH curves for neutralization

General features (titrant added on x-axis; pH on y-axis):

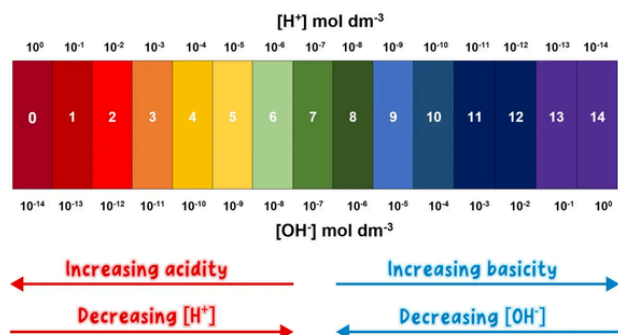
- **Strong acid + strong base:**
 - initial pH low
 - sharp vertical rise near equivalence
 - equivalence at pH ≈ 7
- **Strong base + strong acid:**
 - initial pH high
 - sharp vertical fall near equivalence
 - equivalence at pH ≈ 7
- **Intercepts & equivalence**
 - Initial pH from analyte strength
 - Equivalence point where mol H⁺ = mol OH⁻ (steepest slope).
- **Choice of indicator:** pick one whose range overlaps the steep vertical region.



Quantifying equilibrium compositions (HL)

Definitions (298 K unless stated):

- **pOH** = -log₁₀[OH⁻]
- [OH⁻] = 10^{-(pOH)}
- **pH + pOH = 14.00** (because K_w = [H⁺][OH⁻] = 1.0 × 10⁻¹⁴ at 298 K).
- **Interconvert quickly:** find one of {pH, pOH, [H⁺], [OH⁻]} → get the other three via the two equations above.



Conjugate acid-base pairs (HL)

- For HA ⇌ H⁺ + A⁻ and A⁻ + H₂O ⇌ HA + OH⁻, multiplying K_a and K_b cancels intermediates → K_a · K_b = K_w (at same T).
- **Uses:**
 - Given K_a, find K_b of its conjugate base: K_b = K_w/K_a (and vice versa).
 - Convert pK_a ↔ pK_b: pK_a + pK_b = pK_w (= 14.00 at 298 K).

The pH of a salt solution (HL)

- Decide if **acidic/basic/neutral salt** from parent acid/base strengths:
 - Strong acid + strong base → neutral salt (e.g., NaCl).
 - Strong acid + weak base → acidic salt (e.g., NH₄Cl).
 - Weak acid + strong base → basic salt (e.g., CH₃COONa).
 - Weak acid + weak base → pH depends on relative K_a vs K_b.
- **Hydrolysis equations** (write the reacting ion with water):
 - NH₄⁺ + H₂O ⇌ NH₃ + H₃O⁺ (acidic)
 - RCOO⁻ + H₂O ⇌ RCOOH + OH⁻ (basic)
 - CO₃²⁻ + H₂O ⇌ HCO₃⁻ + OH⁻ (basic)
 - HCO₃⁻ amphiprotic:
 - as base: HCO₃⁻ + H₂O ⇌ H₂CO₃ + OH⁻
 - as acid: HCO₃⁻ + H₂O ⇌ CO₃²⁻ + H₃O⁺

Strength of weak acids and bases (HL)

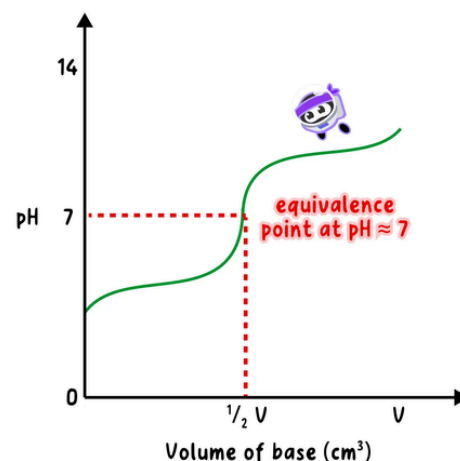
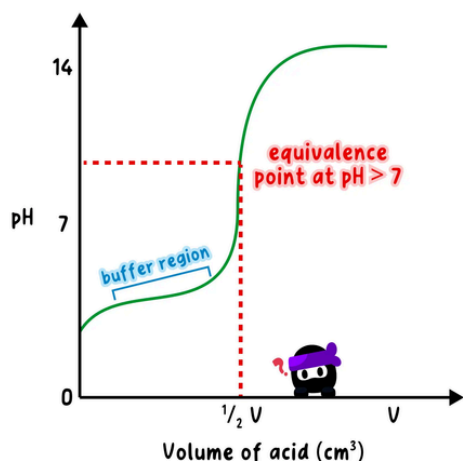
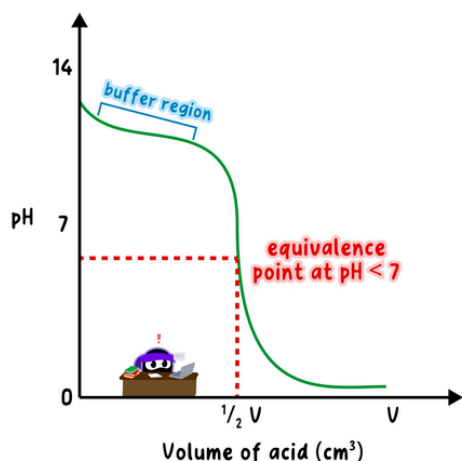
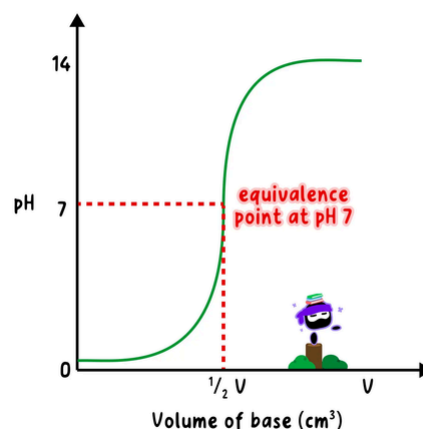
$$K_a = \frac{[H^+][A^-]}{[HA]} \quad K_b = \frac{[BH^+][OH^-]}{[B]}$$

- **Trend sense:**
 - larger K_a / smaller pK_a → stronger acid
 - larger K_b / smaller pK_b → stronger base
- **Comparisons:**
 - If pK_a(HA₁) < pK_a(HA₂) → HA₁ is stronger
 - If pK_b(B₁) < pK_b(B₂) → B₁ is stronger

pH curves of acid-base combinations (HL)

General shapes & landmarks (titrant on x-axis):

- **Strong acid + strong base:** start low pH; equivalence ≈ 7 ; very steep near eq.
- **Weak acid + strong base:** higher initial pH; buffer region; $\frac{1}{2}$ -equivalence: $\text{pH} = \text{pK}_a$; equivalence > 7 .
- **Strong acid + weak base:** lower initial pH than pure base; buffer region; $\frac{1}{2}$ -equivalence: $\text{pOH} = \text{pK}_b$; equivalence < 7 .
- **Weak acid + weak base:** shorter vertical; equivalence pH depends on pK_a vs pK_b ; indicator choice is tricky.



Acid-base indicators and pH changes (HL)

- **Model:** $\text{HInd} \rightleftharpoons \text{H}^+ + \text{Ind}^-$, where HInd and Ind^- are different colors.
- If $\text{pH} \ll \text{pK}(\text{Ind}) \rightarrow \text{HInd}$ color dominates.
- If $\text{pH} \gg \text{pK}(\text{Ind}) \rightarrow \text{Ind}^-$ color dominates.
- **End point** $\approx \text{pK}(\text{Ind})$ (mid-transition).
- **Universal indicator** = mixture \rightarrow wide, multicolor range.



Common Mistake

Don't equate end point with equivalence point, because they should coincide only when the indicator is well chosen.

Choosing an indicator (HL)

- **Rule:** pick an indicator whose transition range overlaps the steep pH jump at equivalence.
- **Equivalence point** = stoichiometric $\text{H}^+ = \text{OH}^-$
- **End point** = observed color change (\approx indicator pK_a).



Common Question

- Which conditions best favour the oxidation of secondary alcohols to ketones?
- Excess acidified potassium dichromate (VI) and reflux
 - Excess acidified potassium dichromate (VI) and distillation
 - Few drops of acidified potassium dichromate (VI) and reflux
 - Few drops of acidified potassium dichromate (VI) and distillation

Buffer solutions (HL)

- **Acidic buffer:** weak acid HA + its salt A^- (e.g., $\text{CH}_3\text{COOH}/\text{CH}_3\text{COONa}$).
- **Basic buffer:** weak base B + its salt BH^+ (e.g., $\text{NH}_3/\text{NH}_4\text{Cl}$).
- **How buffers resist pH change:**
 - Add acid (H^+): A^- consumes $\text{H}^+ \rightarrow \text{HA}$ forms.
 - Add base (OH^-): HA consumes $\text{OH}^- \rightarrow \text{A}^- + \text{H}_2\text{O}$ forms.
- **Buffer capacity** increases with total concentration and with $[\text{A}^-] \approx [\text{HA}]$ (best near $\text{pH} \approx \text{pK}_a$).

pH of buffer solutions (HL)

- **Acidic buffer:**

$$K_a = \frac{[\text{H}^+][\text{A}^-]}{[\text{HA}]} \Rightarrow \text{pH} = \text{pK}_a + \log \frac{[\text{A}^-]}{[\text{HA}]}$$

- **Basic buffer:**

$$\text{pOH} = \text{pK}_b + \log \frac{[\text{BH}^+]}{[\text{B}]}, \quad \text{pH} = 14.00 - \text{pOH} (298 \text{ K})$$

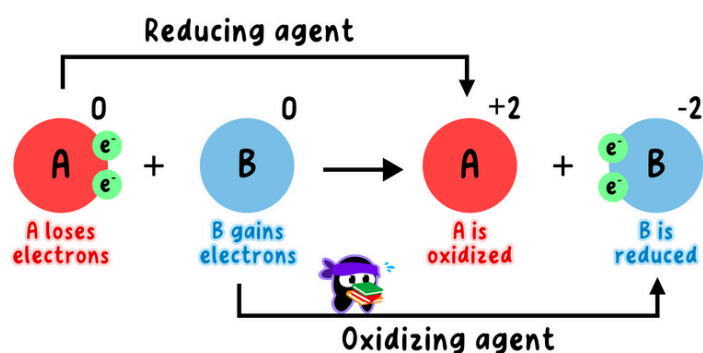
- **Effect of dilution:** if both components diluted by the same factor, the ratio $[\text{A}^-]/[\text{HA}]$ stays \approx constant \rightarrow $\text{pH} \sim$ unchanged, but buffer capacity decreases (less moles to neutralize added acid/base).

IB CHEMISTRY R3.2 ELECTRON TRANSFER REACTIONS



Neutralization

- **Redox lenses:**
 - **Electron:** oxidation = e^- loss; reduction = e^- gain.
 - **O state:** oxidation = increase in oxidation state; reduction = decrease.
 - **O/H:** oxidation = O gain / H loss; reduction = O loss / H gain.
- **Assigning oxidation states** (quick rules): free element = 0; monoatomic ion = charge; Group 1 = +1, Group 2 = +2; F = -1; O = -2 (peroxide -1); H = +1 (metal hydrides -1); sums \rightarrow 0 (molecule) or ion charge.
- **Identify roles in an equation:** the species oxidized (OS \uparrow) is the reducing agent; the species reduced (OS \downarrow) is the oxidizing agent.
- **Variable OS examples:** Fe^{2+}/Fe^{3+} ; Mn from +2 to +7 (e.g., MnO_4^-); S (-2, 0, +4, +6); N (-3 to +5). Names use Roman numerals, e.g., iron(III) oxide.



Acid-metal reactions

- **General:** metal + dilute HCl/ $H_2SO_4 \rightarrow$ salt + H_2 (metals above H in the activity series).

Example:



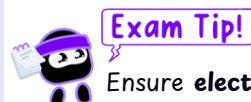
- $Mg + 2HCl \rightarrow MgCl_2 + H_2 \uparrow$
- $Zn + H_2SO_4 \rightarrow ZnSO_4 + H_2 \uparrow$
- $Fe + 2HCl \rightarrow FeCl_2 + H_2 \uparrow$

Primary (voltaic) cell

- **Build:** two half-cells (e.g., $Zn|Zn^{2+}$ and $Cu|Cu^{2+}$), metal electrodes, connecting wire + voltmeter, salt bridge ($KNO_3(aq)$) to maintain charge balance.
- **Flow:** electrons from anode (oxidation) to cathode (reduction).
- In **salt bridge**, anions drift toward anode compartment; cations toward cathode.

Neutralization

- Write **separate oxidation and reduction half-equations**; balance atoms, then charge with e^- ; add to cancel e^- .
- **Acidic solution method:** balance O with H_2O , H with H^+ , then charge with e^- .
- **Neutral (or basic*) shortcut for IB SL:** use the acidic method then (if basic) add same number of OH^- both sides to neutralize H^+ to water.



Exam Tip!

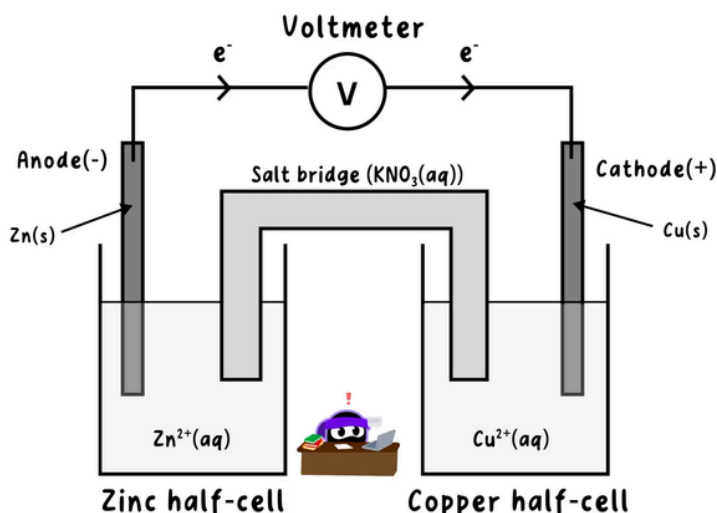
Ensure **electron count** cancels exactly, and then remove any spectator species.

Reactivity of elements based on periodic trends

- **Metals:**
 - **across a period** (to the right) metals become less easily oxidized
 - **down Group 1/2**, larger atoms with lower IE are more easily oxidized.
 - A more reactive metal displaces a less reactive metal from its ion solution.
- **Halogens:** oxidizing power decreases down Group 17; $F_2 > Cl_2 > Br_2 > I_2$ (so Cl_2 oxidizes Br^-/I^- ; Br_2 oxidizes I^-).
- **Using supplied data:** if $M(s) + M^{n+}(aq) \rightarrow$ reaction occurs, M is the stronger reducing agent (easier to oxidize).

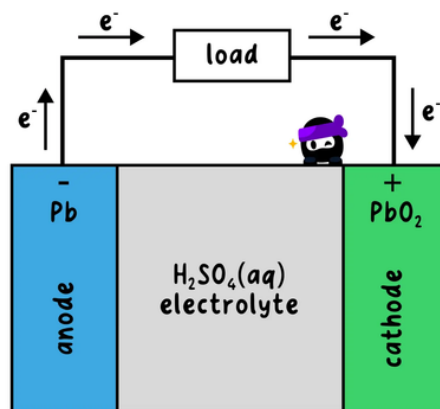
Electrochemical cells: oxidation and reduction

- **Oxidation** at anode, **reduction** at cathode (**always!**).
- **Voltaic** (galvanic, spontaneous): anode is -, cathode is +; e^- flow anode \rightarrow cathode through wire.
- **Electrolytic** (non-spontaneous, power supply): anode is +, cathode is - (polarity set by source).



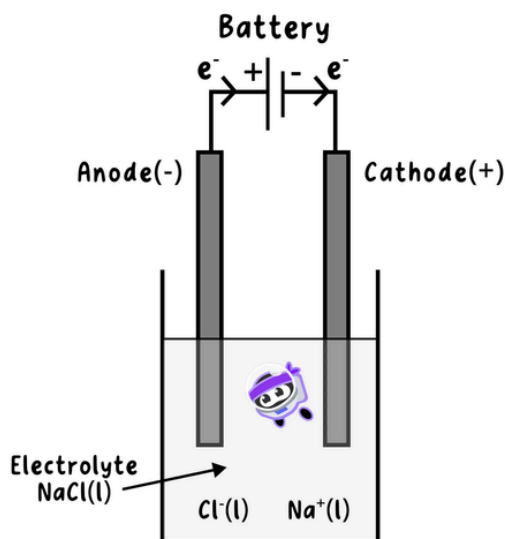
Secondary (rechargeable) cells

- **Secondary cells:** discharge reactions are reversed on charging by applying external voltage $> E(\text{cell})$.
- Given **discharge half-reactions**, reverse them (swap anode/cathode) for charge.
- **Pros/cons (snapshot):**
 - **Primary:** convenient, high energy density, single-use waste.
 - **Secondary:** rechargeable, lower waste, finite cycle life, charging losses.
 - **Fuel cells:** continuous fuel \rightarrow electricity, high efficiency/low local emissions; need fuel supply & infrastructure.



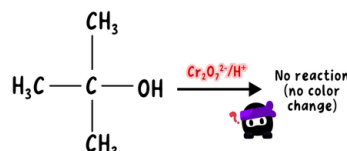
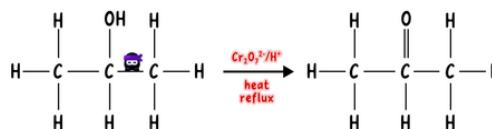
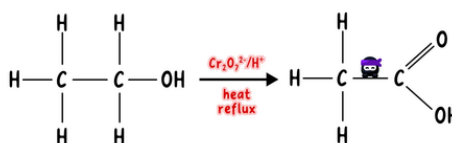
Electrolytic cells

- **Conduction:**
 - **electrons** move in the external circuit
 - **ions** carry charge in the molten/aqueous electrolyte
 - **power source** forces non-spontaneous redox.
- **Products (molten salts, no water present):**
 - **cations** \rightarrow cathode (reduced to metal)
 - **anions** \rightarrow anode (oxidized to non-metal).



Oxidation of organic compounds

- **Primary alcohols (1°):** two-step oxidation
 - 1° alcohol \rightarrow aldehyde (partial oxidation) \rightarrow carboxylic acid (further oxidation); $\text{R-CH}_2\text{-OH} \rightarrow \text{R-CHO} \rightarrow \text{R-COOH}$
- **Secondary alcohols (2°):** $\text{R}_1\text{-CH(OH)-R}_2 \rightarrow$ ketone $\text{R}_1\text{-C(=O)-R}_2$
- **Tertiary alcohols (3°):** no reaction under these conditions (no H on the -C-OH carbon).
- **Setups:**
 - **Distillation** to isolate aldehyde: heat gently with oxidant; aldehyde distilled off as it forms.
 - **Reflux** to drive to acid: heat under condenser so vapors return; maximizes contact with oxidant.



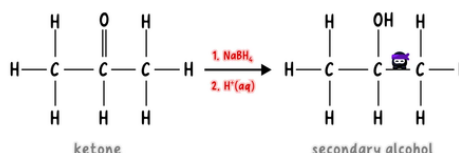
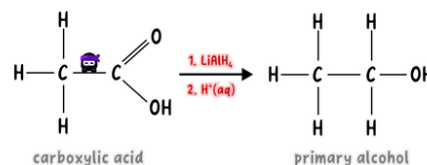
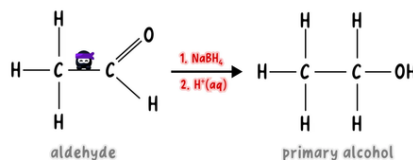
Reduction of functional groups

- **Carboxylic acid** \rightarrow aldehyde \rightarrow 1° alcohol (overall 4 H added: two to C=O , two to O-H stage).
- **Ketone** \rightarrow 2° alcohol.
- **Role of hydride (H^-):** delivers electrons + H to the electrophilic carbonyl carbon (you may write " $+2[\text{H}]$ " per reduction step if reagents are not named).



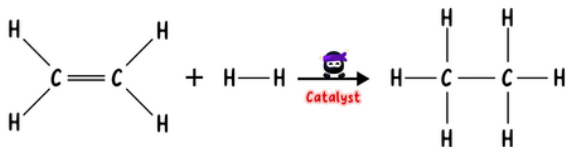
Common Mistake

Don't reduce a **3° alcohol** to a ketone: it is impossible without oxidation; reductions go toward higher H / lower O at carbon.



Hydrogenation of unsaturated compounds

- **Alkenes:** $R-CH=CH-R' + H_2 \rightarrow R-CH_2-CH_2-R'$ (alkane).
- **Alkynes:** $R-C\equiv C-R' + 2 H_2 \rightarrow R-CH_2-CH_2-R'$ (full hydrogenation).
- **"Reduction" view:** C gains H (decrease in oxidation state).



Standard hydrogen electrode (SHE) (HL)

- **SHE half-equation** (reduction form): $2 H^+(aq) + 2 e^- \rightleftharpoons H_2(g)$ assigned $E^\circ = 0.00 \text{ V}$.
- **Interpreting tables:**
 - more positive $E^\circ(\text{reduction}) \rightarrow$ stronger oxidizing agent (easier to reduce)
 - more negative \rightarrow stronger reducing agent.



Exam Tip!

Compare two reductions; the more positive runs as reduction, the other is reversed to give oxidation.

Standard cell potential & spontaneity (HL)

- Compute $E^\circ_{\text{cell}} = E^\circ(\text{cathode, red}) - E^\circ(\text{anode, red})$.
- If $E^\circ_{\text{cell}} > 0$, **forward** reaction is **spontaneous** (under standard conditions)
- If $E^\circ_{\text{cell}} < 0$, **reverse** is **spontaneous**.

Electrolysis of aqueous solutions (HL)

General rule of thumb (use E° and context):

- **Cathode (reduction):**
 - If aqueous NaCl: H_2O/H_2 is typically reduced ($2 H_2O + 2 e^- \rightarrow H_2 + 2 OH^-$) rather than Na^+ .
 - If $CuSO_4(aq)$ with Cu electrodes: $Cu^{2+} + 2 e^- \rightarrow Cu(s)$ plates on cathode.
- **Anode (oxidation):**
 - NaCl(aq): often Cl_2 forms ($2 Cl^- \rightarrow Cl_2 + 2 e^-$) if $[Cl^-]$ high and inert anode; otherwise O_2 from water ($2 H_2O \rightarrow O_2 + 4 H^+ + 4 e^-$).
 - $CuSO_4(aq)$: with inert anode, water/ OH^- oxidized to O_2 ; with Cu anode, $Cu(s) \rightarrow Cu^{2+} + 2 e^-$ (anode dissolves).

Link between ΔG° and E°_{cell} (HL)

$$\Delta G^\circ = -nFE^\circ_{\text{cell}}$$

- where n = moles of electrons transferred; $F \approx 96485 \text{ C mol}^{-1}$.
- **Sign test:** $E^\circ_{\text{cell}} > 0 \rightarrow \Delta G^\circ < 0$ (spontaneous).
- Convert J \rightarrow kJ at the end.

Electroplating (HL)

- **Setup:** object to be plated is cathode (-); source metal is often anode (+) (active), solution contains metal ions M^{n+} .
- **Half-equations** (example: Cu plating with Cu anode):
 - **Cathode:** $Cu^{2+} + 2 e^- \rightarrow Cu(s)$ (coating the object)
 - **Anode (active):** $Cu(s) \rightarrow Cu^{2+} + 2 e^-$ (replenishes ions)
 - If anode is **inert**, add metal salt periodically to maintain $[M^{n+}]$.

IB CHEMISTRY R3.3 ELECTRON SHARING REACTIONS



Radicals

- **Radical** = species with an unpaired electron (\cdot); highly **reactive**; **seeks pairing** via reactions
- **Notation/use**: place a **dot** next to the atom carrying the unpaired electron, e.g., $\text{Cl}\cdot$, $\text{CH}_3\cdot$, tert-butyl $\cdot\text{C}(\text{CH}_3)_3$
- **Representation in mechanisms**: use a **single-barbed "fish-hook" arrow** to show movement of one electron

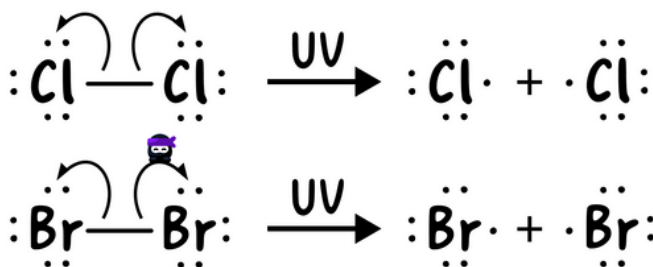


Exam Tip!

Always show the **dot on the correct atom** and conserve total electron count in each step.

Homolytic fission & initiation (UV/heat)

- **Homolytic fission** = breaking a covalent bond so each atom takes one electron; needs **energy** (UV/ Δ); generates **two radicals**
- Initiation step for halogens under UV:
 - $\text{Cl}_2 \rightarrow (h\nu) \rightarrow 2\text{Cl}\cdot$
 - $\text{Br}_2 \rightarrow (h\nu) \rightarrow 2\text{Br}\cdot$



Radical substitution of alkanes

- Alkanes are unreactive (strong C-H/C-C, non-polar) so they need **radical conditions** (UV/ Δ) to undergo substitution with X_2
- **General pattern with methane (chlorination shown)**:
 - Propagation 1: $\text{Cl}\cdot + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3\cdot$
 - Propagation 2: $\text{CH}_3\cdot + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{Cl}\cdot$
 - Net(change): $\text{CH}_4 + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{HCl}$
 - Termination (combine any two radicals to remove them):
 - $\text{CH}_3\cdot + \text{Cl}\cdot \rightarrow \text{CH}_3\text{Cl}$
 - $\text{CH}_3\cdot + \text{CH}_3\cdot \rightarrow \text{C}_2\text{H}_6$
 - $\text{Cl}\cdot + \text{Cl}\cdot \rightarrow \text{Cl}_2$
- **Product mixtures & further substitution**:
 - Once CH_3Cl forms, it can be further chlorinated: $\text{CH}_3\text{Cl} \rightarrow \text{CH}_2\text{Cl}_2 \rightarrow \text{CHCl}_3 \rightarrow \text{CCl}_4$ (under prolonged UV/ Cl_2 excess)
 - In higher alkanes, positional isomers form (e.g., chlorination of propane yields 1-chloropropane and 2-chloropropane)
- **Selectivity & stability**:
 - C-H abstraction forms alkyl radicals;
 - **Stability order**: tertiary > secondary > primary > methyl (more substituted radicals are lower in energy)
 - Br_2 is **more selective** than Cl_2 because endothermic H-abstraction step for $\text{Br}\cdot$ has a larger E_a and favors formation at the most stable radical site)
 - Cl_2 is **less selective/more reactive**



Common Mistake

Don't leave a radical unaccounted for in **propagation** products.

IB CHEMISTRY R3.4 ELECTRON-PAIR SHARING REACTIONS



Nucleophiles

- **Definition:** A **nucleophile** donates a lone pair to make a new σ bond with an electrophile.
- **Typical nucleophiles (neutral):** H_2O , NH_3 , ROH , RNH_2 .
- **Typical nucleophiles (anionic):** HO^- , RO^- , CN^- , HS^- , $\text{Cl}^-/\text{Br}^-/\text{I}^-$, NO_2^- , NH_2^- .
- **Recognition cues:** lone pair(s) and/or negative charge; often attack δ^+ carbons (e.g., C-X in alkyl halides, C=O carbon).

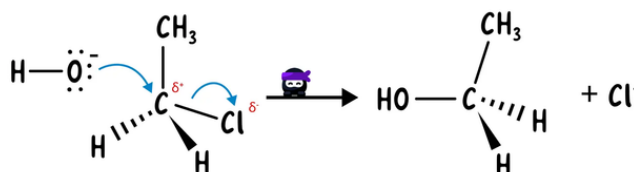
Exam Tip!



Quickly justify: "X has a lone pair/negative charge \rightarrow donates e^- pair \rightarrow nucleophile."

Nucleophilic substitution

- **Core idea:** Nu donates an electron pair to $\text{C}\delta^+$ as C-LG bond breaks \rightarrow leaving group (LG) departs with the bonding pair.
- **Generic equation:** $\text{Nu}^- + \text{R-LG} \rightarrow \text{Nu-R} + \text{LG}^-$ (heterolytic C-LG cleavage).

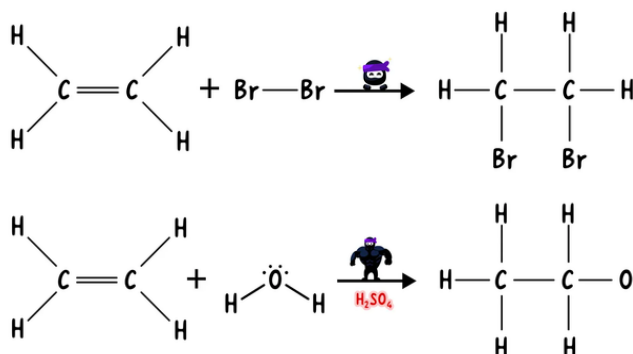


Electrophiles

- **Definition:** An **electrophile** accepts a lone pair from a nucleophile.
- **Typical electrophiles (neutral):** C=O carbon in aldehydes/ketones; SO_3 ; $\text{BF}_3/\text{AlCl}_3$ (Lewis acids).
- **Typical electrophiles (cationic/polarized):** $\text{H}^+/\text{H}_3\text{O}^+$, NO_2^+ , carbocations (R_3C^+), polarized C-X ($\text{C}\delta^+$).
- **Recognition cues:** positive charge, strong δ^+ center, electron-deficient atoms (incomplete octet).

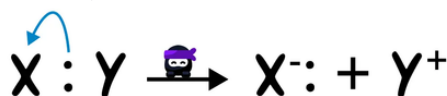
Electrophilic addition to alkenes

- **Alkenes** react with **electrophiles** at the C=C (π electrons donate).
- **Halogenation:** $\text{C}=\text{C} + \text{X}_2 \rightarrow \text{X-C-C-X}$ (e.g., ethene + $\text{Br}_2 \rightarrow$ 1,2-dibromoethane; π electrons attack $\text{X}\delta^+$, X-X breaks).
- **Hydrohalogenation:** $\text{C}=\text{C} + \text{HX} \rightarrow$ haloalkane (Markovnikov product in unsym. alkenes).
- **Hydration (overall):** $\text{C}=\text{C} + \text{H}_2\text{O} \rightarrow$ alcohol (via H^+ catalysis: first add H^+ , then H_2O attacks carbocation, deprotonation gives ROH).



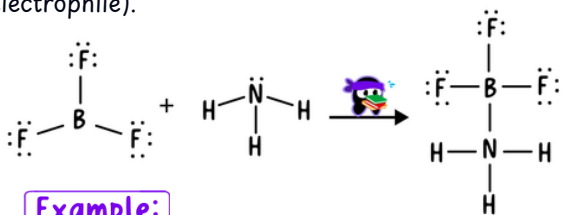
Heterolytic fission

- **Definition:** both bonding electrons go to one fragment when a σ bond breaks \rightarrow ions.
- **Generic:** $\text{R-X} \rightarrow \text{R}^+ + \text{X}^-$ (electrons move toward X if X is more electronegative).
- **Generic equations:**
 - $\text{R-Cl} \rightarrow \text{R}^+ + \text{Cl}^-$ (curly arrow from C-Cl bond to Cl).
 - Proton transfer step: $\text{B}^- + \text{H-A} \rightarrow \text{B-H} + \text{A}^-$ (arrow from B lone pair to H; arrow from H-A bond to A).



Lewis acid and base identification (HL)

- **Lewis base** = electron-pair donor (often the nucleophile).
- **Lewis acid** = electron-pair acceptor (often the electrophile).

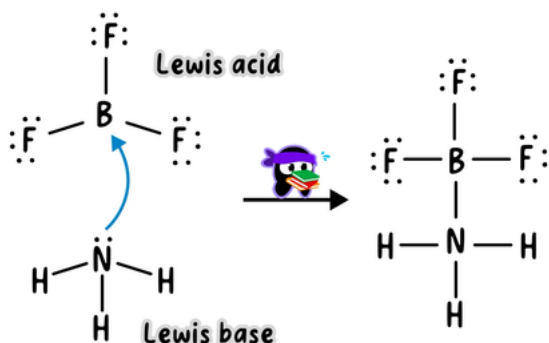


Example:

- **Inorganic examples:**
 - NH_3 (base) + BF_3 (acid) $\rightarrow \text{F}_3\text{B} \leftarrow \text{NH}_3$
 - H_2O (base) + $\text{Al}^{3+}(\text{aq})$ (acidic center) $\rightarrow [\text{Al}(\text{H}_2\text{O})_6]^{3+}$
- **Organic examples:**
 - Carbonyl O donates to BCl_3 (acid); amines donate to metal centers.

Coordination bond formation (HL)

- When a **Lewis base** donates a lone pair to a **Lewis acid**, a **coordinate (dative) bond** forms.
- Draw as an arrow from donor to acceptor in the product (often later shown as a normal line):
 - $\text{BF}_3 + \text{:NH}_3 \rightarrow \text{F}_3\text{B} \leftarrow \text{NH}_3$
 - $[\text{Cu}(\text{H}_2\text{O})_4]^{2+} + 2 \text{NH}_3 \rightarrow [\text{Cu}(\text{H}_2\text{O})_2(\text{NH}_3)_2]^{2+} + 2 \text{H}_2\text{O}$ (N donates to Cu^{2+})
- In **proton transfers**, the $\text{N} \rightarrow \text{H}$ or $\text{O} \rightarrow \text{H}$ donation step is also a coordination bond (e.g., $\text{NH}_3 + \text{H}^+ \rightarrow \text{NH}_4^+$).

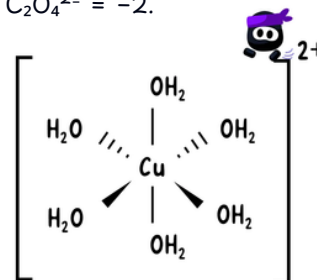


Leaving-group effects on substitution rate (HL)

- Better leaving group** = weaker base & more stable anion → faster substitution.
- Trend (same R):
 - $\text{R-I} > \text{R-Br} > \text{R-Cl} \gg \text{R-F}$ (I⁻ best, F⁻ worst) due to bond strength and anion stability.
- For a given halogen, tertiary > secondary > primary for SN1; primary > secondary > tertiary for SN2 (sterics).

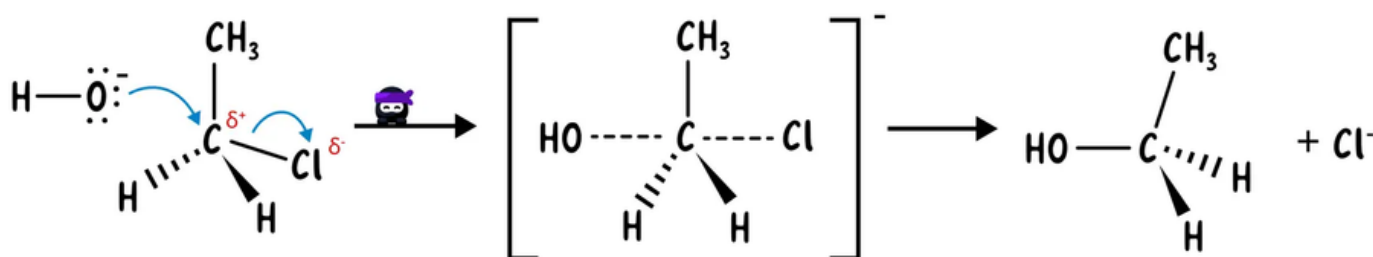
Ligands and coordination bond (HL)

- Ligands** donate a lone pair to a metal cation → coordinate (dative) bonds
- Common ligand charges:** H_2O , NH_3 , CO , en (ethylenediamine) = 0; Cl^- , Br^- , I^- , CN^- , OH^- , NO_2^- = -1; oxalate $\text{C}_2\text{O}_4^{2-}$ = -2.

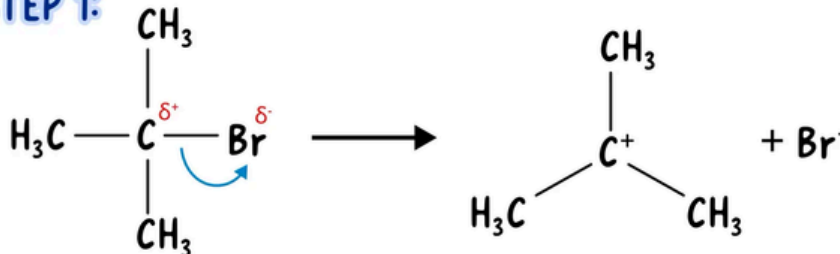


Nucleophilic substitution of halogenoalkanes (HL)

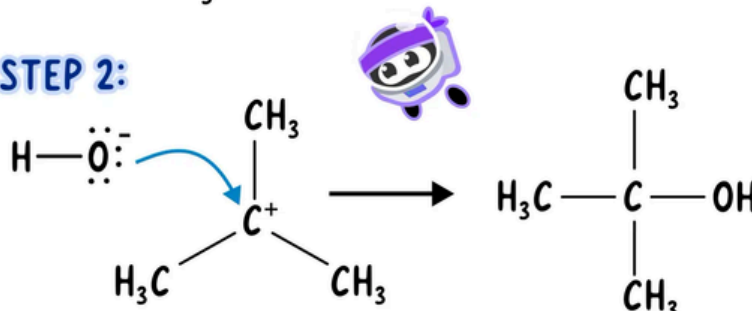
- SN2 (primary RX):**
 - bimolecular
 - concerted one-step backside attack
 - transition state with partial bonds
 - inversion of configuration (stereospecific)
 - bimolecular
- SN1 (tertiary RX):**
 - unimolecular
 - two-step via planar carbocation
 - nucleophile attacks from either side → racemization (often partial)
- Secondary halogenoalkanes:** can go SN1 and/or SN2 depending on conditions (not examined here).



STEP 1:

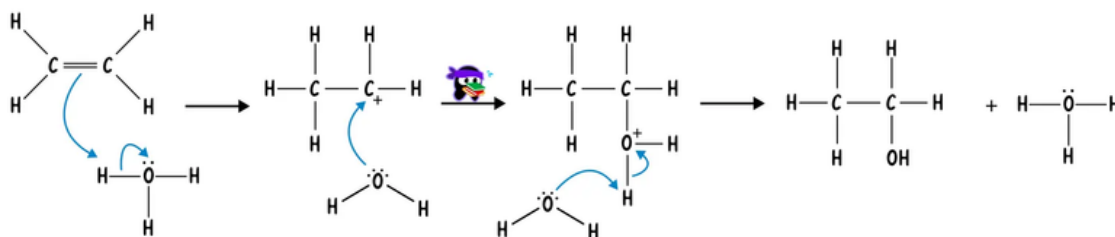
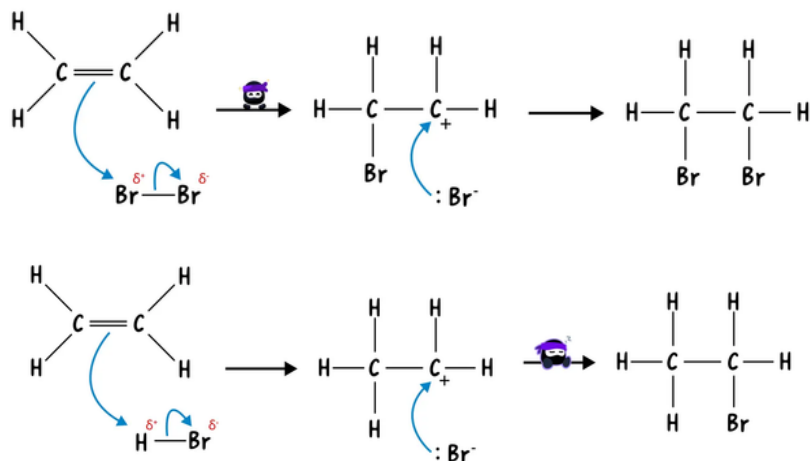


STEP 2:



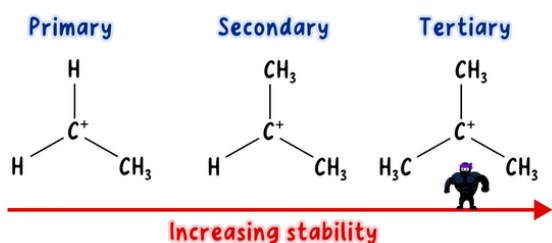
Electrophilic addition(HL)

- **Halogenation:** C=C donates to X₂ → cyclic halonium (not required to name), then X⁻ opens → vicinal dihalide. E.g., ethene + Br₂ → 1,2-dibromoethane.
- **Hydrohalogenation (HX):** π bond → H⁺ adds, then X⁻ adds → haloalkane; for symmetrical alkenes only one product.
- **Hydration (acid-catalyzed):** C=C + H₂O (H⁺ present) → alcohol.



Carbocation stability (HL)

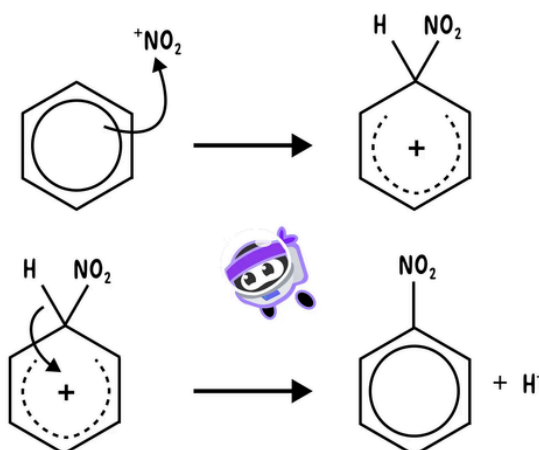
- **Carbocation stability:** 3° > 2° > 1° > methyl (hyperconjugation/inductive effects).
- **Markovnikov orientation:** In HX addition to R¹CH=CHR², H adds to the carbon with more H's; the more substituted carbocation forms, then X⁻ attacks → major product.
- **Water addition** (acid-catalyzed) follows analogous logic → Markovnikov alcohol.



Electrophilic substitution of benzene (HL)

Steps (generic E⁺, formation not examined):

- **Attack:** π system of benzene donates to E⁺ → arenium ion (σ-complex; aromaticity lost).
- **Deprotonation:** base removes H⁺ from the substituted carbon; aromaticity is restored → substituted benzene + H-Base⁺.
- **Arrow pushing:** curved arrow from ring to E⁺; then from C-H bond to ring to re-form π system



Common Question



Which of the following can act as an electrophile?

- H⁺
- NO₂⁺
- NH₃

- I and II only
- I and III only
- II and III only
- I, II and III