Course Companion

International Baccalaureate · IB Diploma · Chemistry · HL

Every topic handout in one volume

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Introduction to the particulate nature of matter

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Structure 1.1, Introduction to the particulate nature of matter, for the course first assessed in 2025. All of it is SL and HL content.

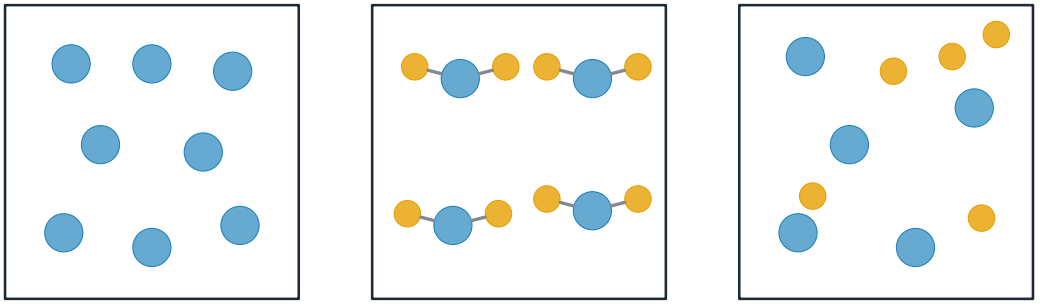
Prerequisites: the idea that matter is made of particles, and reading a temperature–time graph. This is the first unit of the course; the rest of the course builds on it.

Elements, compounds and mixtures

Why is sea water not a pure substance?

Sea water tastes of salt, but heat it in a pan and pure water leaves as steam while the salt stays behind. Sea water is a mixture: water and salt are mixed but not chemically joined, so a physical process can separate them. Water itself cannot be split by boiling; it needs a chemical reaction, such as electrolysis, to give hydrogen and oxygen.

Three kinds of matter



element
only one type of atom

compound
different atoms bonded in a fixed ratio

mixture
not bonded, easy to separate

Elements and compounds are pure substances; a mixture is not

- An **element** contains only one type of atom, for example iron, Fe, or oxygen, O_2.
- A **compound** contains two or more elements **chemically bonded** in a fixed ratio, for example water, H_2O. Its properties differ from those of its elements: sodium and chlorine are dangerous, sodium chloride is table salt.
- A **mixture** contains two or more substances that are not chemically bonded. Its composition can vary, and each part keeps its own properties.

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Homogeneous and heterogeneous mixtures

- A **homogeneous** mixture has the same composition throughout, and you cannot see the parts: salt water, air, an alloy such as brass.
- A **heterogeneous** mixture does not have a uniform composition, and the parts can often be seen: sand in water, oil and water, granite.

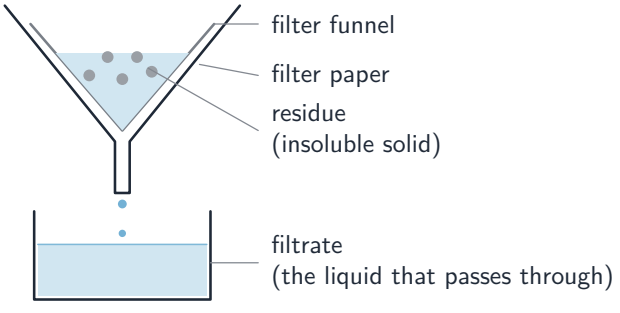
Separating mixtures

Choosing a method

Mixtures are separated by physical methods that use a difference in physical properties: solubility, boiling point, or particle size.

Mixture	Method	Property used
insoluble solid in a liquid (sand and water)	**filtration**	particle size
dissolved solid in a liquid (salt water), solid wanted	**evaporation** or **crystallization**	the solvent evaporates, the solute does not
dissolved solid in a liquid, liquid wanted	simple **distillation**	different boiling points
two miscible liquids (ethanol and water)	fractional distillation	different boiling points
two soluble solids (sand and salt)	**solvation** (dissolve), then filter and evaporate	different solubility
coloured substances in a solution (inks, dyes)	paper chromatography (Structure 2.2)	attraction to two phases

Filtration



The solid that stays in the paper is the residue; the liquid that passes through is the filtrate

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The filter paper has tiny holes. Dissolved particles and the solvent pass through; larger, undissolved particles do not.

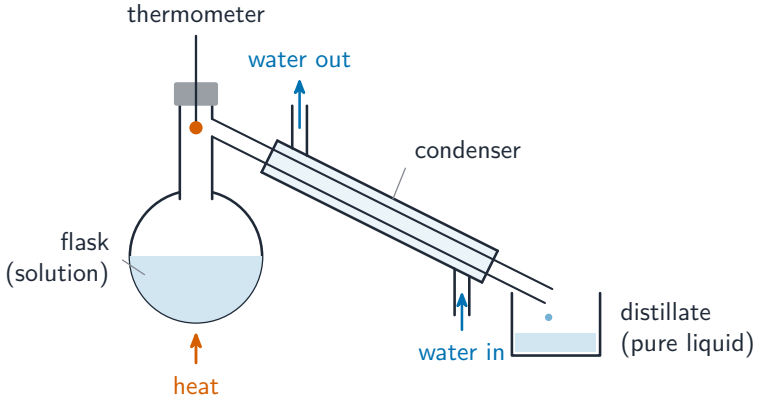
Crystallization

To get crystals of a soluble solid, such as copper(II) sulfate, from its solution:

1. Heat the solution to evaporate some of the water until it is **saturated** : a drop on a cold glass rod forms crystals.
2. Leave it to cool slowly. The solid is less soluble when cold, so crystals form.
3. Filter off the crystals, wash them with a little cold water and dry them.

Evaporating all the water instead gives a powder, and can decompose some solids or remove their water of crystallization.

Distillation



The liquid boils off, condenses in the cold condenser and collects as the distillate

- The liquid with the lower boiling point boils first. The vapour cools in the condenser and turns back into liquid.
- Cold water enters the condenser at the bottom and leaves at the top, so the jacket stays full.
- The thermometer bulb sits level with the side arm, so it reads the temperature of the vapour that is leaving.
- In fractional distillation a column filled with glass beads separates liquids whose boiling points are close: crude oil, or ethanol (78 °C) from water (100 °C).

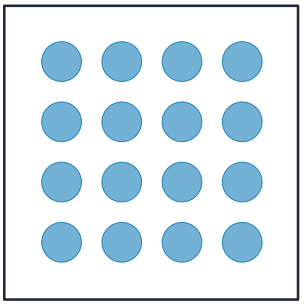
The kinetic molecular theory

Particles in the three states

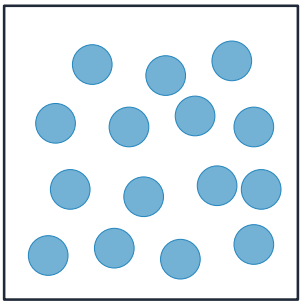
The **kinetic molecular theory** says that all matter is made of particles that are always moving. How the particles are arranged and how they move decides

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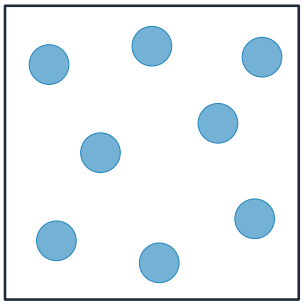
the state.



solid
regular, touching
vibrate in place



liquid
close, random
slide past each other



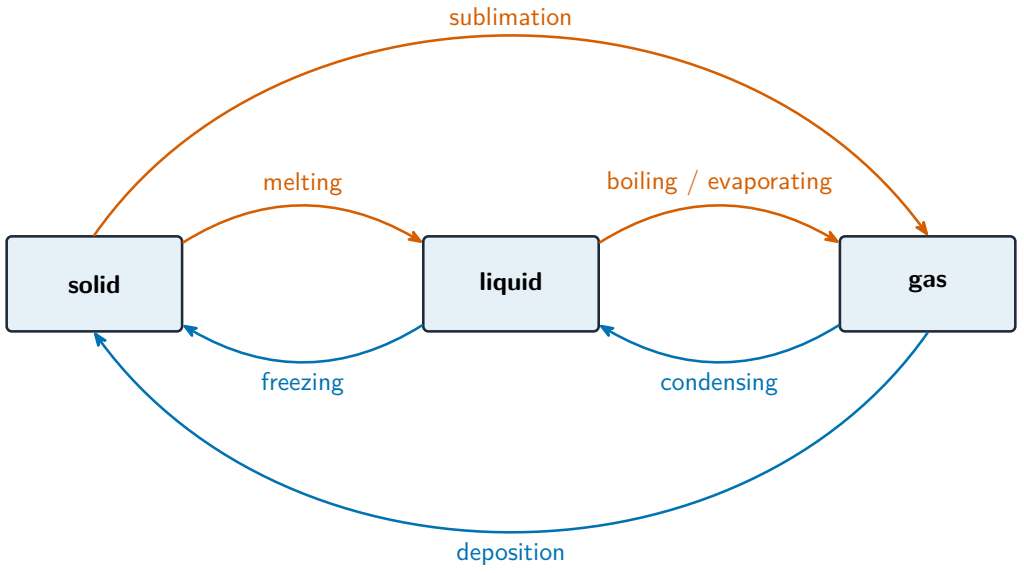
gas
far apart, random
move fast

The state depends on how close the particles are and how freely they move

	Solid	**Liquid**	**Gas**
Arrangement	regular, close together	random, close together	random, far apart
Movement	vibrate about fixed positions	move past each other	move fast in all directions
Forces between particles	strong	weaker	very weak
Shape	fixed	takes the shape of the container	fills the container
Volume	fixed	fixed	fills the container
Compressible?	no	hardly	yes

■ Changes of state

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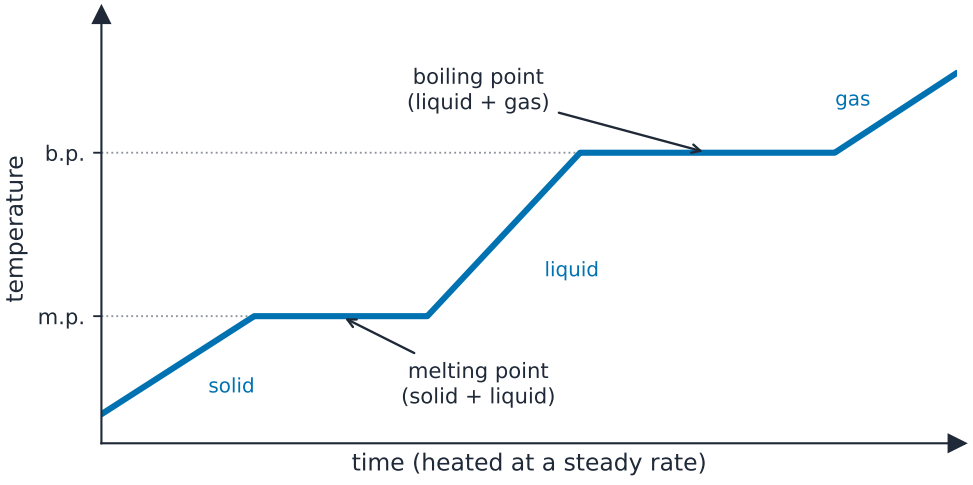
Orange changes need energy; blue changes release it

- Melting, boiling or evaporating, and **sublimation** (solid straight to gas) are **endothermic** : energy is taken in to overcome the forces between particles.
- Freezing, condensing and **deposition** (gas straight to solid) are **exothermic** : energy is released as forces form.
- Dry ice (solid CO_2) and iodine sublime at atmospheric pressure. Frost forming on a cold window is deposition.

Evaporation and boiling are different. Evaporation happens only at the surface and at any temperature: the fastest particles escape. Boiling happens throughout the liquid, at one temperature, the boiling point, and forms bubbles.

The heating curve

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plateau: attractions overcome; temperature constant

On each flat part the energy separates particles instead of making them move faster

- On the sloping parts the energy increases the kinetic energy of the particles, so the temperature rises.
- On the flat parts (the melting point and the boiling point) the energy is used to overcome the attractions between particles. The kinetic energy, and so the temperature, stays the same.
- The boiling plateau is longer than the melting plateau: it takes much more energy to separate the particles completely than to let them slide.
- A pure substance melts and boils at a sharp, fixed temperature. An impure substance melts over a range of temperatures, below the pure melting point. This is a simple test of **purity** .

Temperature and kinetic energy

The kelvin scale

The temperature of a substance is a measure of the **average kinetic energy** of its particles. In kelvin (K), the temperature is directly proportional to the average kinetic energy: double the temperature in K and you double the average kinetic energy.

$$T/\mathrm{K} = \theta/^{\circ}\mathrm{C} + 273$$

- 0 K, **absolute zero** (−273 °C), is the lowest possible temperature: the particles have the minimum possible kinetic energy.
- There are no negative temperatures on the kelvin scale, and no degree sign: write 298 K, not 298 °K.

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- A temperature change of 1 K is the same as a change of 1 °C.

■ **Worked example: converting temperatures**

- 25 °C: $25 + 273 = 298$ K.
- 77 K (liquid nitrogen boils): $77 - 273 = -196$ °C.
- Warming a gas from 27 °C to 327 °C, the temperature goes from 300 K to 600 K, so the average kinetic energy doubles. In degrees Celsius it looks like a twelve-fold rise, which is wrong.

Practice

1. Classify each as an element, a compound or a mixture: (a) carbon dioxide, (b) air, (c) copper, (d) sea water, (e) sodium chloride.
2. Classify each mixture as homogeneous or heterogeneous: (a) vinegar, (b) muddy water, (c) brass, (d) a fruit salad.
3. Describe how to get pure, dry crystals of copper(II) sulfate from a mixture of the solid with sand.
4. Explain why the thermometer bulb in a distillation is placed at the side arm, not in the liquid.
5. Explain how water can be collected from salty water by distillation.
6. Describe the arrangement and movement of particles in a liquid.
7. Explain why gases are easy to compress but liquids are not.
8. Name the change of state when (a) solid iodine turns to a purple vapour, (b) water vapour forms ice on a freezer wall.
9. Explain why the temperature stays constant while ice melts, although it is being heated.
10. A sample melts between 112 °C and 117 °C. The pure substance melts at 122 °C. What does this show?
11. Convert (a) −40 °C to K, (b) 373 K to °C.
12. A gas is heated from 200 K to 400 K. State how its average kinetic energy changes. Explain why heating from 20 °C to 40 °C does not double it.

Answers.

1. (a) compound, (b) mixture, (c) element, (d) mixture, (e) compound.
2. (a) homogeneous, (b) heterogeneous, (c) homogeneous, (d) heterogeneous.
3. Add water and stir (copper sulfate dissolves, sand does not). Filter: sand stays as the residue. Heat the filtrate until saturated, cool so crystals form, filter them off, wash with a little cold water and dry.
4. The thermometer must measure the temperature of the vapour that is distilling over, which tells you which substance is being collected.

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5. Heat the salty water: the water boils and its vapour passes into the condenser, cools and condenses, and drips into the beaker. The salt has a very high boiling point and stays in the flask.
6. Particles are close together in a random arrangement; they move and slide past each other.
7. Gas particles are far apart, with a lot of empty space between them; liquid particles are already close together.
8. (a) sublimation, (b) deposition.
9. The energy is used to overcome the forces between particles in the solid, not to increase their kinetic energy, so the temperature does not change until all the ice has melted.
10. The sample is impure: it melts over a range, below the pure melting point.
11. (a) $-40 + 273 = 233$ K, (b) $373 - 273 = 100$ °C.
12. It doubles, because kinetic energy is proportional to the temperature in K. 20 °C to 40 °C is 293 K to 313 K, an increase of only about 7%.

Exam tips

- "Mixture" means not chemically bonded; "compound" means chemically bonded in a fixed ratio.
- Name the property a separation uses: solubility, particle size or boiling point.
- On a heating curve, say that energy overcomes the forces between particles; the kinetic energy and temperature stay constant.
- Always convert to kelvin before comparing kinetic energies or using a gas law; write K without a degree sign.
- Evaporation happens at the surface at any temperature; boiling happens throughout the liquid at the boiling point.

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The nuclear atom

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

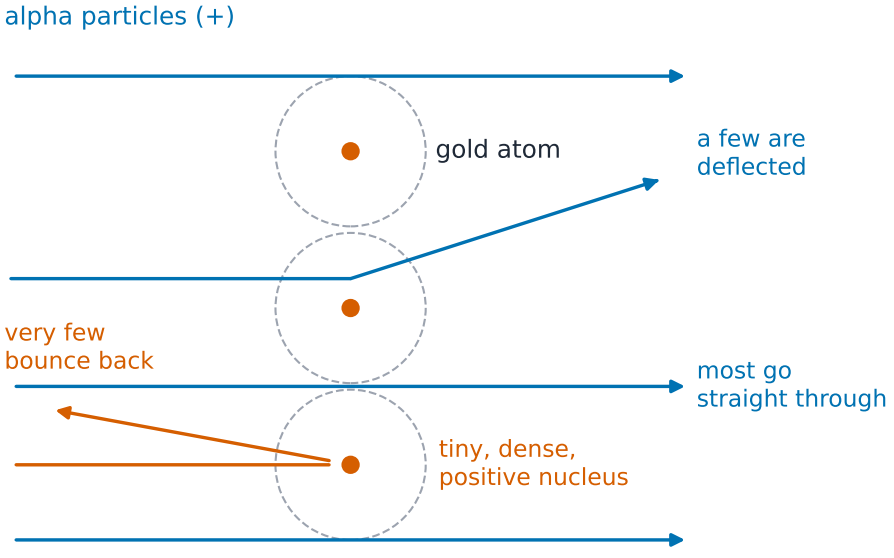
This handout teaches Structure 1.2, The nuclear atom, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: the particle model of matter from Structure 1.1, and positive and negative charge. Use the data booklet for relative atomic masses.

Inside the atom

What did Rutherford see?

In 1909 Geiger and Marsden fired alpha particles, which are small and positive, at a sheet of gold foil only a few hundred atoms thick. Almost all of them went straight through. But about 1 in 8000 bounced back towards the source. Rutherford said it was "as if you fired a 15-inch shell at a piece of tissue paper and it came back and hit you".



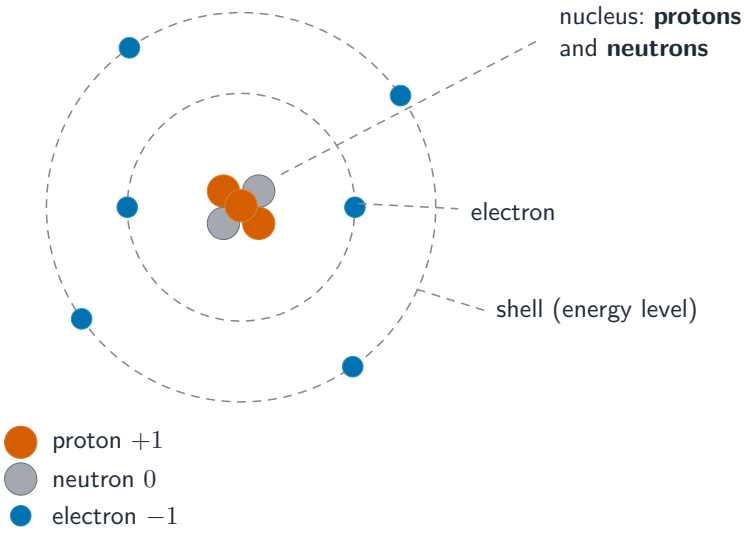
Most of an atom is empty space; its mass and positive charge sit in a tiny nucleus

- Most alpha particles pass straight through, so an atom is mostly empty space.
- A few are deflected, so there is a region of concentrated positive charge that repels them.
- Very few bounce back, so that region, the **nucleus** , is tiny and holds almost all the mass.

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The nucleus is about 10^{-15} m across, and the atom about 10^{-10} m: the atom is about 100 000 times wider than its nucleus.

Protons, neutrons and electrons



Protons and neutrons are in the nucleus; electrons occupy the space around it

Particle	Relative mass	Relative charge	Where
proton	1	+1	nucleus
neutron	1	0	nucleus
electron	1/1836 (about 0.0005)	−1	outside the nucleus

Protons and neutrons together are called **nucleons** . An atom has equal numbers of protons and electrons, so it has no overall charge.

Atomic number and mass number

Nuclear symbols

- The **atomic number** Z is the number of protons. It decides which element the atom is.
- The **mass number** A is the number of protons plus neutrons.
- Number of neutrons $= A - Z$.

The **nuclear symbol** writes A at the top left and Z at the bottom left: ${}^{23}_{11}\text{Na}$ has 11 protons, $23 - 11 = 12$ neutrons and 11 electrons.

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Ions

An **ion** has gained or lost electrons. The number of protons does not change.

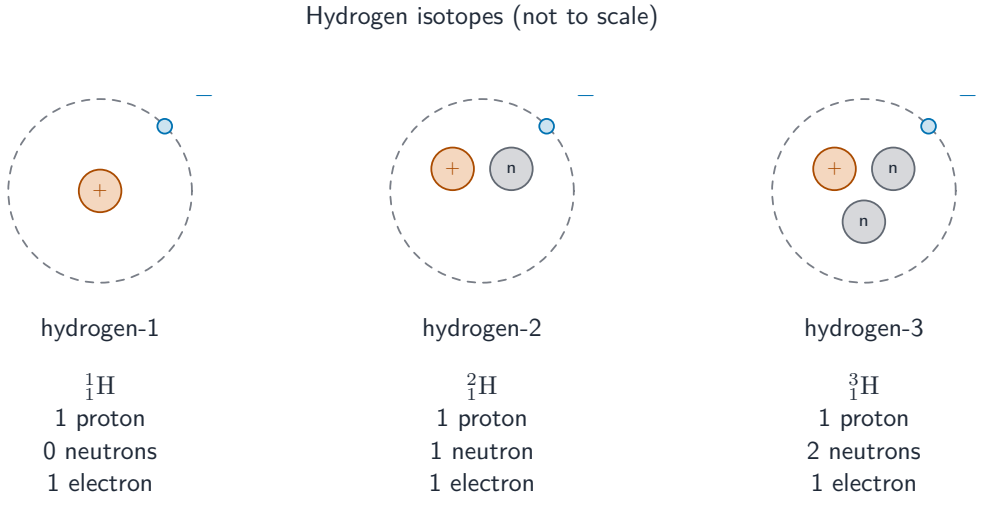
Species	Protons	Neutrons	Electrons
$^{23}_{11}\mathrm{Na}$	11	12	11
$^{23}_{11}\mathrm{Na}^{+}$	11	12	10
$^{32}_{16}\mathrm{S}^{2-}$	16	16	18
$^{27}_{13}\mathrm{Al}^{3+}$	13	14	10

A positive ion has fewer electrons than protons; a negative ion has more.

Isotopes

Same element, different mass

Isotopes are atoms of the same element with different numbers of neutrons: the same Z, a different A.



Isotopes differ only in the number of neutrons

- Isotopes have the same number of electrons, so they have the **same chemical properties**.
- They have different masses, so their **physical properties** differ slightly: density, rate of diffusion, and melting and boiling points. Heavy water, $\mathrm{D_2O}$, boils at 101.4 °C.
- Some isotopes are radioactive. Carbon-14 is used to date old wood and bone; cobalt-60 is used in radiotherapy; iodine-131 is used to treat thyroid disease.

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■ Relative atomic mass from abundances

The relative atomic mass A_r of an element is the weighted mean of the masses of its isotopes, using their **abundances** (percentages in a natural sample).

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

■ Worked example: chlorine

Chlorine is 75.8% ^{35}Cl and 24.2% ^{37}Cl.

$$A_r = \frac{35 \times 75.8 + 37 \times 24.2}{100} = \frac{2653 + 895.4}{100} = 35.5$$

The answer lies nearer 35 because ^{35}Cl is the more abundant isotope.

■ Worked example: finding an abundance

Copper has two isotopes, ^{63}Cu and ^{65}Cu, and $A_r = 63.55$. Let the abundance of ^{63}Cu be x%.

$$63x + 65(100 - x) = 63.55 \times 100$$

$$6500 - 2x = 6355 \quad \Rightarrow \quad x = 72.5$$

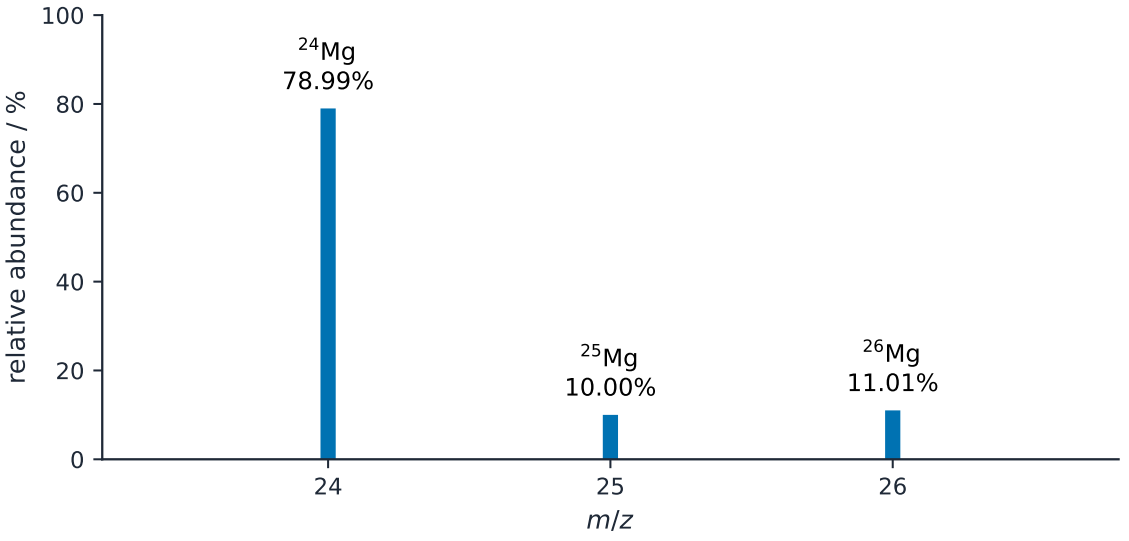
So ^{63}Cu is 72.5% and ^{65}Cu is 27.5%. (Using the exact isotope masses, 62.93 and 64.93, gives the measured 69%; with whole-number masses the answer is approximate.)

AHL: Mass spectra of elements

■ How a mass spectrum is read

A **mass spectrometer** turns atoms into positive ions and separates them by their mass-to-charge ratio, m/z. For ions with a 1+ charge, m/z equals the mass of the isotope.

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Each line is one isotope; its height is the isotope's relative abundance

- The number of lines is the number of isotopes.
- The position of each line gives the isotope's mass.
- The height gives its relative abundance.

Worked example: magnesium

$$A_r = \frac{24 \times 78.99 + 25 \times 10.00 + 26 \times 11.01}{100} = \frac{1895.8 + 250.0 + 286.3}{100} = 24.32$$

The data booklet value is 24.31.

When heights are not percentages

Sometimes the heights are given as relative intensities that do not add up to 100. Then divide by their total instead of by 100. For a spectrum with lines at m/z 10 (height 23) and 11 (height 100):

$$A_r = \frac{10 \times 23 + 11 \times 100}{23 + 100} = \frac{1330}{123} = 10.8$$

This is boron.

Practice

1. State the relative mass, relative charge and position of a proton, a neutron and an electron.
2. Explain what the gold-foil experiment showed about the structure of the atom.
3. Give the numbers of protons, neutrons and electrons in $^{40}_{20}\mathrm{Ca}^{2+}$ and in $^{19}_{9}\mathrm{F}^{-}$.

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4. A species has 26 protons, 30 neutrons and 23 electrons. Write its nuclear symbol with its charge.
5. Explain why ^{35}Cl and ^{37}Cl have the same chemical properties.
6. State one physical property that differs between isotopes, and explain why.
7. Neon is 90.5% ^{20}Ne, 0.3% ^{21}Ne and 9.2% ^{22}Ne. Calculate its A_r to 2 decimal places.
8. Gallium has isotopes ^{69}Ga and ^{71}Ga, and $A_r = 69.8$. Calculate the abundance of each.
9. **AHL.** A spectrum of an element has lines at m/z 79 (50.7%) and 81 (49.3%). Calculate A_r and identify the element.
10. **AHL.** Lines at m/z 28, 29 and 30 have heights 92.2, 4.7 and 3.1. Calculate A_r and identify the element.
11. **AHL.** Explain why the mass spectrum of chlorine gas, Cl_2, has lines at m/z 70, 72 and 74.

Answers.

1. Proton: 1, +1, nucleus. Neutron: 1, 0, nucleus. Electron: 1/1836, −1, outside the nucleus.
2. Most alpha particles passed straight through, so the atom is mostly empty space. A few were deflected or bounced back, so the positive charge and most of the mass are in a tiny, dense nucleus.
3. Ca^{2+}: 20 protons, 20 neutrons, 18 electrons. F^-: 9 protons, 10 neutrons, 10 electrons.
4. $^{56}_{26}Fe^{3+}$.
5. They have the same number of electrons (and the same electron configuration), and chemical reactions involve electrons.
6. Density, rate of diffusion, melting or boiling point: the isotopes have different masses.
7. $(20 \times 90.5 + 21 \times 0.3 + 22 \times 9.2)/100 = (1810 + 6.3 + 202.4)/100 = 20.19$.
8. $69x + 71(100 - x) = 6980$, so $7100 - 2x = 6980$ and $x = 60$: ^{69}Ga 60%, ^{71}Ga 40%.
9. **AHL.** $(79 \times 50.7 + 81 \times 49.3)/100 = 79.99$, about 80: bromine (data booklet 79.90).
10. **AHL.** $(28 \times 92.2 + 29 \times 4.7 + 30 \times 3.1)/(92.2 + 4.7 + 3.1) = 2810.9/100 = 28.11$: silicon.
11. **AHL.** Each Cl_2 molecule holds two atoms, each ^{35}Cl or ^{37}Cl: ^{35}Cl–^{35}Cl is 70, ^{35}Cl–^{37}Cl is 72 and ^{37}Cl–^{37}Cl is 74.

Exam tips

- The atomic number is the number of protons; never say "the number of electrons", which changes in an ion.

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- In an ion, change only the electrons: add for a negative charge, subtract for a positive one.
- Isotopes: "same number of protons, different number of neutrons". Say "same chemical properties because the same electron configuration".
- Give A_r to the precision the data allows, and check that it lies between the lightest and heaviest isotope, nearer the more abundant one.
- **AHL.** If the line heights do not add up to 100, divide by their sum.

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Structure 1.3 · Electron configurations

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Scope and prerequisites

This handout teaches Structure 1.3, Electron configurations, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: protons, neutrons and electrons from Structure 1.2, the atomic number Z, and arithmetic with powers of ten. You will use three relations from the data booklet: $c = f\lambda$, $E = hf$ and the Avogadro constant N_A.

Light, energy and emission spectra

Why do atoms give out coloured light?

Put a little sodium salt in a flame and the flame turns orange-yellow. Pass a high voltage through hydrogen gas in a tube and it glows pink. Each element gives its own colours. The colours tell us how the electrons in the atom are arranged.

Light carries energy in packets

Light is part of the **electromagnetic spectrum** . All of it travels at the same speed $c = 3.00 \times 10^8$ m s^{-1}, and its frequency f and wavelength λ are linked by

$$c = f\lambda$$

Light is given out and taken in as packets of energy called **photons** . The energy of one photon depends only on its frequency:

$$E = hf$$

Here $h = 6.63 \times 10^{-34}$ J s is the Planck constant. So **higher frequency means higher energy and shorter wavelength**.

Region	Wavelength	Frequency and photon energy
infrared	longer than about 700 nm	lowest of the three
visible: red → violet	about 700 nm → 400 nm	rising
ultraviolet	shorter than about 400 nm	highest of the three

In the visible region, red light has the longest wavelength and the lowest energy; violet light has the shortest wavelength and the highest energy.

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Continuous and line spectra

White light from a hot solid, such as a lamp filament, contains every visible wavelength. A prism spreads it into a **continuous spectrum** : a smooth band of colour with no gaps.

Light from excited gas atoms is different. A prism spreads it into a few sharp coloured lines on a dark background. This is a **line emission spectrum** . Every element has its own pattern of lines, so the spectrum works like a fingerprint for the element.

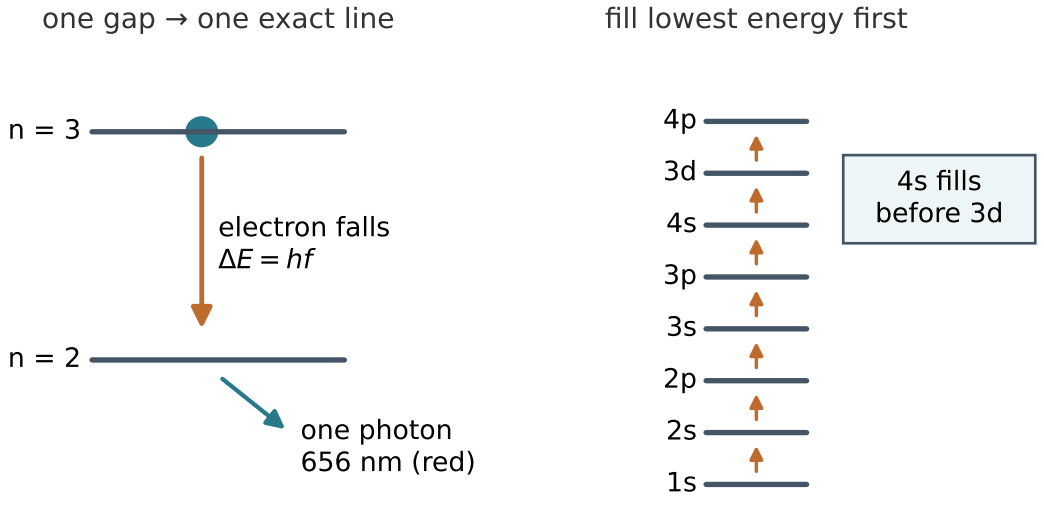
Where the lines come from

An electron in an atom can only have certain fixed energies, called **energy levels** . When the atom absorbs energy (from a flame or an electric current), an electron moves up to a higher level. The atom is now in an **excited state** .

The electron then falls back to a lower level. It gives out the energy difference as **one photon**:

$$\Delta E = E_{\text{upper}} - E_{\text{lower}} = hf$$

Only certain gaps exist, so only certain photon energies, and therefore only certain frequencies, appear. That is why we see separate lines and not a continuous band.



One fixed energy gap gives one line; on the right, sublevels fill lowest energy first, 4s before 3d

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The hydrogen spectrum is evidence for energy levels

Hydrogen has one electron, so its spectrum is the simplest. Two features matter:

- **The lines are separate.** If the electron could have any energy, hydrogen would give a continuous spectrum. The separate lines show that the energy of the electron is **quantized** : it can only take fixed values.
- **The lines get closer together at higher frequency.** The levels themselves get closer together as n increases, so the lines **converge** . Above the **convergence limit** there are no more lines.

Which line appears depends on the level the electron falls to. Falls to $n = 1$ give the largest gaps, so those photons are ultraviolet. Falls to $n = 2$ give visible light, such as the red line at 656 nm. Falls to $n = 3$ give infrared.

> **Worked example.** The red line of hydrogen has $\lambda = 656$ nm. Find the energy gap it comes from.

1. Convert the wavelength: $\lambda = 656 \times 10^{-9}$ m.
2. Find the frequency: $f = \dfrac{c}{\lambda} = \dfrac{3.00 \times 10^{8}}{656 \times 10^{-9}} = 4.57 \times 10^{14}$ Hz.
3. Find the energy: $E = hf = 6.63 \times 10^{-34} \times 4.57 \times 10^{14} = 3.03 \times 10^{-19}$ J.

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

Energy levels, sublevels and orbitals

Main energy levels

The main energy levels are numbered by the **principal quantum number** $n = 1, 2, 3, \ldots$ Level n can hold at most $2n^2$ electrons.

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

Sublevels and orbitals

Each main level is split into **sublevels** called s, p, d and f. Each sublevel is made of **atomic orbitals** . An orbital is a region around the nucleus where there is a high chance of finding an electron. One orbital holds at most two electrons.

Sublevel	**Orbitals**	**Maximum electrons**
s	1	2
p	3	6
d	5	10
f	7	14

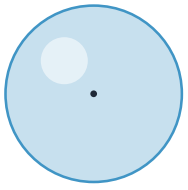
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Check: level $n = 3$ has 3s + 3p + 3d = 2 + 6 + 10 = 18 electrons, which matches $2n^2 = 18$.

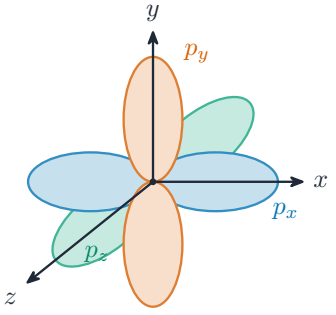
■ Shapes of s and p orbitals

You need to recognise two shapes:

- An **s orbital** is a sphere centred on the nucleus. A 2s orbital is larger than a 1s orbital.
- A **p orbital** has two lobes on opposite sides of the nucleus, like a dumbbell. The three p orbitals of one level point along the x, y and z axes, at right angles to each other. They are named p_x, p_y and p_z.



s orbital
(sphere)



p orbitals
(two lobes each)

An s orbital is a sphere; the three p orbitals are dumbbells along x, y and z

The three p orbitals of one sublevel have the same energy. Orbitals with equal energy are called **degenerate** .

Writing electron configurations

■ Three rules for filling orbitals

1. **Aufbau principle** : electrons go into the lowest-energy orbital available first.
2. **Pauli exclusion principle** : an orbital holds at most two electrons, and they must have **opposite spins** .
3. **Hund's rule** : in a set of degenerate orbitals, electrons go in singly with parallel spins before any orbital gets a second electron. Single electrons in separate orbitals repel each other less.

For atoms up to $Z = 36$, the order of filling is:

$$1s \rightarrow 2s \rightarrow 2p \rightarrow 3s \rightarrow 3p \rightarrow 4s \rightarrow 3d \rightarrow 4p$$

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Notice that 4s fills **before** 3d. In a neutral atom up to calcium, 4s is lower in energy than 3d.

Full and condensed configurations

A **full electron configuration** lists every sublevel with its number of electrons as a superscript:

- sulfur, $Z = 16$: $1s^2\,2s^2\,2p^6\,3s^2\,3p^4$
- iron, $Z = 26$: $1s^2\,2s^2\,2p^6\,3s^2\,3p^6\,4s^2\,3d^6$

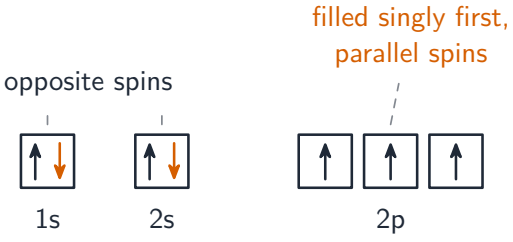
A **condensed configuration** replaces the inner electrons with the symbol of the noble gas before the element, in square brackets:

- sulfur: $[\mathrm{Ne}]\,3s^2\,3p^4$
- iron: $[\mathrm{Ar}]\,4s^2\,3d^6$

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

Orbital diagrams

An **orbital diagram** draws each orbital as a box and each electron as a half-arrow. Two arrows in one box point in opposite directions (Pauli). Within a sublevel, fill every box with one arrow, all pointing the same way, before you add a second arrow to any box (Hund).



Nitrogen, $1s^2\,2s^2\,2p^3$: paired spins in 1s and 2s; the three 2p electrons sit singly with parallel spins

Nitrogen therefore has **three unpaired electrons**. Oxygen, $2p^4$, has one pair and two unpaired electrons in its 2p sublevel.

> **Worked example.** Draw the orbital diagram of the 3d and 4s sublevels of iron.

Iron is $[\mathrm{Ar}]\,4s^2\,3d^6$. The 4s box holds two opposite arrows. Six electrons go into five 3d boxes: one up-arrow in each of the five boxes, then the sixth pairs up in the first box. Iron has **four** unpaired electrons.

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Two exceptions: chromium and copper

Two atoms in the first row of the d-block do not follow the simple order:

- chromium, $Z = 24$: $[\mathrm{Ar}]\,4s^1\,3d^5$, not $4s^2\,3d^4$
- copper, $Z = 29$: $[\mathrm{Ar}]\,4s^1\,3d^{10}$, not $4s^2\,3d^9$

In both, one electron moves from 4s into 3d to give a half-full or full 3d sublevel, which gives a lower total energy for these atoms. Learn these two as facts.

Configurations of ions

- For a **negative ion** , add electrons to the next available orbital. Oxide, O^{2-}: $1s^2\,2s^2\,2p^6$, the same as neon.
- For a **positive ion** of a main-group element, remove electrons from the outermost level. Na^+: $1s^2\,2s^2\,2p^6$.
- For a positive ion of a **transition element** , remove the **4s electrons first**, then 3d electrons. Once 3d is occupied, 4s is no longer the lower level.

Species	Configuration
Fe	$[\mathrm{Ar}]\,4s^2\,3d^6$
Fe^{2+}	$[\mathrm{Ar}]\,3d^6$
Fe^{3+}	$[\mathrm{Ar}]\,3d^5$
Cu^+	$[\mathrm{Ar}]\,3d^{10}$

A common error is to write Fe^{2+} as $[\mathrm{Ar}]\,4s^2\,3d^4$. Remember: **4s fills first and empties first.**

AHL: Ionization energy from the convergence limit

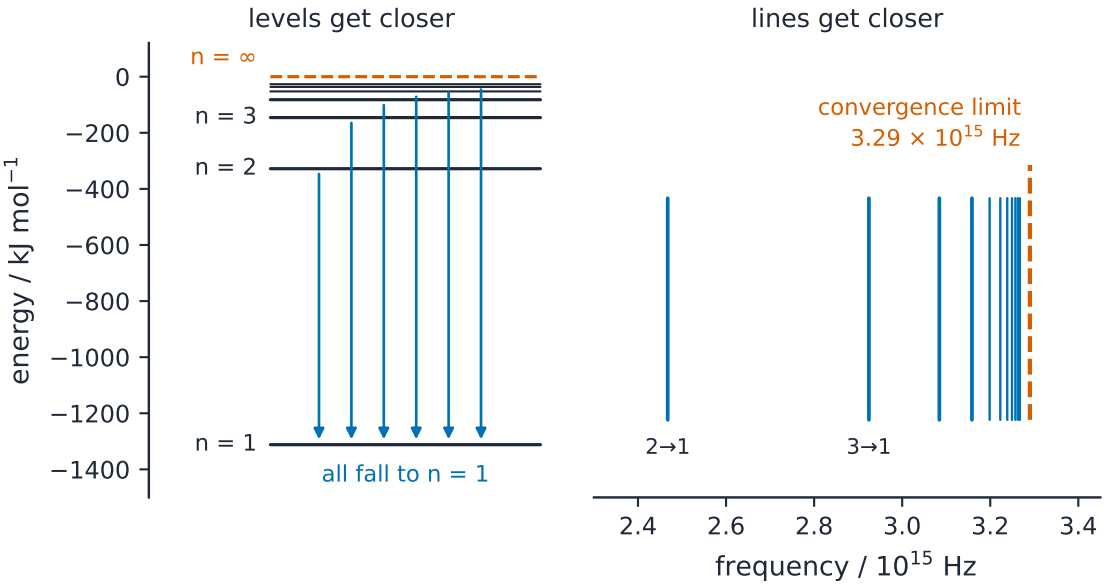
What the convergence limit means

The **first ionization energy** is the minimum energy needed to remove one electron from each atom in one mole of gaseous atoms, in their ground state:

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

Look again at the lines that end on $n = 1$ in hydrogen. As the upper level gets higher, the lines crowd together. At the convergence limit, the electron is falling from $n = \infty$: it starts completely outside the atom. So the photon energy at the convergence limit equals the energy needed to remove the electron from $n = 1$, which is the ionization energy of one atom.

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As the levels crowd together, the lines crowd together; the convergence limit gives the ionization energy

■ Calculating ionization energy from spectral data

The photon energy gives the energy for **one** atom. Multiply by the Avogadro constant to get the value for one mole, then convert to kJ:

$$\text{IE} = hf \times N_A$$

> **Worked example.** The lines in the ultraviolet spectrum of hydrogen converge at $\lambda = 91.2$ nm. Calculate the first ionization energy of hydrogen in kJ mol^{-1}.

1. $f = \dfrac{c}{\lambda} = \dfrac{3.00 \times 10^{8}}{91.2 \times 10^{-9}} = 3.29 \times 10^{15}$ Hz
2. One atom: $E = hf = 6.63 \times 10^{-34} \times 3.29 \times 10^{15} = 2.18 \times 10^{-18}$ J
3. One mole: $2.18 \times 10^{-18} \times 6.02 \times 10^{23} = 1.31 \times 10^{6}$ J mol^{-1}
4. Convert: 1.31×10^{6} J mol^{-1} $= 1310$ kJ mol^{-1}

The data booklet value is 1312 kJ mol^{-1}, so the answer agrees. The two most common lost marks are forgetting N_A and forgetting to divide by 1000.

AHL: Ionization energies as evidence for sublevels

■ What decides the size of an ionization energy

An ionization energy measures how strongly the nucleus holds the electron being removed. Three factors decide it:

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- **Nuclear charge** : more protons pull harder, so the ionization energy is higher.
- **Distance from the nucleus**: an electron in a higher level is further away and held less strongly.
- **Shielding** : inner electrons repel the outer electron and cancel part of the nuclear pull.

Trends across a period and down a group

Across a period, the first ionization energy generally **increases**. The nuclear charge increases by one each time, but the new electron goes into the same main level, so shielding hardly changes. The outer electrons are held more tightly.

Down a group, the first ionization energy **decreases**. Each element has one more occupied level, so the outer electron is further from the nucleus and more shielded. This outweighs the larger nuclear charge.

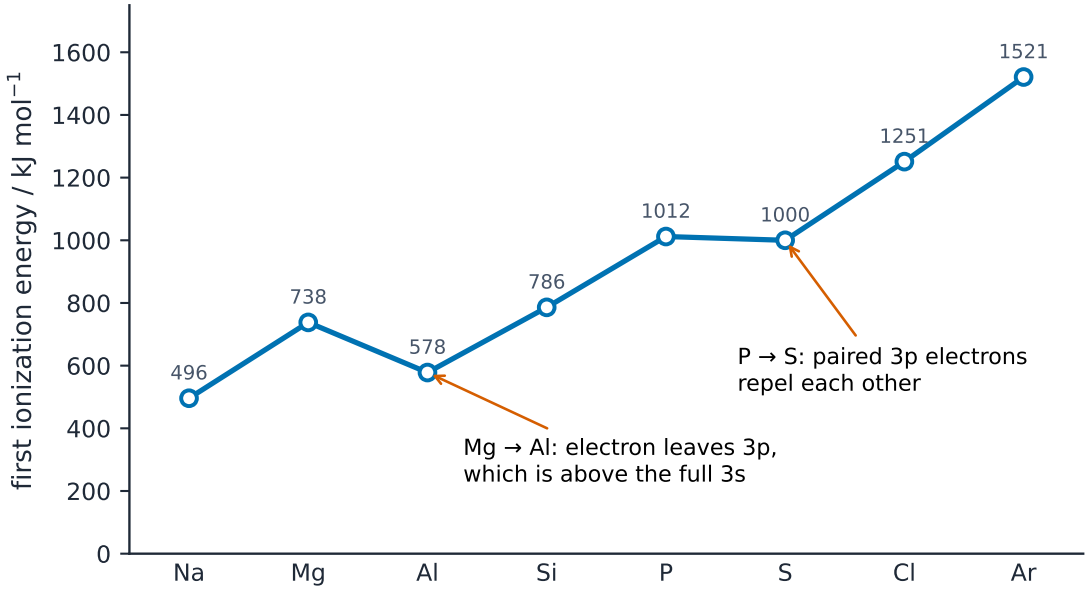
The two dips across a period

The rise across Period 3 is not smooth. There are two small drops, and they are evidence that sublevels exist:

- **Mg → Al.** Magnesium is $[\mathrm{Ne}]\,3s^2$. Aluminium is $[\mathrm{Ne}]\,3s^2\,3p^1$, so its first electron is removed from a 3p orbital. The 3p sublevel is higher in energy than 3s, so less energy is needed.
- **P → S.** Phosphorus is $[\mathrm{Ne}]\,3s^2\,3p^3$ with three unpaired 3p electrons. Sulfur, $3p^4$, has one 3p orbital with two electrons in it. These paired electrons repel each other, so one is easier to remove.

The same two dips appear in Period 2, at B and at O.

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First ionization energy rises across Period 3 but drops at Al (3p above 3s) and at S (paired 3p electrons)

Successive ionization energies

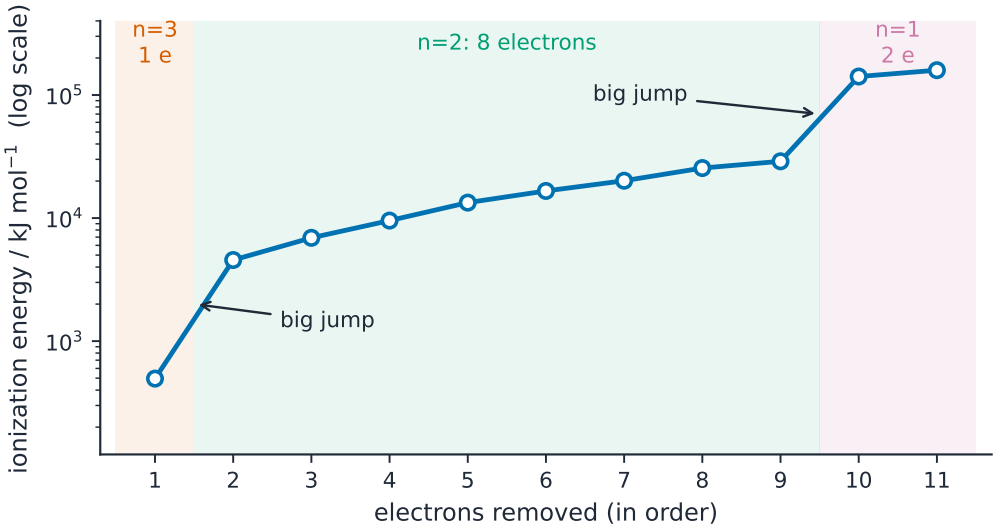
The **second ionization energy** removes an electron from the +1 ion:

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

Removing the electrons one at a time gives the **successive ionization energies** . Each value is larger than the one before, because each electron is removed from an ion that is more positive.

When you plot them, look for **big jumps**. A big jump means the next electron must come from a main level closer to the nucleus. For sodium, the pattern is 1 easy electron, a big jump, 8 more, another big jump, then the last 2. This matches the configuration 2, 8, 1.

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big jump = next electron from a shell closer to the nucleus (shell structure)

Successive ionization energies of sodium (log scale): the big jumps reveal the 2, 8, 1 arrangement

To find the group of a main-group element, count the electrons removed **before** the first big jump. That is the number of outer electrons: 1 means Group 1, 2 means Group 2, 3 means Group 13, and so on up to 8 for Group 18.

> **Worked example.** The first five ionization energies of an element, in kJ mol^{-1}, are 578, 1817, 2745, 11 577 and 14 842. Identify its group.

The values rise steadily for the first three electrons. From the 3rd (2745) to the 4th (11 577) the value more than quadruples: that is the big jump. Three electrons came off before it, so the element has three outer electrons and is in **Group 13**. (These are the values for aluminium.)

Smaller steps inside one main level also show sublevels. In aluminium, the first electron (from 3p) is easier to remove than the next two (from 3s).

Practice

1. A line in the emission spectrum of an element has $\lambda = 589$ nm. Calculate the energy of one photon of this light.
2. State the maximum number of electrons in the $n = 4$ level, and name its sublevels.
3. Write the full configuration of chlorine and the condensed configuration of Cr^{3+}.
4. How many unpaired electrons does a phosphorus atom have? Draw its 3s and 3p orbital diagram.
5. Explain why the emission spectrum of hydrogen is a line spectrum and not a continuous spectrum.

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6. **AHL.** The convergence limit in the spectrum of sodium is at $\lambda = 241$ nm. Calculate the first ionization energy of sodium in kJ mol^{-1}.
7. **AHL.** Explain why the first ionization energy of oxygen is lower than that of nitrogen.

Answers.

1. $f = \dfrac{3.00 \times 10^{8}}{589 \times 10^{-9}} = 5.09 \times 10^{14}$ Hz; $E = 6.63 \times 10^{-34} \times 5.09 \times 10^{14} = 3.38 \times 10^{-19}$ J.
2. $2n^2 = 32$; the sublevels are 4s, 4p, 4d and 4f.
3. Cl: $1s^2\,2s^2\,2p^6\,3s^2\,3p^5$. Cr is $[Ar]\,4s^1\,3d^5$; removing the 4s electron and then two 3d electrons gives Cr^{3+}: $[Ar]\,3d^3$.
4. Three: 3s holds one pair, and each of the three 3p orbitals holds one electron with parallel spins.
5. The electron can only have fixed energies (energy levels). A photon is given out when the electron falls between two levels, so only certain energy gaps, and therefore only certain frequencies, are possible.
6. **AHL.** $f = \dfrac{3.00 \times 10^{8}}{241 \times 10^{-9}} = 1.24 \times 10^{15}$ Hz; $E = 6.63 \times 10^{-34} \times 1.24 \times 10^{15} = 8.25 \times 10^{-19}$ J; $\times\, 6.02 \times 10^{23} = 4.97 \times 10^{5}$ J mol^{-1} $= 497$ kJ mol^{-1}.
7. **AHL.** Oxygen ($2p^4$) has one 2p orbital holding a pair of electrons. The repulsion between the paired electrons makes one of them easier to remove than any electron in nitrogen ($2p^3$), where all three 2p electrons are unpaired.

Exam tips

- Link **frequency, energy and wavelength** in one sentence: higher frequency means higher photon energy and shorter wavelength.
- To explain a line spectrum, mention **both** ideas: electrons occupy fixed energy levels, and a photon is emitted when an electron **falls** to a lower level.
- The lines **converge** at higher frequency because the energy levels get closer together.
- Write 4s before 3d when filling, but **remove 4s first** when forming a transition-metal ion.
- Learn Cr ($4s^1\,3d^5$) and Cu ($4s^1\,3d^{10}$) as exceptions.
- **AHL:** in a convergence-limit calculation, multiply by N_A and convert J to kJ.
- **AHL:** to place an element in a group, count the electrons removed before the first **big jump**.

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Counting particles by mass: the mole

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Structure 1.4, Counting particles by mass: the mole, for the course first assessed in 2025. All of it is SL and HL content.

Prerequisites: atoms, isotopes and ions from Structure 1.2, chemical formulae, and standard form (6.02×10^{23}) on a calculator. Use the relative atomic masses from the data booklet.

The mole

How do you count grains of rice?

Nobody counts rice one grain at a time. A shop sells it by mass: if one grain has a mass of 0.02 g, then 1 kg holds about 50 000 grains. Chemists have the same problem with atoms, which are far too small and too many to count. They also count by weighing.

The Avogadro constant

The **mole** (symbol mol) is the unit of **amount of substance**. One mole contains exactly 6.02×10^{23} particles. This number is the **Avogadro constant**, $N_A = 6.02 \times 10^{23}$ mol^{-1}.

$$N = n \times N_A$$

N is the number of particles and n is the amount in moles.

- Always say which particles you mean: atoms, molecules, ions or **formula units**.
- One mole of H_2O molecules contains 2 mol of H atoms and 1 mol of O atoms.

Worked example: counting particles

How many molecules and how many atoms are in 0.50 mol of water?

- Molecules: $0.50 \times 6.02 \times 10^{23} = 3.01 \times 10^{23}$.
- Each H_2O molecule has 3 atoms, so atoms $= 3 \times 3.01 \times 10^{23} = 9.03 \times 10^{23}$.

Relative masses and molar mass

Relative atomic mass

The **relative atomic mass** A_r is the weighted mean mass of the atoms of an element, relative to one twelfth of the mass of a carbon-12 atom. It has no units.

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$$A_r = \frac{(75 \times 35) + (25 \times 37)}{100} = 35.5$$

A_r is a weighted mean of the isotope masses, so it is rarely a whole number

Natural chlorine is about 75% ^{35}Cl and 25% ^{37}Cl, so its A_r lies closer to 35 than to 37. The data booklet value is 35.45.

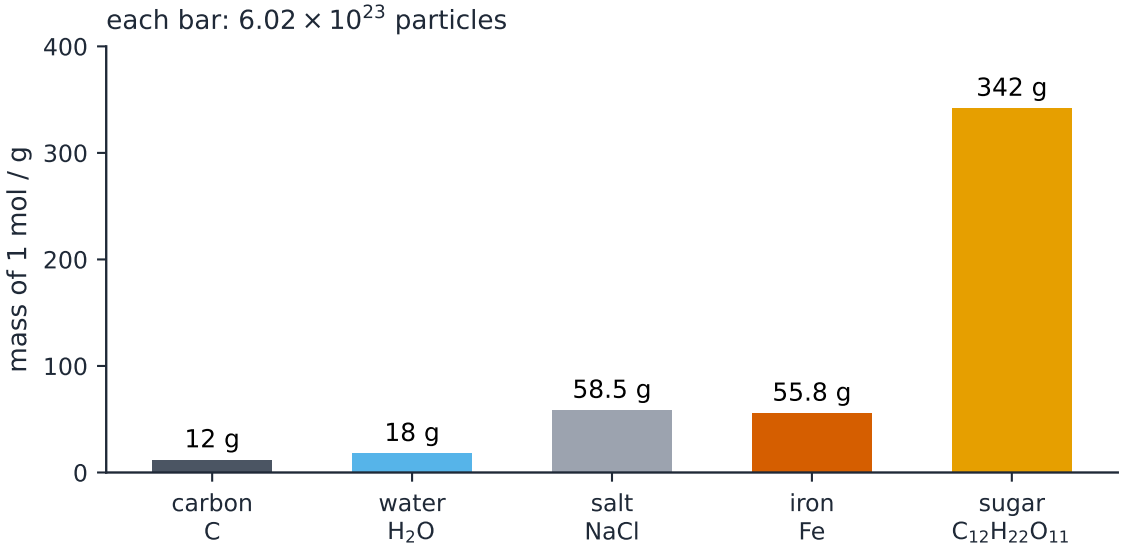
Relative formula mass

The **relative formula mass** M_r is the sum of the A_r values of all the atoms in the formula. "Relative molecular mass" is used for molecules.

$$M_r(\mathrm{CaCO_3}) = 40.08 + 12.01 + 3 \times 16.00 = 100.09$$

Molar mass

The **molar mass** M is the mass of one mole of a substance. It has the same number as M_r, with units g mol^{-1}: $M(\mathrm{CaCO_3}) = 100.09$ g mol^{-1}.



One mole of each substance has the same number of particles but a different mass

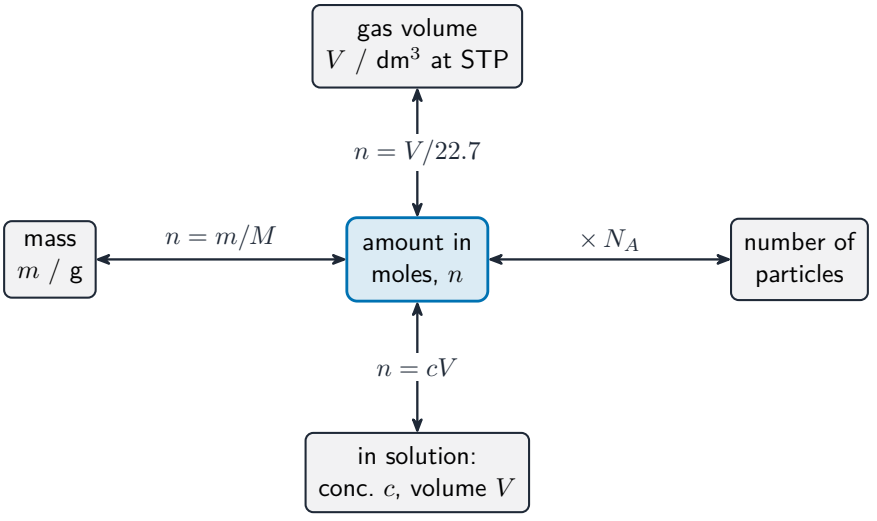
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Moles, mass and the mole map

Mass to moles

$$n = \frac{m}{M}$$

m in g, M in g mol^{-1}, n in mol.



Every route between quantities passes through the amount in moles

Worked example: mass to particles

How many molecules are in 4.4 g of carbon dioxide?

- $M(\mathrm{CO_2}) = 12.01 + 2 \times 16.00 = 44.01$ g mol^{-1}.
- $n = 4.4/44.01 = 0.10$ mol.
- $N = 0.10 \times 6.02 \times 10^{23} = 6.0 \times 10^{22}$ molecules.

Worked example: moles to mass

What is the mass of 0.250 mol of sodium chloride?

- $M(\mathrm{NaCl}) = 22.99 + 35.45 = 58.44$ g mol^{-1}.
- $m = n \times M = 0.250 \times 58.44 = 14.6$ g.

Percentage by mass

$$\%\text{ of element} = \frac{(\text{number of atoms}) \times A_r}{M_r} \times 100$$

For ammonium nitrate, $\mathrm{NH_4NO_3}$: $M_r = 80.06$, and it has 2 N atoms, so % N $= 2 \times 14.01/80.06 \times 100 = 35.0\%$. Farmers compare fertilizers this way.

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Empirical and molecular formulae

Two kinds of formula

- The **empirical formula** is the simplest whole-number ratio of the atoms of each element in a compound.
- The **molecular formula** is the actual number of atoms of each element in one molecule.

Compound	Molecular formula	Empirical formula
ethane	C_2H_6	CH_3
glucose	$C_6H_{12}O_6$	CH_2O
benzene	C_6H_6	CH
water	H_2O	H_2O

The molecular formula is always a whole-number multiple of the empirical formula.

Finding an empirical formula

1. Write the mass (or percentage) of each element.
2. Divide each by its A_r to get moles.
3. Divide every value by the smallest.
4. If a value ends in .5, .33 or .25, multiply all of them to get whole numbers.

element	% by mass	$\div A_r \rightarrow$ moles	$\div$ smallest (3.33)	ratio
C	40.0	$40.0/12 = 3.33$	1.0	1
H	6.7	$6.7/1 = 6.7$	2.0	2
O	53.3	$53.3/16 = 3.33$	1.0	1

empirical formula CH_2O - if $M_r = 180$, it fits $180/30 = 6$ times: molecular formula $C_6H_{12}O_6$

Divide by A_r, then by the smallest number of moles

Worked example: from masses to the molecular formula

A hydrocarbon contains 2.40 g of carbon and 0.60 g of hydrogen. Its M_r is 30.08.

- C: $2.40/12.01 = 0.200$ mol. H: $0.60/1.01 = 0.594$ mol.
- Divide by 0.200: C 1, H $2.97 \approx 3$. Empirical formula CH_3, with $M_r = 15.04$.
- $30.08/15.04 = 2$, so the molecular formula is C_2H_6.

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■ Worked example: water of crystallization

2.50 g of blue hydrated copper(II) sulfate, $CuSO_4 \cdot xH_2O$, is heated until it becomes white. 1.60 g of anhydrous $CuSO_4$ remains.

- Water lost: $2.50 - 1.60 = 0.90$ g; $0.90/18.02 = 0.0499$ mol.
- $CuSO_4$: $1.60/159.62 = 0.0100$ mol.
- Ratio $0.0499/0.0100 = 4.99 \approx 5$, so $x = 5$: $CuSO_4 \cdot 5H_2O$.

Concentration of solutions

■ Molar concentration

A **solution** is a **solute** dissolved in a **solvent** . The **concentration** is the amount of solute per unit volume of solution.

$$c = \frac{n}{V}$$

c in mol dm^{-3}, n in mol, V in dm^3. Remember 1 dm^3 = 1000 cm^3, so divide a volume in cm^3 by 1000.

Concentration can also be given in g dm^{-3}: multiply mol dm^{-3} by the molar mass.

■ Worked example: making a solution

5.85 g of NaCl is dissolved in water and made up to 250 cm^3.

- $n = 5.85/58.44 = 0.100$ mol.
- $V = 250/1000 = 0.250$ dm^3.
- $c = 0.100/0.250 = 0.400$ mol dm^{-3}, which is $0.400 \times 58.44 = 23.4$ g dm^{-3}.

A **standard solution** has an accurately known concentration. Weigh the solid, dissolve it, transfer every drop to a volumetric flask, and make up to the mark with distilled water.

■ Dilution

Adding water does not change the amount of solute, only the volume:

$$c_1V_1 = c_2V_2$$

25.0 cm^3 of 2.00 mol dm^{-3} acid made up to 500 cm^3 gives $c_2 = 2.00 \times 25.0/500 = 0.100$ mol dm^{-3}.

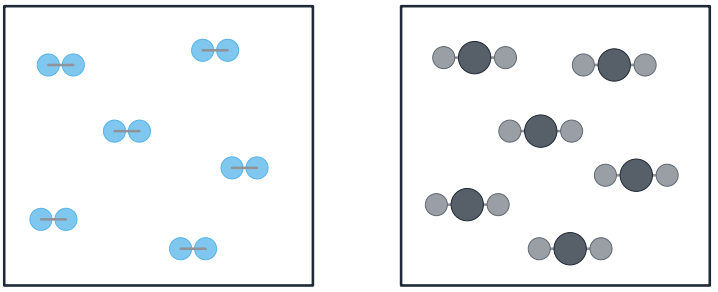
Avogadro's law

■ Equal volumes, equal numbers

Avogadro's law : equal volumes of all gases, at the same temperature and pressure, contain equal numbers of molecules.

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same volume, same temperature and pressure



hydrogen, H_2 carbon dioxide, CO_2

the same **number** of molecules (6 each), even though CO_2 is bigger

Gas molecules are far apart, so their size hardly affects the volume

It works because the molecules in a gas are very far apart. The volume is almost all empty space, so it depends on the number of molecules, not on their size.

At STP (273 K and 100 kPa) one mole of any ideal gas occupies 22.7 dm^3 (data booklet).

■ Volumes of reacting gases

For gases at the same temperature and pressure, the volume ratio equals the mole ratio in the equation.

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$$

20 cm^3 of methane needs 40 cm^3 of oxygen and makes 20 cm^3 of carbon dioxide. The water is a liquid at room temperature, so it is not counted as a gas volume.

Practice

1. Calculate the number of atoms in 0.20 mol of ammonia, NH_3.
2. Natural boron is 20% ^{10}B and 80% ^{11}B. Calculate its A_r.
3. Calculate the molar mass of calcium hydroxide, $Ca(OH)_2$.
4. Calculate the amount in moles in 8.0 g of methane, CH_4.
5. Calculate the mass of 3.01×10^{23} molecules of oxygen, O_2.
6. Calculate the percentage by mass of iron in iron(III) oxide, Fe_2O_3.
7. A compound contains 85.6% carbon and 14.4% hydrogen by mass. Its M_r is 56.12. Find the empirical and molecular formulae.
8. 3.00 g of magnesium burns to give 4.97 g of oxide. Find the empirical formula of the oxide.

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9. 4.80 g of hydrated magnesium sulfate, $MgSO_4 \cdot xH_2O$, loses 2.46 g of water on heating. Find x.
10. Calculate the concentration in mol dm^{-3} of 2.00 g of NaOH in 500 cm^3 of solution.
11. What volume of 0.500 mol dm^{-3} HCl must be diluted to make 250 cm^3 of 0.0200 mol dm^{-3} HCl?
12. 50 cm^3 of propane burns: $C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$. Calculate the volume of oxygen used and of carbon dioxide made, at the same temperature and pressure.

Answers.

1. Molecules $= 0.20 \times 6.02 \times 10^{23} = 1.20 \times 10^{23}$; 4 atoms each, so 4.82×10^{23} atoms.
2. $(20 \times 10 + 80 \times 11)/100 = 10.8$.
3. $40.08 + 2 \times (16.00 + 1.01) = 74.10$ g mol^{-1}.
4. $M = 16.05$ g mol^{-1}; $n = 8.0/16.05 = 0.50$ mol.
5. $n = 3.01 \times 10^{23}/6.02 \times 10^{23} = 0.500$ mol; $m = 0.500 \times 32.00 = 16.0$ g.
6. $M_r = 2 \times 55.85 + 3 \times 16.00 = 159.70$; % Fe $= 111.70/159.70 \times 100 = 69.9\%$.
7. C: $85.6/12.01 = 7.13$; H: $14.4/1.01 = 14.3$; ratio 1 : 2, so CH_2 ($M_r = 14.03$). $56.12/14.03 = 4$, so C_4H_8.
8. O: $4.97 - 3.00 = 1.97$ g. Mg: $3.00/24.31 = 0.123$ mol; O: $1.97/16.00 = 0.123$ mol. Ratio 1 : 1, so MgO.
9. $MgSO_4$: $4.80 - 2.46 = 2.34$ g, $2.34/120.38 = 0.0194$ mol. Water: $2.46/18.02 = 0.137$ mol. $0.137/0.0194 = 7.0$, so $x = 7$.
10. $n = 2.00/40.00 = 0.0500$ mol; $c = 0.0500/0.500 = 0.100$ mol dm^{-3}.
11. $V_1 = 0.0200 \times 250/0.500 = 10.0$ cm^3.
12. Oxygen $5 \times 50 = 250$ cm^3; carbon dioxide $3 \times 50 = 150$ cm^3.

Exam tips

- Say which particle you count: "0.5 mol of O_2 molecules" is 1 mol of O atoms.
- Use the data booklet A_r values and keep them to 2 decimal places; round only the final answer.
- Divide volumes in cm^3 by 1000 before using $c = n/V$.
- For an empirical formula, never round 1.5 or 1.33 to a whole number; multiply all the values instead.
- Gas volume ratios equal mole ratios only for gases at the same temperature and pressure; liquids and solids do not count.

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Ideal gases

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Structure 1.5, Ideal gases, for the course first assessed in 2025. All of it is SL and HL content.

Prerequisites: the amount of substance n in mol and molar mass from Structure 1.4, and rearranging an equation. You will use the gas constant $R = 8.31$ J K^{-1} mol^{-1} and the molar volume 22.7 dm^3 mol^{-1} from the data booklet.

The ideal gas model

Why does a sealed can burst in a fire?

Heat a sealed can and the pressure inside rises until the can splits. Pump air into a bicycle tyre and it gets harder. Squeeze a syringe of air with the end blocked and it pushes back. One simple model explains all three.

Five assumptions

The **kinetic molecular theory** pictures a gas as a huge number of tiny particles in fast, random motion. An **ideal gas** is one that obeys this model exactly:

1. The particles move randomly in straight lines until they collide.
2. The volume of the particles themselves is **negligible** compared with the volume of the container.
3. There are no **intermolecular forces** between the particles.
4. All collisions are **elastic**: no kinetic energy is lost.
5. The average kinetic energy of the particles is proportional to the kelvin temperature.

Pressure is the force per unit area that the particles exert when they hit the walls of the container. More hits per second, or harder hits, mean a higher pressure.

Temperature must be in kelvin

The **kelvin scale** starts at **absolute zero**, the lowest possible temperature, where the particles would have no kinetic energy.

$$T/\mathrm{K} = t/^\circ\mathrm{C} + 273$$

Kelvin temperature is proportional to the average kinetic energy of the particles. Celsius temperature is not: 40 °C is not twice as hot as 20 °C, but 400 K is twice 200 K. **Every gas calculation uses kelvin.**

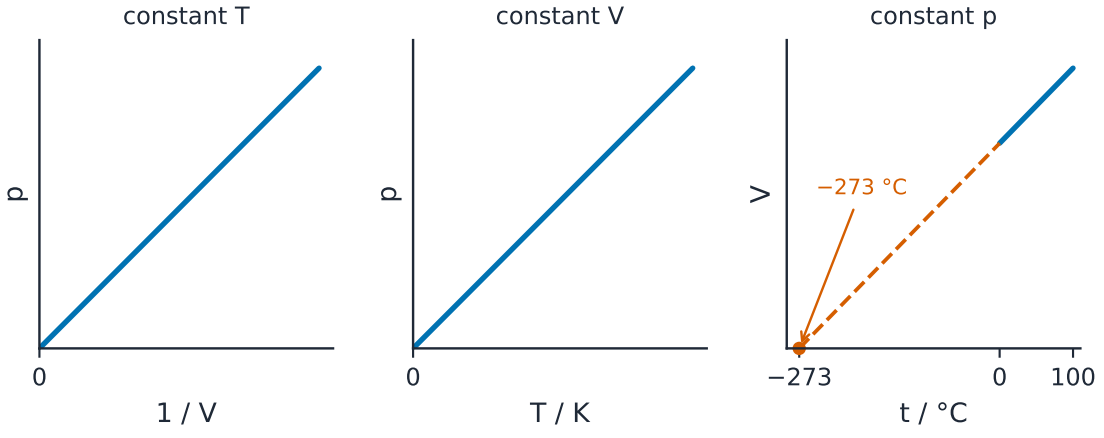
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How pressure, volume and temperature are linked

Three relationships for a fixed amount of gas

Change one quantity, hold one fixed, and watch the third. Each result has a particle explanation.

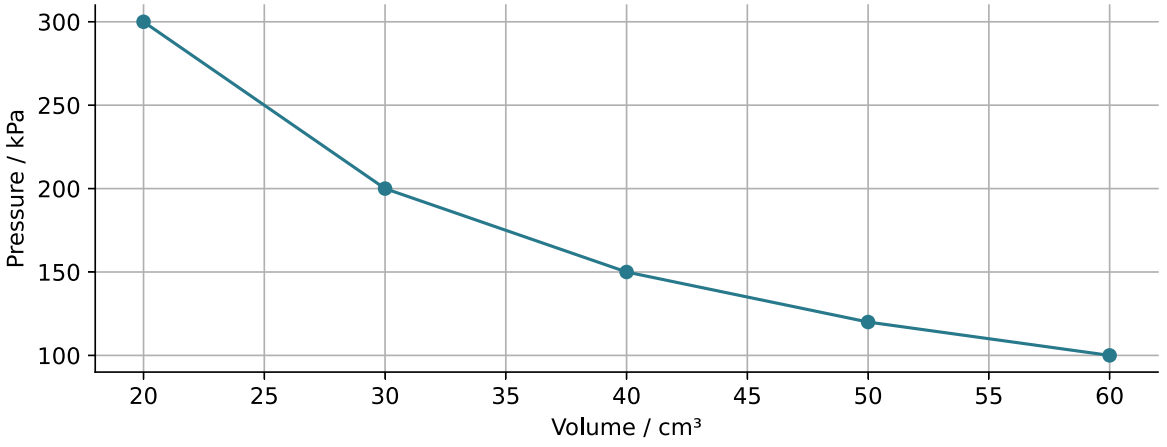
Held fixed	Relationship	Particle explanation
T	$p \propto \frac{1}{V}$, so pV is constant	smaller volume → particles hit the walls more often
V	$p \propto T$	hotter particles move faster, hit more often and harder
p	$V \propto T$	faster particles push the walls out until the pressure is back to its old value



Straight lines through the origin show proportionality; the volume line meets zero at $-273\ °C$, absolute zero

A plot of p against V is a curve, so it is hard to test. Plot p against $\frac{1}{V}$ instead: a straight line through the origin shows that $p \propto \frac{1}{V}$.

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At constant temperature pV stays constant: $300 \times 20 = 100 \times 60 = 6000$

The combined gas law

The three relationships combine into one equation for a fixed amount of gas:

$$\frac{p_1 V_1}{T_1} = \frac{p_2 V_2}{T_2}$$

Any units of pressure and volume work, as long as both sides use the same ones. Temperature must be in kelvin.

> **Worked example.** A gas occupies 250 cm^3 at 20 °C and 100 kPa. It is heated to 80 °C and the pressure rises to 150 kPa. Find the new volume.

1. Convert to kelvin: $T_1 = 293$ K, $T_2 = 353$ K.
2. Rearrange: $V_2 = \dfrac{p_1 V_1 T_2}{p_2 T_1}$.
3. Substitute: $V_2 = \dfrac{100 \times 250 \times 353}{150 \times 293} = 201$ cm^3.
4. Check: the higher pressure squeezes the gas and the higher temperature expands it. The two effects nearly cancel, so a volume close to 250 cm^3 is sensible.

Molar volume and the ideal gas equation

Equal volumes, equal numbers of particles

In an ideal gas the particles have negligible volume, so the volume of a gas depends only on **how many** particles there are, not on what they are. **Avogadro's law** : equal volumes of all gases at the same temperature and pressure contain the same number of particles.

So one mole of any ideal gas has the same volume at a given temperature and pressure. This is the **molar volume** . At standard temperature and pressure (STP: 273 K and 100 kPa):

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$$V_m = 22.7 \text{ dm}^3 \text{ mol}^{-1}$$

$$n = \frac{V}{V_m}$$

For example, 0.500 mol of oxygen or of carbon dioxide at STP each occupy $0.500 \times 22.7 = 11.4$ dm^3.

Because volume is proportional to amount, the coefficients in a balanced equation for gases give their **volume ratio** too. In $N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$, 10 cm^3 of nitrogen reacts with 30 cm^3 of hydrogen to give 20 cm^3 of ammonia, all measured at the same temperature and pressure.

The ideal gas equation

Putting amount into the combined law gives the **ideal gas equation** :

$$pV = nRT$$

R is the **gas constant** , 8.31 J K^{-1} mol^{-1}. The units must fit R:

Quantity	SI unit	Convert from
p	Pa	1 kPa = 10^3 Pa
V	m^3	1 dm^3 = 10^{-3} m^3; 1 cm^3 = 10^{-6} m^3
T	K	add 273 to °C

A useful shortcut: kPa multiplied by dm^3 also gives joules, so you may use kPa with dm^3 in the same equation.

Worked example: finding a molar mass. A 0.320 g sample of a gas occupies 180 cm^3 at 300 K and 100 kPa. Find its molar mass.

1. Convert: $p = 1.00 \times 10^5$ Pa, $V = 180 \times 10^{-6} = 1.80 \times 10^{-4}$ m^3.
2. Amount: $n = \dfrac{pV}{RT} = \dfrac{1.00 \times 10^5 \times 1.80 \times 10^{-4}}{8.31 \times 300} = 7.22 \times 10^{-3}$ mol.
3. Molar mass: $M = \dfrac{m}{n} = \dfrac{0.320}{7.22 \times 10^{-3}} = 44.3$ g mol^{-1}.
4. Interpret: this is close to 44.0 g mol^{-1}, so the gas could be carbon dioxide or propane.

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Real gases

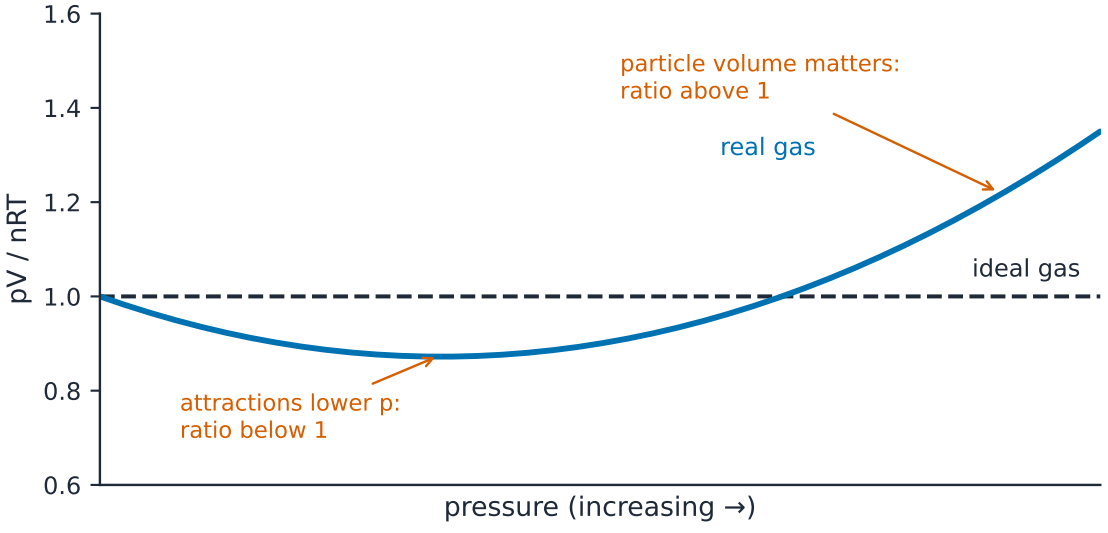
When the model breaks down

A **real gas** behaves almost ideally at high temperature and low pressure. It deviates most at **low temperature and high pressure**, because two assumptions stop being true.

- **High pressure.** The particles are pushed close together, so their own volume is no longer negligible. The space they can move in is smaller than the container volume, and the measured volume is **larger** than $pV = nRT$ predicts.
- **Low temperature.** The particles move slowly, so intermolecular attractions have time to act. A particle about to hit the wall is pulled back by its neighbours, so it hits less hard and the pressure is **lower** than predicted.

Gases with strong intermolecular forces, such as ammonia and water vapour, deviate more than gases with weak forces, such as helium and hydrogen.

We can compare a real gas with the model by plotting $\frac{pV}{nRT}$ against pressure. For an ideal gas this ratio is exactly 1 at every pressure.



Below 1, attractions win; above 1, the particles' own volume wins

Measuring gas behaviour in the lab

To test $p \propto T$, warm a sealed flask of air in a water bath connected to a pressure sensor. Let the gas reach the temperature of the bath before each reading, and keep within the temperature and pressure limits your teacher sets. **Never heat a sealed vessel that is not designed for it.**

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Practice

1. Convert -23 °C and 127 °C to kelvin.
2. A gas at 300 K and 120 kPa in a rigid container is cooled to 250 K. Find the new pressure.
3. Calculate the volume of 0.0400 mol of a gas at STP, in cm^3.
4. Calculate the volume, in dm^3, of 0.500 mol of gas at 298 K and 101 kPa.
5. 1.00 g of a gas occupies 0.763 dm^3 at 273 K and 100 kPa. Find its molar mass and suggest the gas.
6. Explain, in terms of particles, why the pressure of a gas rises when it is heated at constant volume.
7. State two assumptions of the ideal gas model, and explain why each fails at high pressure or low temperature.

Answers.

1. 250 K and 400 K.
2. $p_2 = 120 \times \dfrac{250}{300} = 100$ kPa.
3. $0.0400 \times 22.7 = 0.908\ \text{dm}^3 = 908\ \text{cm}^3$.
4. $V = \dfrac{nRT}{p} = \dfrac{0.500 \times 8.31 \times 298}{101} = 12.3\ \text{dm}^3$ (kPa with dm^3).
5. $n = \dfrac{0.763}{22.7} = 0.0336$ mol; $M = \dfrac{1.00}{0.0336} = 29.8\ \text{g mol}^{-1}$, close to 30: ethane, C_2H_6, or nitrogen monoxide, NO.
6. The particles gain kinetic energy and move faster. They hit the walls more often and with more force, so the force per unit area rises.
7. Particle volume is negligible: at high pressure the particles are close together and their own volume is a large share of the container. No intermolecular forces: at low temperature the particles move slowly and attractions pull them together, lowering the pressure.

Exam tips

- Convert every temperature to **kelvin** before you substitute.
- In $pV = nRT$, use Pa with m^3, or kPa with dm^3; never mix kPa with m^3.
- In the combined gas law, any unit of p and V works as long as both sides match.
- "Deviates at high pressure and low temperature" earns a mark only with the reason: particle volume and intermolecular attractions.
- The molar volume 22.7 $\text{dm}^3\ \text{mol}^{-1}$ applies at STP (273 K, 100 kPa) only.

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The ionic model

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Structure 2.1, The ionic model, for the course first assessed in 2025. All of it is SL and HL content.

Prerequisites: electron configurations and the periodic table groups from Structure 1.3. You will use lattice enthalpy values from the data booklet.

Ions and their charges

Why does salt conduct only when it melts?

Push two electrodes into solid table salt and no current flows. Melt the salt, or dissolve it in water, and it conducts at once. Nothing has been added: the same particles are there. The **ionic model** explains this with one idea: salt is made of charged particles that are locked in place in the solid and free to move in the liquid.

How ions form

An **ion** is an atom or group of atoms with an electric charge. Atoms form ions by losing or gaining electrons until they reach a stable arrangement, usually the configuration of a noble gas.

- Metal atoms **lose** electrons and form positive ions, called **cations**. Sodium, $[\mathrm{Ne}]\,3s^1$, loses one electron to form Na^+, [Ne].
- Non-metal atoms **gain** electrons and form negative ions, called **anions**. Chlorine, $[\mathrm{Ne}]\,3s^2\,3p^5$, gains one electron to form Cl^-, [Ar].

In an ionic compound the electrons lost by the metal are the electrons gained by the non-metal, so the total charge is zero.

Predicting the charge from the group

For main-group elements, the group number tells you the charge:

Group	1	2	13	15	16	17
Electrons lost or gained	lose 1	lose 2	lose 3	gain 3	gain 2	gain 1
Ion charge	+1	+2	+3	−3	−2	−1
Example	Li^+	Mg^{2+}	Al^{3+}	N^{3-}	O^{2-}	F^-

Transition elements can form ions with different charges, so the name gives the charge as a Roman numeral: iron(II) is Fe^{2+} and iron(III) is Fe^{3+}; copper(I)

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is Cu^{+} and copper(II) is Cu^{2+}.

■ Polyatomic ions

A **polyatomic ion** is a group of covalently bonded atoms that carries an overall charge. Learn these:

Ion	Formula	Ion	Formula
ammonium	NH_4^+	carbonate	CO_3^{2-}
hydroxide	OH^-	hydrogencarbonate	HCO_3^-
nitrate	NO_3^-	sulfate	SO_4^{2-}
		phosphate	PO_4^{3-}

Ionic bonding, formulas and names

■ The ionic bond

An **ionic bond** is the **electrostatic attraction** between oppositely charged ions. The attraction acts in every direction, so each ion attracts all the oppositely charged ions around it, not just one partner.

Ionic bonding happens between elements with a large difference in **electronegativity** : typically a metal on the left of the periodic table and a non-metal on the right. The larger the difference, the more ionic the bond. (Structure 2.4 shows bonding as a scale, not three separate boxes.)

■ Writing the formula

The formula shows the simplest ratio of ions that makes the total charge zero.

1. Write the two ions with their charges.
2. Find the smallest numbers of each that make the charges add up to zero.
3. Write the ratio as subscripts. Put a polyatomic ion in brackets if you need more than one.

Ions	Balance	Formula	Name
Na^+, Cl^-	$1 \times (+1) + 1 \times (-1) = 0$	$NaCl$	sodium chloride
Mg^{2+}, Cl^-	$1 \times (+2) + 2 \times (-1) = 0$	$MgCl_2$	magnesium chloride
Al^{3+}, O^{2-}	$2 \times (+3) + 3 \times (-2) = 0$	Al_2O_3	aluminium oxide
Ca^{2+}, NO_3^-	$1 \times (+2) + 2 \times (-1) = 0$	$Ca(NO_3)_2$	calcium nitrate
NH_4^+, SO_4^{2-}	$2 \times (+1) + 1 \times (-2) = 0$	$(NH_4)_2SO_4$	ammonium sulfate

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Naming ionic compounds

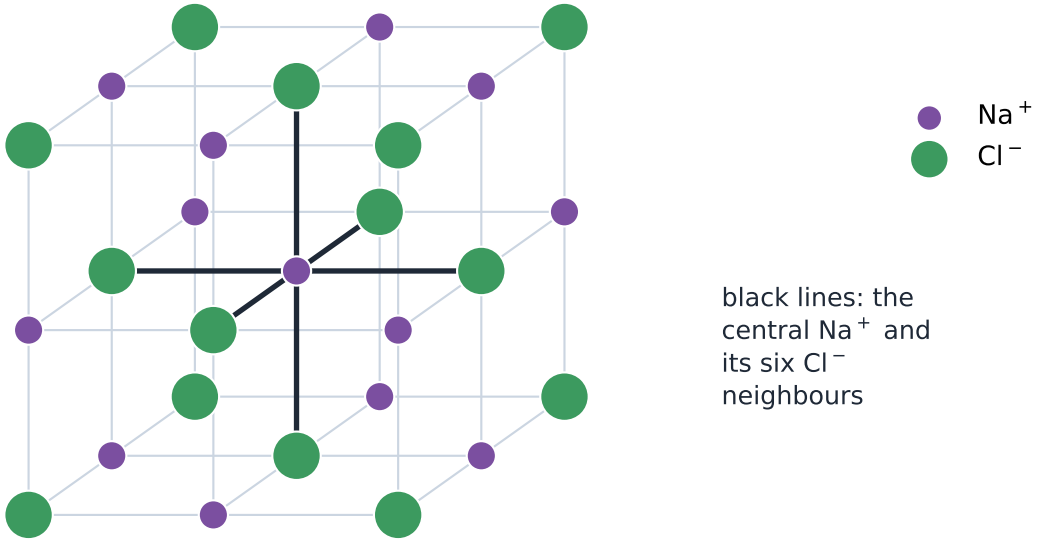
Name the cation first, then the anion. A simple anion ends in **-ide**: chloride, oxide, nitride, sulfide. A polyatomic ion keeps its own name: sulfate, nitrate. Give a transition-metal charge as a Roman numeral: $FeCl_3$ is iron(III) chloride.

Ionic lattices and lattice enthalpy

A giant three-dimensional lattice

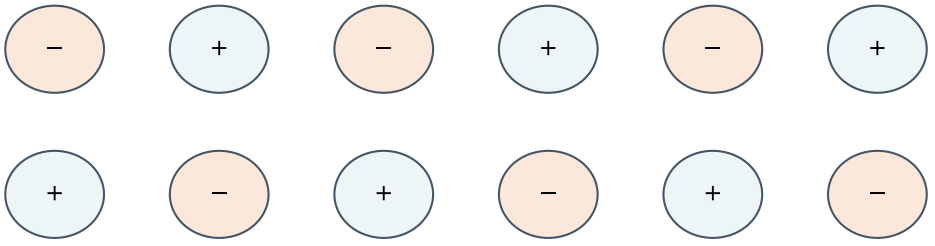
Ionic compounds do not form molecules. The ions pack into a regular, repeating three-dimensional arrangement called a **lattice** . The formula NaCl gives only the **ratio** of ions, 1 : 1, not a molecule.

In sodium chloride each Na^+ ion is surrounded by six Cl^- ions, and each Cl^- ion by six Na^+ ions.



In NaCl every ion has six nearest neighbours of the opposite charge

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Alternating charges in an ionic lattice

Each ion is surrounded by ions of opposite charge: ionic bonding acts in every direction

Lattice enthalpy measures the strength of the bonding

The **lattice enthalpy** is the enthalpy change when one mole of a solid ionic compound is separated into its gaseous ions:

$$\mathrm{NaCl(s)} \rightarrow \mathrm{Na^+(g)} + \mathrm{Cl^-(g)} \qquad \Delta H_{\mathrm{lattice}} = +790\ \mathrm{kJ\ mol^{-1}}$$

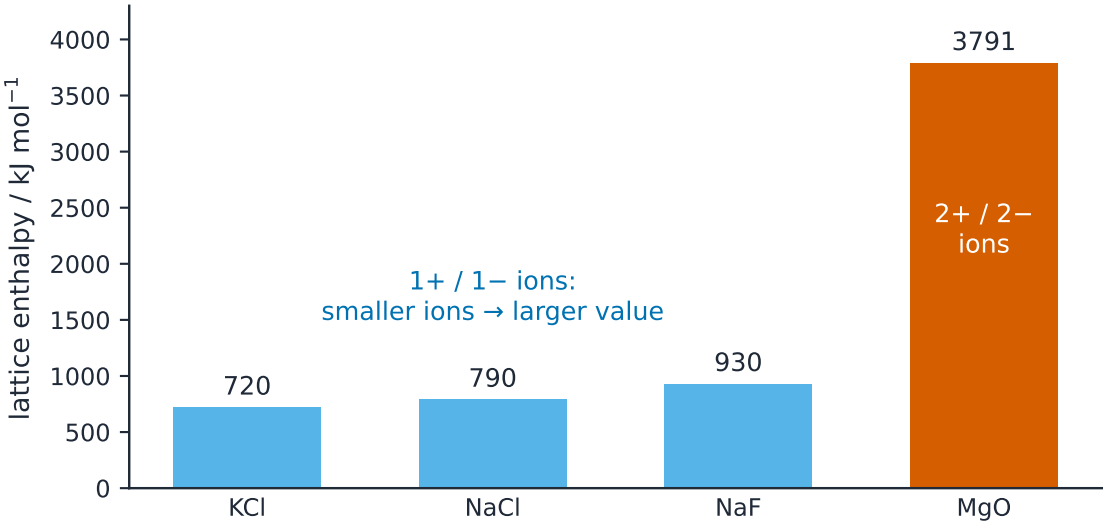
Breaking the attractions always needs energy, so lattice enthalpy is always positive (endothermic). A larger value means stronger ionic bonding.

Two factors decide its size, because the attraction between two ions is stronger when the charges are larger and the ions are closer together:

- **Ionic charge:** larger charges attract more strongly, so the lattice enthalpy is larger.
- **Ionic radius:** smaller ions sit closer together, so the lattice enthalpy is larger.

Compound	Ions	Lattice enthalpy / kJ mol^{-1}	Reason
KCl	K^+, Cl^-	720	K^+ is larger than Na^+
NaCl	Na^+, Cl^-	790	reference
NaF	Na^+, F^-	930	F^- is smaller than Cl^-
MgO	Mg^{2+}, O^{2-}	3791	both charges are doubled

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Doubling both charges has a far bigger effect than changing the radius

Worked example. Explain why magnesium oxide melts at 2852 °C but sodium chloride melts at 801 °C.

Both are giant ionic lattices, so melting means overcoming electrostatic attractions between ions. Mg^{2+} and O^{2-} carry twice the charges of Na^{+} and Cl^{-}, and they are also smaller. So the attraction between the ions is much stronger, the lattice enthalpy is much larger (3791 against 790 kJ mol^{-1}), and more energy is needed to separate the ions.

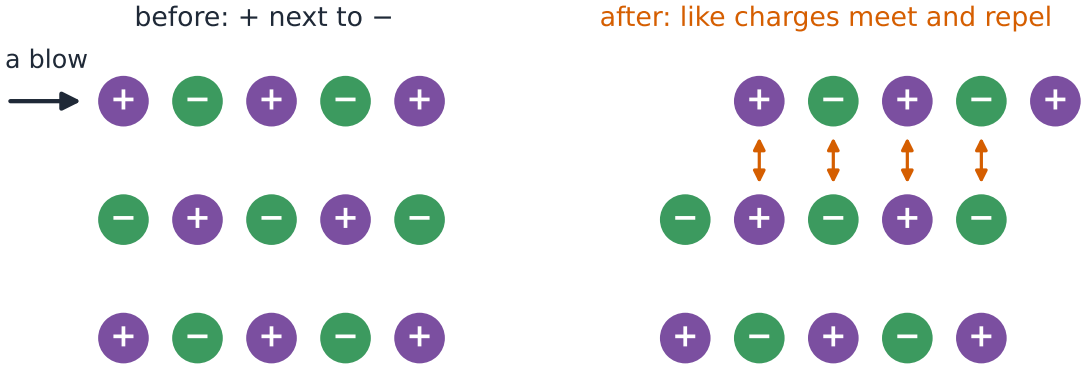
Properties of ionic compounds

Explaining properties from the structure

To explain any property, name the **structure**, the **particles**, the **forces** between them, and whether there are **mobile charged particles**.

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Property	Typical behaviour	Explanation
melting and boiling point	high; low **volatility**	many strong electrostatic attractions in a giant lattice must be overcome
electrical conductivity	none as a solid; conducts when molten or in solution	ions are fixed in the solid; they can move and carry charge when molten or dissolved
solubility	often soluble in water, insoluble in non-polar solvents such as hexane	polar water molecules attract and surround the ions; non-polar molecules cannot
brittleness	shatters when hit	a blow shifts a layer so that like charges line up and repel



Shift one layer by one ion and like charges meet: the lattice splits apart

Note that an ionic compound conducts by **moving ions**, not by moving electrons. Electrolysis of a molten salt shows this: the ions move to the electrodes and are discharged there.

■ Use a pattern of evidence

One property alone rarely proves a structure. A giant covalent solid such as silicon dioxide also has a very high melting point, and some simple molecular substances dissolve in water. Look for the full pattern: high melting point, **and** no conduction as a solid, **and** conduction when molten.

> **Worked example.** Substance X melts at 801 °C, does not conduct as a solid, conducts when molten, and dissolves in water. Substance Y melts at 60 °C and does not conduct as a solid or as a liquid. Which is ionic?

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X fits every part of the ionic pattern: a high melting point from strong attractions in a lattice, and conduction only when the ions are free to move. Y does not: its low melting point and lack of conduction suggest a simple molecular substance with weak forces between neutral molecules.

Practice

1. Give the charge on the ion formed by: (a) potassium, (b) sulfur, (c) aluminium, (d) nitrogen.
2. Write the formulas of: (a) calcium fluoride, (b) sodium oxide, (c) aluminium sulfate, (d) iron(III) hydroxide, (e) ammonium carbonate.
3. Name: (a) K_2S, (b) Mg_3N_2, (c) $CuSO_4$ (copper is +2), (d) $NaHCO_3$.
4. Write the equation for the lattice enthalpy of calcium oxide, including state symbols.
5. Put these in order of increasing lattice enthalpy and explain: NaCl, CaO, KBr.
6. Explain why sodium chloride conducts electricity when dissolved in water but not when solid.
7. Explain why an ionic crystal shatters when hit with a hammer.

Answers.

1. (a) +1, (b) −2, (c) +3, (d) −3.
2. (a) CaF_2, (b) Na_2O, (c) $Al_2(SO_4)_3$, (d) $Fe(OH)_3$, (e) $(NH_4)_2CO_3$.
3. (a) potassium sulfide, (b) magnesium nitride, (c) copper(II) sulfate, (d) sodium hydrogencarbonate.
4. $CaO(s) \rightarrow Ca^{2+}(g) + O^{2-}(g)$
5. KBr < NaCl < CaO. KBr has the largest ions with single charges, so the weakest attraction. CaO has 2+ and 2− ions, so by far the strongest attraction.
6. In the solid the ions are held in fixed positions in the lattice. In solution the ions are free to move, so they can carry charge through the liquid.
7. The blow shifts one layer of ions by one position. Ions of the same charge then line up next to each other, they repel, and the crystal splits along that plane.

Exam tips

- Define an ionic bond as "electrostatic attraction between **oppositely charged ions**". "Transfer of electrons" describes how ions form, not the bond.
- An ionic formula is a **ratio**: never call NaCl a molecule.
- Ionic compounds conduct by **mobile ions**, never by "free electrons".
- For lattice enthalpy, compare **charge** first, then **radius**, and say that both change the electrostatic attraction.
- Write lattice enthalpy as the solid going to **gaseous** ions, with a positive value.

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- Put brackets around a polyatomic ion when you need two or more of it: $Ca(OH)_2$, not $CaOH_2$.

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The covalent model

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

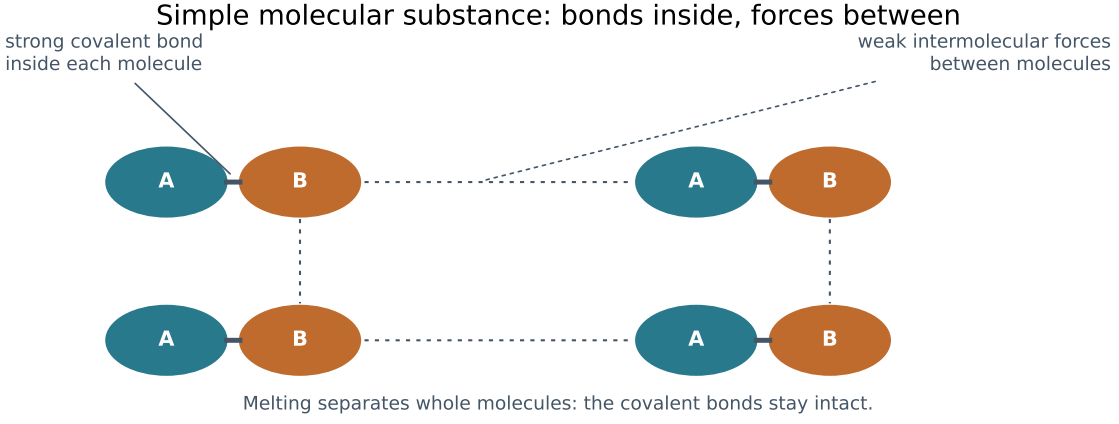
This handout teaches Structure 2.2, The covalent model, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: electron configurations and valence electrons from Structure 1.3, and the ionic model from Structure 2.1. You will use electronegativity values from the data booklet.

The covalent bond

Why does iodine melt so easily?

Iodine is made of I_2 molecules. The bond that holds the two iodine atoms together is strong: it takes 151 kJ mol^{-1} to break it. Yet solid iodine melts at only 114 °C and turns to a purple vapour with gentle heating. The vapour is still I_2: no bonds were broken. This unit explains the difference between the strong **covalent bonds** inside a molecule and the weak **intermolecular forces** between molecules.



Bonds inside molecules are strong; forces between them are weak, so melting leaves the molecules intact

What a covalent bond is

A covalent bond is the electrostatic attraction between a **shared pair** of electrons and the positively charged nuclei of the two bonded atoms. Covalent bonds form between non-metal atoms, which have similar, high electronegativities: neither atom can take an electron completely, so they share.

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- Most atoms in covalent molecules end with eight electrons in their outer shell. This is the **octet rule** . Hydrogen is the exception: it is full with two.
- Some small atoms have fewer than eight. In BF_3 boron has only six outer electrons, and in $BeCl_2$ beryllium has only four. These are **incomplete octets** .
- Pairs of outer electrons that are not shared are **lone pairs** . They matter for shape and for hydrogen bonding.

Lewis formulas

A **Lewis formula** shows every valence electron: shared pairs as lines (or dot-cross pairs) and lone pairs as pairs of dots. To draw one:

1. Add up the valence electrons of all the atoms. Add one for each negative charge and subtract one for each positive charge.
2. Put the least electronegative atom in the centre (never H) and join each outer atom with a single bond.
3. Complete the octets of the outer atoms with lone pairs, then put any electrons left on the central atom.
4. If the central atom still has fewer than eight, move a lone pair from an outer atom to make a double or triple bond.

For CO_2: $4 + 2(6) = 16$ valence electrons. Two C–O single bonds and full octets on both O use all 16, but C has only four. Moving one lone pair from each O gives O = C = O, with two lone pairs on each O and eight electrons round C.

Single, double and triple bonds

Two atoms can share one, two or three pairs. More shared pairs pull the nuclei closer together and hold them more strongly.

Bond	Shared pairs	Length / pm	Bond enthalpy / kJ mol^{-1}
C–C	1	154	346
C=C	2	134	614
C≡C	3	120	839

So a triple bond is the **shortest** and **strongest**. Note that a double bond is not twice as strong as a single bond.

Coordination bonds

In a **coordination bond** (a dative covalent bond) both shared electrons come from the same atom. Once it has formed, it is identical to any other covalent bond.

- $NH_3 + H^+ \rightarrow NH_4^+$: the lone pair on N bonds to the H^+ ion. All four N–H bonds in NH_4^+ are the same.
- $H_2O + H^+ \rightarrow H_3O^+$, the oxonium ion in every acid solution.

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- Carbon monoxide, C ≡ O: two of the three shared pairs come from both atoms, but one comes from oxygen alone.

Draw a coordination bond as an arrow from the donor atom to the acceptor atom.

Shapes of molecules: VSEPR

Electron domains repel

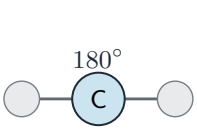
The **valence shell electron pair repulsion** (VSEPR) model predicts shape from one idea: groups of electrons round the central atom repel and spread as far apart as possible. Each group is an **electron domain**: a single bond, a double bond, a triple bond or a lone pair each counts as **one** domain.

1. Draw the Lewis formula.
2. Count the electron domains round the central atom: this gives the **electron domain geometry**.
3. Count how many domains are bonds: the positions of the atoms give the **molecular geometry** (the shape).

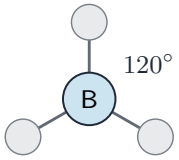
Lone pairs repel more strongly than bonding pairs, because they sit closer to the central atom. Each lone pair squeezes the bond angle by about 2.5°.

Domains	Lone pairs	Shape	Angle	Example
2	0	linear	180°	CO_2, $BeCl_2$
3	0	trigonal planar	120°	BF_3, CO_3^{2-}
3	1	bent (V-shaped)	below 120°	SO_2, O_3
4	0	tetrahedral	109.5°	CH_4, NH_4^+
4	1	trigonal pyramidal	107°	NH_3
4	2	bent (V-shaped)	104.5°	H_2O

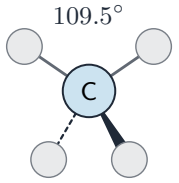
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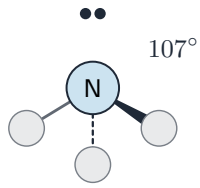
linear
CO_2



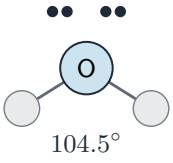
trigonal planar
BF_3



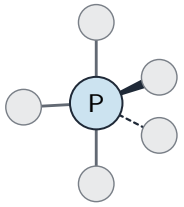
tetrahedral
CH_4



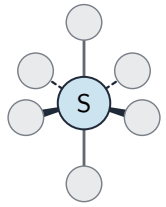
pyramidal
NH_3



bent
H_2O



trig. bipyramidal
PF_5, 120° & 90°



octahedral
SF_6, 90°

Wedges point towards you and dashed bonds away. The last two shapes, with five and six domains, are part of the HL course.

■ Worked example: the shape of NH_3

- Valence electrons: $5 + 3(1) = 8$, so four pairs round N.
- Three are N–H bonds and one is a lone pair: four domains, so the electron domain geometry is tetrahedral.
- Only three positions hold atoms, so the shape is **trigonal pyramidal**.
- The lone pair repels more strongly than the bonds, so the angle closes from 109.5° to 107°.

Bond polarity and molecular polarity

■ Polar bonds

Electronegativity is the ability of an atom to attract a shared pair of electrons. When the two bonded atoms have different electronegativities, the shared pair sits closer to the more electronegative atom. That atom gains a small negative charge, $\delta-$, and the other a small positive charge, $\delta+$. The bond is a **polar bond** and has a **bond dipole**.

Atom	H	C	N	O	F	Cl
Electronegativity	2.2	2.6	3.0	3.4	4.0	3.2

The larger the electronegativity difference, the more polar the bond. O–H (difference 1.2) is much more polar than C–H (difference 0.4). With a very large difference, around

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1.8 or more, the bonding is mostly ionic: bonding is a continuum, not two separate boxes.

Polar molecules

A molecule is **polar** when its bond dipoles do not cancel, so it has a net **dipole moment**. Whether they cancel depends on the shape.

- CO_2 has two polar C=O bonds, but the molecule is linear: the two dipoles point in opposite directions and cancel. CO_2 is **non-polar**.
- H_2O has two polar O–H bonds, but the molecule is bent: the dipoles add up towards the oxygen. Water is **polar**.
- CH_4 and CCl_4 are symmetrical tetrahedra, so they are non-polar. In CH_3Cl one bond is different, the dipoles no longer cancel, and the molecule is polar.

A quick test: a molecule with no lone pairs on the central atom and all outer atoms the same is non-polar. Anything less symmetrical is usually polar.

Giant covalent structures

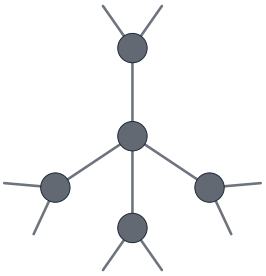
Networks instead of molecules

In a **covalent network structure** (giant covalent structure) every atom is joined to its neighbours by covalent bonds in a continuous lattice. There are no separate molecules, so melting means breaking strong covalent bonds. These substances have very high melting points and do not dissolve in any solvent.

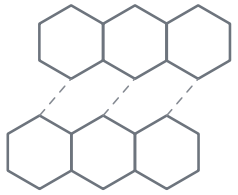
Carbon has several **allotropes**: different structural forms of the same element in the same state.

Allotrope	Bonding of each C	Structure	Key properties
diamond	4 C, tetrahedral	3D network	hardest natural substance; does not conduct
graphite	3 C, trigonal planar	flat hexagonal layers, weak forces between them	soft, slippery; conducts along the layers
graphene	3 C, trigonal planar	a single layer of graphite	very strong and light; conducts very well
fullerene C_{60}	3 C	hollow ball of 60 atoms	a molecule, so soft with low melting point; poor conductor

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diamond
every C bonded to 4:
rigid 3D network, very hard



graphite
layers slide; spare
electrons let it conduct

Diamond is a rigid 3D network. In graphite one electron per carbon is free to move along each layer.

In graphite, graphene and C_{60} each carbon uses three electrons in bonds. The fourth is **delocalized** : spread over many atoms rather than held between two. Mobile delocalized electrons explain why graphite and graphene conduct.

■ Silicon and silicon dioxide

- **Silicon** has the same tetrahedral network as diamond, but the Si–Si bond is longer and weaker, so silicon melts lower (1414 °C) and is a semiconductor.
- **Silicon dioxide** , SiO_2 (quartz, sand), is a network in which each Si bonds to four O atoms and each O bonds to two Si atoms. The ratio 1 : 2 gives the formula. Compare it with CO_2: carbon dioxide is a small molecule and a gas at room temperature, while silicon dioxide melts above 1600 °C.

Intermolecular forces

■ Four kinds of attraction between molecules

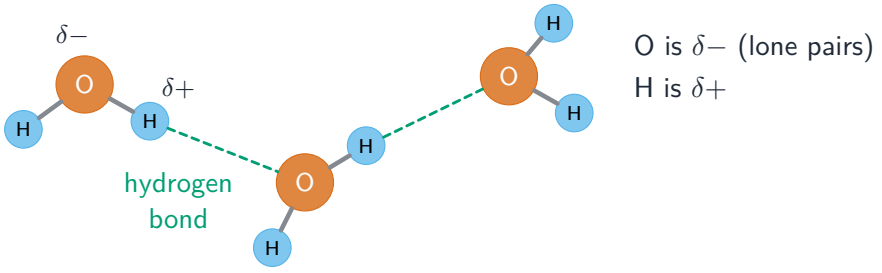
Intermolecular forces act between molecules in simple molecular substances. From weakest to strongest for molecules of similar size:

1. **London forces** (dispersion forces) act between all molecules. Electrons move, so at any instant one side of a molecule may have more electrons than the other: an **instantaneous dipole**. It induces a dipole in the next molecule, and the two attract. London forces grow with the number of electrons (larger molar mass) and with greater surface contact between molecules.
2. **Dipole–induced dipole forces** act between a polar molecule and a non-polar one: the permanent dipole distorts the electrons of its neighbour.
3. **Dipole–dipole forces** act between polar molecules: the $\delta+$ end of one attracts the $\delta-$ end of the next, in addition to London forces.

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4. **Hydrogen bonding** is the strongest. It forms when H is bonded to N, O or F, and is attracted to a lone pair on an N, O or F atom of another molecule.

These three forces together, London, dipole–induced dipole and dipole–dipole, are called **van der Waals forces** .

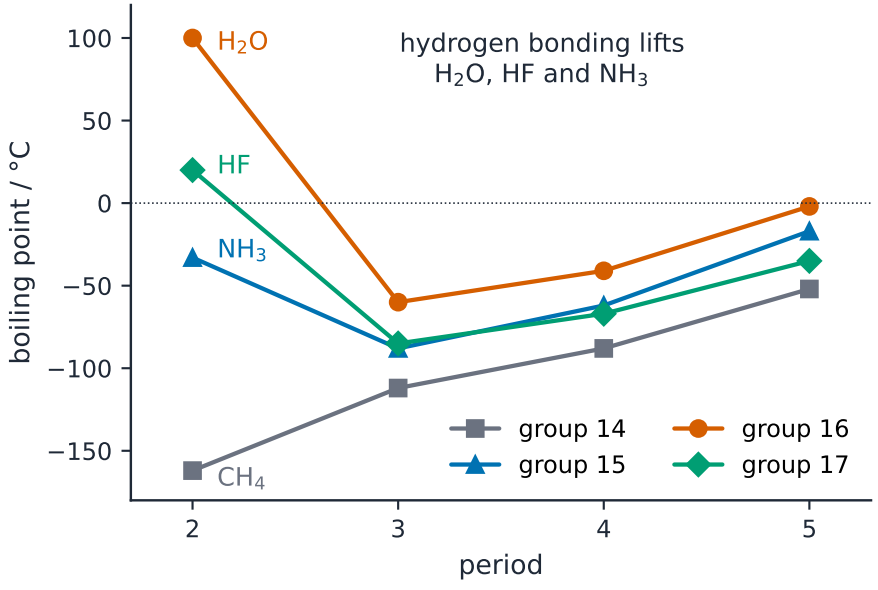


Each water molecule can form up to four hydrogen bonds: two through its H atoms and two through its lone pairs

Hydrogen bonding is strong because N, O and F are very electronegative, which leaves the H almost a bare proton, and because H is so small that the lone pair can come very close.

■ Evidence from boiling points

Down each group the hydrides boil higher, because the molecules have more electrons and stronger London forces. Three hydrides break the pattern.



Hydrogen bonding lifts H_2O, HF and NH_3 far above the trend. CH_4 has no hydrogen bonding and follows it.

Water boils at 100 °C; without hydrogen bonding, the trend in group 16 suggests

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about −80 °C.

Properties of covalent substances

Explaining a property

To explain a physical property, name the structure, the particles, the forces that must be overcome and any mobile charged particles.

Property	Simple molecular	Covalent network
melting and boiling point	low: only weak intermolecular forces are overcome	very high: strong covalent bonds must break
volatility	often high	very low
conductivity	none: no ions or delocalized electrons (except graphite-like structures)	none, except graphite and graphene
solubility	depends on polarity	insoluble

Comparing boiling points: a method

1. Check the type of structure. A network always beats a simple molecular substance.
2. For molecular substances, list every force present, then compare the strongest one.
3. If the strongest force is the same kind, compare London forces through the number of electrons and the shape.

Example: propane, C_3H_8 ($M = 44$), boils at −42 °C; ethanal, CH_3CHO ($M = 44$), at 20 °C; ethanol, C_2H_5OH ($M = 46$), at 78 °C. Similar masses mean similar London forces. Ethanal adds dipole–dipole forces; ethanol adds hydrogen bonding through its O–H group.

Shape matters too: pentane (a straight chain) boils at 36 °C but its branched isomer 2,2-dimethylpropane at 10 °C, because the compact molecules touch over a smaller surface.

Solubility: like dissolves like

A substance dissolves well when the new attractions between solvent and solute are similar in strength to the ones that must be broken.

- Polar and hydrogen-bonding substances dissolve in water: ethanol and glucose form hydrogen bonds with water molecules.
- Non-polar substances such as iodine or hexane dissolve in non-polar solvents but hardly in water: they cannot replace the hydrogen bonds between water molecules.
- In a series such as methanol, ethanol, propanol, butanol, solubility in water falls as the non-polar hydrocarbon chain grows longer.

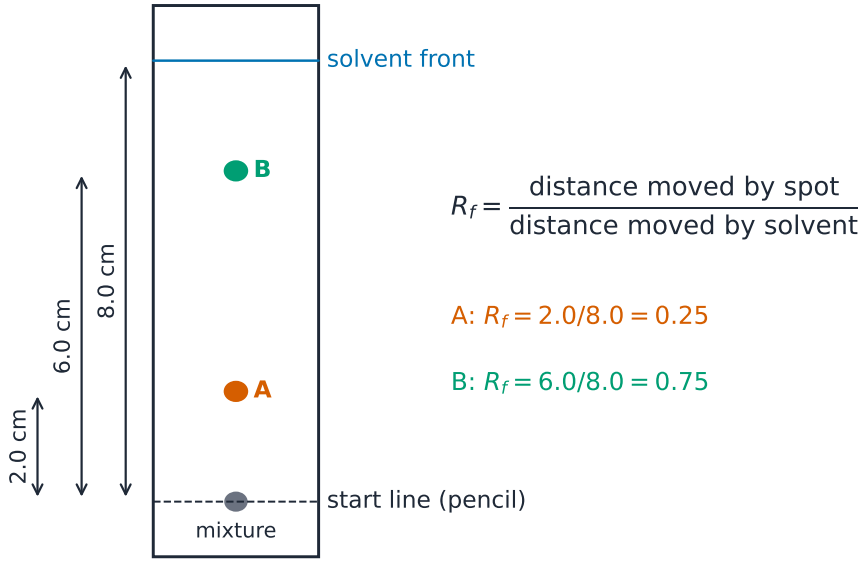
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Chromatography

Chromatography separates the components of a mixture by how strongly each one is attracted to two phases:

- the **stationary phase**, which does not move: water held in the fibres of the paper, or a thin layer of silica on a plate in thin-layer chromatography (TLC);
- the **mobile phase**, the solvent that moves through it.

A component that is more attracted to the mobile phase moves further. A component that is more attracted to the stationary phase stays near the start. Because these attractions are intermolecular forces, polarity decides the result: on polar silica with a non-polar solvent, polar components move least.



Measure every distance from the start line, to the centre of each spot

The **retardation factor**, R_f, is

$$R_f = \frac{\text{distance moved by the component}}{\text{distance moved by the solvent front}}$$

R_f always lies between 0 and 1 and has no units. Under the same conditions (paper, solvent, temperature) a substance always has the same R_f, so you can identify a component by comparing it with known samples. Draw the start line in pencil, because ink would itself separate, and keep it above the level of the solvent. Colourless spots are shown with a UV lamp or a locating agent such as ninhydrin.

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AHL: Resonance and delocalization

When one Lewis formula is not enough

Ozone, O_3, can be drawn as O = O − O or as O − O = O. One drawing predicts one short and one long bond. Experiments show both O–O bonds are the **same** length, 128 pm, between an O–O single bond (148 pm) and an O=O double bond (121 pm).

The real molecule is a single structure in between the two drawings. The drawings are **resonance structures** , joined by a double-headed arrow. The electrons of the extra bond are **delocalized** over all three atoms.

- The carbonate ion, CO_3^{2-}, has three resonance structures. All three C–O bonds are equal, each with a **bond order** of $4/3 \approx 1.33$ (four shared pairs across three bonds).
- Other examples: NO_3^-, NO_2^-, SO_2 and the carboxylate ion, $RCOO^-$.

Delocalization spreads electrons over more atoms, and this lowers the energy: delocalized structures are more stable than any single resonance structure suggests.

Benzene

Benzene , C_6H_6, is a flat ring of six carbon atoms. A structure with alternating single and double bonds (the Kekulé structure) does not match the evidence:

Evidence	Alternating C–C and C=C predicts	Benzene shows
bond lengths	three at 154 pm and three at 134 pm	six equal bonds of 140 pm
enthalpy of hydrogenation	three times cyclohexene: $3(-120) = -360$ kJ mol^{-1}	-208 kJ mol^{-1}, so about 150 kJ more stable
reactions	addition, like alkenes (decolourizes bromine water)	substitution; keeps the ring
isomers of $C_6H_4Br_2$	two different 1,2-isomers	only one 1,2-isomer

Each carbon uses three electrons in sigma bonds (two C–C, one C–H). The six remaining p electrons form one delocalized ring of electron density above and below the plane. That is why benzene is drawn as a hexagon with a circle inside.

AHL: Expanded octets and formal charge

Five and six electron domains

Atoms in period 3 and below can hold more than eight electrons in their outer shell, an **expanded octet** , because they have empty d orbitals close in energy. VSEPR still works: count domains, then lone pairs.

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Domains	Lone pairs	Shape	Angles	Example
5	0	trigonal bipyramidal	90°, 120°	PCl_5
5	1	see-saw	about 87°, 102°	SF_4
5	2	T-shaped	about 88°	ClF_3
5	3	linear	180°	XeF_2, I_3^-
6	0	octahedral	90°	SF_6
6	1	square pyramidal	about 84°	BrF_5
6	2	square planar	90°	XeF_4

With five domains, lone pairs always go in the **equatorial** positions (round the middle), where they have more room. With six, two lone pairs sit opposite each other.

Worked example, XeF_4: Xe has 8 valence electrons; four go into Xe–F bonds and four remain as two lone pairs. Six domains give an octahedral electron domain geometry; the lone pairs sit opposite, so the four F atoms form a **square planar** shape. The molecule is non-polar, because the four Xe–F dipoles cancel.

Formal charge

When you can draw more than one Lewis formula, **formal charge** (FC) helps you choose. For each atom:

$$\text{FC} = V - \tfrac{1}{2}B - L$$

where V is the number of valence electrons in the free atom, B the number of bonding (shared) electrons round it, and L the number of non-bonding (lone-pair) electrons. The formal charges add up to the charge on the species.

The preferred structure has formal charges **closest to zero**; if a negative formal charge is needed, it should sit on the most electronegative atom.

Worked example, CO_2:

- O = C = O: each O has $6 - \frac{1}{2}(4) - 4 = 0$; C has $4 - \frac{1}{2}(8) - 0 = 0$. All zero.
- O ≡ C − O: the triple-bonded O has $6 - 3 - 2 = +1$; C has 0; the single-bonded O has $6 - 1 - 6 = -1$.

The first structure has all formal charges zero, so it is preferred, which matches the two equal C=O bonds found by experiment.

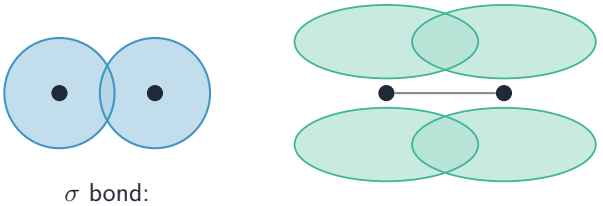
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AHL: Sigma and pi bonds and hybridization

Two ways for orbitals to overlap

A covalent bond forms where atomic orbitals overlap.

- A **sigma bond** (σ) forms by head-on overlap along the line between the nuclei. Every single bond is a sigma bond.
- A **pi bond** (π) forms by sideways overlap of parallel p orbitals, above and below that line. It is weaker than a sigma bond, because the overlap is smaller.



σ bond: head-on overlap

π bond: sideways overlap of p orbitals

Sigma overlap lies on the axis between the nuclei; pi overlap lies above and below it

A double bond is one σ and one π; a triple bond is one σ and two π. This is why C=C (614) is less than twice C–C (346): the second bond is a weaker pi bond. Rotation about a double bond would break the pi overlap, so it does not happen at room temperature.

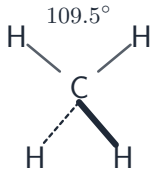
Ethene, $CH_2 = CH_2$, has five sigma bonds (four C–H, one C–C) and one pi bond.

Hybridization

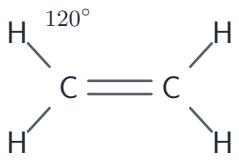
Carbon's ground state, $2s^2\,2p^2$, has only two unpaired electrons, yet carbon forms four equal bonds in methane. **Hybridization** explains this: atomic orbitals on one atom mix to form the same number of new, equal **hybrid orbitals** that point in the directions VSEPR predicts.

Hybridization	Orbitals mixed	Domains	Geometry	Example
sp^3	one s, three p	4	tetrahedral, 109.5°	CH_4; also N in NH_3, O in H_2O
sp^2	one s, two p	3	trigonal planar, 120°	each C in C_2H_4; C in benzene
sp	one s, one p	2	linear, 180°	each C in C_2H_2; C in CO_2

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sp^3: 4 single bonds
tetrahedral



sp^2: 1 double + 2 single
planar (flat)



sp: 1 triple bond
linear

The number of electron domains tells you the hybridization

Hybrid orbitals form sigma bonds or hold lone pairs. The p orbitals left unhybridized form the pi bonds: one in sp^2 carbon, two in sp carbon. To find the hybridization of any atom, count its electron domains: 4 is sp^3, 3 is sp^2, 2 is sp.

Practice

1. Draw the Lewis formula of: (a) N_2, (b) HCN, (c) NH_4^+, showing the coordination bond.
2. State and explain which is shorter and stronger: the C–O bond in methanol or the C=O bond in methanal.
3. Predict the shape and bond angle of: (a) PH_3, (b) BCl_3, (c) H_2S, (d) CS_2.
4. Explain why CCl_4 is non-polar but $CHCl_3$ is polar.
5. Explain why diamond is hard and does not conduct electricity, but graphite is soft and conducts.
6. Put these in order of increasing boiling point and explain: CH_3OCH_3, C_2H_5OH, C_3H_8 (all have $M \approx 44$–46).
7. Explain why ethanol mixes with water but hexane does not.
8. In a chromatogram the solvent front is 9.0 cm from the start line. Spot X has moved 3.6 cm. Calculate its R_f.
9. **AHL.** Draw two resonance structures of the nitrate ion and state the bond order of each N–O bond.
10. **AHL.** Predict the shape and bond angles of: (a) SF_4, (b) SF_6, (c) ICl_4^-.
11. **AHL.** Use formal charges to decide which Lewis formula of SCN^- is preferred: $[S=C=N]^-$ or $[S-C\equiv N]^-$.
12. **AHL.** For propene, $CH_2=CH-CH_3$, count the sigma and pi bonds and state the hybridization of each carbon.

Answers.

1. (a) $N\equiv N$ with one lone pair on each N. (b) $H-C\equiv N$ with one lone pair on N. (c) N in the centre with four N–H bonds; one is drawn as an arrow from N to H; overall charge +1, shown with square brackets.

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2. The C=O bond in methanal: two shared pairs pull the nuclei closer together and attract them more strongly than one.
3. (a) trigonal pyramidal, less than 109.5° (four domains, one lone pair; VSEPR predicts about 107°). (b) trigonal planar, 120°. (c) bent, less than 109.5° (two lone pairs). (d) linear, 180°.
4. Both are tetrahedral. In CCl_4 the four equal C–Cl dipoles cancel by symmetry. In $CHCl_3$ the C–H bond has a much smaller dipole, so the dipoles do not cancel and there is a net dipole moment.
5. In diamond every C forms four strong covalent bonds in a rigid 3D network, and all outer electrons are in bonds, so there are no mobile charged particles. In graphite each C bonds to three others in layers held by weak London forces, so layers slide; the fourth electron of each C is delocalized and moves along the layers.
6. C_3H_8 (−42 °C) < CH_3OCH_3 (−24 °C) < C_2H_5OH (78 °C). Similar masses give similar London forces. Methoxymethane is polar and adds dipole–dipole forces. Ethanol has an O–H group and forms hydrogen bonds, the strongest intermolecular force.
7. Ethanol forms hydrogen bonds with water molecules through its O–H group, so the new attractions replace the ones broken. Hexane is non-polar and can only form London forces with water, too weak to replace the hydrogen bonds between water molecules.
8. $R_f = 3.6/9.0 = 0.40$.
9. **AHL.** N in the centre, one N=O and two N–O bonds (each single-bonded O carries a negative formal charge; overall −1); the double bond can sit on any of the three O atoms. Bond order $4/3 \approx 1.33$ for every N–O bond.
10. **AHL.** (a) see-saw (five domains, one equatorial lone pair), about 87° and 102°. (b) octahedral, 90°. (c) square planar (six domains, two opposite lone pairs), 90°.
11. **AHL.** $[S=C=N]^-$: S $6-2-4=0$, C 0, N $5-2-4=-1$. $[S-C\equiv N]^-$: S $6-1-6=-1$, C 0, N $5-3-2=0$. Both have charges closest to zero, so the preferred one puts the −1 on the more electronegative atom: N (3.0) is more electronegative than S (2.6), so $[S=C=N]^-$ is preferred.
12. **AHL.** Eight sigma bonds (six C–H, two C–C) and one pi bond. The two carbons of the C=C are sp^2; the CH_3 carbon is sp^3.

Exam tips

- Define a covalent bond as the attraction between a **shared pair** of electrons and the **nuclei** of the bonded atoms.
- In VSEPR count **domains**, not bonds: a double bond is one domain. Then name the shape from the atoms only.
- Lone pairs repel more than bonding pairs: write this whenever you explain an angle below 109.5°.

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- A polar molecule needs polar bonds **and** an unsymmetrical shape; always say whether the dipoles cancel.
- Melting a simple molecular substance overcomes **intermolecular forces**; never write that it breaks covalent bonds.
- Hydrogen bonding needs H bonded **directly** to N, O or F; CH_3F has no hydrogen bonding.
- For R_f, measure to the **centre** of the spot and from the start line, not from the bottom of the paper.
- **AHL.** Resonance structures are not switching between forms: there is one real structure with delocalized electrons.
- **AHL.** In five-domain shapes, lone pairs go in the **equatorial** positions.

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The metallic model

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Structure 2.3, The metallic model, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: electron configurations and ionization energy from Structure 1.3, and the ionic and covalent models from Structures 2.1 and 2.2. You will compare melting points from the data booklet.

The metallic bond

Why can a copper wire bend and conduct?

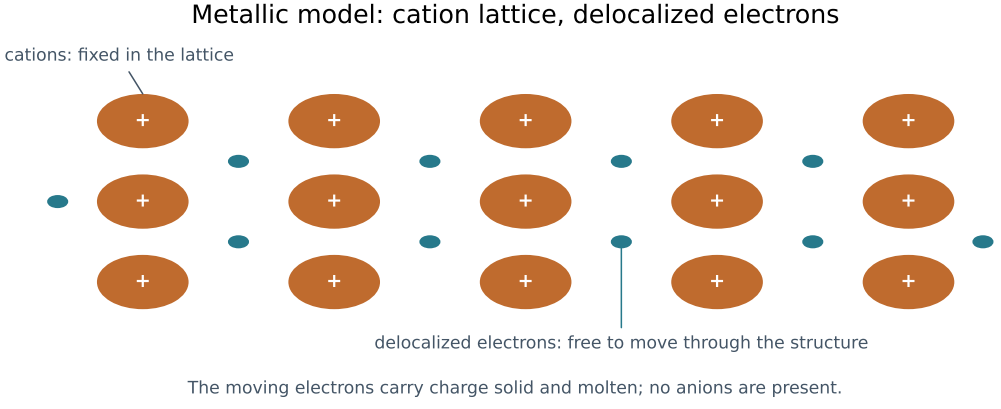
A copper wire carries current when it is cold and when it is red hot. You can bend it, hammer it flat or pull it into a thinner wire, and it does not shatter. An ionic crystal does neither: it conducts only when molten and it breaks under a hammer. The **metallic model** explains both properties of metals with one picture.

Cations in a sea of electrons

Metal atoms have few outer electrons and low ionization energies, so they lose their outer electrons easily. In a solid metal:

- the atoms lose their outer electrons and become positive ions, **cations**, packed in a regular **lattice**;
- the lost electrons are not attached to any one ion. They are **delocalized electrons**, free to move through the whole structure, often called a "sea" of electrons.

The **metallic bond** is the electrostatic attraction between a lattice of cations and the delocalized electrons.



Fixed cations in a sea of delocalized electrons; the moving electrons conduct

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Three points the examiners look for:

- There are **no anions** in a metal. The negative charge is carried by electrons.
- The attraction acts in every direction: the bonding is **non-directional**
  .
- Each ion is attracted to many electrons, and each electron to many ions, so there are no separate bonds between pairs of atoms.

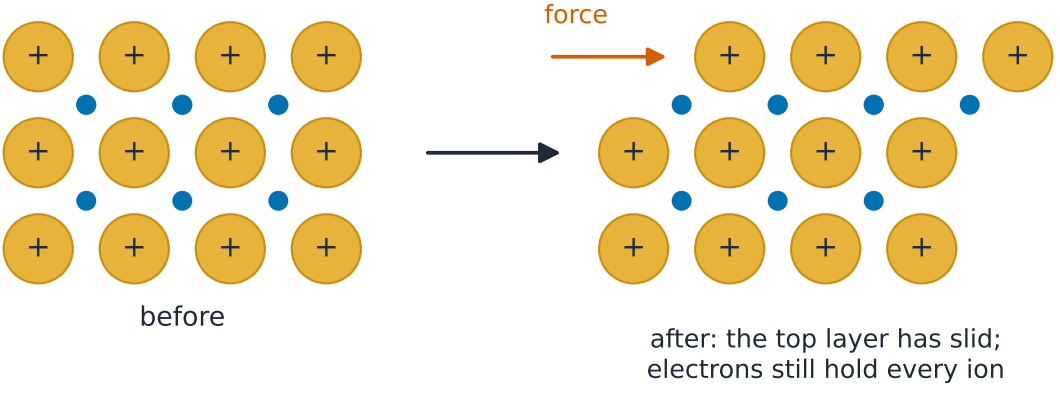
Properties of metals

Explaining each property

To explain any property, name the structure, the particles, the force and the mobile charge carriers.

Property	Explanation
electrical conductivity in solid and liquid	delocalized electrons move through the lattice when a voltage is applied
thermal conductivity	delocalized electrons (and vibrating ions) pass kinetic energy quickly through the metal
malleability and **ductility**	layers of cations can slide over each other; the electrons move with them, so the bonding is unchanged
high melting and boiling points (most metals)	strong attraction between many cations and the electron sea in a giant lattice
shiny (lustre)	delocalized electrons absorb and re-emit light

Malleable means it can be hammered into shape; ductile means it can be drawn into a wire.



The bonding is non-directional, so a shifted layer is held just as strongly as before

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Metals compared with ionic compounds

	Metal	Ionic compound
particles	cations and delocalized electrons	cations and anions
conducts when solid	yes, by electrons	no: ions are fixed
conducts when molten	yes, by electrons	yes, by ions
effect of a blow	layers slide, metal bends	like charges meet, crystal shatters

Notice the different charge carriers: always say **electrons** for a metal and **ions** for a molten ionic compound.

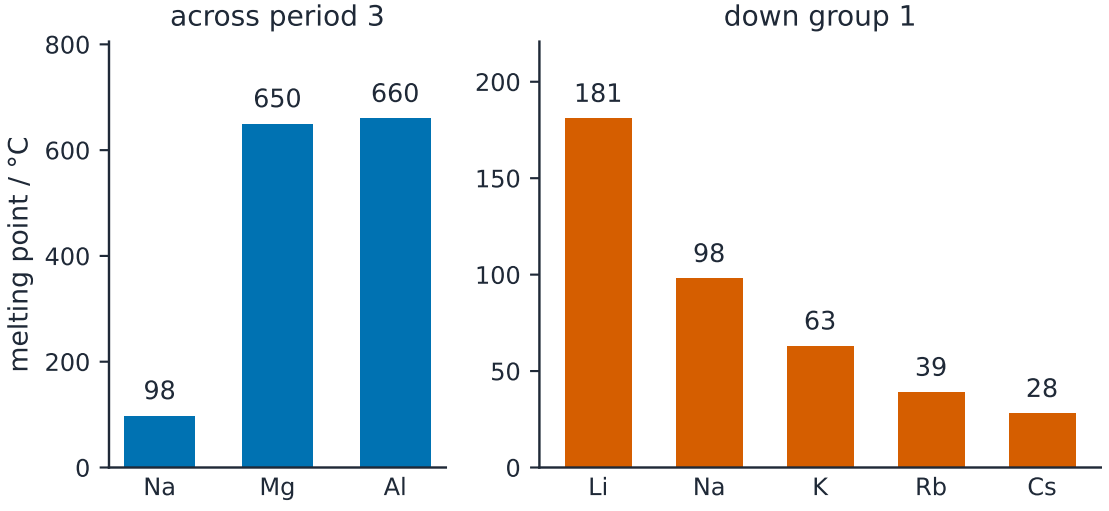
Strength of the metallic bond

What makes the bond stronger

The metallic bond is stronger when the attraction between the cations and the electron sea is stronger. Two factors decide this:

1. **Charge of the cation and number of delocalized electrons.** A larger charge gives more delocalized electrons per ion and a stronger attraction.
2. **Radius of the cation.** A smaller ion lets the electrons come closer to the nucleus, so the attraction is stronger.

A stronger metallic bond means a higher melting point and boiling point.



The two charts use different vertical scales. Charge raises the melting point across period 3; size lowers it down group 1.

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Across period 3: Na, Mg, Al

- Na^+ gives one delocalized electron per ion, Mg^{2+} two and Al^{3+} three.
- The ions also get smaller: Na^+ 102 pm, Mg^{2+} 72 pm, Al^{3+} 54 pm.
- Both changes strengthen the attraction, so the melting point rises from 98 °C to 650 °C and 660 °C.

Boiling points show the trend more clearly than melting points: Na 883 °C, Mg 1090 °C, Al 2519 °C. Melting only loosens the lattice, but boiling separates the ions from each other completely.

Down group 1: Li to Cs

Every group 1 metal gives one delocalized electron per ion. Down the group the cations get larger, so the delocalized electrons are further from each nucleus and the attraction is weaker. The melting point falls from 181 °C (Li) to 28 °C (Cs): caesium melts in a warm hand.

Worked example

Explain why magnesium has a higher melting point than sodium.

- **Structure:** both are giant metallic lattices; melting overcomes the metallic bonding.
- **Ions:** Mg^{2+} has a higher charge than Na^+ and is smaller.
- **Electrons:** magnesium has two delocalized electrons per atom, sodium only one.
- **Conclusion:** the attraction between cations and delocalized electrons is stronger in magnesium, so more energy is needed to melt it.

AHL: Transition elements

Delocalized d electrons

The **transition elements** have partly filled 3d sublevels. The 4s and 3d sublevels are very close in energy, so both the 4s and some of the 3d electrons can become delocalized. More delocalized electrons per ion and a high ionic charge give a much stronger metallic bond than in the s-block metals.

Metal	Block	Delocalized electrons per atom (approx.)	Melting point / °C
potassium	s	1	63
calcium	s	2	842
iron	d	more than 2 (4s and 3d)	1538
chromium	d	more than 2 (4s and 3d)	1907

So transition metals have:

- **high melting points** and high boiling points;

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- high **density** , because the ions are small and heavy and pack closely;
- high **electrical conductivity**, because there are many delocalized electrons to carry charge;
- great strength and hardness, which is why iron, titanium and their alloys are used for structures.

Zinc, with a full 3d sublevel, does not use d electrons in this way: it melts at only 420 °C, much lower than its neighbours.

Practice

1. Define the metallic bond.
2. Explain why solid copper conducts electricity but solid copper(II) chloride does not.
3. Explain why a metal bends when hammered, but a crystal of sodium chloride shatters.
4. Explain why aluminium has a higher boiling point than sodium.
5. Explain why the melting point of the group 1 metals decreases from lithium to caesium.
6. Predict, with a reason, which has the higher melting point: potassium or calcium.
7. **AHL.** Explain why iron has a much higher melting point than calcium.

Answers.

1. The electrostatic attraction between a lattice of positive ions (cations) and delocalized electrons.
2. Copper contains delocalized electrons that can move through the lattice and carry charge. In solid copper(II) chloride the ions are held in fixed positions and there are no mobile electrons, so no charge can move.
3. In a metal the bonding is non-directional: layers of cations slide and the delocalized electrons move with them, so the attraction holds the new arrangement. In NaCl a shift brings ions of the same charge next to each other, they repel and the crystal splits.
4. Al^{3+} has a higher charge and a smaller radius than Na^{+}, and aluminium has three delocalized electrons per atom against one. The attraction between cations and delocalized electrons is stronger, so more energy is needed to separate the ions.
5. Each ion gives one delocalized electron, but the ions get larger down the group. The delocalized electrons are further from the nucleus, the attraction is weaker, and less energy is needed to melt the metal.
6. Calcium: Ca^{2+} has a higher charge and is smaller than K^{+}, and gives two delocalized electrons per atom, so its metallic bond is stronger (842 °C against 63 °C).

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7. **AHL.** Iron is a transition element. Its 4s and 3d electrons are close in energy, so 3d electrons are delocalized as well as 4s ones. More delocalized electrons and small, highly charged ions make the metallic bond much stronger.

Exam tips

- Define the metallic bond as an attraction between **cations** and **delocalized electrons**; never mention anions or "molecules".
- Metals conduct by **delocalized electrons** in both solid and liquid states; molten ionic compounds conduct by **ions**.
- For malleability, say that layers **slide** and the **non-directional** bonding is kept.
- Compare metallic bond strength with **charge** (number of delocalized electrons) and **ionic radius**, and link it to the energy needed.
- **AHL.** For transition metals, say that **d electrons** are delocalized too.

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Structure 2.4 · From models to materials

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

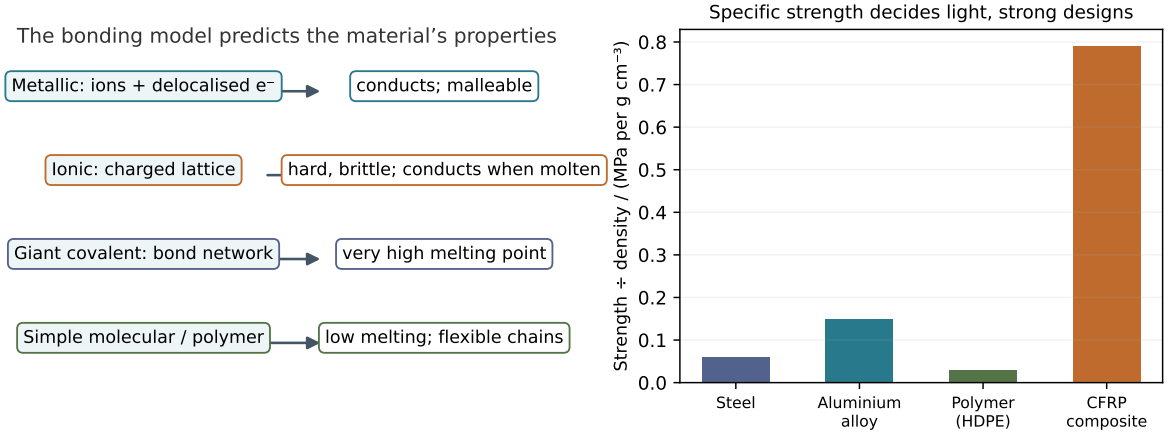
This handout teaches Structure 2.4, From models to materials, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: the ionic, covalent and metallic models from Structures 2.1 to 2.3, and electronegativity values from the data booklet. You will draw structural formulas of simple organic molecules.

Bonding is a continuum

■ Why is a bicycle frame made of carbon fibre?

A racing bicycle frame must be strong, stiff and light. Steel is strong but heavy. Aluminium alloy is lighter. Carbon-fibre composite, long chains of covalently bonded carbon held in a polymer, is stronger than steel for its mass. Choosing a **material** means choosing a type of bonding, because the bonding decides the properties.



The bonding model predicts properties; strength per unit density decides light, strong designs

■ Three models, one continuum

Ionic, covalent and metallic bonding are models: ideal cases. Real substances often sit between them.

- **Ionic** bonding needs a large difference in electronegativity: one atom takes electrons from the other.
- **Covalent** bonding happens between atoms that both have high electronegativity: they share electrons.

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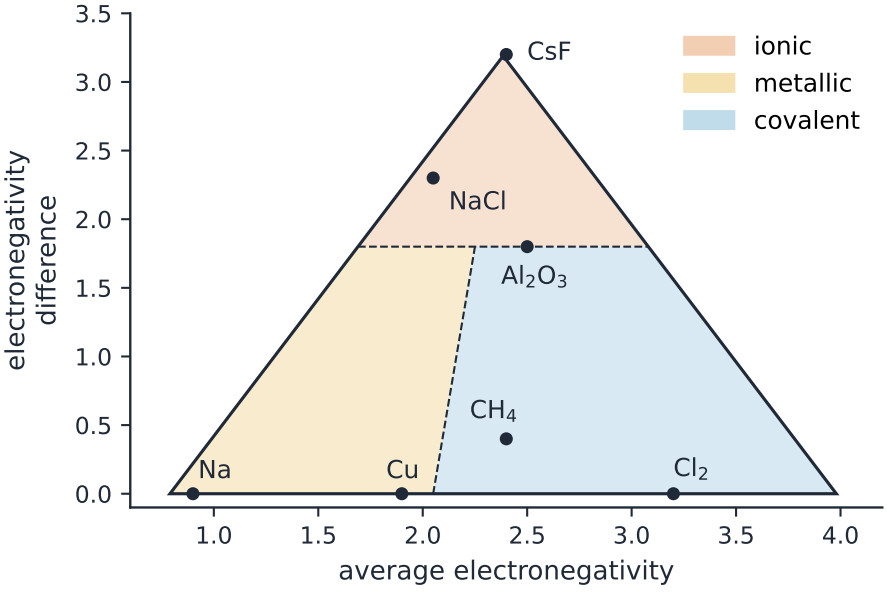
- **Metallic** bonding happens between atoms that both have low electronegativity: they release electrons into a shared sea.

Most bonds have some character of more than one type. In aluminium oxide the bonding is mainly ionic, but the small, highly charged Al^{3+} ion pulls the electrons of the oxide ion towards it, giving the bond some covalent character.

The bonding triangle

The **bonding triangle** (the van Arkel–Ketelaar triangle in the data booklet) places a binary substance by two numbers:

- the **average electronegativity** of the two elements on the x-axis;
- the **electronegativity difference** on the y-axis.



The boundaries are approximate: bonding changes gradually across the triangle

Worked example: placing a compound

Use the triangle to predict the bonding in magnesium oxide. Electronegativities: Mg 1.3, O 3.4.

- Average: $(1.3 + 3.4)/2 = 2.35$.
- Difference: $3.4 - 1.3 = 2.1$.
- The point (2.35, 2.1) is in the ionic region, so MgO is predicted to be mainly ionic: a high melting point, and conduction only when molten.

For silicon dioxide (Si 1.9, O 3.4): average 2.65, difference 1.5. The point lies in the covalent region, which fits its giant covalent structure.

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From position to properties

Region	Typical properties
ionic (top)	high melting point, brittle, conducts only when molten or dissolved, often soluble in water
covalent (bottom right)	molecular: low melting point, no conduction; network: very high melting point, no conduction
metallic (bottom left)	conducts when solid, malleable, shiny, most melt high

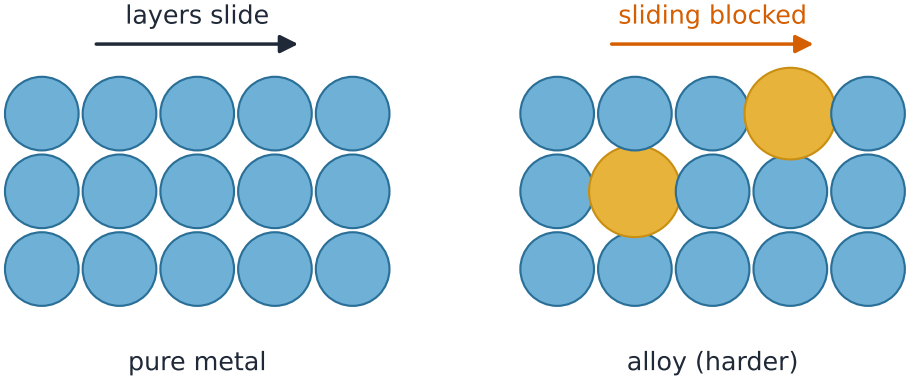
The triangle predicts bonding; it does not decide between a molecular and a network covalent structure. Use other evidence, such as the melting point, for that.

Alloys

Metals mixed with other elements

An **alloy** is a mixture of a metal with other metals, or with a non-metal such as carbon. Alloys are made by mixing the molten elements and letting them cool. They still have metallic bonding: cations of different elements in a sea of delocalized electrons.

Pure metals are often too soft. In a pure metal all the cations are the same size, so the layers slide easily. In an alloy, atoms of a different size distort the regular layers. The layers can no longer slide easily, so the alloy is **harder** and stronger.



Different-sized atoms distort the layers, so they cannot slide past each other easily

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Alloy	Composition	Improved property	Use
steel	iron with up to about 2% carbon	harder and stronger than iron	buildings, bridges
stainless steel	iron with chromium and nickel	resists corrosion	cutlery, medical tools
brass	copper and zinc	harder than copper, resists corrosion	taps, musical instruments
bronze	copper and tin	harder, resists corrosion	statues, bearings
duralumin	aluminium with copper and magnesium	stronger, still light	aircraft bodies

Alloys can also change other properties: some melt at lower temperatures than any of their parts (solder), and some resist corrosion because the added element forms a protective oxide layer (chromium in stainless steel).

Polymers

Long chains from small units

A **polymer** is a very large molecule (a macromolecule) made of many small units joined in a chain. The small molecules that join are **monomers**, and the part of the chain that repeats is the **repeating unit**.

Polymers can be natural, such as starch, cellulose, proteins and DNA, or synthetic, such as poly(ethene) and nylon. Most plastics are synthetic polymers.

Properties of plastics

The properties of a plastic come from its long chains:

- Chains are held together by intermolecular forces. Longer chains have more contact between them, so the forces are stronger and the plastic is stronger and melts higher.
- Chains with no side branches pack closely (high-density poly(ethene), HDPE); branched chains pack loosely (low-density poly(ethene), LDPE), so LDPE is softer and more flexible.
- Plastics are light, cheap, easy to shape and unreactive. Most do not conduct electricity, so they are good insulators.

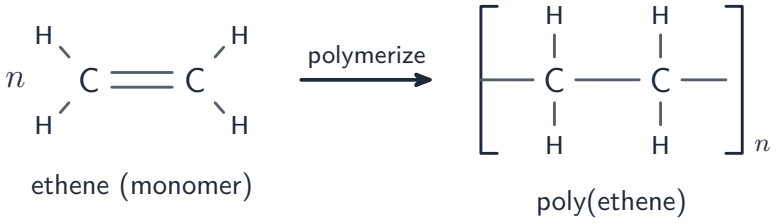
The same unreactive covalent bonds cause a problem: most plastics are not **biodegradable**. They last for hundreds of years in landfill and in the oceans. Burning them releases carbon dioxide and, for PVC, toxic hydrogen chloride. Recycling sorts plastics by type, using the resin identification code printed on them.

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Addition polymers

Joining alkenes

In **addition polymerization** monomers with a C=C double bond join together. The pi bond in each double bond breaks, and the electrons form new single bonds to the neighbouring monomers. No other product forms: every atom of the monomers ends up in the polymer.



The double bond opens; the repeating unit has the same atoms as the monomer, joined by single bonds

To draw the repeating unit from a monomer:

1. Draw the two carbons of the C=C with a **single** bond between them.
2. Keep every group that was attached to those carbons in the same place.
3. Add a continuation bond on each side, through square brackets, and write n after the bracket.

Monomer	Formula	Polymer	Repeating unit
ethene	$CH_2 = CH_2$	poly(ethene)	$-CH_2 - CH_2-$
propene	$CH_2 = CHCH_3$	poly(propene)	$-CH_2 - CH(CH_3)-$
chloroethene	$CH_2 = CHCl$	poly(chloroethene), PVC	$-CH_2 - CHCl-$
tetrafluoroethene	$CF_2 = CF_2$	PTFE (Teflon)	$-CF_2 - CF_2-$

To go backwards from a polymer to its monomer, find the two-carbon repeating unit and put a double bond between those two carbons.

Note that the side group (such as CH_3 or Cl) hangs **off** the main chain; it is never part of the chain itself.

AHL: Condensation polymers

Joining two functional groups

In **condensation polymerization** each new bond forms between two functional groups, and a small molecule, usually water or hydrogen chloride, is released. Each monomer must have **two** functional groups, one at each end, so that the chain can keep growing in both directions.

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polyester: -C(=O)-OH + H-O- → -C(=O)-O- + H_2O

polyamide: -C(=O)-OH + H-N(H)- → -C(=O)-NH- + H_2O

every new ester or amide link loses a small molecule (condensation)

Every new ester or amide link releases one small molecule

- **Polyesters** form from a dicarboxylic acid and a diol. Each link is an **ester link**, −COO−. Example: PET, from benzene-1,4-dicarboxylic acid and ethane-1,2-diol, used for drinks bottles and polyester fibres.
- **Polyamides** form from a dicarboxylic acid (or a diacyl chloride) and a diamine. Each link is an **amide link**, −CONH−. Examples: nylon-6,6 from hexanedioic acid and hexane-1,6-diamine; Kevlar, whose flat chains form many hydrogen bonds, which makes it strong enough for body armour.
- With a diacyl chloride, $ClOC - R - COCl$, the small molecule released is HCl instead of water.

Biological condensation polymers

Many natural polymers are condensation polymers:

- **Proteins** are polyamides made from amino acids, each joined by an amide (peptide) link with loss of water.
- **Polysaccharides**, such as starch and cellulose, are made from glucose units joined with loss of water.
- **Nucleic acids** (DNA and RNA) are made from nucleotides joined with loss of water.

Addition against condensation

	Addition polymer	Condensation polymer
monomer	contains C=C	two functional groups per monomer (or two different monomers)
other product	none	a small molecule (H_2O or HCl)
main chain	C–C bonds only	contains ester or amide links
breaking down	very slow; not hydrolysed	ester and amide links can be hydrolysed, so many are more biodegradable

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Hydrolysis is the reverse of condensation: water breaks the ester or amide link and gives back the monomers. This is how the body digests proteins and starch, and how some polyesters can be chemically recycled.

Practice

1. Electronegativities: Na 0.9, Cl 3.2, C 2.6, H 2.2, Cu 1.9, Zn 1.6. Use the bonding triangle to predict the main type of bonding in: (a) NaCl, (b) CH_4, (c) CuZn (brass).
2. Explain why aluminium oxide is described as ionic with some covalent character.
3. Explain why steel is harder than pure iron.
4. Draw the repeating unit of poly(propene), and the monomer of a polymer with repeating unit $-CH_2-CH(CN)-$.
5. State two properties that make poly(ethene) useful for packaging and one environmental problem it causes.
6. Explain why HDPE is stronger and denser than LDPE.
7. **AHL.** Name the two monomers needed to make nylon-6,6, state the link formed and name the other product.
8. **AHL.** Give two differences between addition and condensation polymerization.

Answers.

1. (a) average 2.05, difference 2.3: ionic. (b) average 2.4, difference 0.4: covalent. (c) average 1.75, difference 0.3: metallic.
2. The electronegativity difference (Al 1.6, O 3.4: difference 1.8) is on the boundary of the ionic region. The small Al^{3+} ion with a high charge distorts the electron cloud of O^{2-}, pulling electron density between the ions, so the bond has some covalent character.
3. Steel contains carbon atoms of a different size among the iron cations. They distort the regular layers, so the layers cannot slide over each other easily.
4. Poly(propene): $-CH_2-CH(CH_3)-$ in square brackets with continuation bonds and n. The monomer is $CH_2=CHCN$ (propenenitrile).
5. Any two of: light, cheap, flexible, waterproof, unreactive, easy to shape. Problem: not biodegradable, so it stays in landfill and the oceans for hundreds of years (or: burning releases CO_2).
6. HDPE chains have no branches, so they pack closely together. There is more contact between chains, so the London forces are stronger and more mass fits in the same volume.
7. **AHL.** Hexanedioic acid and hexane-1,6-diamine. An amide link, $-CONH-$, forms and water is released.
8. **AHL.** Any two: addition monomers contain C=C, condensation monomers have two functional groups; addition gives only the polymer, condensation also releases a small molecule such as water; the addition polymer chain has only C–C bonds,

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the condensation chain contains ester or amide links that can be hydrolysed.

Exam tips

- Use the bonding triangle with **both** numbers: the average electronegativity and the difference.
- Say that bonding is a **continuum**: the triangle regions have no sharp boundaries.
- For alloys, explain hardness with **different-sized atoms** that **distort the layers** so they cannot slide.
- When drawing an addition repeating unit, change C=C to C–C, keep the side groups off the chain, and add continuation bonds with n.
- **AHL.** For condensation polymers, always name the **small molecule** lost and the **link** formed.

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Structure 3.1 · The periodic table: classification of elements

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

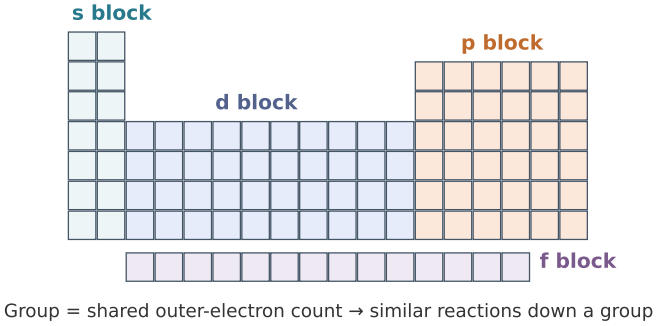
This handout teaches Structure 3.1, The periodic table: classification of elements, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

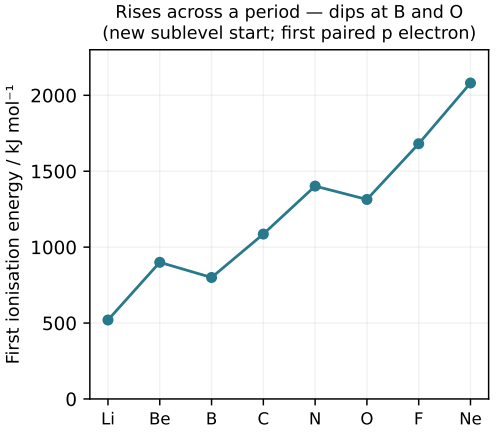
Prerequisites: electron configurations and ionization energy from Structure 1.3, and ionic and covalent bonding from Structures 2.1 and 2.2. You will use the periodic table, ionic radii and electronegativity values from the data booklet.

Organizing the periodic table

One table, many predictions

In 1869 Dmitri Mendeleev arranged the known elements in order of atomic mass and left gaps where the pattern said an element should be. He predicted the properties of "eka-silicon", and germanium, found in 1886, matched them closely. The **periodic table** works because the properties of elements repeat in a regular way: **periodicity** .





The table follows the order in which sublevels fill: s, p, d and f blocks

Periods, groups and blocks

The modern table orders the elements by atomic number Z.

- A **period** is a horizontal row. The period number is the number of the outer energy level: sodium, $[\mathrm{Ne}]\,3s^1$, is in period 3.

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- A **group** is a vertical column, numbered 1 to 18. Elements in a group have the same number of outer electrons, so they react in similar ways. For groups 1 and 2 the number of valence electrons equals the group number; for groups 13 to 18 it is the group number minus 10.
- A **block** is named after the sublevel being filled: s (groups 1 and 2), p (groups 13 to 18), d (groups 3 to 12) and f (the lanthanoids and actinoids).

Worked example: chlorine is $1s^2\,2s^2\,2p^6\,3s^2\,3p^5$. The outer level is $n = 3$, so period 3; the last electron enters a p sublevel, so p block; seven outer electrons, so group 17.

Metals, metalloids and non-metals

Metals are on the left and in the middle of the table; non-metals are on the right. A diagonal band of **metalloids** (B, Si, Ge, As, Sb, Te) separates them. Metalloids have some properties of both: silicon looks shiny but is brittle, and it is a semiconductor.

Some groups have names: group 1 the **alkali metals**, group 2 the alkaline earth metals, group 17 the **halogens** and group 18 the noble gases.

Periodic trends

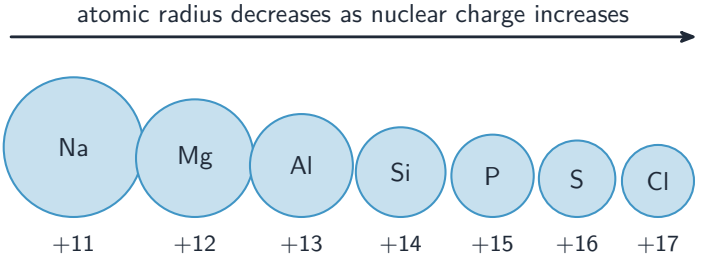
Two ideas explain every trend

Every trend in this section comes from the balance of two effects on the outer electrons:

- **nuclear charge**: more protons pull the electrons more strongly;
- **shielding**: inner electrons repel the outer electrons and reduce the pull they feel.

Across a period, the nuclear charge rises by one each time but the electrons go into the **same** energy level, so shielding hardly changes. The outer electrons feel a stronger pull. Down a group, each element has one more full **inner** level: the outer electrons are further away and more shielded, so they feel a weaker pull, even though the nuclear charge is larger.

Atomic radius



Across period 3 the growing nuclear charge pulls the same outer level closer

- **Across a period** the atomic radius decreases: Na 186 pm to Cl 102 pm.
- **Down a group** the atomic radius increases: one extra occupied energy level each time.

Ionic radius

- A **cation** is smaller than its atom: it has lost its whole outer level, and the remaining electrons are pulled in more strongly. Na 186 pm, Na^+ 102 pm.
- An **anion** is larger than its atom: the extra electrons repel each other, and the same nuclear charge holds more electrons. Cl 102 pm, Cl^- 181 pm.
- For ions with the **same electron configuration** (isoelectronic ions), the radius falls as the nuclear charge rises: $N^{3-} > O^{2-} > F^- > Na^+ > Mg^{2+} > Al^{3+}$, all with the configuration of neon.

Ionization energy, electron affinity and electronegativity

Property	Meaning	Across a period	Down a group
first ionization energy	energy to remove one mole of electrons from one mole of gaseous atoms	generally increases	decreases
electron affinity	energy change when one mole of gaseous atoms each gain one electron	generally more negative (more released)	generally less negative
electronegativity	ability of an atom to attract a shared pair of electrons	increases	decreases

All three follow from the same idea: a stronger pull on the outer electrons makes them harder to remove and makes the atom attract extra electrons more strongly. The first electron affinity is usually negative (exothermic), because the incoming electron is attracted by the nucleus.

Fluorine is the most electronegative element (4.0); caesium and francium are the least.

Metallic and non-metallic character

Metals react by **losing** electrons. Metallic character therefore increases as ionization energy decreases: **down** a group and **to the left** across a period. Non-metallic character increases up and to the right. This is why the most reactive metals (Cs, Fr) are at the bottom left and the most reactive non-metal (F) is at the top right.

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Group 1 and group 17

The alkali metals

Group 1 metals are soft, have low melting points and react quickly with water to give a hydroxide and hydrogen:

$$2\mathrm{Na(s)} + 2\mathrm{H_2O(l)} \rightarrow 2\mathrm{NaOH(aq)} + \mathrm{H_2(g)}$$

Reactivity **increases** down the group. The outer electron is further from the nucleus and more shielded, so it is lost more easily. Lithium fizzes steadily; potassium melts, catches fire and burns with a lilac flame.

The halogens

Halogens exist as diatomic molecules: F_2 and Cl_2 are gases, Br_2 a liquid and I_2 a solid at room temperature (London forces increase down the group). Halogens react by **gaining** an electron, so their reactivity **decreases** down the group: the incoming electron is further from the nucleus and more shielded.

A more reactive halogen **displaces** a less reactive one from a solution of its halide ions:

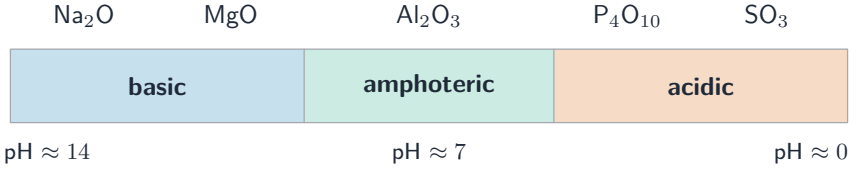
$$\mathrm{Cl_2(aq)} + 2\mathrm{Br^-(aq)} \rightarrow 2\mathrm{Cl^-(aq)} + \mathrm{Br_2(aq)}$$

The solution turns orange-yellow as bromine forms. Bromine cannot displace chloride ions, because chlorine is more reactive.

Oxides of the elements

From basic to acidic

Metal oxides are mostly ionic and **basic** : they react with acids, and those that dissolve give alkaline solutions. Non-metal oxides are covalent and **acidic** : they react with bases and dissolve to give acidic solutions.



metal oxides (left) are basic; non-metal oxides (right) are acidic

Across period 3 the oxides change from basic through amphoteric to acidic

Oxide	Bonding	Reaction with water	Character
Na_2O	ionic	$Na_2O + H_2O \rightarrow 2NaOH$	basic
MgO	ionic	$MgO + H_2O \rightarrow Mg(OH)_2$ (slightly soluble)	basic
Al_2O_3	ionic with covalent character	insoluble	**amphoteric**
SiO_2	giant covalent	insoluble	acidic (reacts with hot NaOH)
P_4O_{10}	molecular covalent	$P_4O_{10} + 6H_2O \rightarrow 4H_3PO_4$	acidic
SO_3	molecular covalent	$SO_3 + H_2O \rightarrow H_2SO_4$	acidic

An amphoteric oxide reacts with both acids and bases:

$$Al_2O_3 + 6HCl \rightarrow 2AlCl_3 + 3H_2O \qquad Al_2O_3 + 2NaOH + 3H_2O \rightarrow 2NaAl(OH)_4$$

■ Acid deposition and ocean acidification

Non-metal oxides in the air make rain more acidic. Burning fuels that contain sulfur forms SO_2, and the high temperature in engines forms nitrogen oxides. In the air they form sulfuric and nitric acid:

$$SO_2 + H_2O \rightarrow H_2SO_3 \qquad 4NO_2 + O_2 + 2H_2O \rightarrow 4HNO_3$$

This **acid deposition** damages limestone buildings, forests and lakes. Carbon dioxide dissolving in the oceans forms carbonic acid, $CO_2 + H_2O \rightleftharpoons H_2CO_3$, which lowers the pH of seawater: **ocean acidification** . It makes it harder for corals and shellfish to build calcium carbonate shells.

Oxidation states

■ Rules for assigning oxidation states

An **oxidation state** is the charge an atom would have if all its bonds were ionic. It is written with the sign first: +2, −1.

1. An uncombined element is 0: Fe, O_2, Cl_2.
2. A simple ion has its charge: Na^+ is +1, O^{2-} is −2.
3. In a compound, oxygen is usually −2 (except in peroxides, −1, and with fluorine), hydrogen is usually +1 (except in metal hydrides, −1), and fluorine is always −1.
4. The oxidation states add up to zero in a compound, and to the charge in an ion.

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Worked example: the oxidation state of Mn in MnO_4^-. Four oxygens give $4(-2) = -8$. The total must be -1, so $Mn + (-8) = -1$, and Mn is $+7$.

Naming with Roman numerals

When an element can have more than one oxidation state, the name shows it in Roman numerals: iron(II) chloride is $FeCl_2$, iron(III) chloride is $FeCl_3$. Oxyanions are named the same way: SO_4^{2-} is sulfate(VI) and SO_3^{2-} is sulfate(IV), commonly called sulfite; NO_3^- is nitrate(V).

AHL: Transition elements

What makes an element a transition element

A **transition element** is an element that has an incomplete d sublevel, or that forms at least one stable ion with an incomplete d sublevel. In the first row, titanium to copper are transition elements.

- Scandium forms only Sc^{3+}, [Ar], with an empty d sublevel: **not** a transition element.
- Zinc forms only Zn^{2+}, $[Ar]\,3d^{10}$, with a full d sublevel: **not** a transition element.

When a transition element forms an ion, it loses its **4s electrons first**: Fe is $[Ar]\,3d^6\,4s^2$ and Fe^{2+} is $[Ar]\,3d^6$.

Characteristic properties

Transition elements share four properties:

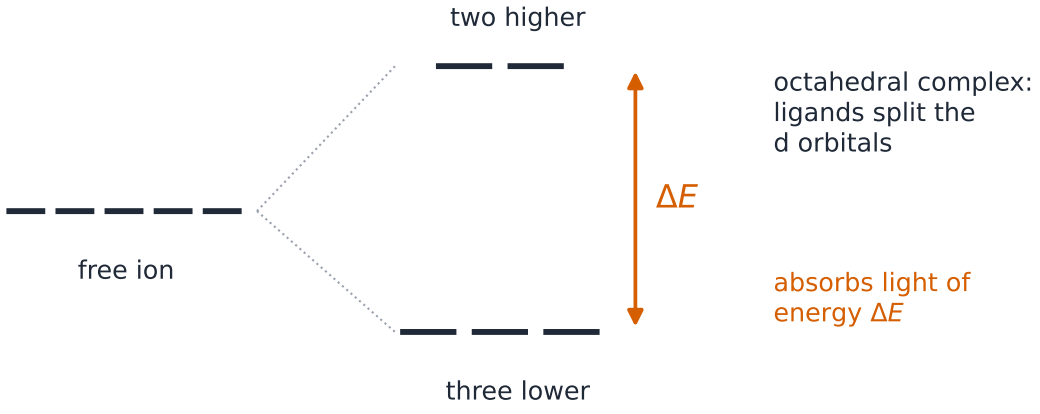
1. **Variable oxidation states.** The 4s and 3d sublevels are close in energy, so successive ionization energies rise gradually and different numbers of electrons can be lost. Manganese shows every state from +2 to +7, as in Mn^{2+}, MnO_2 and MnO_4^-.
2. **Complex ions.** A central metal ion bonds to **ligands** : molecules or ions with a lone pair that form coordination bonds to the metal, such as H_2O, NH_3, Cl^- and CN^-. The number of coordination bonds is the **coordination number** . Example: $[Cu(H_2O)_6]^{2+}$ is octahedral, with coordination number 6.
3. **Coloured compounds**, explained below.
4. **Catalytic activity.** Variable oxidation states and the ability to adsorb molecules on the surface make transition elements good catalysts: iron in the Haber process, V_2O_5 in the Contact process, nickel in the hydrogenation of alkenes, and MnO_2 in the decomposition of hydrogen peroxide.

The charge on a complex ion is the oxidation state of the metal plus the charges of the ligands. In $[CuCl_4]^{2-}$, four Cl^- give -4, so copper is $+2$.

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Why transition metal complexes are coloured

In a free ion the five d orbitals have the same energy. In a complex, the lone pairs of the ligands repel the d electrons. In an octahedral complex, two of the d orbitals point straight at the ligands and are raised in energy; the other three are lowered. The d orbitals **split** into two sets separated by an energy gap ΔE.



An electron absorbs light of energy ΔE to move to a higher d orbital

An electron in a lower d orbital absorbs a photon of visible light with energy equal to ΔE and moves to a higher d orbital. The light that is **not** absorbed passes through, so we see the **complementary colour** . $[Cu(H_2O)_6]^{2+}$ absorbs orange-red light and looks blue.

The size of ΔE, and so the colour, depends on:

- the **metal** and its **oxidation state**: Fe^{2+} solutions are pale green, Fe^{3+} yellow-brown;
- the **ligand**: adding ammonia to blue $[Cu(H_2O)_6]^{2+}$ gives deep blue $[Cu(NH_3)_4(H_2O)_2]^{2+}$, because NH_3 splits the d orbitals more strongly;
- the **coordination number** and shape of the complex.

There is no colour if no d-to-d transition is possible: Sc^{3+} ($3d^0$) and Zn^{2+} ($3d^{10}$) compounds are white or colourless.

Magnetic properties

Electrons spin, and an unpaired electron behaves like a tiny magnet.

- A substance with **unpaired** electrons is **paramagnetic** : it is attracted into a magnetic field. The more unpaired electrons, the stronger the attraction. Fe^{3+}, $3d^5$, has five unpaired electrons and is strongly paramagnetic.
- A substance with **all electrons paired** is **diamagnetic** : it is weakly repelled by a magnetic field. Zn^{2+}, $3d^{10}$, is diamagnetic.

Iron, cobalt and nickel are also **ferromagnetic**: the unpaired electrons of neighbouring atoms line up, so the metals can become permanent magnets.

Practice

1. Without a periodic table, state the period, group and block of the element with configuration $1s^2\,2s^2\,2p^6\,3s^2\,3p^4$.
2. Explain why the atomic radius decreases from sodium to chlorine.
3. Put these in order of increasing radius and explain: Mg^{2+}, Na^+, F^-, O^{2-}.
4. Explain why potassium reacts more vigorously with water than sodium.
5. Write an equation for the reaction of chlorine with aqueous potassium iodide, and state what you would see.
6. Write equations to show the reaction of (a) sodium oxide and (b) sulfur trioxide with water, and state the effect of each on the pH.
7. Deduce the oxidation state of: (a) Cr in $Cr_2O_7^{2-}$, (b) S in $Na_2S_2O_3$, (c) N in NH_4^+.
8. **AHL.** Explain why zinc is a d-block element but not a transition element.
9. **AHL.** State the oxidation state of the metal and the coordination number in $[Fe(CN)_6]^{3-}$.
10. **AHL.** Explain why $[Cu(H_2O)_6]^{2+}$ is blue, and why the colour changes when ammonia is added.
11. **AHL.** Deduce the number of unpaired electrons in Mn^{2+} and state whether it is paramagnetic or diamagnetic.

Answers.

1. Period 3 (outer level $n = 3$), group 16 (six outer electrons), p block. It is sulfur.
2. The nuclear charge increases from +11 to +17, but the outer electrons stay in the same energy level, with about the same shielding. The outer electrons are pulled closer to the nucleus.
3. $Mg^{2+} < Na^+ < F^- < O^{2-}$. All four have the neon configuration (10 electrons). The nuclear charges are 12, 11, 9 and 8; the larger the nuclear charge, the more strongly the same electrons are pulled in.
4. Potassium's outer electron is in the fourth energy level, further from the nucleus and more shielded than sodium's. It is held less strongly, so it is lost more easily.
5. $Cl_2(aq) + 2KI(aq) \to 2KCl(aq) + I_2(aq)$. The colourless solution turns brown as iodine forms.
6. (a) $Na_2O + H_2O \to 2NaOH$: the pH rises (alkaline, about 14). (b) $SO_3 + H_2O \to H_2SO_4$: the pH falls (strongly acidic, about 0 to 1).
7. (a) $2Cr + 7(-2) = -2$, so Cr is +6. (b) $2(+1) + 2S + 3(-2) = 0$, so S is +2. (c) $N + 4(+1) = +1$, so N is −3.

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8. **AHL.** Zinc is in the d block because its last electrons fill the 3d sublevel. But its only ion, Zn^{2+}, is $[Ar]\,3d^{10}$, and the atom is $[Ar]\,3d^{10}\,4s^2$: neither has an incomplete d sublevel.
9. **AHL.** Six CN^- ligands give -6; the total is -3, so iron is $+3$. Coordination number 6.
10. **AHL.** The water ligands split the 3d orbitals of Cu^{2+}. An electron absorbs orange-red light of energy ΔE to move to a higher d orbital, and we see the complementary colour, blue. Ammonia ligands split the d orbitals by a different amount, so a different wavelength is absorbed and the colour changes to deep blue.
11. **AHL.** Mn is $[Ar]\,3d^5\,4s^2$; Mn^{2+} loses the 4s electrons, giving $3d^5$. The five electrons occupy the five d orbitals singly: five unpaired electrons, so it is paramagnetic.

Exam tips

- Explain every trend with **nuclear charge**, **shielding** and **distance**; say what happens to the attraction for the outer electrons.
- Across a period, electrons go into the **same** energy level; down a group, a **new** level is added.
- Isoelectronic ions: compare nuclear charge only; the electron number is the same.
- Metal oxides are basic, non-metal oxides acidic, Al_2O_3 amphoteric; write equations for both of its reactions.
- Write oxidation states with the sign **first** ($+3$), and charges with the sign last ($3+$).
- **AHL.** Transition metals lose **4s** electrons before 3d electrons.
- **AHL.** For colour, say that the d orbitals **split**, light of energy ΔE is **absorbed**, and the **complementary** colour is seen; never say the complex "emits" its colour.

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Functional groups: classification of organic compounds

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Structure 3.2, Functional groups: classification of organic compounds, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: covalent bonding and molecular shapes from Structure 2.2, intermolecular forces and hydrogen bonding, and the mole and empirical formulae from Structure 1.4. Use the data booklet for infrared and ^{1}H NMR data.

Representing organic molecules

Same formula, different substances

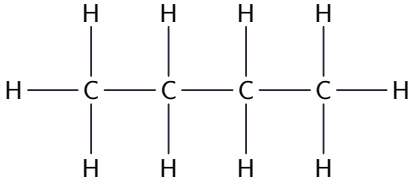
Ethanol and methoxymethane both have the formula C_2H_6O. Ethanol is the liquid in alcoholic drinks and boils at 78 °C; methoxymethane is a gas used in aerosol sprays and boils at −24 °C. The atoms are the same, but they are joined in a different order. In organic chemistry the formula alone is not enough: you need to show the structure.

Types of formula

molecular C_4H_{10}

condensed $CH_3CH_2CH_2CH_3$

full structural



skeletal



Each type of formula shows less detail than the one above it

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Formula	What it shows	Butan-1-ol
molecular	the number of atoms of each element	$C_4H_{10}O$
empirical	the simplest whole-number ratio	$C_4H_{10}O$
condensed structural	the atoms on each carbon, in order	$CH_3CH_2CH_2CH_2OH$
full structural	every atom and every bond	all 15 atoms and 14 bonds drawn
skeletal	carbon chain as a zigzag; C and H on carbon left out	a zigzag of 4 corners with OH at one end

In a **skeletal formula** each corner and each line end is a carbon atom, and each carbon has enough hydrogen atoms to make four bonds. Atoms other than C and H (and H atoms on them, as in OH) are always written.

A benzene ring, C_6H_6, is drawn as a hexagon with a circle inside, which shows the delocalized electrons. A benzene ring attached to a chain is a **phenyl** group, C_6H_5–.

Functional groups and homologous series

Functional groups

A **functional group** is the atom or group of atoms that gives a compound its typical reactions. Compounds with the same functional group react in similar ways.

Class	Functional group	Suffix or prefix	Example
alkane	C–C only	-ane	propane, $CH_3CH_2CH_3$
alkene	C=C	-ene	propene, $CH_2{=}CHCH_3$
alkyne	C≡C	-yne	ethyne, HC≡CH
halogenoalkane	–X (F, Cl, Br, I)	fluoro-, chloro-, bromo-, iodo-	bromoethane, CH_3CH_2Br
alcohol	–OH (hydroxyl)	-ol	ethanol, CH_3CH_2OH
aldehyde	–CHO (carbonyl at the chain end)	-al	ethanal, CH_3CHO

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Class	Functional group	Suffix or prefix	Example
ketone	C=O inside the chain (carbonyl)	-one	propanone, CH_3COCH_3
carboxylic acid	–COOH (carboxyl)	-oic acid	ethanoic acid, CH_3COOH
ether	C–O–C (ether)	alkoxy-	methoxymethane, CH_3OCH_3
ester	–COO– (ester)	-yl -oate	methyl ethanoate, CH_3COOCH_3
amine	$–NH_2$ (amino)	-amine	ethylamine, $CH_3CH_2NH_2$
amide	$–CONH_2$ (amido)	-amide	ethanamide, CH_3CONH_2
nitrile	–C≡N	-nitrile	ethanenitrile, CH_3CN

Homologous series

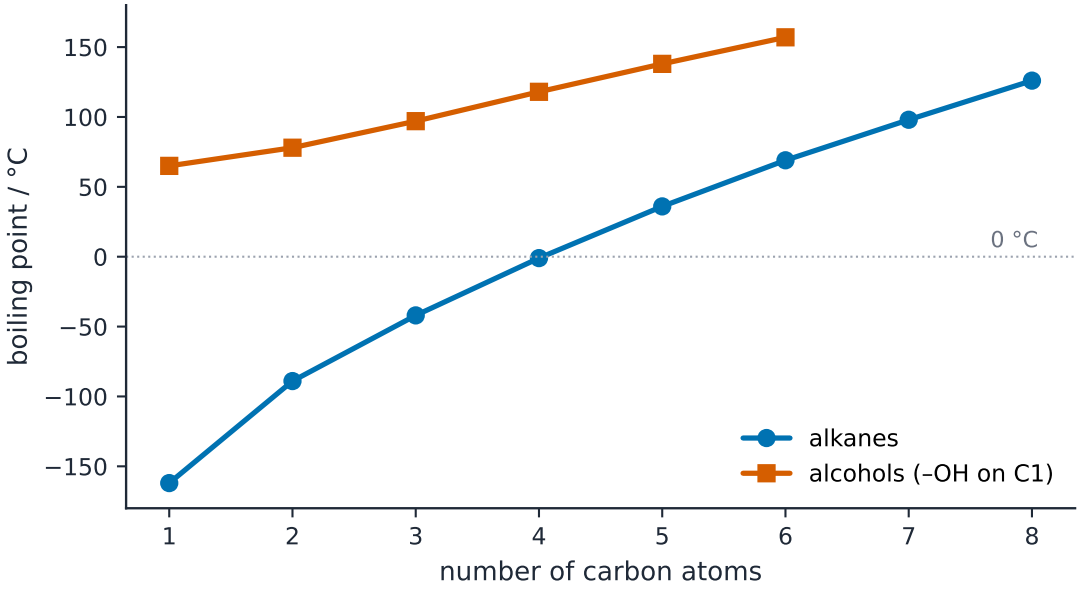
A **homologous series** is a family of compounds with the same functional group and the same general formula.

- Each member differs from the next by CH_2.
- They have similar chemical properties.
- Physical properties, such as boiling point, change gradually along the series.

Series	General formula
alkanes	C_nH_{2n+2}
alkenes	C_nH_{2n}
alcohols	$C_nH_{2n+1}OH$
carboxylic acids	$C_nH_{2n+1}COOH$

Trends in boiling point

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Each extra CH_2 raises the boiling point; hydrogen bonding lifts the whole alcohol series

- Each extra CH_2 adds electrons and surface area, so London forces between molecules get stronger and the boiling point rises.
- Branched isomers have lower boiling points than straight chains: the molecules touch over a smaller area.
- Alcohols and carboxylic acids boil much higher than alkanes of similar mass because their molecules form hydrogen bonds.

Naming organic compounds

The IUPAC rules

The IUPAC system gives each compound one name built from three parts: prefix, stem and suffix.

1. Find the longest carbon chain that contains the functional group. Its length gives the stem.

Carbons	**1**	**2**	**3**	**4**	**5**	**6**
Stem	meth-	eth-	prop-	but-	pent-	hex-

1. Add the suffix of the main functional group (-ene, -ol, -al, -one, -oic acid).
2. Number the chain from the end that gives the functional group the lowest number. Put the number before the suffix: but-1-ene, propan-2-ol.
3. Name side chains (methyl-, ethyl-) and halogens (chloro-, bromo-) as prefixes with their position numbers, in alphabetical order.
4. Use di-, tri- for repeated groups: 2,2-dimethylpropane.

Worked examples

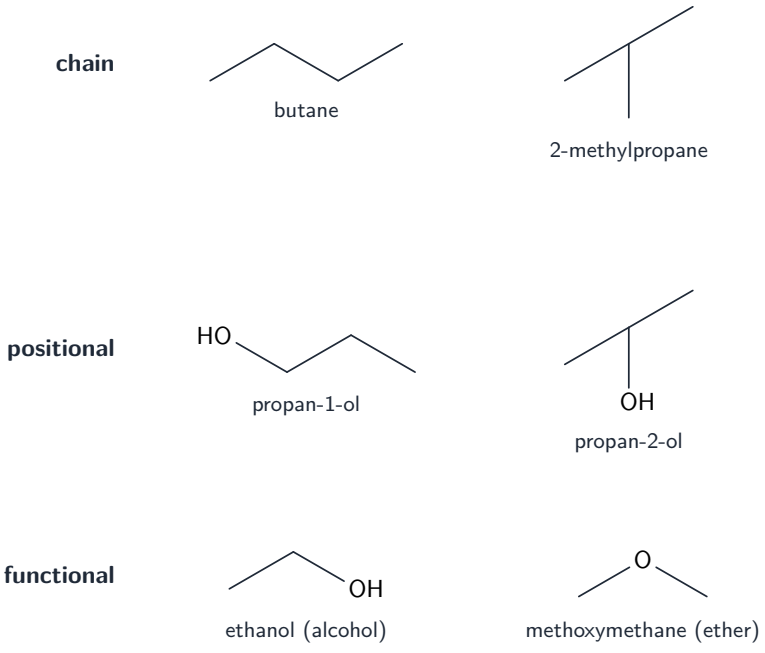
- $CH_3CH(OH)CH_3$: 3 carbons, –OH on carbon 2 → **propan-2-ol**.
- $CH_3CH_2CH(CH_3)CH_3$: longest chain 4 carbons, methyl on carbon 2 → **2-methylbutane** (not 3-methylbutane).
- $CH_2{=}CHCH_2CH_3$: 4 carbons, C=C starting at carbon 1 → **but-1-ene**.
- $CH_3CHBrCH_3$: **2-bromopropane**.
- CH_3CH_2COOH: 3 carbons including the COOH carbon → **propanoic acid**.

An aldehyde or carboxylic acid group is always on carbon 1, so it needs no number.

Structural isomers

Same molecular formula, different structure

Structural isomers have the same molecular formula but a different structural formula: the atoms are joined in a different order.



Structural isomers differ in their chain, in the position of a group, or in the functional group itself

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Type	What changes	Example, C_n...
chain	the carbon skeleton is branched differently	butane and 2-methylpropane, C_4H_{10}
position	the functional group sits on a different carbon	propan-1-ol and propan-2-ol, C_3H_8O
functional group	the atoms form a different functional group	ethanol and methoxymethane, C_2H_6O

Alcohols are classified by the carbon that holds the –OH: **primary** (that carbon has one other carbon attached), **secondary** (two) or **tertiary** (three). Propan-1-ol is primary; propan-2-ol is secondary; 2-methylpropan-2-ol is tertiary. Halogenoalkanes are classified the same way.

Identifying compounds

Index of hydrogen deficiency

The **index of hydrogen deficiency** (IHD) counts how many rings and π bonds a molecule has. Each ring or double bond counts 1; a triple bond counts 2. For a compound $C_cH_hN_nO_oX_x$ (X = halogen):

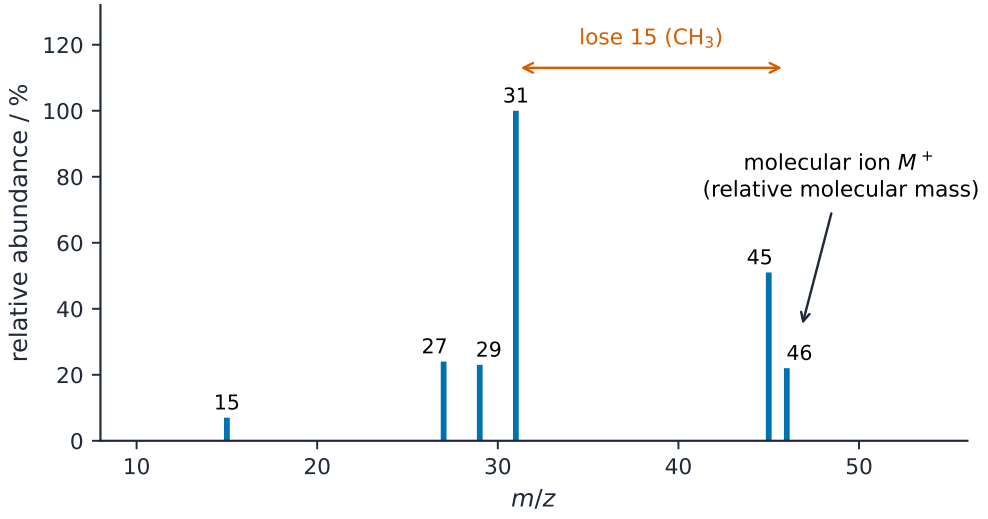
$$\text{IHD} = \frac{2c + 2 + n - h - x}{2}$$

Oxygen does not affect the IHD. For C_3H_6O: $(6+2-6)/2 = 1$, so one C=C, one C=O or one ring. Benzene, C_6H_6: $(12 + 2 - 6)/2 = 4$ (one ring and three double bonds).

Mass spectrometry

In a **mass spectrometer** molecules are ionized and break into fragments. The spectrum shows each ion's mass-to-charge ratio, m/z.

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M^+ (highest m/z) $\approx M_r$ · gaps = masses lost

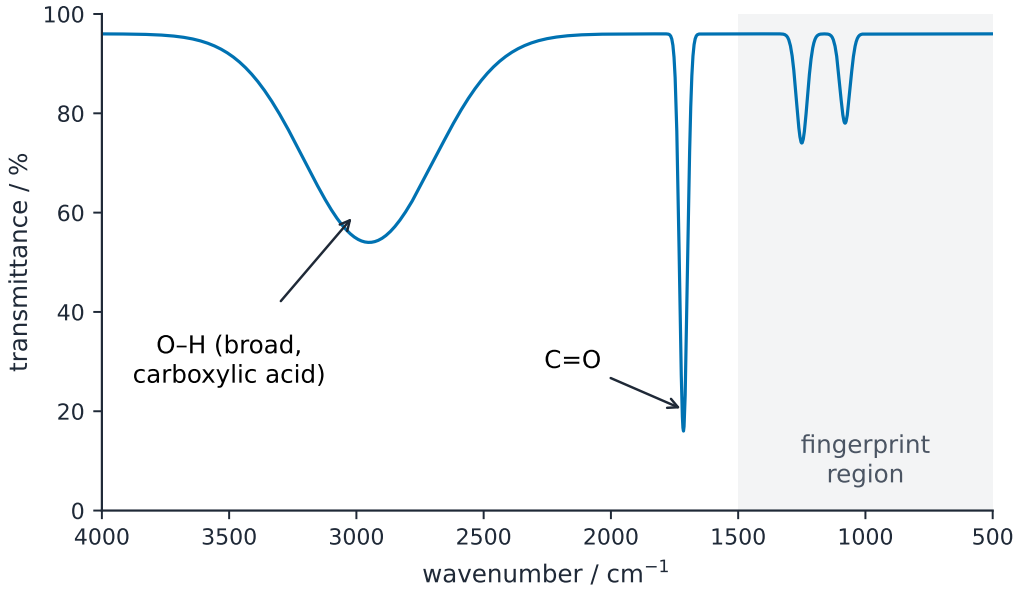
The molecular ion gives M_r; the gaps between peaks show which pieces broke off

- The **molecular ion** peak, at the highest m/z, gives the relative molecular mass: 46 for ethanol.
- Fragment peaks show what was lost. Common losses: 15 (CH_3), 17 (OH), 29 (C_2H_5 or CHO), 31 (CH_3O), 45 (COOH).
- For ethanol, 31 is CH_2OH^+: the molecule lost CH_3 (46 − 15).

Infrared spectroscopy

Bonds absorb infrared radiation at frequencies that make them vibrate. Each type of bond absorbs in its own range, so an IR spectrum shows which **bonds**, and so which functional groups, are present. The x-axis is the **wavenumber** in cm^{-1}; absorptions appear as dips in transmittance.

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A broad O–H band and a strong C=O band together mean a carboxylic acid

Bond	**Wavenumber / cm^{-1} (data booklet)**	**Look**
O–H in alcohols	3200–3600	broad
O–H in carboxylic acids	2500–3000	very broad
N–H	3300–3500	medium
C–H	2850–3090	strong, in most organic molecules
C=O	1700–1750	strong, sharp
C=C	1620–1680	medium
C–O	1050–1410	strong

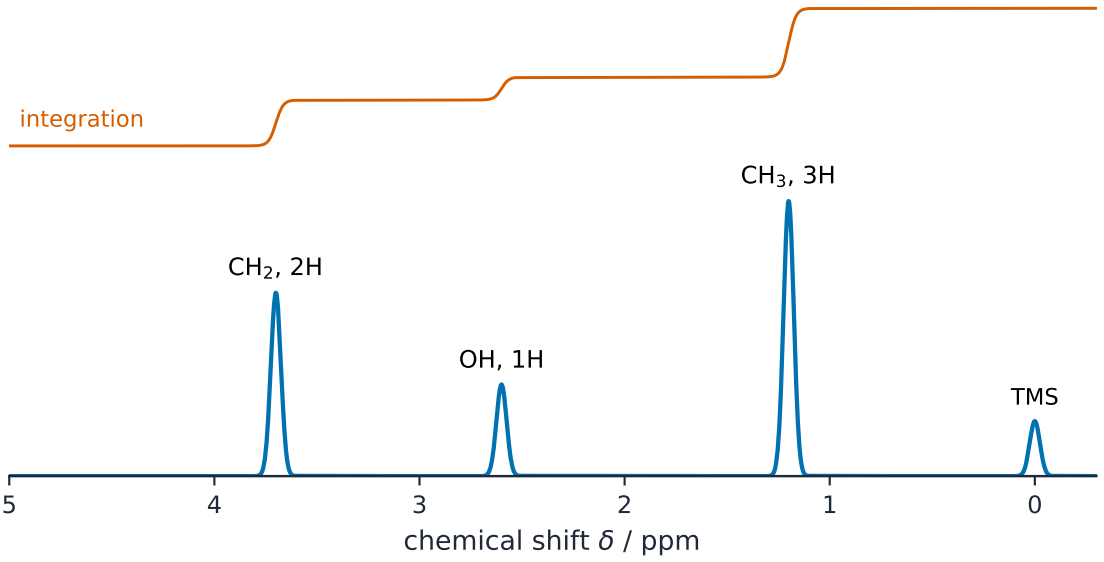
Below about 1500 cm^{-1} lies the **fingerprint region** : a complex pattern that is unique to each compound and can be matched to a database.

^{1}H NMR spectroscopy

What the spectrum shows

In ^{1}H **nuclear magnetic resonance** (NMR) spectroscopy, hydrogen nuclei in a strong magnetic field absorb radio waves. Hydrogen atoms in different surroundings absorb at slightly different frequencies.

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Three peaks for three hydrogen environments; the integration gives their ratio

- **Number of peaks** = the number of different hydrogen environments. Ethanol, CH_3CH_2OH, has three.
- **Chemical shift** , δ in ppm, tells you what each hydrogen is near. Electronegative atoms nearby move the peak to a higher shift.
- **Integration** : the area under each peak is proportional to the number of hydrogen atoms in that environment: 2 : 1 : 3 for ethanol.
- **TMS**, tetramethylsilane, $Si(CH_3)_4$, is the reference at $\delta = 0$. It gives one strong peak away from most others, and it is inert.

Hydrogen type	δ **/ ppm (data booklet)**
R–CH_3	0.9–1.0
CH next to C=O (–CH_2–CO–)	2.2–2.7
CH next to O (–O–CH_2–)	3.3–3.7
CH next to the O of an ester (–COO–CH_2–)	3.7–4.8
R–OH	1.0–6.0
on a benzene ring	6.9–9.0
–CHO	9.4–10.0
–COOH	9.0–13.0

■ Worked example: using several techniques

A compound has molecular formula $C_3H_6O_2$.

- IHD $= (6 + 2 - 6)/2 = 1$: one C=O (or C=C or ring).
- IR: strong peak at 1740 cm^{-1} (C=O), no broad band at 2500–3600 cm^{-1}, so no O–H: not an acid. An ester is likely.
- MS: molecular ion at m/z 74, which matches M_r for $C_3H_6O_2$.
- ^{1}H NMR: three peaks at 3.7 (3H), 2.3 (2H) and 1.1 (3H). The 3.7 peak is CH_3 next to O; the 2.3 peak is CH_2 next to C=O.

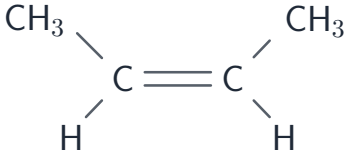
The compound is methyl propanoate, $CH_3CH_2COOCH_3$.

AHL: Stereoisomers

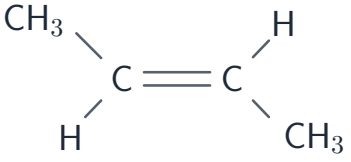
■ What stereoisomers are

Stereoisomers have the same structural formula (the same atoms joined in the same order) but a different arrangement of the atoms in space.

■ Cis–trans isomers



cis: both CH_3 on the same side



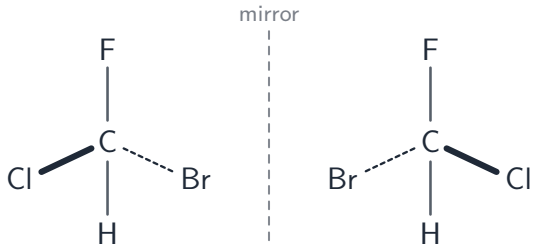
trans: CH_3 on opposite sides

Rotation about C=C is restricted, so the two forms do not interconvert

- A C=C double bond cannot rotate, because rotation would break the π bond.
- **Cis–trans isomers** form when each carbon of the C=C has two different groups.
- **Cis**: the same groups on the same side. **Trans**: on opposite sides.
- Ring compounds can show the same isomerism, because a ring also stops rotation: cis- and trans-1,2-dichlorocyclopropane.
- Cis and trans isomers often have different physical properties. Cis-but-2-ene boils at 4 °C and trans-but-2-ene at 1 °C.

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Optical isomers



enantiomers: mirror images that cannot be superimposed
(the central carbon has 4 different groups)

A carbon with four different groups has two mirror-image forms

- A **chiral** carbon atom (a stereocentre) has four different atoms or groups attached.
- A molecule with one chiral carbon exists as two **enantiomers** : mirror images that cannot be superimposed, like a left and a right hand.
- Enantiomers have the same physical properties and the same chemical reactions, except with other chiral substances.
- Enantiomers rotate **plane-polarized light** by the same angle in opposite directions. A polarimeter measures this rotation.
- A **racemic mixture** has equal amounts of the two enantiomers. Their rotations cancel, so it does not rotate the light.

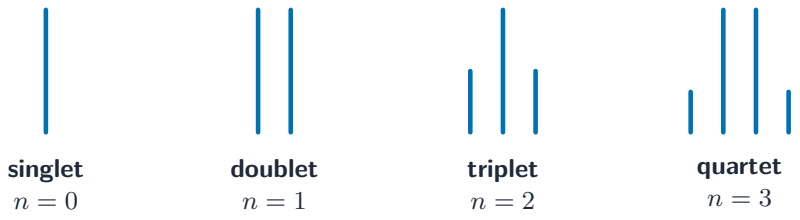
Example: butan-2-ol, $CH_3CH(OH)CH_2CH_3$. Carbon 2 carries H, OH, CH_3 and C_2H_5, four different groups, so it is chiral. Many drugs are chiral, and the two enantiomers can act very differently in the body.

AHL: Splitting in ^{1}H NMR

The n + 1 rule

In a high-resolution spectrum each peak can be split into several lines. The splitting comes from hydrogen atoms on the **neighbouring** carbon atoms (spin–spin coupling).

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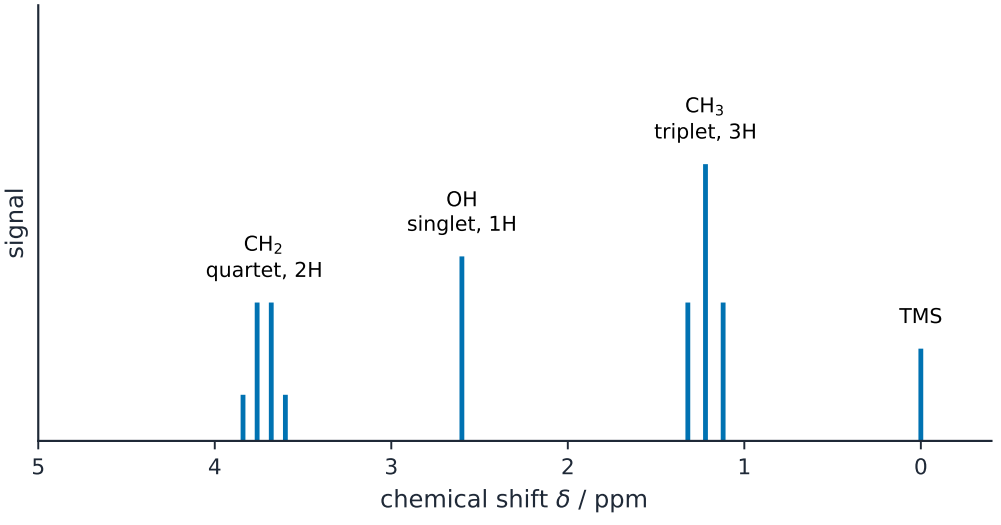
n equivalent neighbours split a peak into $n + 1$ lines

A peak with n equivalent neighbouring H atoms splits into $n + 1$ lines

Neighbouring H	Lines	Name	Line heights
0	1	singlet	1
1	2	doublet	1 : 1
2	3	triplet	1 : 2 : 1
3	4	quartet	1 : 3 : 3 : 1

- Hydrogen atoms in the same environment do not split each other.
- The O–H hydrogen usually appears as a singlet: it exchanges quickly between molecules and does not couple.

■ Reading a high-resolution spectrum



n+1 rule · integration 3 : 2 : 1 · TMS = 0 ppm

CH_3 next to CH_2 gives a triplet; CH_2 next to CH_3 gives a quartet

In ethanol, CH_3 has 2 neighbouring H (on CH_2), so it is a triplet; CH_2 has 3 neighbouring H (on CH_3), so it is a quartet. A triplet with a quartet is the sign of an ethyl

group, CH_3CH_2–.

In methyl propanoate from the worked example, the 3.7 peak (O–CH_3) is a singlet, because its carbon is joined to O, which carries no H; the CH_2 is a quartet and the CH_3 at 1.1 is a triplet.

Practice

1. Draw the skeletal formula of pentan-2-ol and write its condensed structural formula.
2. Name: (a) $CH_3CH_2CH_2CHO$, (b) $CH_3COCH_2CH_3$, (c) $CH_3CH_2COOCH_2CH_3$, (d) $(CH_3)_3CBr$.
3. Give the general formula of the alkenes and the formula of the alkene with 5 carbon atoms.
4. Explain why butan-1-ol (117 °C) boils at a much higher temperature than pentane (36 °C), although their M_r values are similar.
5. Draw and name the structural isomers of $C_4H_{10}O$ that are alcohols, and classify each as primary, secondary or tertiary.
6. Calculate the IHD of $C_4H_8O_2$ and of C_6H_5Cl.
7. A mass spectrum has peaks at m/z 58 (molecular ion) and 43. Suggest the ion at 43 and what was lost, for propanone.
8. An IR spectrum has a broad band at 3350 cm^{-1} and no absorption at 1700–1750 cm^{-1}. Which functional group is present, and which is absent?
9. How many peaks, and in what ratio, are in the ^1H NMR spectrum of (a) propanone, (b) propan-1-ol, (c) methyl ethanoate?
10. Explain why TMS is used as the reference in ^1H NMR.
11. **AHL.** Explain why but-2-ene shows cis–trans isomerism but but-1-ene does not.
12. **AHL.** Identify the chiral carbon in 2-chlorobutane and describe how its two enantiomers could be told apart.
13. **AHL.** Predict the splitting of each peak in the ^1H NMR spectrum of chloroethane, CH_3CH_2Cl.
14. **AHL.** $C_4H_8O_2$ shows IR absorptions at 1740 cm^{-1} and no O–H band. Its ^1H NMR spectrum has a singlet (3H) at 2.0, a quartet (2H) at 4.1 and a triplet (3H) at 1.3. Identify the compound.

Answers.

1. Zigzag of 5 carbons with OH on the second carbon; $CH_3CH(OH)CH_2CH_2CH_3$.
2. (a) butanal, (b) butanone, (c) ethyl propanoate, (d) 2-bromo-2-methylpropane.
3. C_nH_{2n}; C_5H_{10} (for example pent-1-ene).
4. Both have London forces of similar strength, but butan-1-ol molecules also form hydrogen bonds through their –OH groups. More energy is needed to separate them.

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5. Butan-1-ol, $CH_3CH_2CH_2CH_2OH$ (primary); butan-2-ol, $CH_3CH(OH)CH_2CH_3$ (secondary); 2-methylpropan-1-ol, $(CH_3)_2CHCH_2OH$ (primary); 2-methylpropan-2-ol, $(CH_3)_3COH$ (tertiary).
6. $C_4H_8O_2$: $(8 + 2 - 8)/2 = 1$. C_6H_5Cl: $(12 + 2 - 5 - 1)/2 = 4$.
7. 43 is CH_3CO^+; a CH_3 group (15) was lost: $58 - 15 = 43$.
8. O–H of an alcohol is present (broad, 3200–3600 cm^{-1}); C=O is absent.
9. (a) 1 peak. (b) 4 peaks, 3 : 2 : 2 : 1 (CH_3, CH_2, CH_2, OH). (c) 2 peaks, 3 : 3.
10. TMS gives one strong peak (12 equivalent H) at a shift away from most organic signals; it is inert and volatile, so it is easy to remove.
11. **AHL.** In but-2-ene each C of the C=C carries two different groups (H and CH_3), and the C=C cannot rotate. In but-1-ene one carbon of the C=C carries two H atoms, so the two "isomers" would be identical.
12. **AHL.** Carbon 2 (bonded to H, Cl, CH_3 and C_2H_5). The enantiomers rotate plane-polarized light by the same angle in opposite directions, measured with a polarimeter.
13. **AHL.** CH_3: triplet (2 neighbouring H); CH_2: quartet (3 neighbouring H), at a higher shift because it is next to Cl.
14. **AHL.** Ethyl ethanoate, $CH_3COOCH_2CH_3$: the singlet at 2.0 is CH_3 next to C=O (no neighbouring H), the quartet at 4.1 is O–CH_2 next to CH_3, the triplet at 1.3 is the CH_3 of the ethyl group.

Exam tips

- Write the IUPAC name with numbers and hyphens exactly: propan-2-ol, not 2-propanol.
- Choose the longest chain that includes the functional group, and number from the end nearer to it.
- In IR, quote the bond and its wavenumber range from the data booklet, not just the functional group.
- In ^{1}H NMR, the number of peaks is the number of environments; the integration ratio is not the splitting pattern.
- **AHL.** For cis–trans isomerism, check that both carbons of the C=C carry two different groups.
- **AHL.** Splitting counts the H atoms on the next carbon, not on the carbon itself.

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Measuring enthalpy change

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 1.1, Measuring enthalpy changes, for the course first assessed in 2025. This unit has the same content at SL and HL; there are no additional higher-level understandings here.

Prerequisites: balancing equations, $n = m/M$, $n = cV$, limiting reactants and the particle model. All experimental data and questions are original, invented teaching examples.

Energy transfer: choose the system

A reacting mixture warms an insulated cup. Has energy been created? No: energy has been transferred from chemical stores into thermal motion. Total energy is conserved.

The **system** is the part studied; everything else is the **surroundings**. Here the chemical reaction is the system; the solution and cup are the thermal surroundings. The solution contains the reacting particles while also absorbing heat from their reaction.

Heat is energy transferred because of a temperature difference, measured in joules. **Temperature** relates to average particle kinetic energy, not an amount of energy. Two water samples at the same temperature can require different heat transfers for the same rise because their masses differ.

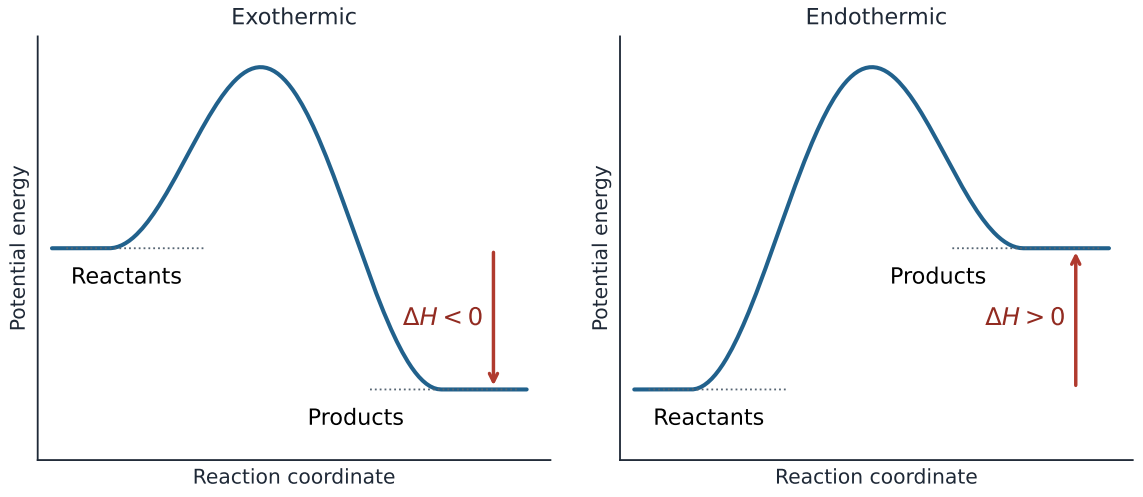
An **exothermic** reaction transfers energy from the system to the surroundings: the solution normally warms and the reaction has a negative **enthalpy change**. An **endothermic** reaction takes energy from its surroundings: the solution normally cools and the reaction has a positive enthalpy change. A cooling solution has lost thermal energy even though the reaction has gained energy.

At constant pressure, with only pressure–volume work, the heat transferred to the reacting system equals its enthalpy change. We measure an enthalpy *difference*, not the absolute enthalpy of a substance.

Reaction profiles and relative stability

An energy profile plots **potential energy** against **reaction coordinate**: progress along a pathway, not time. Label both axes and the reactant and product levels; connect the levels through a peak.

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The sign of the enthalpy change comes from the product level minus the reactant level, not from the height of the peak.

- Exothermic: products have lower potential energy and are more stable in this energetic sense than reactants; $\Delta H < 0$.
- Endothermic: products have higher potential energy and are less stable in this energetic sense; $\Delta H > 0$.
- The peak represents a barrier. Its height above the reactants relates to **activation energy** ; it does not equal the enthalpy change. An exothermic fuel may still need ignition.

Bond breaking requires energy; bond formation releases energy. The net balance determines the sign. Do not say that burning releases energy because bonds are broken. Quantitative bond-energy calculations belong to the next unit. Nor does a negative enthalpy change, by itself, tell us how fast a reaction occurs or fully determine whether it is thermodynamically favourable.

Worked comparison. On an arbitrary common energy scale, reactants are at 80 kJ, products at 30 kJ and the peak at 140 kJ for one stated reaction amount. The endpoint change is $\Delta H = 30 - 80 = -50$ kJ: exothermic. The forward barrier is $140 - 80 = 60$ kJ. Reversing the reaction gives +50 kJ, not −60 kJ.

Standard enthalpy changes

A **standard enthalpy change** refers to a specified reaction at constant pressure with substances in their standard states. Standard pressure is 100 kPa (1 bar). A temperature must also be stated; tables commonly use 298 K. Standard does not mean 0 °C, and 298 K is not part of the definition of standard pressure.

Specify physical states; for a solution, the school-level standard concentration is 1 $\text{mol}\,\text{dm}^{-3}$. Include state symbols in thermochemical equations: producing water vapour rather than liquid water changes the enthalpy change.

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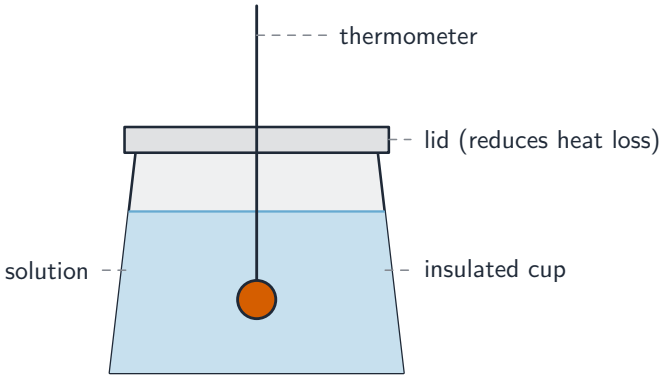
A quoted molar reaction enthalpy is tied to the equation as written. Double every coefficient and the heat change for that reaction amount doubles; reverse the equation and its sign reverses. Always explain the basis of "per mole": per mole of fuel burned, salt dissolved, water formed, or reaction as written. A cup experiment at other conditions yields an experimental estimate; do not attach a standard symbol merely because a thermometer was used.

Calorimetry: from temperature to energy

Calorimetry measures heat transfer through a temperature change. For a substance whose specific heat capacity is approximately constant over the range,

$$q = mc\Delta T, \qquad \Delta T = T_{\text{final}} - T_{\text{initial}}.$$

Here m is the mass being heated or cooled, c its specific heat capacity and q the heat it gains. Specific heat capacity is the energy needed to raise the temperature of unit mass by 1 K. With m in grams and $c = 4.18\ \text{J}\,\text{g}^{-1}\,\text{K}^{-1}$, q is in joules. A temperature *difference* of 1 °C equals 1 K: no 273 conversion is needed for a difference.



Measure the mass and temperature change of the material that absorbs the heat; reduce exchange with the room.

For dilute aqueous mixtures we often approximate density as $1.00\ \text{g}\,\text{cm}^{-3}$ and specific heat capacity as that of water. Use the **total** solution mass, not just the acid volume or the mass of solid added. If dissolving a solid and the stated model includes it, add its mass to the water mass. These are assumptions to justify, not universal properties of all solutions.

If heat exchange with the room and the cup's heat capacity are neglected,

$$q_{\text{reaction}} = -q_{\text{solution}}, \qquad \Delta H_{\text{r}} = -\frac{q_{\text{solution}}}{1000\, n_{\text{reaction}}}.$$

Convert J to kJ before division. The smallest reactant amount/coefficient ratio gives n_{reaction}; for 1:1 equations, use the **limiting reactant** amount.

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■ Worked example: neutralization with unequal amounts

Mix 25.0 cm^3 of 2.00 mol dm^{-3} HCl with 40.0 cm^3 of 1.00 mol dm^{-3} NaOH. Both start at 21.0 °C and the mixture reaches 28.0 °C. Use the water approximations above and neglect the cup.

The equation is $\text{HCl(aq)} + \text{NaOH(aq)} \rightarrow \text{NaCl(aq)} + \text{H}_2\text{O(l)}$.

$$n_{\text{HCl}} = cV = 2.00 \times 0.0250 = 0.0500 \text{ mol}.$$

$$n_{\text{NaOH}} = cV = 1.00 \times 0.0400 = 0.0400 \text{ mol}.$$

NaOH limits this 1:1 reaction; 0.0400 mol of water forms. The heated solution mass is $(25.0 + 40.0) \times 1.00 = 65.0$ g, and $\Delta T = 7.0$ K.

$$q_{\text{solution}} = mc\Delta T = 65.0 \times 4.18 \times 7.0 = 1901.9 \text{ J}.$$

$$\Delta H_{\text{r}} = -\frac{q_{\text{solution}}}{1000n} = -\frac{1901.9}{1000 \times 0.0400} \approx -48 \text{ kJ mol}^{-1}.$$

The solution gains heat; the reaction loses heat. Dividing by 0.0500 mol would include unreacted acid. The result is an experimental estimate, not evidence that heat loss was absent.

■ Worked example: an endothermic dissolution

Dissolve 4.00 g of a salt of molar mass 80.0 g mol^{-1} in 100.0 g water. The temperature falls from 22.0 to 18.5 °C. Include the salt in the solution mass and assume $c = 4.18 \text{ J g}^{-1} \text{ K}^{-1}$.

$$n = \frac{m_{\text{salt}}}{M} = \frac{4.00}{80.0} = 0.0500 \text{ mol}.$$

$$q_{\text{solution}} = mc\Delta T = 104.0 \times 4.18 \times (-3.5) = -1521.52 \text{ J}.$$

$$\Delta H_{\text{solution}} = -\frac{q_{\text{solution}}}{1000n} = -\frac{-1521.52}{1000 \times 0.0500} \approx +30 \text{ kJ mol}^{-1}.$$

Keep the negative temperature change through the calculation. The solution loses heat while the dissolving process gains it.

■ If the cup absorbs appreciable heat

A calibrated calorimeter heat capacity C_{cal} is in J K^{-1}, so it needs no mass factor. When cup and solution undergo the same temperature change,

$$q_{\text{surroundings}} = (mc + C_{\text{cal}})\Delta T.$$

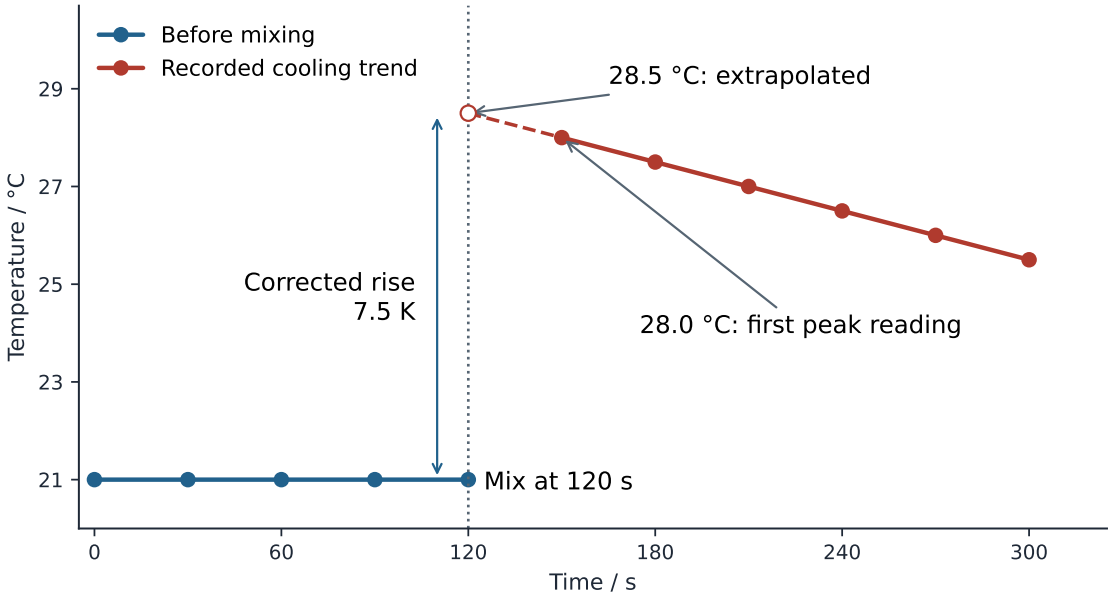
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For 100.0 g solution, $c = 4.18\ \mathrm{J\,g^{-1}\,K^{-1}}$, $C_{\mathrm{cal}} = 32.0\ \mathrm{J\,K^{-1}}$ and a 5.00 K rise, $q_{\mathrm{surroundings}} = (418 + 32.0) \times 5.00 = 2250$ J. If 0.0500 mol reacts, $\Delta H = -45.0\ \mathrm{kJ\,mol^{-1}}$. Ignoring the cup gives $-41.8\ \mathrm{kJ\,mol^{-1}}$, a smaller magnitude.

Designing and interpreting an experiment

Use approved apparatus, eye protection and teacher-specified reagents and quantities. An insulated cup and lid reduce heat exchange; a stirrer makes temperature more uniform. Immerse the thermometer bulb without touching the cup. Bring solutions to the same initial temperature, or account for their different starting temperatures; averaging them without regard to their masses and heat capacities is not generally valid.

Record temperature regularly before mixing, note the mixing time, then record through the rise or fall and subsequent return towards room temperature. A single observed maximum may miss heat already lost while mixing and reading.



Extrapolate suitable pre- and post-reaction trends to the same mixing time; do not read the extrapolated value at a later time.

In this simplified invented example, mixing is at 120 s, the baseline is 21.0 °C, and the later cooling trend extrapolates to 28.5 °C at mixing. The corrected rise is $28.5 - 21.0 = 7.5$ K rather than the observed $28.0 - 21.0 = 7.0$ K. If all else is unchanged, the corrected heat and enthalpy magnitude are $7.5/7.0 \approx 1.07$ times larger. The cooling trend must represent heat exchange during the short reaction. Slow reaction, evaporation or changing conditions can invalidate that assumption.

For combustion, heat water above a spirit burner and weigh the capped burner before and after. The fuel amount comes from mass *lost* divided by molar mass; the heated

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mass in $mc\Delta T$ is the water. Keep the burner–container distance consistent and reduce draughts without restricting oxygen. A flame shield must not turn the apparatus into a sealed vessel. Extinguish before weighing; never refill a hot burner.

Heat escaping to the air, heat absorbed by apparatus and incomplete combustion commonly make a measured combustion enthalpy less negative than the complete-combustion value. Soot suggests incomplete combustion. Fuel evaporation increases apparent fuel use without supplying the measured heat and also reduces the calculated magnitude. Repetition reduces random uncertainty, not systematic heat-loss bias.

Distinguish **uncertainty** from percentage disagreement with a reference. If each temperature reading has a stated maximum uncertainty of ±0.1 °C, conservative addition gives ±0.2 K in the difference. A 2.0 K rise has 10% temperature-difference uncertainty; a 10.0 K rise has 2%. Do not increase quantities beyond safe limits merely to improve this percentage.

Practice

Use $c = 4.18\ \mathrm{J\,g^{-1}\,K^{-1}}$ unless stated otherwise. Neglect apparatus heat capacity except in question 8. All data are invented.

1. Explain the difference between heat and temperature. Compare the heat needed to warm 50 g and 100 g of water by the same 4 K.
2. A reaction cools its solution. State the signs of q_{solution} and $\Delta H_{\mathrm{reaction}}$, and identify the direction of energy transfer.
3. An energy profile has reactants at 40 kJ, products at 90 kJ and a peak at 130 kJ for a stated reaction amount. Find the forward enthalpy change, forward barrier and reverse enthalpy change. State which endpoint is lower in energy.
4. A student calls any reaction measured at 25 °C "standard" and omits state symbols. Explain two problems with this claim.
5. A 75.0 g solution warms from 20.0 to 24.0 °C. Calculate the heat it gains and the molar reaction enthalpy if 0.0250 mol reacts.
6. Mix 30.0 $\mathrm{cm^3}$ of 1.00 mol $\mathrm{dm^{-3}}$ HCl with 20.0 $\mathrm{cm^3}$ of 1.00 mol $\mathrm{dm^{-3}}$ NaOH. Both start at 20.0 °C; the final temperature is 25.0 °C. Use density 1.00 g $\mathrm{cm^{-3}}$. Determine the limiting reactant and enthalpy change per mole of water formed.
7. A 2.00 g salt, molar mass 100 g $\mathrm{mol^{-1}}$, dissolves in 50.0 g water. Temperature falls by 2.0 K. Include the salt in the heated/cooled mass. Calculate the molar enthalpy of solution.
8. A 100.0 g solution and calorimeter of heat capacity 40.0 J $\mathrm{K^{-1}}$ warm by 4.00 K when 0.0400 mol reacts. Calculate the enthalpy change including the calorimeter. Explain the effect of ignoring it.
9. An alcohol of molar mass 46.0 g $\mathrm{mol^{-1}}$ loses 0.460 g from a burner while 200.0 g water warms by 12.0 K. Calculate the experimental molar combustion enthalpy. Explain why using 0.460 g in $mc\Delta T$ is wrong.

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10. A reaction starts at 20.0 °C. The observed peak is 26.0 °C; extrapolation to mixing gives 26.8 °C. Find both temperature rises and the factor by which the calculated enthalpy magnitude changes.
11. Give two separate reasons why a spirit-burner result may be less negative than a complete-combustion reference, and one appropriate improvement for each. Would repeating the unmodified experiment remove these biases?
12. Two temperature readings each have a maximum uncertainty of ±0.1 °C. Find the conservative percentage uncertainty in a 3.0 K rise. Distinguish this from percentage disagreement when an experimental enthalpy is −42.0 kJ mol^{-1} and the stated reference is −50.0 kJ mol^{-1}.
13. In the equation $H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l)$, the stated enthalpy change is −286 kJ per mole of reaction. Find the heat transferred by the reaction when 0.250 mol water forms, then state the enthalpy changes for the doubled equation and the reversed original equation.

■ Worked answers

1. Heat is energy transferred because of a temperature difference; temperature relates to average particle kinetic energy. $q = mc\Delta T$: the 50 g sample needs $50 \times 4.18 \times 4 =$ 836 J and the 100 g sample needs 1672 J. Doubling the mass doubles the required heat, although both temperature rises are equal.
2. $q_{\text{solution}} < 0$, so $q_{\text{reaction}} > 0$ and $\Delta H_{\text{reaction}} > 0$: endothermic. Energy transfers from the thermal surroundings to the reacting system.
3. $\Delta H = H_{\text{products}} - H_{\text{reactants}} = 90 - 40 = +50$ kJ; forward barrier $= 130 - 40 = 90$ kJ. The reverse enthalpy change is −50 kJ. Reactants are lower in potential energy; the forward reaction is endothermic.
4. Temperature alone does not establish standard states: pressure, solution concentration where applicable and physical states matter. State symbols distinguish different initial and final states, whose enthalpies differ. The temperature must be specified too.
5. $q = mc\Delta T = 75.0 \times 4.18 \times 4.0 = 1254$ J. $\Delta H = -q/(1000n) = -1254/(1000 \times 0.0250) \approx -50$ kJ mol^{-1}; the reaction supplies the heat gained by solution.
6. $n = cV$: HCl is $1.00 \times 0.0300 = 0.0300$ mol; NaOH is $1.00 \times 0.0200 = 0.0200$ mol. NaOH limits the 1:1 reaction, giving 0.0200 mol water. Total mass is 50.0 g. $q = mc\Delta T = 50.0 \times 4.18 \times 5.0 = 1045$ J. $\Delta H = -q/(1000n) = -1045/20.0 \approx -52$ kJ mol^{-1}.
7. $n = m/M = 2.00/100 = 0.0200$ mol. $q = mc\Delta T = 52.0 \times 4.18 \times (-2.0) = -434.72$ J. $\Delta H = -q/(1000n) = +434.72/20.0 \approx +22$ kJ mol^{-1}. The dissolution absorbs energy.
8. $q = (mc + C_{\text{cal}})\Delta T = (100.0 \times 4.18 + 40.0) \times 4.00 = 1832$ J. $\Delta H = -q/(1000n) = -1832/40.0 = -45.8$ kJ mol^{-1}. Ignoring the calorimeter gives −41.8 kJ mol^{-1}, underestimating the magnitude because it omits energy gained by the cup.

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9. $q = mc\Delta T = 200.0 \times 4.18 \times 12.0 = 10032$ J. $n = m_{\text{fuel}}/M = 0.460/46.0 = 0.0100$ mol. $\Delta H = -q/(1000n) = -10032/10.0 \approx -1.00 \times 10^3$ kJ mol^{-1}. The water is the material whose temperature rise is measured; fuel mass instead determines how many moles burned.
10. $\Delta T_{\text{observed}} = 26.0 - 20.0 = 6.0$ K; $\Delta T_{\text{corrected}} = 26.8 - 20.0 = 6.8$ K. The magnitude increases by a factor $6.8/6.0 \approx 1.13$ (about 13%); the exothermic sign stays negative.
11. Heat escapes to the room: insulation or a suitable draught shield reduces that transfer. Incomplete combustion produces less heat than complete combustion: ensure an adequate oxygen supply and inspect for soot. Repetition alone does not eliminate either systematic bias; a shield that restricts oxygen could worsen combustion.
12. Conservative uncertainty in the difference is $0.1 + 0.1 = 0.2$ K, so percentage uncertainty is $(0.2/3.0) \times 100 \approx 6.7\%$. Percentage disagreement is $|-42.0 - (-50.0)|/50.0 \times 100 = 16\%$. The first quantifies measurement uncertainty; the second compares a result with a specified reference and may reflect systematic effects.
13. $q_{\text{reaction}} = n\Delta H = 0.250 \times (-286) = -71.5$ kJ: 71.5 kJ transfers to the surroundings. For $2H_2 + O_2 \rightarrow 2H_2O(l)$, the enthalpy change is -572 kJ per mole of the doubled reaction. Reversing the original equation gives $+286$ kJ per mole of that reversed reaction.

Exam tips

- Balance the equation and find the limiting amount; use all the solution mass in $mc\Delta T$. Name the system before assigning a sign: warming solution means a negative reaction enthalpy in this model.
- Show the J-to-kJ conversion, retain guard digits and state the mole basis. A standard symbol needs standard conditions and states; a negative sign does not prove a fast reaction.
- Label profile axes and draw ΔH between endpoints. Explain an experimental error through its cause, direction of bias and a specific improvement; "human error" is insufficient.

Reference: IB Chemistry guide, Reactivity 1.1.

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Reactivity 1.2 · Energy cycles in reactions

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 1.2, Energy cycles in reactions, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: enthalpy change, exothermic and endothermic reactions, and calorimetry from Reactivity 1.1; covalent bonds from Structure 2.2; lattice enthalpy and ionization energy from Structures 2.1 and 1.3. You will use bond enthalpies and enthalpy data from the data booklet.

Bond enthalpy

Where does the energy of a reaction come from?

Burning one mole of methane in a gas cooker releases about 800 kJ. No atoms are created or destroyed, so the energy must come from the bonds: the bonds in the products are stronger than the bonds in the reactants. This unit shows how to calculate enthalpy changes from bond data and from **energy cycles** when they cannot be measured directly.

Breaking and making bonds

- Breaking a bond **needs** energy: bond breaking is **endothermic**.
- Making a bond **releases** energy: bond making is **exothermic**.

The **bond enthalpy** is the energy needed to break one mole of a covalent bond, with the substances in the **gaseous** state. It is always positive. For example, $H_2(g) \rightarrow 2H(g)$, $\Delta H = +436$ kJ mol^{-1}.

The value for a bond such as C–H differs a little from one molecule to another, so the data booklet gives an **average bond enthalpy** : the mean over many compounds.

Calculating ΔH from bond enthalpies

$$\Delta H = \sum(\text{bonds broken}) - \sum(\text{bonds formed})$$

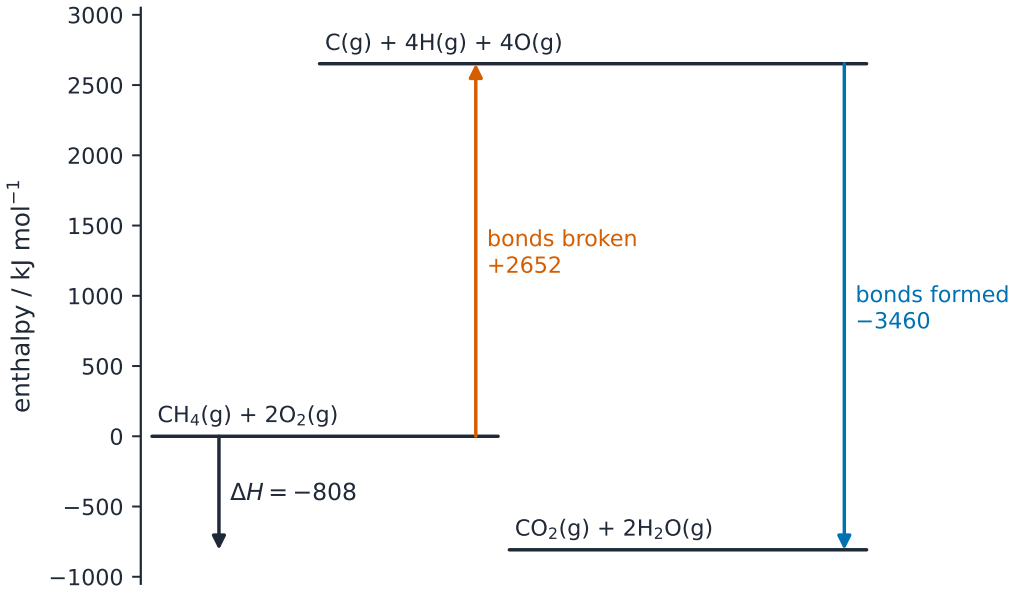
Worked example: $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$.

Bonds broken	Energy / kJ	Bonds formed	Energy / kJ
4 C–H: 4×414	1656	2 C=O: 2×804	1608
2 O=O: 2×498	996	4 O–H: 4×463	1852
total	2652	total	3460

$\Delta H = 2652 - 3460 = -808$ kJ mol^{-1}. More energy is released by forming bonds than

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is needed to break them, so the reaction is exothermic.



Every bond is broken to gaseous atoms, then the new bonds form; ΔH is the difference

Why the answer is only approximate

The measured value for this reaction is -802 kJ mol^{-1} (with water as a gas). The bond enthalpy answer differs because:

- **average** bond enthalpies are used, not the values for these exact molecules;
- bond enthalpies apply only to **gases**. If a substance is a liquid or solid, the energy to change its state is missing. With liquid water as a product the true value is -890 kJ mol^{-1}.

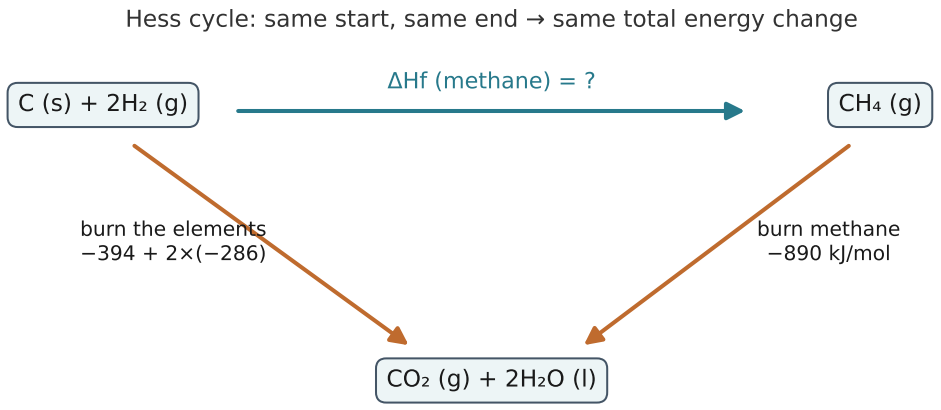
Hess's law

Same start, same end

Hess's law : the enthalpy change of a reaction is the same whatever route is taken, as long as the initial and final conditions are the same. Enthalpy is a **state function**: it depends only on where you start and where you finish, like the difference in height between the bottom and the top of a mountain, whichever path you climb.

This lets you calculate enthalpy changes that cannot be measured directly. Build an **energy cycle** with the target reaction on one route and reactions with known ΔH on the other.

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Same start, same end: $\Delta Hf = -394 + 2(-286) - (-890) = -76$ kJ/mol

Working with equations

You can also combine equations directly, like algebra:

- If you **reverse** an equation, change the sign of ΔH.
- If you **multiply** an equation by a number, multiply ΔH by the same number.
- Add the equations and their ΔH values; species that appear on both sides cancel.

Worked example: find ΔH for $\mathrm{C(s)} + \frac{1}{2}\mathrm{O_2(g)} \rightarrow \mathrm{CO(g)}$, which cannot be measured because some $\mathrm{CO_2}$ always forms.

- (1) $\mathrm{C(s)} + \mathrm{O_2(g)} \rightarrow \mathrm{CO_2(g)}$, $\Delta H = -394$ kJ mol^{-1}
- (2) $\mathrm{CO(g)} + \frac{1}{2}\mathrm{O_2(g)} \rightarrow \mathrm{CO_2(g)}$, $\Delta H = -283$ kJ mol^{-1}

Keep (1) and reverse (2): $\mathrm{CO_2} \rightarrow \mathrm{CO} + \frac{1}{2}\mathrm{O_2}$, $\Delta H = +283$. Adding them, $\mathrm{CO_2}$ cancels and $\frac{1}{2}\mathrm{O_2}$ is left on the left:

$$\Delta H = -394 + 283 = -111 \text{ kJ mol}^{-1}$$

Worked example: three equations

Find ΔH for $\mathrm{2C(s) + H_2(g) \rightarrow C_2H_2(g)}$, given:

- (1) $\mathrm{C(s) + O_2(g) \rightarrow CO_2(g)}$, $\Delta H = -394$
- (2) $\mathrm{H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l)}$, $\Delta H = -286$
- (3) $\mathrm{C_2H_2(g) + \frac{5}{2}O_2(g) \rightarrow 2CO_2(g) + H_2O(l)}$, $\Delta H = -1301$

Take $2 \times$ (1) (two C on the left), $1 \times$ (2), and reverse (3) ($\mathrm{C_2H_2}$ on the right):

$$\Delta H = 2(-394) + (-286) + 1301 = +227 \text{ kJ mol}^{-1}$$

Check that the oxygen, $\mathrm{CO_2}$ and water cancel: $\frac{5}{2}\mathrm{O_2}$ on each side, $2\mathrm{CO_2}$ on each side, one $\mathrm{H_2O}$ on each side.

AHL: Formation and combustion cycles

Standard enthalpy changes

Standard conditions are 100 kPa and a stated temperature, usually 298 K, written with the symbol $\ominus$.

- The **standard enthalpy change of formation** , $\Delta H_f^\ominus$, is the enthalpy change when one mole of a substance forms from its elements in their standard states. For an element in its standard state, $\Delta H_f^\ominus = 0$.
- The **standard enthalpy change of combustion** , $\Delta H_c^\ominus$, is the enthalpy change when one mole of a substance burns completely in oxygen under standard conditions.

Using formation data

When $\Delta H_f^\ominus$ values are known for every substance, use the products-minus-reactants rule, which comes from a cycle through the elements:

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

Worked example: the combustion of ethanol, $C_2H_5OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l)$. Data: $\Delta H_f^\ominus$ ethanol -278, CO_2 -394, $H_2O(l)$ -286 kJ mol^{-1}; O_2 is an element, so 0.

$$\Delta H_c^\ominus = [2(-394) + 3(-286)] - [(-278) + 0] = -1646 + 278 = -1368 \text{ kJ mol}^{-1}$$

Using combustion data

When combustion values are known, the arrows of the cycle point **down** to the combustion products, and the rule turns round:

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

Worked example: the formation of methane, $C(s) + 2H_2(g) \rightarrow CH_4(g)$. Data: $\Delta H_c^\ominus$ carbon -394, hydrogen -286, methane -890 kJ mol^{-1}.

$$\Delta H_f^\ominus = [(-394) + 2(-286)] - (-890) = -966 + 890 = -76 \text{ kJ mol}^{-1}$$

This is the cycle in the Hess's law figure above.

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AHL: Born–Haber cycles

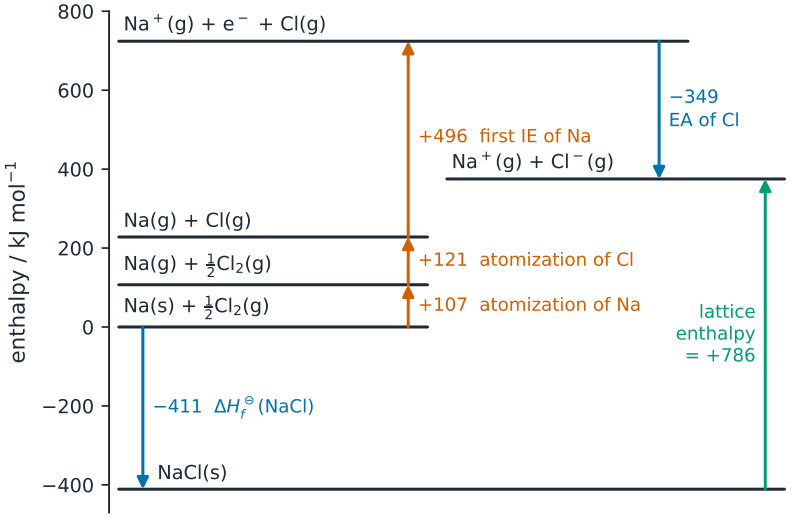
Lattice enthalpy from a cycle

Lattice enthalpy cannot be measured directly, because you cannot separate a crystal into gaseous ions in one step. A **Born–Haber cycle** - is an energy cycle for forming an ionic compound from its elements, through gaseous atoms and gaseous ions. All the other steps can be measured, so the lattice enthalpy can be calculated.

The steps for sodium chloride:

Step	Process	ΔH / kJ mol^{-1}
atomization of Na	$Na(s) \rightarrow Na(g)$	+107
atomization of Cl	$\frac{1}{2}Cl_2(g) \rightarrow Cl(g)$	+121
first ionization energy of Na	$Na(g) \rightarrow Na^+(g) + e^-$	+496
first electron affinity of Cl	$Cl(g) + e^- \rightarrow Cl^-(g)$	−349
formation of NaCl	$Na(s) + \frac{1}{2}Cl_2(g) \rightarrow NaCl(s)$	−411
lattice enthalpy	$NaCl(s) \rightarrow Na^+(g) + Cl^-(g)$	?

The **enthalpy of atomization** is the enthalpy change to form one mole of gaseous atoms from the element in its standard state. For chlorine it is half the Cl–Cl bond enthalpy, because one mole of Cl atoms comes from half a mole of Cl_2.



Two routes from NaCl(s) to the gaseous ions have the same total enthalpy change

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Calculating the lattice enthalpy

Going round the cycle, the route from NaCl(s) to the gaseous ions directly must equal the route back through the elements:

$$\Delta H_{\text{latt}} = -\Delta H_f^{\ominus} + \Delta H_{\text{at}}(\text{Na}) + \Delta H_{\text{at}}(\text{Cl}) + \text{IE}(\text{Na}) + \text{EA}(\text{Cl})$$

$$\Delta H_{\text{latt}} = 411 + 107 + 121 + 496 - 349 = +786 \text{ kJ mol}^{-1}$$

The data booklet value, 790 kJ mol^{-1}, differs only by rounding in the data.

For a group 2 compound such as MgO, the cycle includes the first **and** second ionization energies of magnesium, and the first **and** second electron affinities of oxygen. The second electron affinity is positive: adding an electron to O^- means pushing it against the negative charge already there.

Practice

1. Explain, in terms of bonds, why the combustion of methane is exothermic.
2. Use bond enthalpies (H–H 436, Cl–Cl 242, H–Cl 431 kJ mol^{-1}) to calculate ΔH for $H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$.
3. Use bond enthalpies (C=C 614, H–H 436, C–C 346, C–H 414 kJ mol^{-1}) to calculate ΔH for $C_2H_4(g) + H_2(g) \rightarrow C_2H_6(g)$.
4. Give two reasons why an enthalpy change calculated from average bond enthalpies differs from the measured value.
5. State Hess's law.
6. Given $S(s) + O_2(g) \rightarrow SO_2(g)$, $\Delta H = -297$, and $2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$, $\Delta H = -198$ kJ mol^{-1}, calculate ΔH for $S(s) + \frac{3}{2}O_2(g) \rightarrow SO_3(g)$.
7. **AHL.** Use $\Delta H_f^{\ominus}$ values (NH_3 −46, NO +90, $H_2O(g)$ −242 kJ mol^{-1}) to calculate $\Delta H^{\ominus}$ for $4NH_3(g) + 5O_2(g) \rightarrow 4NO(g) + 6H_2O(g)$.
8. **AHL.** Use $\Delta H_c^{\ominus}$ values (C −394, H_2 −286, C_2H_6 −1560 kJ mol^{-1}) to calculate $\Delta H_f^{\ominus}$ of ethane.
9. **AHL.** Write the equations, with state symbols, for the first electron affinity of oxygen and the lattice enthalpy of magnesium oxide.
10. **AHL.** Data for KCl: ΔH_{at}(K) +89, ΔH_{at}(Cl) +121, IE(K) +419, EA(Cl) −349, $\Delta H_f^{\ominus}$(KCl) −437 kJ mol^{-1}. Calculate the lattice enthalpy of KCl.

Answers.

1. Bonds broken: 4 C–H and 2 O=O need 2652 kJ. Bonds formed: 2 C=O and 4 O–H release 3460 kJ. More energy is released forming the new bonds than is needed to break the old ones.
2. Broken: $436 + 242 = 678$. Formed: $2 \times 431 = 862$. $\Delta H = 678 - 862 = -184$ kJ mol^{-1}.

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3. Broken: C=C 614 and H–H 436, total 1050 (the four C–H bonds are not broken). Formed: C–C 346 and two new C–H $2 \times 414 = 828$, total 1174. $\Delta H = 1050 - 1174 = -124$ kJ mol^{-1}.
4. Average bond enthalpies are means over many compounds, not the values for these molecules; bond enthalpies apply to gases, so any liquid or solid needs extra energy for the change of state.
5. The enthalpy change of a reaction is independent of the route taken, provided the initial and final conditions are the same.
6. Keep the first equation and halve the second: $\Delta H = -297 + \frac{1}{2}(-198) = -297 - 99 = -396$ kJ mol^{-1}.
7. **AHL.** $[4(+90)+6(-242)]-[4(-46)+0] = (360-1452)-(-184) = -1092+184 = -908$ kJ mol^{-1}.
8. **AHL.** $2C + 3H_2 \rightarrow C_2H_6$: $\Delta H_f^\ominus = [2(-394) + 3(-286)] - (-1560) = -1646 + 1560 = -86$ kJ mol^{-1}.
9. **AHL.** $O(g) + e^- \rightarrow O^-(g)$; $MgO(s) \rightarrow Mg^{2+}(g) + O^{2-}(g)$.
10. **AHL.** $\Delta H_{\text{latt}} = 437 + 89 + 121 + 419 - 349 = +717$ kJ mol^{-1} (data booklet 720).

Exam tips

- Bond breaking is endothermic and bond making exothermic; write "**broken minus formed**" before you substitute numbers.
- Count every bond: draw the structural formula, and leave out bonds that are not broken.
- Bond enthalpies are for **gases**; say so when you explain why a calculated value differs.
- When you reverse an equation, change the **sign**; when you multiply it, multiply ΔH.
- **AHL.** Formation data: products minus reactants. Combustion data: **reactants minus products**.
- **AHL.** Elements in their standard states have $\Delta H_f^\ominus = 0$; do not forget the coefficients.
- **AHL.** In the IB convention, lattice enthalpy is the endothermic separation of the solid into gaseous ions, so it is positive.

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Energy from fuels

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 1.3, Energy from fuels, for the course first assessed in 2025. The understandings in this unit are shared by SL and HL. It also develops the life-cycle comparisons and functional-unit reasoning in the course objectives.

Prerequisites: balancing equations, mole calculations, enthalpy changes and oxidation–reduction. Numerical scenarios are original and invented unless a reference value is explicitly identified. They are not official examination questions.

Combustion: where the energy comes from

A **fuel** stores chemical energy that can be transferred in a useful process. During **combustion**, a substance reacts with oxygen. Many metals, non-metals and organic substances burn when sufficiently heated. Examples include

$$2\mathrm{Mg(s)} + \mathrm{O_2(g)} \rightarrow 2\mathrm{MgO(s)},$$

$$\mathrm{C(s)} + \mathrm{O_2(g)} \rightarrow \mathrm{CO_2(g)},$$

$$\mathrm{CH_4(g)} + 2\mathrm{O_2(g)} \rightarrow \mathrm{CO_2(g)} + 2\mathrm{H_2O(l)}.$$

These reactions release energy overall because forming the product bonds releases more energy than breaking the reactant bonds requires. The energy is not released simply by "breaking the fuel's bonds". An ignition source overcomes an activation barrier; a fuel that releases much energy can still be relatively unreactive during safe storage.

Complete combustion of a hydrocarbon or an alcohol produces carbon dioxide and water. Balance carbon first, hydrogen second and oxygen last. An alcohol already contains oxygen, so include that oxygen when calculating the external oxygen supply.

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■ **Worked example: ethanol**

Ethanol is C_2H_5OH, with two carbon atoms, six hydrogen atoms and one oxygen atom per molecule. Two carbon atoms give $2CO_2$; six hydrogen atoms give $3H_2O$. The products contain seven oxygen atoms. One comes from ethanol, leaving six to be supplied by three oxygen molecules:

$$C_2H_5OH(l) + 3O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l).$$

Water may leave a hot flame as vapour. If using a tabulated combustion enthalpy, match its specified water state; a value for liquid water includes the additional energy released on condensation. Do not compare fuel values defined with different product states without accounting for that difference.

Limited oxygen and incomplete combustion

Incomplete combustion occurs when carbon is not fully oxidized to carbon dioxide. Carbon monoxide and/or solid carbon can form, usually alongside some carbon dioxide and water. The following equations are idealized limiting cases, not a claim that a real flame produces only one carbon-containing product:

$$2CH_4(g) + 3O_2(g) \rightarrow 2CO(g) + 4H_2O(g),$$

$$CH_4(g) + O_2(g) \rightarrow C(s) + 2H_2O(g).$$

Carbon monoxide is colourless and odourless and is toxic because it binds strongly to haemoglobin, impairing oxygen transport. Soot consists of carbon-rich particles; inhaled particles damage health. A yellow, sooty flame can indicate incomplete combustion, but the absence of visible soot does not prove the absence of carbon monoxide.

Hydrocarbons with higher carbon-to-hydrogen ratios, such as longer-chain alkanes, tend to soot more under comparable burning conditions. Oxygen delivery, vaporization and mixing also affect the outcome.

More chemical energy remains in CO or carbon than in fully oxidized products, so incomplete combustion releases less heat per mole of original fuel than complete combustion to the same final water state. It wastes fuel as well as increasing health risks. Provide a suitable oxygen supply and ventilation; never use an unvented flame in an enclosed room. This is a reason to improve apparatus, not an instruction to experiment with unsafe oxygen restrictions.

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■ Worked example: balancing an incomplete reaction

For ethanol producing only CO and water as the carbon/hydrogen products, begin with $C_2H_5OH \rightarrow 2CO + 3H_2O$. Products contain five oxygen atoms; ethanol supplies one, so two O_2 molecules supply the remaining four:

$$C_2H_5OH(l) + 2O_2(g) \rightarrow 2CO(g) + 3H_2O(g).$$

Check every atom after balancing. A smaller oxygen coefficient than in the complete-combustion equation is consistent with incomplete oxidation.

Compare fuels on the same basis

A more negative molar enthalpy does not automatically identify the most useful fuel. A large molecule can release more energy per mole simply because it contains more atoms. **Specific energy** compares energy per unit mass; **energy density** compares energy per unit volume. Storage volume, safety, cost, availability, transport and conversion efficiency also matter.

Use positive magnitudes when comparing energy released. For molar mass M and molar combustion enthalpy ΔH_c,

$$\text{specific energy} = \frac{|\Delta H_c|}{M}.$$

If ΔH_c is in kJ mol^{-1} and M in g mol^{-1}, the result is in kJ g^{-1}, numerically equal to MJ kg^{-1}.

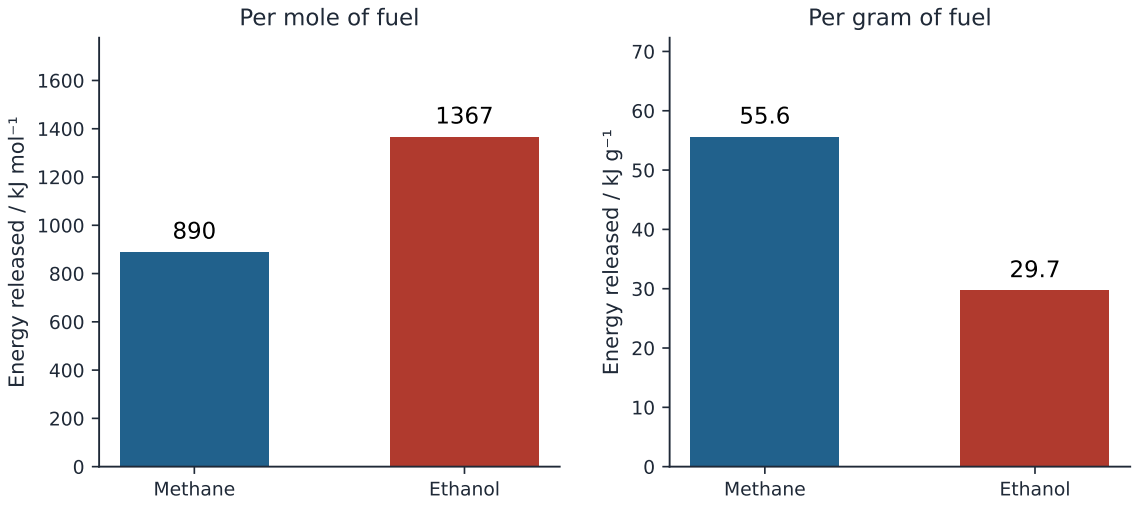
■ Worked comparison: methane and ethanol

Use rounded comparison values of $-890\ \text{kJ mol}^{-1}$ for methane and $-1367\ \text{kJ mol}^{-1}$ for liquid ethanol, both for complete combustion to liquid water. Use $M = 16.0$ and $46.0\ \text{g mol}^{-1}$, respectively.

$$E_{\text{methane}} = \frac{890}{16.0} = 55.6\ \text{kJ g}^{-1},$$

$$E_{\text{ethanol}} = \frac{1367}{46.0} = 29.7\ \text{kJ g}^{-1}.$$

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The denominator changes the question being answered; use a common basis before comparing fuels.

Ethanol releases more per mole, but methane more per gram. Methane is a gas under ordinary conditions, requiring a storage strategy such as compression; ethanol is a liquid. The mass comparison alone does not settle a vehicle-storage decision.

■ Carbon dioxide per unit energy

From the balanced equations, one mole methane makes one mole CO_2, while one mole ethanol makes two. With $M_{CO_2} = 44.0\ \text{g mol}^{-1}$,

$$I_{\text{methane}} = \frac{44.0}{0.890} = 49.4\ \text{g CO}_2\,\text{MJ}^{-1},$$

$$I_{\text{ethanol}} = \frac{88.0}{1.367} = 64.4\ \text{g CO}_2\,\text{MJ}^{-1}.$$

These are **direct combustion** emissions per energy released, not full life-cycle emissions. The carbon source in ethanol and energy used during production have not yet been counted.

A **functional unit** specifies a common service, such as 1 MJ of useful heat, rather than one mole or one tank. If a heater transfers only a fraction η of the fuel energy usefully,

$$\text{direct CO}_2 \text{ per useful MJ} = \frac{\text{direct CO}_2 \text{ per released MJ}}{\eta}.$$

For invented efficiencies of 80% for methane and 90% for ethanol, the respective intensities become $49.4/0.80 \approx 61.8$ and $64.4/0.90 \approx 71.6$ g per useful MJ. Write percentages as fractions. Comparing released energy on one side with useful energy on the other is unfair.

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Fossil fuels and biofuels

Fossil fuels are formed from ancient biological material over geological timescales and are non-renewable on human timescales. Coal is a carbon-rich solid with impurities; crude oil is a mixture refined into useful fractions; natural gas is methane-rich, with composition varying by source.

- Coal can be stored as a solid but produces substantial direct CO_2 per released energy; impurities and ash create additional pollution concerns.
- Oil-derived liquid fuels are convenient for transport and energy storage, but combustion emits CO_2 and spills can damage ecosystems.
- Natural gas generally emits less direct CO_2 per released energy than coal, but extraction and transport can leak methane, itself a greenhouse gas. Lower combustion emissions do not remove the need for life-cycle assessment.

CO_2 absorbs and emits infrared radiation at particular wavelengths. Increasing its atmospheric concentration initially reduces net energy escaping to space; warming changes the energy balance towards a new equilibrium. This enhanced greenhouse effect is distinct from ozone depletion. Direct CO_2 accounting therefore addresses a climate impact, while CO and soot introduce additional health and pollution effects.

A **renewable** source is replenished on a timescale relevant to its use; a finite source is not made renewable merely by using it more slowly. Solar energy captured by plants can become a **biofuel**. Photosynthesis fixes atmospheric carbon into biological material:

$$6CO_2 + 6H_2O \rightarrow C_6H_{12}O_6 + 6O_2.$$

Light supplies energy; photosynthesis is not an energy source independent of sunlight. Fermentation can convert glucose into ethanol and carbon dioxide:

$$C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2.$$

Biomass can regrow, but this does not guarantee that a biofuel is carbon neutral. Growing, harvesting, fertilizer production, processing and transport consume energy and may emit greenhouse gases. Land-use change can release stored carbon or displace food production; regrowth and land availability matter. Waste-derived fuels may have different impacts from crops grown specifically for fuel. Carbon taken up during growth must be counted consistently with carbon released later, without counting the same uptake twice.

Life-cycle assessment and a defensible decision

A **life-cycle assessment** follows impacts from raw materials and production through transport, use and end-of-life processes. Specify the boundary

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and functional unit before comparing options. Carbon dioxide alone does not describe water demand, land use, toxicity, local air pollution or waste.

■ Worked comparison: useful heat with upstream emissions

In an invented comparison per 1 MJ of useful heat, fuel A has 62 g direct CO_2 and 14 g CO_2-equivalent upstream emissions. Fuel B has 72 g direct CO_2; its stated accounting credits 60 g of uptake during feedstock growth, and assigns 25 g CO_2-equivalent upstream emissions.

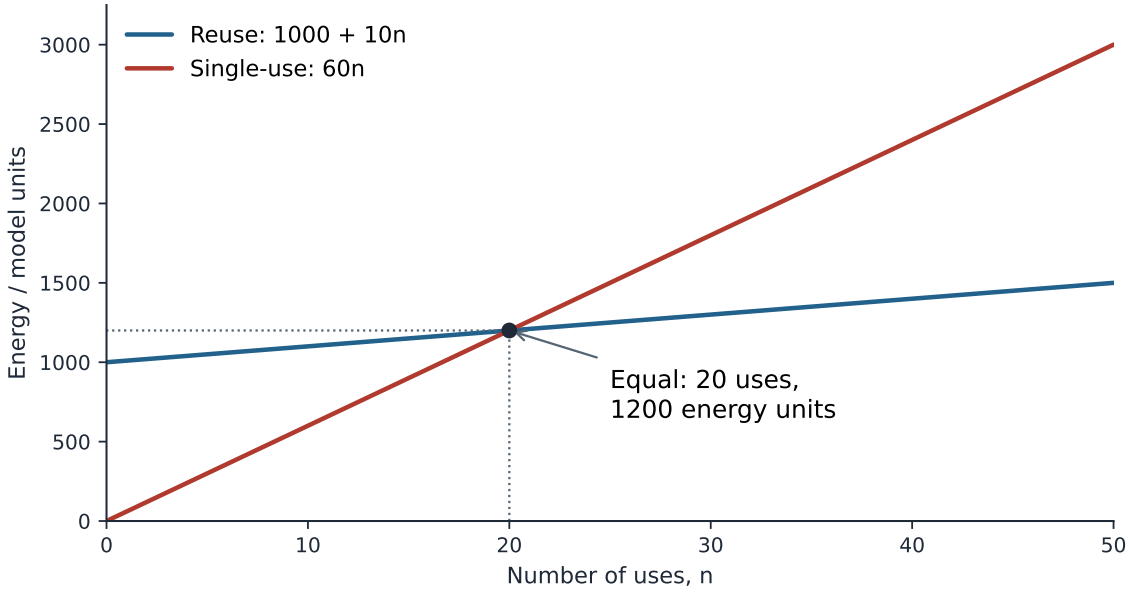
$$I_A = 62 + 14 = 76 \text{ g } CO_2\text{-equivalent},$$

$$I_B = 72 - 60 + 25 = 37 \text{ g } CO_2\text{-equivalent}.$$

B has lower net greenhouse-gas emissions under these assumptions, despite higher direct CO_2. This is a conditional result: the uptake credit, land-use boundary and upstream data must be justified. CO_2-equivalent is an accounting measure combining greenhouse gases on a stated basis; it is not a claim that the exhaust contains that mass of CO_2 alone.

The same logic applies beyond fuels. In a simplified invented reusable-container model, manufacturing costs 1000 energy units and cleaning costs 10 per use, whereas a disposable costs 60 per use. With the same delivered service,

$$E_{\text{reuse}} = 1000 + 10n, \qquad E_{\text{single}} = 60n.$$



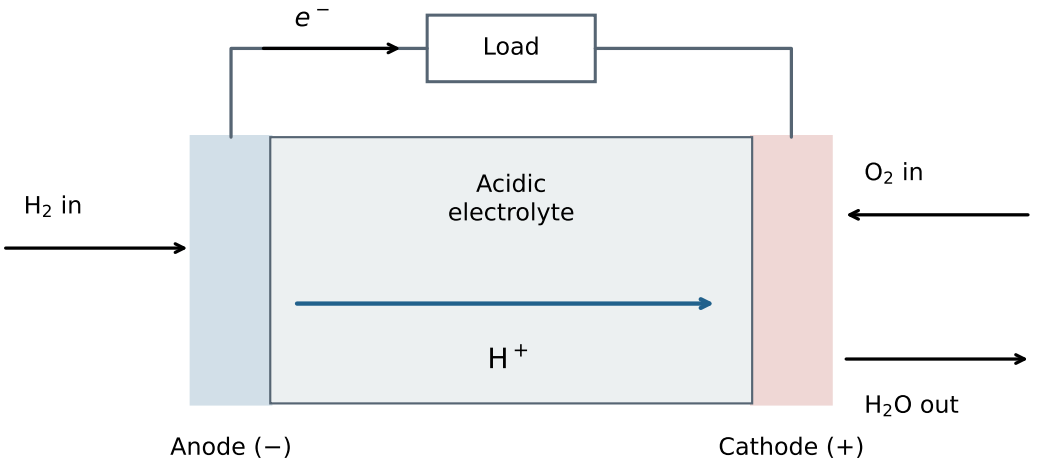
Equal at 20 uses; the reusable option uses less energy after that point.

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Equality occurs at $n = 1000/(60 - 10) = 20$ uses. The reusable option uses less energy only **after** 20 uses. Cleaning assumptions, transport and disposal can change the crossover; energy break-even does not establish break-even for water or emissions. "Recyclable" describes a possibility, not proof of collection and recycling. State which impacts and priorities support the final judgement.

Fuel cells: chemical energy directly to electricity

A **fuel cell** separates fuel oxidation from oxygen reduction at electrodes. Electrons travel through an external circuit and can do electrical work; ions carry charge through an electrolyte. The electrolyte must not provide an electron short circuit. Fuel and oxidant are supplied continuously, unlike the finite stored reactants of a primary cell. A fuel cell is not simply a battery that must be recharged after consuming its original reactants.



Oxidation supplies electrons; reduction consumes them.

Oxidation at the anode supplies electrons to the external circuit; oxygen is reduced at the cathode.

Hydrogen in acidic conditions

At the anode, hydrogen is oxidized:

$$\mathrm{H_2} \rightarrow 2\mathrm{H^+} + 2\mathrm{e^-}.$$

At the cathode, oxygen is reduced:

$$\tfrac{1}{2}\mathrm{O_2} + 2\mathrm{H^+} + 2\mathrm{e^-} \rightarrow \mathrm{H_2O}.$$

Add and cancel electrons and hydrogen ions to obtain $\mathrm{H_2} + \tfrac{1}{2}\mathrm{O_2} \rightarrow \mathrm{H_2O}$. Check both

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atoms and charge in each half-equation. In this operating cell the anode is negative and the cathode positive; the definitions oxidation/anode and reduction/cathode remain valid in other electrochemical cells too.

In alkaline conditions, balance using hydroxide ions. At the anode:

$$H_2 + 2OH^- \rightarrow 2H_2O + 2e^-.$$

At the cathode:

$$\tfrac{1}{2}O_2 + H_2O + 2e^- \rightarrow 2OH^-.$$

The overall reaction is unchanged. Keep both half-equations in the same medium.

■ Methanol as a fuel

For a direct methanol cell in acidic conditions, anode oxidation is

$$CH_3OH + H_2O \rightarrow CO_2 + 6H^+ + 6e^-.$$

Multiply the acidic oxygen-reduction equation by three:

$$\tfrac{3}{2}O_2 + 6H^+ + 6e^- \rightarrow 3H_2O.$$

After cancelling species, the overall reaction is $CH_3OH + \tfrac{3}{2}O_2 \rightarrow CO_2 + 2H_2O$. Methanol is a convenient liquid to store, but it is toxic and its use produces CO_2. It is incorrect to say all fuel cells emit only water.

Hydrogen cells have no direct CO_2 from the hydrogen–oxygen reaction. However, hydrogen is an **energy carrier**: producing, compressing, transporting and storing it require resources and energy. Emissions depend on the production pathway and energy supply. Fuel cells can avoid an intermediate combustion heat engine, but still have losses; neither direct conversion nor a water-only cell product proves 100% efficiency or zero life-cycle impact.

Practice

Use the rounded fuel data above where needed. All additional scenarios are invented.

1. Balance complete combustion equations for propane, C_3H_8, and methanol, CH_3OH. Include water as a liquid.
2. Balance separate idealized equations for propane forming (a) only CO and water vapour and (b) only carbon and water vapour as products. Why can a real flame differ from both equations?
3. Explain why an exothermic fuel can need ignition. Identify the error in “energy is released when fuel bonds break”.

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4. Compare methane and ethanol on energy released per mole and per gram, using the given data. Why do the rankings differ?
5. Calculate direct CO_2 produced when methane releases 4.45 MJ and when ethanol releases 4.101 MJ. Then express each as g per released MJ.
6. A methane heater has efficiency 70%. Calculate direct CO_2 per useful MJ and the mass of methane required to deliver 7.00 MJ useful heat.
7. Explain one advantage and one limitation each of coal, oil-derived fuels and natural gas. Distinguish a combustion-emissions comparison from a life-cycle comparison.
8. Write the photosynthesis and ethanol-fermentation equations. Explain two reasons why crop-derived ethanol need not be carbon neutral.
9. A reusable product needs 900 energy units to manufacture and 6 per use; a disposable needs 36 per use. Find the equality point and the first whole number of uses for which reuse consumes less energy. State two model limitations.
10. For the life-cycle example, suppose B's upstream emissions rise to 70 g CO_2-equivalent and its uptake credit falls to 50 g, all per useful MJ. Recalculate B's total and compare with A. What does this show about the decision?
11. Write and add acidic hydrogen-cell half-equations. Identify the electron direction, the oxidation electrode and the species carrying charge through the electrolyte.
12. Derive the acidic methanol-cell overall equation from its two half-equations. Explain why "fuel cells have no carbon emissions" is too broad.
13. A cell receives 100 kJ chemical energy and supplies 58 kJ electricity and 30 kJ useful heat. Find electrical efficiency and total useful-energy efficiency. Explain why neither value alone establishes the lower-impact fuel supply.

■ Worked answers

1. $C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O(l)$; $2CH_3OH + 3O_2 \rightarrow 2CO_2 + 4H_2O(l)$. Carbon and hydrogen balance first; then count oxygen already present in methanol.
2. (a) $2C_3H_8 + 7O_2 \rightarrow 6CO + 8H_2O(g)$. (b) $C_3H_8 + 2O_2 \rightarrow 3C + 4H_2O(g)$. Real flames can produce mixtures of CO_2, CO, soot and unburned fuel because mixing and oxygen availability vary.
3. Ignition supplies the activation energy needed to begin a pathway. Bond breaking absorbs energy; product bond formation releases energy. A negative net enthalpy does not imply a negligible barrier.
4. Per mole: ethanol 1367 > methane 890 kJ mol^{-1}. Per gram: $E = |\Delta H_c|/M$ gives methane $890/16.0 = 55.6$ and ethanol $1367/46.0 = 29.7$ kJ g^{-1}. The molar masses differ; neither ranking alone describes storage or life-cycle impact.
5. Methane: $n = 4450/890 = 5.00$ mol, giving $m_{CO_2} = 5.00 \times 44.0 = 220$ g; $220/4.45 = 49.4$ g MJ^{-1}. Ethanol: $n = 4101/1367 = 3.00$ mol, giving $m_{CO_2} = 2 \times 3.00 \times 44.0 = 264$ g; $264/4.101 = 64.4$ g MJ^{-1}.

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6. Intensity = 49.4/0.70 ≈ 70.6 g per useful MJ. Released energy = E_{useful}/η = 7.00/0.70 = 10.0 MJ. $n = 10000/890 = 11.24$ mol and $m = nM = 11.24 \times 16.0 \approx$ 180 g methane. Guard digits avoid premature rounding.
7. Coal: solid storage is straightforward, but combustion and impurities create CO_2/pollution concerns. Oil fuels: convenient liquid transport, but CO_2 and spills matter. Gas: lower direct CO_2 per released energy than coal in a suitable comparison, but methane leakage and storage/infrastructure matter. Life-cycle assessment also counts production, transport and other upstream/downstream impacts.
8. $6CO_2 + 6H_2O \rightarrow C_6H_{12}O_6 + 6O_2$ using light; $C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$. Fossil energy in production and transport can emit CO_2; fertilizer use and land-use change can add greenhouse-gas emissions. Biomass uptake must be assessed over the stated boundary and timescale.
9. $900 + 6n = 36n$, so $n = 900/30 = 30$. Totals are equal at 30 uses; reuse uses less from 31 whole uses onwards. Cleaning and transport assumptions may change the result; energy equality does not establish equality in water use or waste impacts.
10. $I_B = 72 - 50 + 70 = 92$ g CO_2-equivalent per useful MJ, exceeding A's 76. The ranking reverses when the assumptions change. State the boundary, uncertain inputs and priorities rather than declaring one fuel universally preferable.
11. Anode: $H_2 \rightarrow 2H^+ + 2e^-$. Cathode: $\frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O$. Overall: $H_2 + \frac{1}{2}O_2 \rightarrow H_2O$. Electrons travel from the oxidation anode through the load to the reduction cathode; hydrogen ions carry charge through the acidic electrolyte in this model.
12. Add $CH_3OH + H_2O \rightarrow CO_2 + 6H^+ + 6e^-$ to $\frac{3}{2}O_2 + 6H^+ + 6e^- \rightarrow 3H_2O$. Cancel electrons, hydrogen ions and one water: $CH_3OH + \frac{3}{2}O_2 \rightarrow CO_2 + 2H_2O$. Methanol cells directly produce CO_2; even hydrogen cells can have upstream emissions.
13. Electrical efficiency = 58/100×100 = 58%. Total useful efficiency = (58+30)/100× 100 = 88%; the remaining 12 kJ is not useful output in this boundary. A full comparison also needs fuel production emissions, storage/transport and a common service; useful heat is only credited if there is an actual use for it.

Exam tips

- Balance all atoms, including oxygen already in alcohols, and check charge in half-equations. Use one electrolyte medium consistently.
- Compare the same functional unit. Distinguish direct emissions from life-cycle impacts, and renewable supply from a justified carbon-neutral claim.
- Support a conditional judgement with data, boundaries and uncertain assumptions. Hydrogen cells have no direct CO_2, but fuel production can emit it; methanol cells directly produce CO_2.

References: IB guide, R1.3; NIST ethanol data; DOE fuel cells.

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Entropy and spontaneity

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 1.4, Entropy and spontaneity, for the course first assessed in 2025. The whole unit is additional higher level (AHL); there is no SL counterpart. Prerequisites: enthalpy changes, balanced equations, equilibrium and logarithms. Numerical model reactions are original teaching examples, not experimental measurements or official examination questions.

AHL: Entropy and accessible arrangements

An endothermic change can occur without continuous external driving: enthalpy alone cannot predict the favoured direction. The second ingredient is **entropy** , a state property related to the ways matter and energy can be distributed among accessible microscopic arrangements. “Disorder” is a rough analogy, not a sufficient explanation. A state with more accessible arrangements has higher entropy.

Imagine four labelled, independently moving model particles, each able to occupy the left or right half of a box. There is one arrangement with all four on the left but six distinct arrangements with two on each side. A spread-out distribution is more probable because more microscopic arrangements produce it, not because particles actively seek disorder. These counts illustrate the idea; they are not a quantitative entropy calculation for a real gas.

For the same substance under comparable conditions, the gas generally has higher entropy than the liquid, and the liquid higher than the solid: particles and energy have more accessible arrangements. Melting, vaporization and expansion of a gas normally increase entropy; freezing, condensation and compression at constant temperature normally decrease it.

In a reaction, an increase in the total amount of gas often suggests a positive system entropy change. For $N_2O_4(g) \rightarrow 2NO_2(g)$, one mole of gas becomes two, suggesting an increase. This is a useful qualitative guide, not a replacement for entropy data when gas amounts are unchanged or different substances must be compared.

A standard molar entropy S° is an entropy per mole under specified standard conditions, usually tabulated in $\mathrm{J\,K^{-1}\,mol^{-1}}$. Unlike standard enthalpies of formation, the standard molar entropies of elements at room temperature are **not zero**. The third-law reference is a perfect crystal at 0 K, with zero entropy in that ideal limit.

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AHL: Calculating a reaction entropy change

Use coefficients from the balanced equation:

$$\Delta S^\circ = \sum \nu S^\circ_{\text{products}} - \sum \nu S^\circ_{\text{reactants}}.$$

Multiply each molar entropy by its stoichiometric coefficient before subtracting. Reversing the reaction reverses the sign; doubling the equation doubles its reaction entropy change.

■ **Worked example: a model dissociation**

For the invented model reaction $\mathrm{AB(g)} \rightarrow \mathrm{A(g)} + \mathrm{B(g)}$, assign $S^\circ_{\mathrm{AB}} = 220$, $S^\circ_{\mathrm{A}} = 150$ and $S^\circ_{\mathrm{B}} = 160\ \mathrm{J\,K^{-1}\,mol^{-1}}$.

$$\Delta S^\circ = (150 + 160) - 220 = +90\ \mathrm{J\,K^{-1}\,mol^{-1}}.$$

The positive sign agrees with the increase in gas amount. It describes the reacting **system**, not system plus surroundings. A negative system entropy change is possible when the surroundings gain sufficient entropy.

For rounded example data $S^\circ_{\mathrm{N_2}} = 192$, $S^\circ_{\mathrm{H_2}} = 131$ and $S^\circ_{\mathrm{NH_3}} = 193$ in the same units, the equation $\mathrm{N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)}$ gives

$$\Delta S^\circ = 2(193) - [192 + 3(131)] = -199\ \mathrm{J\,K^{-1}\,mol^{-1}}.$$

The negative sign is consistent with four moles of gas becoming two. The value refers to the equation as written, forming two moles of ammonia; it is not automatically the change per mole of ammonia.

AHL: Gibbs energy and spontaneity

Gibbs energy combines the system's enthalpy and entropy changes. At constant temperature and pressure,

$$\Delta G = \Delta H - T\Delta S.$$

Here T is absolute temperature in kelvin. Use one energy unit throughout: either all J or all kJ. If ΔH is in $\mathrm{kJ\,mol^{-1}}$ and ΔS in $\mathrm{J\,K^{-1}\,mol^{-1}}$, divide the entropy value by 1000 before substitution.

- $\Delta G < 0$: the forward change is thermodynamically spontaneous for the **current composition and conditions**.
- $\Delta G > 0$: the reverse change is favoured; the forward direction would require coupling or external driving.
- $\Delta G = 0$: there is no net thermodynamic driving force; a reacting mixture is at equilibrium.

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Spontaneous does not mean instantaneous, complete, explosive or requiring no initial activation. An activation barrier can make a favourable change extremely slow. A catalyst changes the pathway and rates, not the initial/final thermodynamic states: it does not change ΔG° or the equilibrium constant at a fixed temperature.

The criterion includes the surroundings indirectly. At constant pressure, an exothermic system transfers heat to its surroundings, increasing their entropy. The relationship $\Delta S_{\text{total}} = -\Delta G/T$ under the stated constant-temperature/pressure conditions explains why the system's entropy may decrease while the total entropy increases.

■ **Worked example: an endothermic change**

Assign $\Delta H^\circ = +20.0\ \text{kJ mol}^{-1}$, $\Delta S^\circ = +100\ \text{J K}^{-1}\,\text{mol}^{-1}$ and $T = 300\ \text{K}$ to an invented reaction.

$$\Delta S^\circ = \frac{100}{1000} = 0.100\ \text{kJ K}^{-1}\,\text{mol}^{-1}.$$

$$\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ = 20.0 - 300(0.100) = -10.0\ \text{kJ mol}^{-1}.$$

The positive entropy contribution outweighs the positive enthalpy term. The negative **standard** Gibbs energy change favours products in the equilibrium sense, but the actual direction at an arbitrary composition also depends on the reaction quotient, developed below.

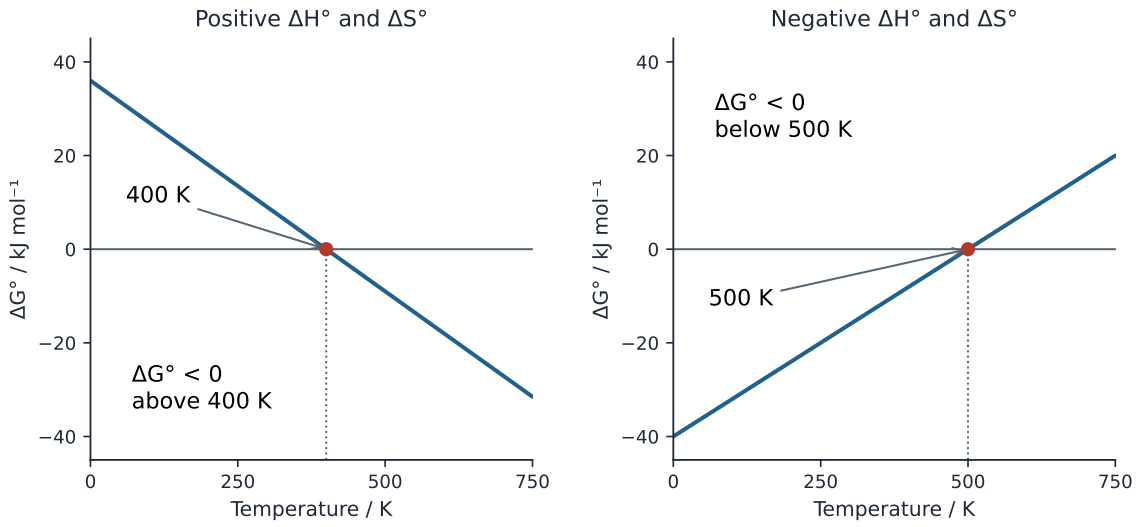
AHL: Temperature thresholds

If ΔH° and ΔS° are approximately constant over a temperature range, a plot of ΔG° against T is a straight line. Its intercept is ΔH° and gradient is $-\Delta S^\circ$. Set $\Delta G^\circ = 0$ to find a crossing:

$$T_{\text{cross}} = \frac{\Delta H^\circ}{\Delta S^\circ}.$$

Convert units first. A crossing is a boundary, not an interval of negative Gibbs energy. Test a temperature on either side, or reason from the gradient, before writing an inequality.

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Temperature trends assume constant enthalpy and entropy and unchanged phases over the range shown.

Worked comparison: opposite slopes

For model A, $\Delta H^\circ = +36.0\ \text{kJ mol}^{-1}$ and $\Delta S^\circ = +90.0\ \text{J K}^{-1}\,\text{mol}^{-1}$:

$$T_{\text{cross}} = 36.0/0.0900 = 400\ \text{K}.$$

At 300 K, $\Delta G^\circ = 36.0 - 300(0.0900) = +9.0\ \text{kJ mol}^{-1}$; at 500 K it is $-9.0\ \text{kJ mol}^{-1}$. Thus $\Delta G^\circ < 0$ above 400 K in this model.

For model B, $\Delta H^\circ = -40.0\ \text{kJ mol}^{-1}$ and $\Delta S^\circ = -80.0\ \text{J K}^{-1}\,\text{mol}^{-1}$:

$$\Delta G^\circ = -40.0 + 0.0800T, \qquad T_{\text{cross}} = 500\ \text{K}.$$

At 300 K the value is -16.0 kJ mol^{-1}; at 600 K it is $+8.0$ kJ mol^{-1}. The negative-entropy model instead has $\Delta G^\circ < 0$ **below** 500 K.

Sign of ΔH°	**Sign of ΔS°**	**When $\Delta G^\circ < 0$**
$-$	$+$	all positive temperatures in the model
$+$	$-$	no positive temperature in the model
$+$	$+$	above the positive crossing
$-$	$-$	below the positive crossing

These predictions are conditional. Enthalpy and entropy vary with temperature; phase changes can invalidate a straight-line extrapolation. A mathematically calculated

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threshold outside the stated range of stable phases is not proof of a real operating condition.

AHL: Composition, reaction quotient and equilibrium

Standard and actual Gibbs energy changes answer different questions. For the current mixture,

$$\Delta G = \Delta G^\circ + RT \ln Q.$$

Q is the reaction quotient, built from the current composition with stoichiometric powers. Rigorous thermodynamic Q uses dimensionless activities; school ideal-mixture calculations use concentrations or pressures relative to their standard values. Pure solids and pure liquids have activity approximately one and do not appear as variable concentration factors. Do not take a logarithm of a quantity carrying units.

For an ideal model $\mathrm{A(g)} \rightleftharpoons \mathrm{B(g)}$, Q is the ratio of the activities of B to A. As B accumulates relative to A, Q rises and the forward driving force becomes less negative. Equilibrium means $Q = K$ and $\Delta G = 0$, giving

$$\Delta G^\circ = -RT \ln K.$$

Use $R = 8.314\ \mathrm{J\,K^{-1}\,mol^{-1}}$ with ΔG° in $\mathrm{J\ mol^{-1}}$, or $R = 0.008314$ with $\mathrm{kJ\ mol^{-1}}$. The logarithm is natural, not base ten.

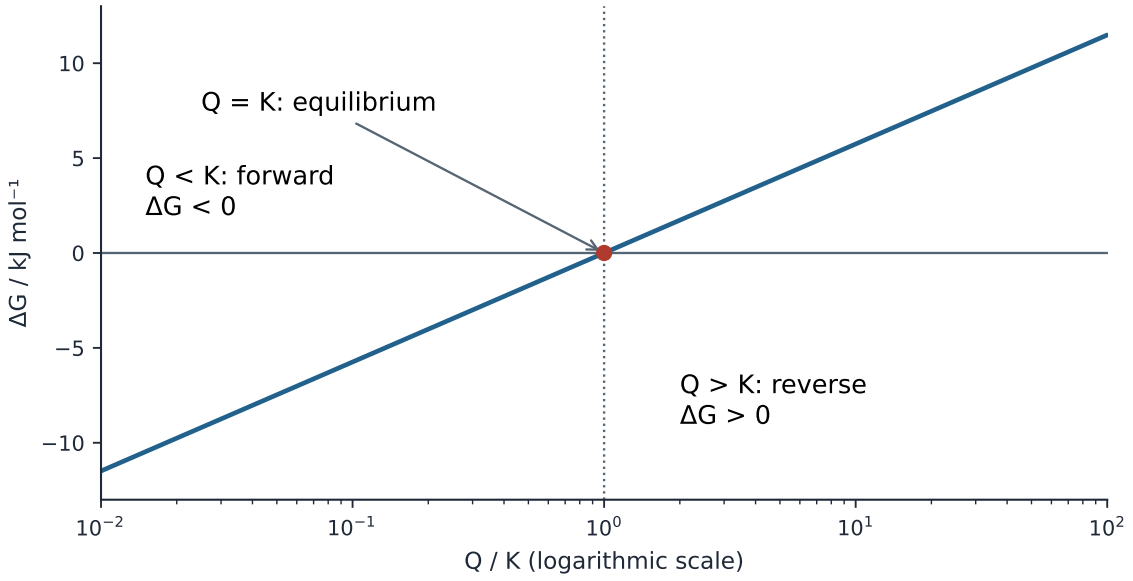
- $K > 1$ means $\ln K > 0$ and $\Delta G^\circ < 0$.
- $K < 1$ means $\Delta G^\circ > 0$; reactants are favoured in the equilibrium ratio, not the exclusive species present.
- $K = 1$ means $\Delta G^\circ = 0$. It does not imply equal concentrations of every species for every possible equation.

Combining the equations gives a particularly useful direction test:

$$\Delta G = RT \ln \left(\frac{Q}{K} \right).$$

If $Q < K$, the forward change is favoured; if $Q > K$, the reverse change is favoured. At equilibrium, $\Delta G = 0$ even when ΔG° is nonzero.

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The standard value can stay unchanged while composition changes the actual driving force.

■ **Worked example: an unfavourable standard value, but forward change**

For an invented reaction at 300 K, let $\Delta G^\circ = +6.00\ \text{kJ mol}^{-1}$ and $Q = 0.0100$.

$$\Delta G = 6.00 + 0.008314(300)\ln(0.0100) = -5.49\ \text{kJ mol}^{-1}.$$

The forward change is favoured at this composition even though the standard value is positive. Separately, $K = \exp[-6000/(8.314\times300)] \approx 0.0902$, so $Q < K$, confirming the direction independently. Do not replace the actual ΔG with the standard value.

Practice

All model data are invented unless identified as rounded example data. Use $R = 8.314\ \text{J K}^{-1}\,\text{mol}^{-1}$.

1. Explain entropy using accessible arrangements, and explain why "particles want to become disordered" is inadequate. Compare liquid and gas of the same substance under suitable comparable conditions.
2. Predict the sign of the system entropy change for water freezing, isothermal compression of a gas, and $2N_2O_5(g) \rightarrow 4NO_2(g) + O_2(g)$. State the reasoning and one limitation of gas-amount counting.
3. Use the rounded ammonia data above to calculate ΔS° for the balanced synthesis equation. Give the value for the reversed equation and for forming one mole of ammonia.

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4. A student sets the standard molar entropy of nitrogen at 298 K to zero because it is an element. Correct the error and identify the relevant zero-entropy reference.
5. Calculate ΔG° at 300 K for $\Delta H^\circ = +20.0$ kJ mol^{-1} and $\Delta S^\circ = +100$ J K^{-1} mol^{-1}. Explain why an endothermic standard change can have a negative standard Gibbs energy change.
6. For $\Delta H^\circ = +40.0$ kJ mol^{-1} and $\Delta S^\circ = +80.0$ J K^{-1} mol^{-1}, find ΔG° at 400 K. Find the crossing temperature and the interval with $\Delta G^\circ < 0$ under the constant-value approximation.
7. State the sign combinations giving $\Delta G^\circ < 0$ at all positive temperatures and at no positive temperature in the simple model. Explain each from $\Delta H^\circ - T\Delta S^\circ$.
8. For $\Delta H^\circ = -40.0$ kJ mol^{-1} and $\Delta S^\circ = -80.0$ J K^{-1} mol^{-1}, determine the interval with $\Delta G^\circ < 0$. Check it using 300 K and 600 K.
9. A model has $\Delta H^\circ = +18.0$ kJ mol^{-1} and $\Delta G^\circ = -6.00$ kJ mol^{-1} at 300 K. Calculate ΔS° in J K^{-1} mol^{-1}.
10. An equilibrium has $K = 1000$ at 298 K. Calculate ΔG° and explain what its sign says about K, without claiming the reaction goes to completion.
11. At 300 K, $\Delta G^\circ = +6.00$ kJ mol^{-1} and $Q = 0.0100$. Calculate the actual ΔG. Calculate K as a separate check of the predicted direction.
12. A model reaction has $K = 10.0$ at 300 K. Use $\Delta G = RT\ln(Q/K)$ to find ΔG for $Q = 0.100$, 10.0 and 100. Identify the direction favoured in each case.
13. Explain why a catalyst does not change K at fixed temperature, why a spontaneous reaction can be slow, and why a temperature crossing calculated from constant thermodynamic values may fail outside the stated range.

■ Worked answers

1. Entropy relates to the number of accessible ways matter/energy can be distributed, a state property rather than an intention of particles. A gas generally has more accessible arrangements than the same substance as a liquid; qualitative "disorder" alone does not explain the microscopic counting.
2. Freezing: negative, fewer accessible arrangements in the solid. Isothermal gas compression: negative, less available spatial distribution. Decomposition: positive is expected as 2 mol gas becomes 5 mol. Gas amount is a guide; compare entropy data when changes of substance or similar gas amounts make the prediction uncertain.
3. $\Delta S^\circ = 2(193) - [192 + 3(131)] = -199$ J K^{-1} mol^{-1} per equation as written. Reverse: $+199$ J K^{-1} mol^{-1}. For $\frac{1}{2}N_2 + \frac{3}{2}H_2 \rightarrow NH_3$, halve the value: -99.5 J K^{-1} mol^{-1}.
4. The zero convention for elemental standard enthalpy of formation is not an entropy convention. Nitrogen gas at 298 K has nonzero molar entropy. The ideal third-law reference is a perfect crystal at 0 K.

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5. Convert $\Delta S^\circ = 0.100$ kJ K^{-1} mol^{-1}. $\Delta G^\circ = \Delta H^\circ - T\Delta S^\circ = 20.0 - 300(0.100) = -10.0$ kJ mol^{-1}. The positive entropy term outweighs the endothermic enthalpy term; the actual direction also depends on composition.
6. $\Delta G^\circ = 40.0 - 400(0.0800) = +8.00$ kJ mol^{-1}. $T_{\text{cross}} = 40.0/0.0800 = 500$ K. Because the gradient is negative, $\Delta G^\circ < 0$ for $T > 500$ K; equality at 500 K is not a negative value.
7. Negative enthalpy and positive entropy: both terms make ΔG° negative at every positive T. Positive enthalpy and negative entropy: subtracting $T\Delta S^\circ$ adds a positive term, so no positive T makes it negative in this model.
8. $\Delta G^\circ = -40.0 + 0.0800T$; it is negative below 500 K. At 300 K it is -16.0 kJ mol^{-1}; at 600 K it is $+8.0$ kJ mol^{-1}. The direction of the inequality differs from question 6 because ΔS° is negative.
9. $\Delta S^\circ = (\Delta H^\circ - \Delta G^\circ)/T = [18.0 - (-6.00)]/300 = 0.0800$ kJ K^{-1} mol^{-1} $= 80.0$ J K^{-1} mol^{-1}.
10. $\Delta G^\circ = -RT\ln K = -8.314(298)\ln(1000) = -17114$ J mol^{-1}, or -17.1 kJ mol^{-1}. The negative standard value corresponds to $K > 1$; finite K does not mean all reactants disappear.
11. $\Delta G = \Delta G^\circ + RT\ln Q = 6.00 + 0.008314(300)\ln(0.0100) = -5.49$ kJ mol^{-1}: forward change is favoured. $K = \exp[-6000/(8.314 \times 300)] \approx 0.0902$; $0.0100 < K$ independently gives the same direction.
12. At $Q = 0.100$, $\Delta G = 0.008314(300)\ln(0.0100) = -11.5$ kJ mol^{-1}: forward. At $Q = 10.0$, $\Delta G = RT\ln 1 = 0$: equilibrium. At $Q = 100$, $\Delta G = 0.008314(300)\ln 10 = +5.74$ kJ mol^{-1}: reverse.
13. A catalyst lowers a kinetic barrier but does not change the Gibbs-energy difference of the states, so ΔG° and K are unchanged at fixed T. A high barrier can make a favourable process slow. Thermodynamic values change with temperature and phases can change, invalidating a constant-value extrapolation.

Exam tips

- Write T in kelvin. Convert J to kJ before combining entropy with a kJ enthalpy; keep R consistent too.
- Use products minus reactants, including all coefficients, for entropy changes. Elements at 298 K do not have zero standard molar entropy.
- A crossing needs an inequality and stated assumptions. For negative entropy, increasing temperature makes ΔG° more positive.
- Distinguish ΔG from ΔG°: equilibrium requires the first to be zero, not generally the second. Use natural logarithms and dimensionless Q and K.
- State spontaneity separately from rate and completion. A catalyst changes neither K nor the thermodynamic direction at a specified composition.

Reference: IB Chemistry guide, Reactivity 1.4.

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How much? The amount of chemical change

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 2.1, How much? The amount of chemical change, for the course first assessed in 2025. All of it is SL and HL content.

Prerequisites: the mole, molar mass and concentration from Structure 1.4, and the molar volume of a gas from Structure 1.5. Use the relative atomic masses from the data booklet.

Balanced equations

A recipe for a reaction

A cake recipe says 2 eggs for every 250 g of flour. With 6 eggs you need 750 g of flour, and if you have only 500 g of flour, the flour runs out first. A balanced equation is a recipe for a reaction, but it counts particles, not eggs.

Conservation of mass

In a chemical reaction atoms are rearranged, never made or destroyed. This is the **conservation of mass** : the total mass of the products equals the total mass of the reactants. So a balanced equation has the same number of atoms of each element on both sides.

Balancing an equation

Change only the numbers in front of the formulae, the **coefficients** . Never change a formula itself.

Propane burns in oxygen:

- Unbalanced: $C_3H_8 + O_2 \rightarrow CO_2 + H_2O$.
- Balance C: 3 C on the left, so $3CO_2$.
- Balance H: 8 H on the left, so $4H_2O$.
- Balance O last: $3 \times 2 + 4 \times 1 = 10$ O atoms on the right, so $5O_2$.

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$

State symbols: (s) solid, (l) liquid, (g) gas, (aq) dissolved in water.

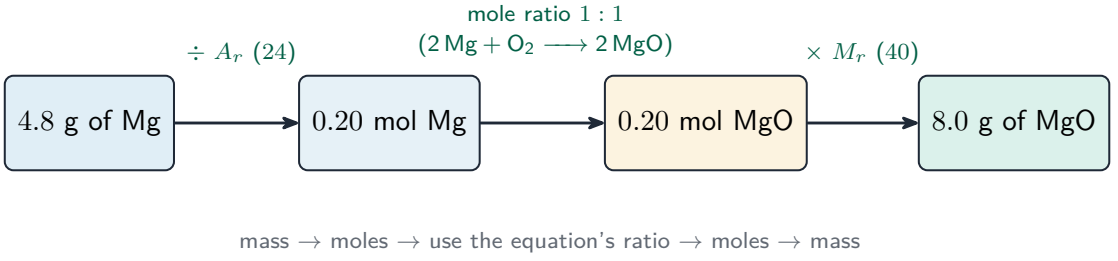
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What the coefficients mean

The coefficients give the **mole ratio** of the reaction. For propane: 1 mol of C_3H_8 reacts with 5 mol of O_2 to give 3 mol of CO_2 and 4 mol of H_2O. The study of these amounts is **stoichiometry** .

Reacting masses

Three steps



Mass → moles → use the equation's ratio → moles → mass

1. Convert the mass you know to moles: $n = m/M$.
2. Use the mole ratio from the balanced equation.
3. Convert the moles you want back to a mass: $m = n \times M$.

Worked example: lime from limestone

What mass of calcium oxide forms when 50.0 g of calcium carbonate is heated?

$$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$$

- $n(CaCO_3) = 50.0/100.09 = 0.500$ mol.
- Ratio 1 : 1, so $n(CaO) = 0.500$ mol.
- $m(CaO) = 0.500 \times 56.08 = 28.0$ g.

Worked example: iron from iron ore

What mass of iron forms from 16.0 g of iron(III) oxide?

$$Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(l) + 3CO_2(g)$$

- $n(Fe_2O_3) = 16.0/159.70 = 0.100$ mol.
- Ratio Fe_2O_3 : Fe = 1 : 2, so $n(Fe) = 0.200$ mol.
- $m(Fe) = 0.200 \times 55.85 = 11.2$ g.

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Reacting gas volumes

Using the molar volume

At STP (273 K, 100 kPa) one mole of any ideal gas occupies 22.7 dm^3. This is the **molar volume** (data booklet).

$$n = \frac{V}{22.7} \quad (V \text{ in } dm^3 \text{ at STP})$$

Worked example: gas from a reaction

What volume of carbon dioxide, at STP, forms when 2.50 g of calcium carbonate reacts with excess hydrochloric acid?

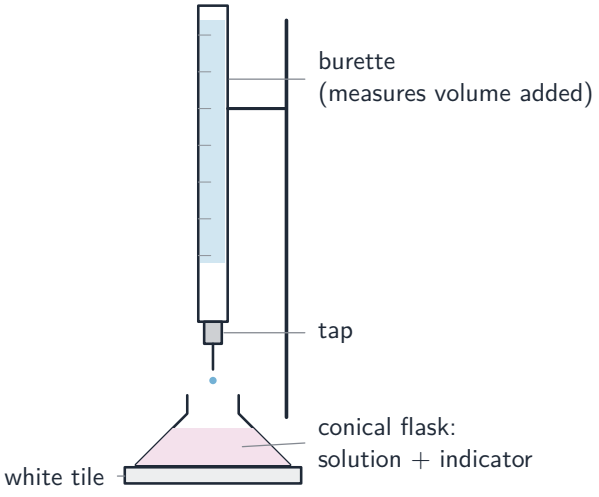
$$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(aq) + H_2O(l) + CO_2(g)$$

- $n(CaCO_3) = 2.50/100.09 = 0.0250$ mol.
- Ratio 1 : 1, so $n(CO_2) = 0.0250$ mol.
- $V = 0.0250 \times 22.7 = 0.567\ dm^3 = 567\ cm^3$.

For two gases at the same temperature and pressure you do not need the molar volume: the volume ratio is the mole ratio (Avogadro's law, Structure 1.4).

Titrations

What a titration does



The titre is the final burette reading minus the initial reading

A **titration** finds the concentration of a solution by reacting it with a **standard solution** of known concentration.

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- A **pipette** delivers an exact volume, often 25.00 cm^3, of one solution into a conical flask.
- Add a few drops of **indicator** .
- Add the other solution from a **burette** until the indicator just changes colour: the **end point** .
- The volume added from the burette is the **titre** .

Good technique

- Rinse the burette with the solution it will hold, and the pipette with the solution it will deliver. Rinse the flask with distilled water only; extra water does not change the amount in it.
- Stand the flask on a white tile so the colour change is easy to see.
- Do a rough titration first. Then add the solution drop by drop near the end point, swirling the flask.
- Read the bottom of the meniscus at eye level, to the nearest 0.05 cm^3.
- Repeat until two or more titres are **concordant** , within 0.10 cm^3 of each other, and average only those.

Worked example: a titration calculation

25.00 cm^3 of sodium hydroxide solution is titrated with 0.100 mol dm^{-3} sulfuric acid.

Titration	**rough**	**1**	**2**	**3**
Final reading / cm^3	22.10	43.65	21.45	42.95
Initial reading / cm^3	0.00	22.10	0.00	21.45
Titre / cm^3	22.10	21.55	21.45	21.50

The concordant titres are 21.55, 21.45 and 21.50 cm^3; the mean is 21.50 cm^3. The rough titre is left out.

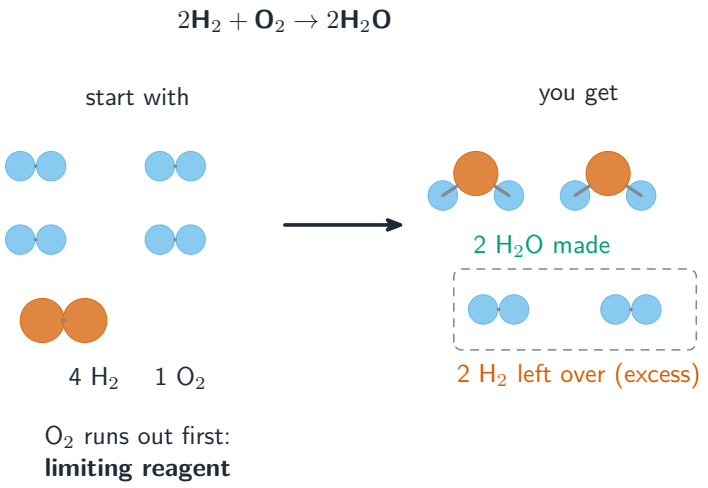
$$H_2SO_4(aq) + 2NaOH(aq) \rightarrow Na_2SO_4(aq) + 2H_2O(l)$$

- $n(H_2SO_4) = 0.100 \times 21.50/1000 = 2.150 \times 10^{-3}$ mol.
- Ratio 1 : 2, so $n(NaOH) = 4.300 \times 10^{-3}$ mol.
- $c(NaOH) = 4.300 \times 10^{-3}/0.02500 = 0.172$ mol dm^{-3}.

Limiting reactant and yield

The limiting reactant

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The reactant that runs out first decides how much product forms

The **limiting reactant** is used up first and stops the reaction. The other reactant is **in excess**: some of it is left over.

To find the limiting reactant, work out the amount of each reactant in moles and **divide by its coefficient** in the equation. The smaller result is the limiting reactant.

Worked example: aluminium and chlorine

5.40 g of aluminium is heated with 14.2 g of chlorine.

$$2Al(s) + 3Cl_2(g) \rightarrow 2AlCl_3(s)$$

- $n(Al) = 5.40/26.98 = 0.200$ mol; $0.200/2 = 0.100$.
- $n(Cl_2) = 14.2/70.90 = 0.200$ mol; $0.200/3 = 0.0667$.
- 0.0667 is smaller, so chlorine is the limiting reactant and aluminium is in excess.
- $n(AlCl_3) = 0.200 \times 2/3 = 0.133$ mol; $m = 0.133 \times 133.33 = 17.8$ g.

Equal amounts in moles do not mean neither is limiting. Always use the coefficients.

Percentage yield

The **theoretical yield** is the mass of product calculated from the limiting reactant. The mass you actually collect is the actual yield.

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

If 14.2 g of $AlCl_3$ is collected in the example above: $14.2/17.8 \times 100 = 79.8\%$.

Yields are less than 100% because:

- the reaction may be reversible and reach equilibrium;
- side reactions make other products;

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- product is lost when it is filtered, transferred or purified.

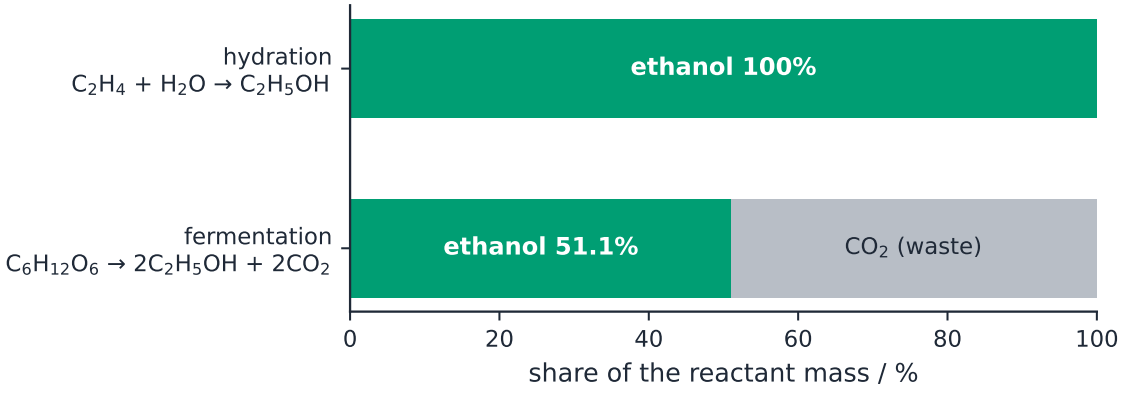
Atom economy

How much of the reactants ends up as product?

Atom economy measures how much of the mass of the reactants ends up in the product you want.

$$\text{atom economy} = \frac{\text{molar mass of the desired product}}{\text{total molar mass of all reactants}} \times 100$$

Use the coefficients from the balanced equation in both totals.



An addition reaction has no waste product, so its atom economy is 100%

Worked example: two routes to ethanol

- Hydration: $C_2H_4 + H_2O \rightarrow C_2H_5OH$. Every atom ends up in ethanol: atom economy 100%.
- Fermentation: $C_6H_{12}O_6 \rightarrow 2C_2H_5OH + 2CO_2$. Atom economy $= 2 \times 46.08/180.18 \times 100 = 51.1\%$.

A high atom economy means less waste, less raw material and often less cost; it is one idea of green chemistry. It is not the same as percentage yield: a reaction can have a 100% atom economy but a poor yield.

Practice

1. Balance: $Al + O_2 \rightarrow Al_2O_3$.
2. Balance: $C_2H_6 + O_2 \rightarrow CO_2 + H_2O$.
3. Calculate the mass of magnesium oxide made by burning 6.08 g of magnesium: $2Mg + O_2 \rightarrow 2MgO$.
4. Calculate the mass of oxygen needed to burn 11.0 g of propane completely (equation in the handout).

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5. Calculate the volume of hydrogen at STP made when 0.654 g of zinc reacts with excess acid: $Zn + 2HCl \rightarrow ZnCl_2 + H_2$.
6. 25.00 cm^3 of hydrochloric acid needs 18.40 cm^3 of 0.150 mol dm^{-3} sodium hydroxide for neutralization. Calculate the concentration of the acid.
7. Titres of 24.30, 23.80, 23.70 and 23.75 cm^3 were recorded; the first was the rough titration. Calculate the mean titre to use.
8. Explain why the conical flask is rinsed with distilled water but the burette is rinsed with the solution it holds.
9. 4.00 g of hydrogen reacts with 16.0 g of oxygen: $2H_2 + O_2 \rightarrow 2H_2O$. Find the limiting reactant and the mass of water made.
10. 10.0 g of $CaCO_3$ is heated and 4.80 g of CaO is collected. Calculate the percentage yield.
11. Calculate the atom economy for making hydrogen from methane: $CH_4 + H_2O \rightarrow CO + 3H_2$.
12. Give two reasons why the actual yield of a reaction is often less than the theoretical yield.

Answers.

1. $4Al + 3O_2 \rightarrow 2Al_2O_3$.
2. $2C_2H_6 + 7O_2 \rightarrow 4CO_2 + 6H_2O$.
3. $n(Mg) = 6.08/24.31 = 0.250$ mol, so 0.250 mol MgO; $m = 0.250 \times 40.31 = 10.1$ g.
4. $n(C_3H_8) = 11.0/44.11 = 0.249$ mol; $n(O_2) = 5 \times 0.249 = 1.25$ mol; $m = 1.25 \times 32.00 = 39.9$ g.
5. $n(Zn) = 0.654/65.38 = 0.0100$ mol, so 0.0100 mol H_2; $V = 0.0100 \times 22.7 = 0.227$ dm^3 (227 cm^3).
6. $n(NaOH) = 0.150 \times 0.01840 = 2.76 \times 10^{-3}$ mol; ratio 1 : 1; $c(HCl) = 2.76 \times 10^{-3}/0.02500 = 0.110$ mol dm^{-3}.
7. Concordant titres 23.80, 23.70, 23.75; mean 23.75 cm^3.
8. Water in the flask does not change the amount of solute it holds. Water left in the burette would dilute the solution and make the titre too large.
9. $n(H_2) = 4.00/2.02 = 1.98$ mol, $\div 2 = 0.990$; $n(O_2) = 16.0/32.00 = 0.500$ mol, $\div 1 = 0.500$. Oxygen limits. $n(H_2O) = 1.00$ mol; $m = 1.00 \times 18.02 = 18.0$ g.
10. $n(CaCO_3) = 10.0/100.09 = 0.0999$ mol; theoretical CaO $= 0.0999 \times 56.08 = 5.60$ g; yield $= 4.80/5.60 \times 100 = 85.7\%$.
11. Reactants $16.05 + 18.02 = 34.07$; desired product $3 \times 2.02 = 6.06$; atom economy $= 6.06/34.07 \times 100 = 17.8\%$.
12. Any two: the reaction is reversible; side reactions; product lost in transfer, filtering or purification; the reaction does not go to completion.

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Exam tips

- Balance the equation before any calculation, and change only the coefficients.
- Show the mole ratio as a separate line; it is where most marks are lost.
- Divide cm^3 by 1000 before using $c = n/V$, and use 22.7 dm^3 only at STP.
- Average only concordant titres, and leave out the rough titration.
- For the limiting reactant, divide moles by the coefficient; never compare masses.
- Percentage yield compares masses of product; atom economy compares molar masses in the equation.

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How fast? The rate of chemical change

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 2.2, How fast? The rate of chemical change, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: concentration and moles from Structure 1.4, enthalpy changes and energy profiles from Reactivity 1.1, and drawing tangents to curves. At Higher Level you will also use natural logarithms and the Arrhenius equation from the data booklet.

Measuring the rate of reaction

Why does food last longer in a fridge?

Milk goes sour in two days on a warm table but lasts a week in a fridge. A firework burns in a second, iron rusts over months. Chemists need to know not only what forms but how fast, and how to make a reaction faster or slower.

What rate means

The **rate of reaction** is the change in the amount or concentration of a reactant or product per unit time.

$$\text{rate} = \frac{\Delta[\text{product}]}{\Delta t} \quad \text{or} \quad -\frac{\Delta[\text{reactant}]}{\Delta t}$$

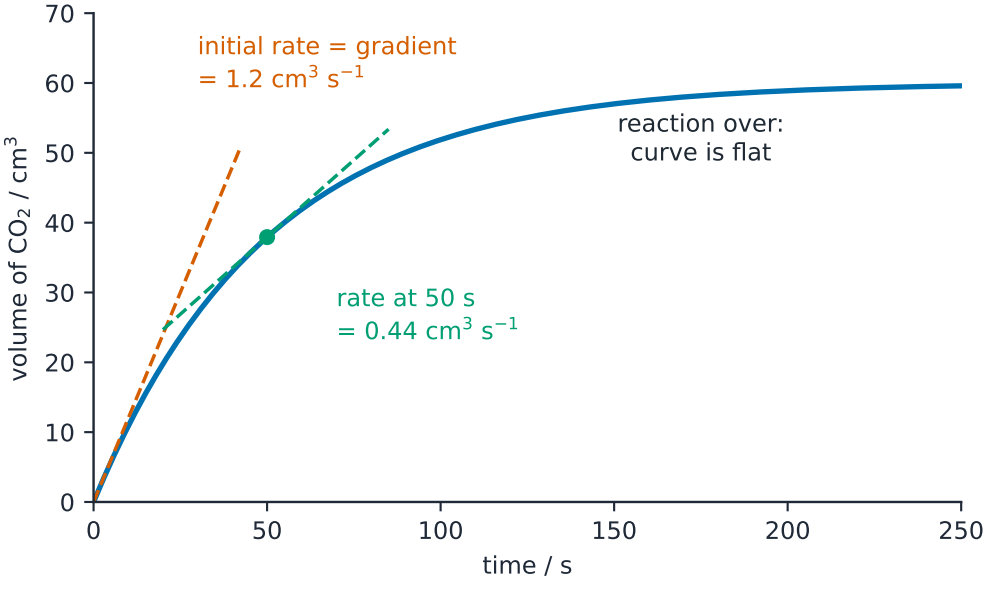
The unit is usually mol dm^{-3} s^{-1}. If you follow something else, such as a gas volume, the unit follows it: cm^3 s^{-1} or g s^{-1}.

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Ways to follow a reaction

What changes	Method	Example
gas is given off	collect the gas in a gas syringe; read the volume every 10 s	$CaCO_3$ + HCl
gas escapes	stand the flask on a balance; read the mass loss	$CaCO_3$ + HCl
colour	colorimeter: measure how much light passes through	bromine reacting with methanoic acid
ions form or are used	conductivity or pH meter	ester hydrolysis
a precipitate forms	time until a cross under the flask disappears	sodium thiosulfate + HCl

Reading a rate from a graph



The rate at any moment is the gradient of the tangent to the curve

- The rate at any time is the gradient of the curve at that time. Draw a **tangent** and find its gradient.
- The curve is steepest at the start, where reactant concentrations are highest. The **initial rate** is the gradient of the tangent at $t = 0$.
- The rate falls as reactants are used up. When the curve is flat, the reaction has stopped.

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Collision theory

Three conditions for a reaction

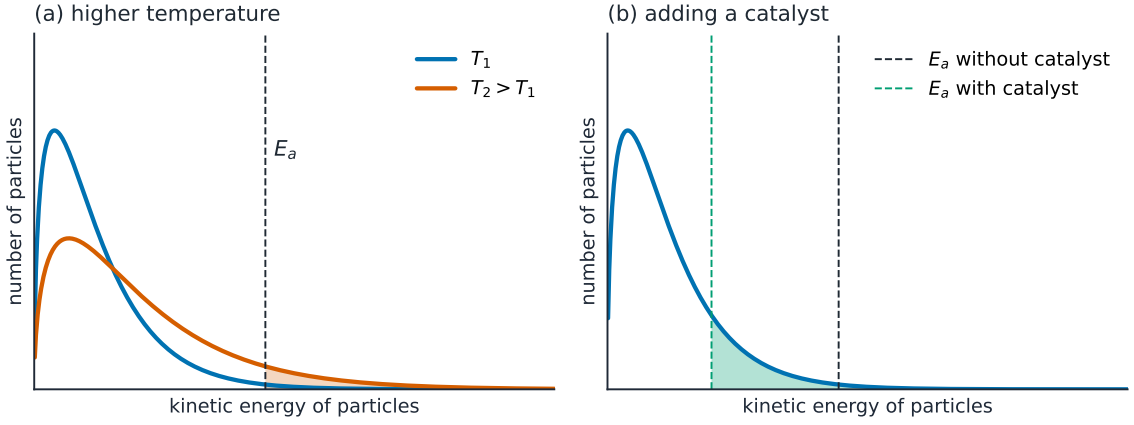
Collision theory says that particles react only when they collide, and only some collisions work. A successful collision needs:

1. A collision: the particles must meet.
2. Enough energy: the collision energy must be at least the **activation energy**, E_a, the minimum energy needed for a reaction.
3. The right orientation: the reacting parts of the particles must meet.

The rate depends on how many successful collisions happen each second.

The Maxwell–Boltzmann distribution

The particles in a gas or solution do not all have the same energy. The **Maxwell–Boltzmann distribution** - shows how many particles have each energy.



The shaded areas are the particles with at least enough energy to react

- The curve starts at the origin: no particle has zero energy.
- It has no maximum energy: the curve never meets the x-axis.
- The area under the curve is the total number of particles. At a higher temperature the area stays the same, so the peak moves right and falls.
- Only particles in the shaded area beyond E_a can react.

Factors that affect the rate

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Concentration, pressure and surface area

Change	Effect on collisions	Effect on rate
higher concentration of a solution	more particles per dm^3, so more frequent collisions	faster
higher pressure of a gas	particles closer together, so more frequent collisions	faster
smaller pieces of a solid (larger **surface area**)	more particles exposed, so more frequent collisions	faster

These three change only the **frequency** of collisions. The fraction of collisions with enough energy stays the same.

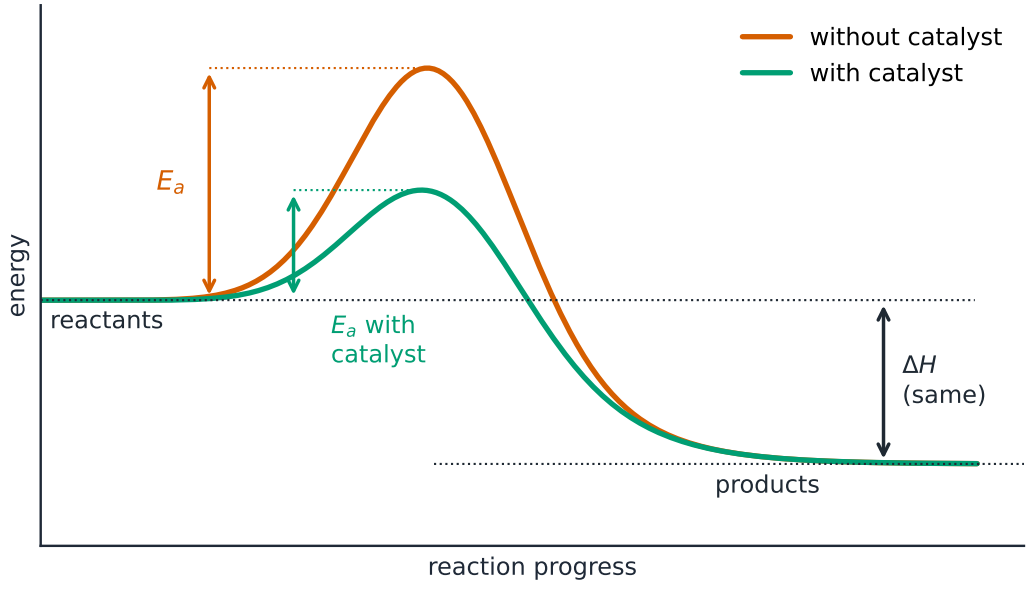
Temperature

A temperature rise of 10 K often roughly doubles the rate. Two effects add together:

1. Particles move faster, so collisions are a little more frequent.
2. Much more important: more particles have energy at least E_a (panel (a) above), so a much larger fraction of collisions succeeds.

Catalysts

A **catalyst** increases the rate of a reaction without being used up. It gives an **alternative reaction pathway** with a lower activation energy.



A catalyst lowers E_a but does not change ΔH

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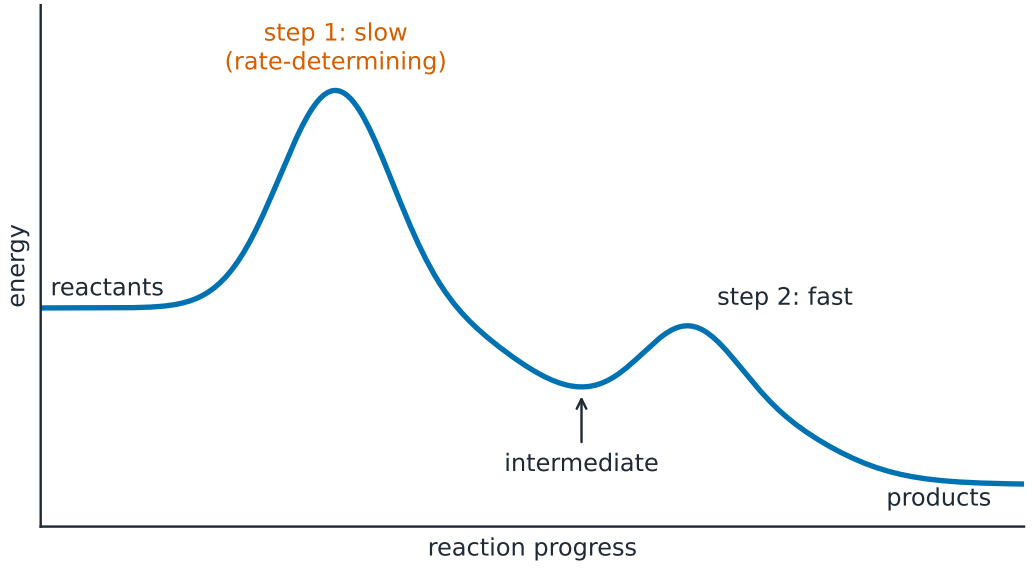
- With a lower E_a, more particles have enough energy (panel (b) above), so more collisions succeed.
- A catalyst does not change ΔH, and it does not change the position of an equilibrium.
- Examples: iron in the Haber process, MnO_2 for the decomposition of hydrogen peroxide, enzymes in living cells.

AHL: Rate equations

Elementary steps and mechanisms

Most reactions happen in a series of simple steps called **elementary steps** . The list of steps is the **reaction mechanism** .

- The **molecularity** of a step is the number of particles that collide in it: unimolecular (1), bimolecular (2) or, rarely, termolecular (3).
- An **intermediate** is made in one step and used up in a later step. It does not appear in the overall equation.
- The slowest step is the **rate-determining step** . The overall reaction cannot go faster than it.



The step with the highest barrier is the rate-determining step

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The rate equation

For a reaction A + B → products, experiments give a **rate equation** of the form:

$$\text{rate} = k[\text{A}]^m[\text{B}]^n$$

- m and n are the **orders** with respect to A and B. They are usually 0, 1 or 2, and they can only be found by experiment, not from the balanced equation.
- The overall order is $m + n$.
- k is the **rate constant** . It is constant at one temperature, and it increases when the temperature rises.

Units of k

Work out the units from rate = $k\times$ concentrations:

Overall order	**Units of k**
0	mol dm^{-3} s^{-1}
1	s^{-1}
2	dm^3 mol^{-1} s^{-1}
3	dm^6 mol^{-2} s^{-1}

Finding orders from initial rates

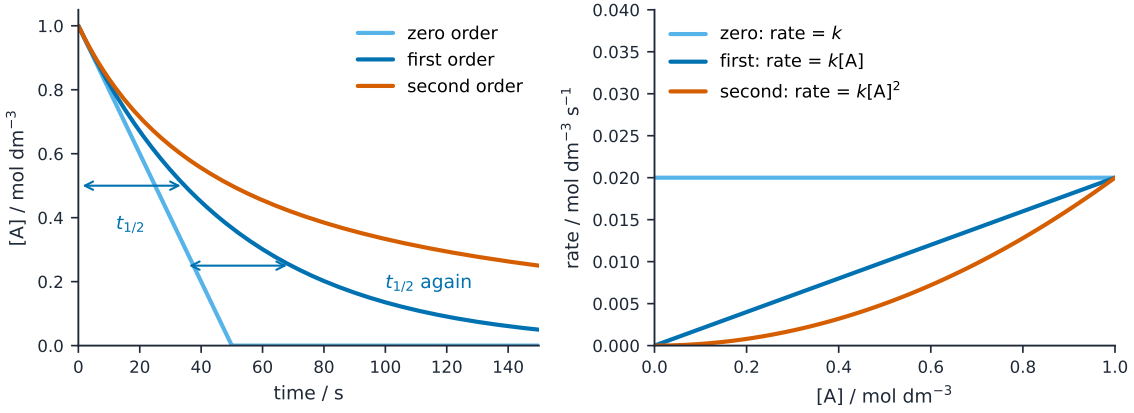
Worked example. For $2\text{NO(g)} + \text{Br}_2\text{(g)} \rightarrow 2\text{NOBr(g)}$:

Experiment	**[NO] / mol dm^{-3}**	**[Br_2] / mol dm^{-3}**	**Initial rate / mol dm^{-3} s^{-1}**
1	0.10	0.10	1.2×10^{-3}
2	0.20	0.10	4.8×10^{-3}
3	0.10	0.20	2.4×10^{-3}

1. Experiments 1 and 2: [NO] doubles, [Br_2] is the same, and the rate goes up 4 times $= 2^2$. Second order in NO.
2. Experiments 1 and 3: [Br_2] doubles and the rate doubles $= 2^1$. First order in Br_2.
3. Rate $= k[\text{NO}]^2[\text{Br}_2]$, third order overall.
4. $k = \dfrac{1.2 \times 10^{-3}}{(0.10)^2 \times 0.10} = 1.2$ dm^6 mol^{-2} s^{-1}.

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Graphs of each order



The shape of each graph shows the order

- **Zero order:** [A] falls in a straight line; the rate does not depend on [A].
- **First order:** the rate is proportional to [A]. The **half-life** , the time for [A] to halve, is constant: $t_{1/2} = \dfrac{0.693}{k}$.
- **Second order:** the rate–concentration graph is a curve; doubling [A] makes the rate four times faster.

Linking the rate equation and the mechanism

The rate equation contains only the species in the rate-determining step and the steps before it.

> **Worked example.** Below 500 K, $NO_2 + CO \rightarrow NO + CO_2$ has rate $= k[NO_2]^2$. A mechanism that fits:

$$\text{step 1 (slow): } 2NO_2 \rightarrow NO_3 + NO$$

$$\text{step 2 (fast): } NO_3 + CO \rightarrow NO_2 + CO_2$$

- The slow step involves two NO_2, so the rate is second order in NO_2.
- CO only appears in the fast step after it, so it is zero order and is not in the rate equation.
- NO_3 is an intermediate. The steps add up to the overall equation.

A mechanism must agree with the rate equation and add up to the overall equation. Agreement makes it possible, not proven.

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AHL: The Arrhenius equation

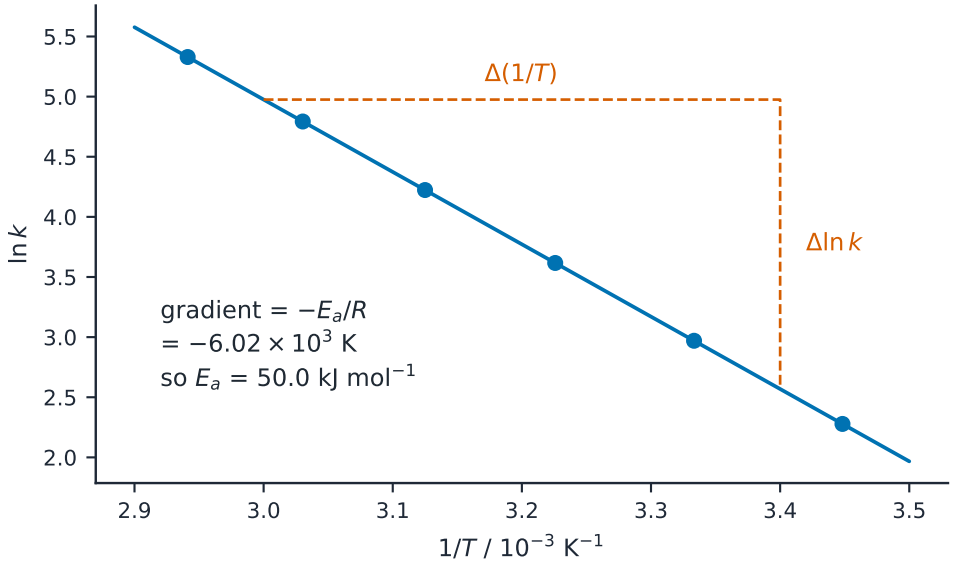
How k depends on temperature

$$k = Ae^{-E_a/RT} \qquad \ln k = -\frac{E_a}{RT} + \ln A$$

- A is the **frequency factor** (also called the pre-exponential factor). It takes account of how often particles collide and with the right orientation. It has the same units as k.
- $e^{-E_a/RT}$ is the fraction of collisions with at least E_a. It rises steeply with T.
- $R = 8.31$ J K^{-1} mol^{-1} and T is in kelvin, so E_a must be in J mol^{-1}.

Finding E_a from a graph

A graph of $\ln k$ against $1/T$ is a straight line. The gradient is $-E_a/R$ and the y-intercept is $\ln A$.



$$Gradient = -E_a/R$$

Here the gradient is -6.02×10^3 K, so $E_a = 6.02 \times 10^3 \times 8.31 = 5.00 \times 10^4$ J mol^{-1} $= 50.0$ kJ mol^{-1}.

Two temperatures

With rate constants at two temperatures, use the data booklet form:

$$\ln \frac{k_1}{k_2} = \frac{E_a}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Worked example. The rate constant doubles from 298 K to 308 K. Find E_a.

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1. $k_2 = 2k_1$, so $\ln\dfrac{k_2}{k_1} = \ln 2 = 0.693$.
2. $\dfrac{1}{298} - \dfrac{1}{308} = 1.0895 \times 10^{-4}$ K^{-1} (keep all the digits).
3. $E_a = \dfrac{8.31 \times 0.693}{1.0895 \times 10^{-4}} = 5.29 \times 10^{4}$ J mol^{-1} $= 52.9$ kJ mol^{-1}.

This is where the rule "a 10 K rise doubles the rate" comes from: it holds for E_a near 50 kJ mol^{-1} at room temperature.

Practice

1. In an experiment, 0.050 mol dm^{-3} of a reactant is used up in 25 s. Calculate the mean rate in mol dm^{-3} s^{-1}.
2. Describe how to follow the rate of the reaction between magnesium ribbon and hydrochloric acid.
3. State the three conditions for a successful collision.
4. Use collision theory to explain why powdered calcium carbonate reacts faster with acid than the same mass of lumps.
5. Sketch Maxwell–Boltzmann curves at two temperatures and use them to explain why a small rise in temperature gives a large rise in rate.
6. Explain how a catalyst increases the rate, with reference to an energy profile and a Maxwell–Boltzmann curve.
7. From the gas–time graph in this handout, explain why the rate at 50 s is lower than the initial rate.
8. **AHL.** For A + 2B → C, rate $= k[\mathrm{A}][\mathrm{B}]^2$. State the overall order and the units of k, and the factor by which the rate changes when [B] is tripled.
9. **AHL.** Initial-rate data for X + Y → Z: [X] 0.10, [Y] 0.10, rate 2.0×10^{-4}; [X] 0.30, [Y] 0.10, rate 6.0×10^{-4}; [X] 0.10, [Y] 0.20, rate 2.0×10^{-4}. Deduce the rate equation and calculate k.
10. **AHL.** The hydrolysis of 2-bromo-2-methylpropane has rate $= k[(\mathrm{CH_3})_3\mathrm{CBr}]$. Suggest a two-step mechanism and identify the rate-determining step and the intermediate.
11. **AHL.** A first-order reaction has $k = 0.0231$ s^{-1}. Calculate its half-life.
12. **AHL.** k is 3.0×10^{-4} s^{-1} at 300 K and 1.2×10^{-3} s^{-1} at 320 K. Calculate E_a.
13. **AHL.** State what the gradient and the intercept of a $\ln k$ against $1/T$ graph represent.

Answers.

1. $0.050/25 = 2.0 \times 10^{-3}$ mol dm^{-3} s^{-1}.
2. Collect the hydrogen in a gas syringe and read the volume every 10 s (or measure the mass loss on a balance); keep the temperature, acid concentration and volume the same.

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3. The particles collide, with energy at least equal to E_a, and with the correct orientation.
4. Powder has a larger surface area, so more particles are exposed and collisions with acid particles are more frequent.
5. At the higher temperature the curve is lower and broader with the same area; the area beyond E_a is much larger, so a much larger fraction of collisions has enough energy.
6. It gives an alternative pathway with a lower E_a (a lower peak on the profile, the same ΔH). On the Maxwell–Boltzmann curve the lower E_a line has more particles beyond it, so more collisions succeed.
7. Reactants have been used up, so their concentration is lower and collisions are less frequent; the tangent is less steep.
8. **AHL.** Third order; $\text{dm}^6\ \text{mol}^{-2}\ \text{s}^{-1}$; $3^2 = 9$ times faster.
9. **AHL.** Tripling [X] triples the rate: first order in X. Doubling [Y] has no effect: zero order in Y. Rate $= k[\text{X}]$; $k = 2.0 \times 10^{-4}/0.10 = 2.0 \times 10^{-3}\ \text{s}^{-1}$.
10. **AHL.** Step 1 (slow, rate-determining): $(\text{CH}_3)_3\text{CBr} \rightarrow (\text{CH}_3)_3\text{C}^+ + \text{Br}^-$. Step 2 (fast): $(\text{CH}_3)_3\text{C}^+ + \text{OH}^- \rightarrow (\text{CH}_3)_3\text{COH}$. The intermediate is the carbocation $(\text{CH}_3)_3\text{C}^+$.
11. **AHL.** $t_{1/2} = 0.693/0.0231 = 30.0$ s.
12. **AHL.** $\ln(1.2 \times 10^{-3}/3.0 \times 10^{-4}) = \ln 4 = 1.386$. $1/300 - 1/320 = 2.08 \times 10^{-4}\ \text{K}^{-1}$. $E_a = 8.31 \times 1.386/2.08 \times 10^{-4} = 5.53 \times 10^4\ \text{J mol}^{-1} = 55.3\ \text{kJ mol}^{-1}$.
13. **AHL.** Gradient $= -E_a/R$; intercept $= \ln A$.

Exam tips

- Rate is measured from the gradient of a tangent; draw the tangent long and read two far-apart points.
- Concentration, pressure and surface area change the collision frequency; temperature and catalysts change the fraction of collisions with enough energy.
- On a Maxwell–Boltzmann curve: start at the origin, never touch the x-axis, keep the same area at the higher temperature.
- A catalyst does not change ΔH or the equilibrium position.
- **AHL.** Orders come from experiments, never from the balanced equation.
- **AHL.** In the Arrhenius equation, use T in K and E_a in J mol^{-1}; divide by 1000 at the end.

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How far? The extent of chemical change

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 2.3, How far? The extent of chemical change, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: concentration in mol dm^{-3} from Structure 1.4, exothermic and endothermic reactions from Reactivity 1.1, and rates and catalysts from Reactivity 2.2. At Higher Level you will also use Gibbs energy from Reactivity 1.4 and natural logarithms.

Dynamic equilibrium

Why does a sealed bottle of cola stay fizzy?

In a closed bottle, carbon dioxide gas sits above the drink. Molecules of CO_2 leave the liquid and others dissolve back into it, all the time. The two rates are equal, so the amount of gas in the drink does not change and the drink stays fizzy for months. Open the bottle and the gas escapes: the balance is gone, and the drink goes flat.

Many chemical reactions behave the same way. They do not go to completion; they stop at a mixture of reactants and products.

Reversible reactions

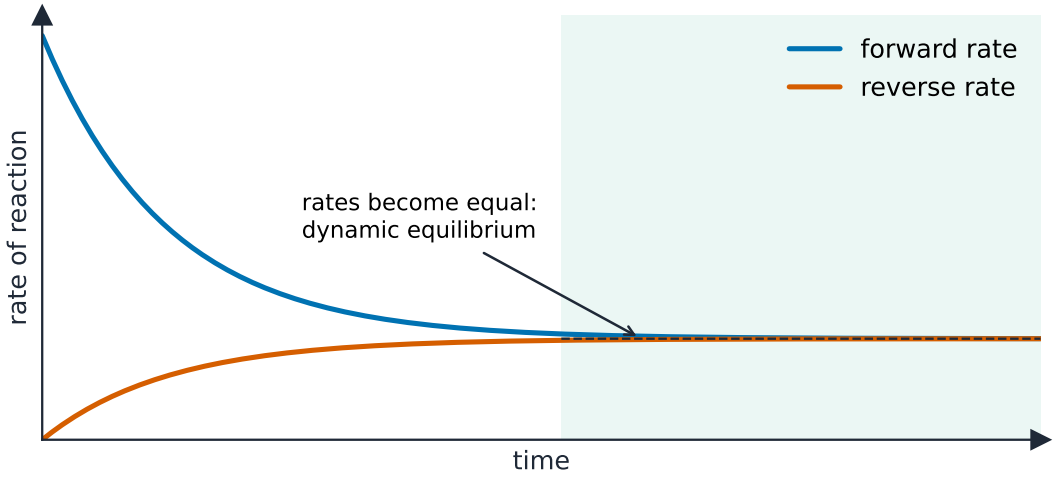
A **reversible reaction** can go in both directions. The sign $\rightleftharpoons$ shows this.

$$H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$$

- The **forward reaction** goes from left to right; the **reverse reaction** goes from right to left.
- At the start only the forward reaction happens. As soon as some HI forms, the reverse reaction starts too.

What dynamic equilibrium means

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$$\text{at equilibrium: } \text{rate}_f = \text{rate}_r \cdot K_c = \frac{[\text{products}]}{[\text{reactants}]}$$

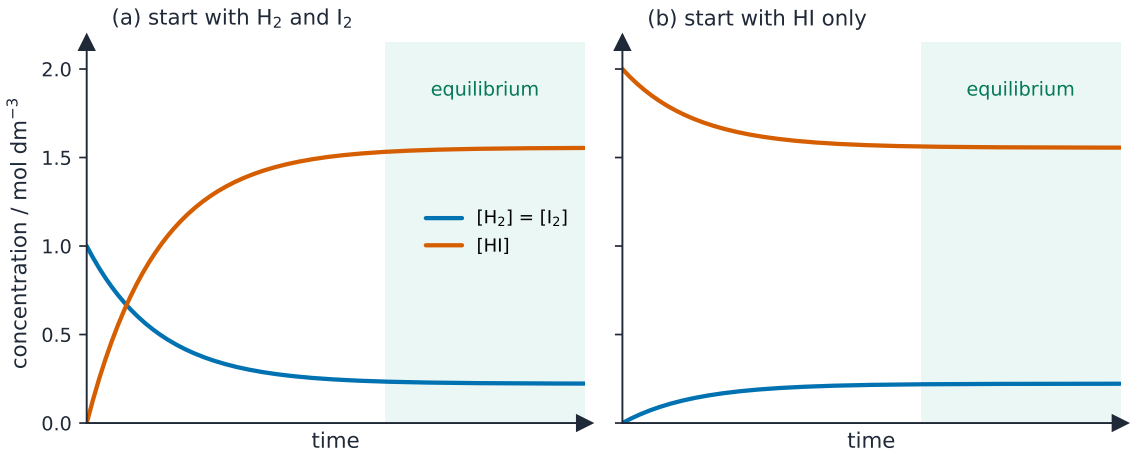
At equilibrium the two rates are equal, but neither is zero

A **dynamic equilibrium** is reached in a **closed system** when the rate of the forward reaction equals the rate of the reverse reaction.

- **Dynamic:** both reactions keep going. Particles still react, but the forward and reverse changes cancel.
- **Constant concentrations:** the amounts of reactants and products no longer change.
- **Not equal concentrations:** "constant" does not mean "the same". At equilibrium a mixture can be mostly products or mostly reactants.
- **Closed system:** nothing enters or leaves. If a product escapes, as CO_2 escapes from an open bottle, equilibrium is never reached.

The same equilibrium from both sides

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Under the same conditions you reach the same equilibrium mixture from either direction

At 700 K, 1.00 mol dm^{-3} each of H_2 and I_2 reacts until [HI] = 1.56 mol dm^{-3} and $[H_2] = [I_2]$ = 0.22 mol dm^{-3}. Starting with 2.00 mol dm^{-3} of HI alone gives the same final mixture.

Evidence that equilibrium is dynamic. Add a little D_2 (hydrogen-2, a heavier **isotope** of hydrogen) to an equilibrium mixture of H_2, I_2 and HI. The concentrations do not change, but soon DI appears in the mixture. Molecules are still reacting in both directions.

■ Physical equilibria

Equilibrium is not only for reactions. In a closed flask of bromine, liquid evaporates and vapour condenses at equal rates, so the brown colour of the vapour stays constant:

$$Br_2(l) \rightleftharpoons Br_2(g)$$

The equilibrium constant

■ The equilibrium law

For the general reaction

$$aA + bB \rightleftharpoons cC + dD$$

the **equilibrium constant** K_c is

$$K_c = \frac{[C]^c\,[D]^d}{[A]^a\,[B]^b}$$

- Square brackets mean concentration in mol dm^{-3} **at equilibrium**.
- Products go on top, reactants underneath.

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- Each concentration is raised to the power of its coefficient in the balanced equation.
- For a given reaction, K_c has the same value at a given temperature, whatever the starting amounts. It changes only when the temperature changes.

■ Worked example: calculating K_c

At 700 K the equilibrium mixture for $H_2 + I_2 \rightleftharpoons 2HI$ contains $[H_2] = [I_2] = 0.020$ mol dm^{-3} and $[HI] = 0.14$ mol dm^{-3}.

$$K_c = \frac{[HI]^2}{[H_2][I_2]} = \frac{0.14^2}{0.020 \times 0.020} = \frac{0.0196}{0.00040} = 49$$

IB questions usually give and expect K_c as a number, without units.

■ Writing K_c for other equations

Equation	K_c
$N_2 + 3H_2 \rightleftharpoons 2NH_3$	$\frac{[NH_3]^2}{[N_2][H_2]^3}$
$2SO_2 + O_2 \rightleftharpoons 2SO_3$	$\frac{[SO_3]^2}{[SO_2]^2[O_2]}$
$2HI \rightleftharpoons H_2 + I_2$ (reverse of the example)	$\frac{[H_2][I_2]}{[HI]^2} = \frac{1}{49} = 0.020$

- Reversing an equation gives $1/K_c$.
- Doubling every coefficient squares K_c: for $2H_2 + 2I_2 \rightleftharpoons 4HI$, $K_c = 49^2 = 2401$.

■ What the size of K tells you

The **position of equilibrium** says whether the mixture is mainly reactants or mainly products.

Value of K	Equilibrium mixture	Example
$K \gg 1$ (say 10^{10})	almost all products; the reaction "goes to completion"	burning methane
$K \approx 1$	similar amounts of reactants and products	ester formation, $K_c \approx 4$
$K \ll 1$ (say 10^{-10})	almost all reactants; hardly any reaction	$N_2 + O_2 \rightarrow 2NO$ at room temperature

K tells you **how far** a reaction goes, not **how fast**. A reaction with a huge K can still be very slow, for example the burning of a diamond at room temperature.

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Le Chatelier's principle

The principle

Le Chatelier's principle : when a system at equilibrium is disturbed, the position of equilibrium shifts to reduce the effect of the change.

To predict a shift, first write the balanced equation with state symbols and the sign of ΔH for the forward reaction.

Changing a concentration

Add more of a reactant: the system uses some of it up, so the equilibrium shifts to the right and more product forms. Remove a product: the system makes more of it, again a shift to the right.

K_c does **not** change. The concentrations rearrange until the fraction in the K_c expression has its old value again.

Changing the pressure

Pressure matters only for gases. Count the moles of gas on each side.

- Increase the pressure: the equilibrium shifts to the side with **fewer** gas molecules, which lowers the pressure.
- Decrease the pressure: the equilibrium shifts to the side with **more** gas molecules.
- Same number on both sides, as in $H_2 + I_2 \rightleftharpoons 2HI$ (2 and 2): pressure has no effect on the position.

For $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g)$ there are 4 gas molecules on the left and 2 on the right, so a higher pressure shifts the equilibrium to the right and gives more ammonia.

Changing the temperature

Temperature is the only change that alters the value of K.

- Raise the temperature: the equilibrium shifts in the **endothermic** direction, which takes in heat.
- Lower the temperature: it shifts in the **exothermic** direction.

$$N_2O_4(g) \rightleftharpoons 2NO_2(g) \qquad \Delta H = +57 \text{ kJ mol}^{-1}$$

N_2O_4 is colourless and NO_2 is brown. The forward reaction is endothermic, so heating the gas shifts the equilibrium to the right: the gas turns darker brown and K_c becomes larger. In ice water the gas turns pale.

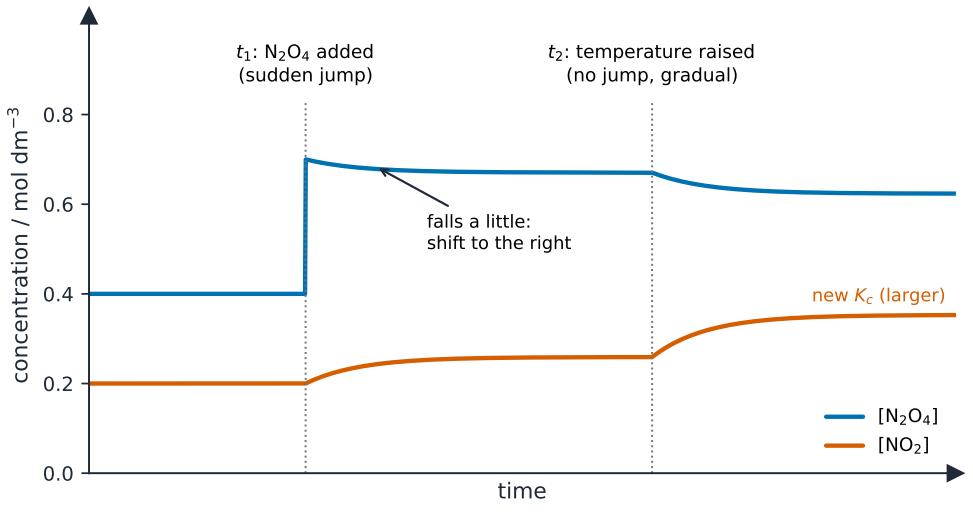
For an exothermic forward reaction the opposite is true: a higher temperature gives a smaller K and less product.

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Adding a catalyst

A catalyst speeds up the forward and reverse reactions by the same factor. Equilibrium is reached sooner, but the position of equilibrium and K do not change.

Summary



$N_2O_4(g) \rightleftharpoons 2NO_2(g)$, forward endothermic · NO_2 changes twice as much as N_2O_4

A concentration change gives a sudden jump; a temperature change gives smooth curves and a new K_c

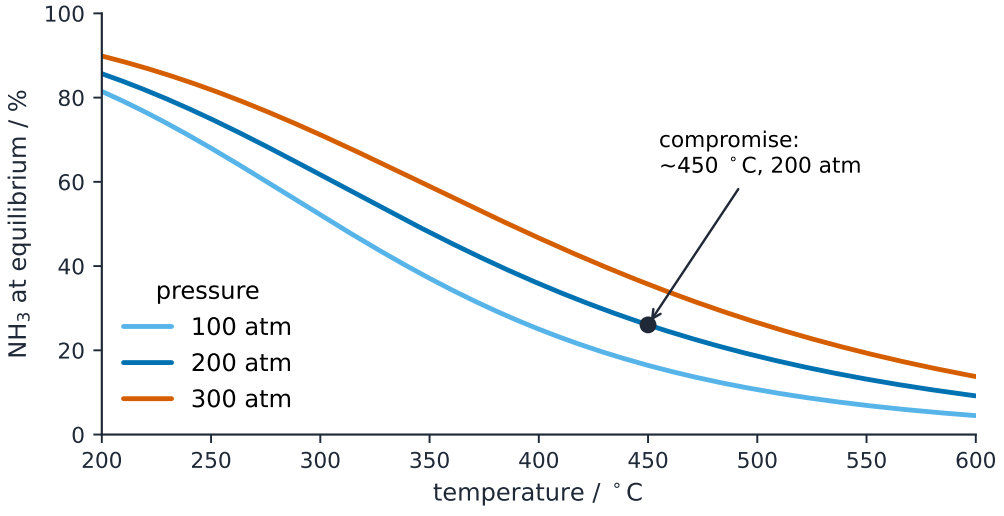
Change	Shift in position	Effect on K
add a reactant or remove a product	to the right	none
increase the pressure (gases)	to the side with fewer gas molecules	none
raise the temperature	in the endothermic direction	changes
add a catalyst	none; equilibrium is reached sooner	none

Industry: making ammonia

The Haber process makes ammonia for fertilizers:

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \qquad \Delta H = -92 \text{ kJ mol}^{-1}$$

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exothermic: lower T ↑ yield · higher P ↑ yield

The equilibrium yield is highest at low temperature and high pressure

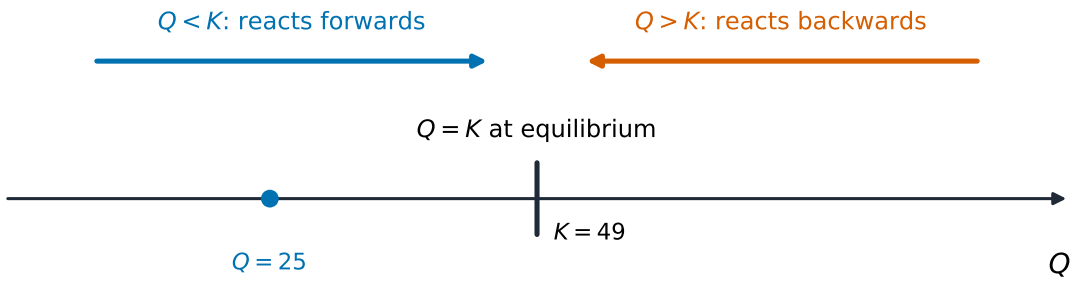
- **Pressure about 200 atm.** Fewer gas molecules on the right, so high pressure gives a higher **yield** . Even higher pressure would cost too much in equipment and energy.
- **Temperature about 450 °C.** The forward reaction is exothermic, so a low temperature gives a higher yield, but the reaction would be far too slow. 450 °C is a **compromise** between yield and rate.
- **Iron catalyst.** It makes the reaction faster; it does not change the yield.
- **Ammonia is removed** by cooling it to a liquid, and unreacted N_2 and H_2 are recycled. Removing the product keeps shifting the equilibrium to the right.

AHL: The reaction quotient

■ Q for a mixture that is not at equilibrium

The **reaction quotient** Q has the same expression as K, but uses the concentrations at any moment, not only at equilibrium.

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Compare Q with K to see which way the mixture will react

- $Q < K$: too little product. The forward reaction goes faster until $Q = K$.
- $Q > K$: too much product. The reverse reaction goes faster until $Q = K$.
- $Q = K$: the mixture is already at equilibrium.

Worked example: which way?

At 700 K, $K_c = 49$ for $H_2 + I_2 \rightleftharpoons 2HI$. A flask contains $[H_2] = [I_2] = 0.10$ mol dm^{-3} and $[HI] = 0.50$ mol dm^{-3}.

$$Q = \frac{0.50^2}{0.10 \times 0.10} = \frac{0.25}{0.010} = 25$$

Q (25) is less than K (49), so the mixture is not at equilibrium. It reacts forwards: [HI] rises and $[H_2]$ and $[I_2]$ fall until Q reaches 49.

AHL: Equilibrium calculations

The ICE table

To find equilibrium amounts, set out three rows:

- **I**nitial amounts.
- **C**hange, in the mole ratio of the equation.
- **E**quilibrium amounts = initial + change.

Worked example: finding K_c

1.00 mol of ethanoic acid and 1.00 mol of ethanol are heated with a little acid catalyst until equilibrium. The mixture then contains 0.67 mol of ethyl ethanoate.

	CH_3COOH	C_2H_5OH	$CH_3COOC_2H_5$	H_2O
Initial / mol	1.00	1.00	0	0
Change / mol	−0.67	−0.67	+0.67	+0.67
Equilibrium / mol	0.33	0.33	0.67	0.67

The volume V is the same for every substance, and there are 2 particles on each side, so V cancels:

$$K_c = \frac{(0.67/V)(0.67/V)}{(0.33/V)(0.33/V)} = \frac{0.67^2}{0.33^2} = 4.1$$

■ Worked example: finding equilibrium concentrations

At 700 K, $K_c = 49$ for $H_2 + I_2 \rightleftharpoons 2HI$. Start with 1.00 mol dm^{-3} each of H_2 and I_2 and no HI. Let x mol dm^{-3} of H_2 react.

	H_2	I_2	HI
Initial	1.00	1.00	0
Change	$-x$	$-x$	$+2x$
Equilibrium	$1.00 - x$	$1.00 - x$	$2x$

$$49 = \frac{(2x)^2}{(1.00 - x)^2}$$

Both sides are perfect squares, so take the square root:

$$7.0 = \frac{2x}{1.00 - x} \quad \Rightarrow \quad 7.0 - 7.0x = 2x \quad \Rightarrow \quad x = 0.78$$

So [HI] = 1.56 mol dm^{-3} and [H_2] = [I_2] = 0.22 mol dm^{-3}. These are the values in the concentration–time graphs above.

■ When K is very small

If K is very small, very little reactant is used up. You may then take the equilibrium concentration of each reactant as equal to its initial concentration. This **approximation** avoids solving a quadratic.

At a high temperature, $K_c = 4.0 \times 10^{-4}$ for $N_2(g) + O_2(g) \rightleftharpoons 2NO(g)$. Start with [$N_2$] = [$O_2$] = 0.50 mol dm^{-3}.

$$K_c = \frac{[NO]^2}{[N_2][O_2]} \approx \frac{[NO]^2}{0.50 \times 0.50} = 4.0 \times 10^{-4}$$

$$[NO]^2 = 1.0 \times 10^{-4} \quad \Rightarrow \quad [NO] = 0.010 \text{ mol dm}^{-3}$$

Only 0.005 mol dm^{-3} of N_2 was used, 1% of 0.50, so the approximation was fair. State the assumption in your answer.

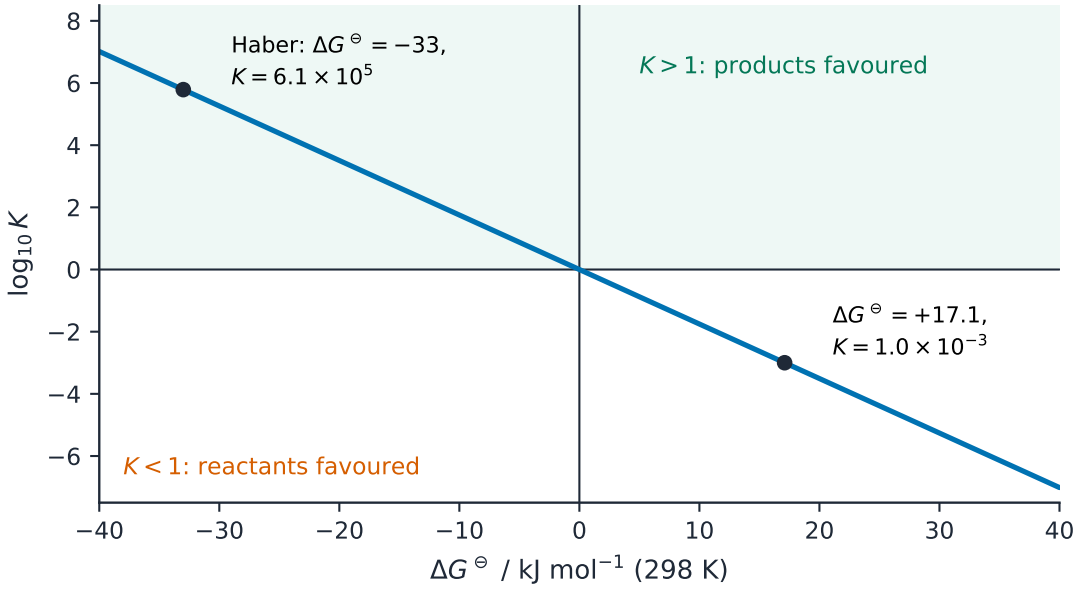
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■ Linking $\Delta G^{\ominus}$ and K

The standard **Gibbs energy** change of a reaction and its equilibrium constant are linked (data booklet):

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

$R = 8.31$ J K^{-1} mol^{-1}, T in K, $\Delta G^{\ominus}$ in J mol^{-1}.



A negative $\Delta G^{\ominus}$ means $K > 1$; a positive $\Delta G^{\ominus}$ means $K < 1$

$\Delta G^{\ominus}$	K	**Equilibrium mixture**
negative	greater than 1	mainly products
zero	1	similar amounts
positive	less than 1	mainly reactants

At equilibrium the mixture has the lowest Gibbs energy it can reach, so $\Delta G = 0$ for any further change. A reaction with a positive $\Delta G^{\ominus}$ still happens a little: it reaches an equilibrium that lies to the left.

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■ **Worked example: K from $\Delta G^\ominus$**

For the Haber process, $\Delta G^\ominus = -33$ kJ mol^{-1} at 298 K.

$$\ln K = \frac{-\Delta G^\ominus}{RT} = \frac{33\,000}{8.31 \times 298} = 13.3 \quad \Rightarrow \quad K = e^{13.3} = 6.1 \times 10^5$$

At room temperature the equilibrium lies far to the right. Industry still heats the gases, because at 298 K the reaction is far too slow.

■ **Worked example: $\Delta G^\ominus$ from K**

A reaction has $K = 1.0 \times 10^{-3}$ at 298 K.

$\Delta G^\ominus = -8.31 \times 298 \times \ln(1.0 \times 10^{-3}) = -2476 \times (-6.91) = +17\,100$ J mol^{-1} $= +17.1$ kJ mol^{-1}

Practice

1. State two features of a dynamic equilibrium.
2. Explain why a mixture of calcium carbonate and its decomposition products in an open container never reaches equilibrium.
3. Write the K_c expression for $4NH_3(g) + 5O_2(g) \rightleftharpoons 4NO(g) + 6H_2O(g)$.
4. For $PCl_5 \rightleftharpoons PCl_3 + Cl_2$, the equilibrium concentrations are $[PCl_5] = 0.040$, $[PCl_3] = 0.020$ and $[Cl_2] = 0.080$ mol dm^{-3}. Calculate K_c.
5. $K_c = 2.5 \times 10^{-31}$ for a reaction at 298 K. Describe the equilibrium mixture.
6. $CO(g) + 2H_2(g) \rightleftharpoons CH_3OH(g)$, $\Delta H = -91$ kJ mol^{-1}. Predict the effect on the yield of methanol of (a) raising the pressure, (b) raising the temperature, (c) adding a catalyst.
7. A sealed syringe of N_2O_4 and NO_2 is put into hot water. State and explain the colour change.
8. Explain why the Haber process runs at about 450 °C and not at room temperature.
9. **AHL.** For $H_2 + I_2 \rightleftharpoons 2HI$, $K_c = 49$. A mixture has $[H_2] = [I_2] = 0.050$ and $[HI] = 0.60$ mol dm^{-3}. Calculate Q and state the direction of change.
10. **AHL.** 2.00 mol of SO_2 and 1.00 mol of O_2 are mixed in a 1.00 dm^3 flask. At equilibrium, 1.60 mol of SO_3 is present. Calculate K_c for $2SO_2 + O_2 \rightleftharpoons 2SO_3$.
11. **AHL.** $K_c = 4.0$ for $CH_3COOH + C_2H_5OH \rightleftharpoons CH_3COOC_2H_5 + H_2O$. Starting with 1.00 mol of acid and 1.00 mol of ethanol, calculate the amount of ester at equilibrium.
12. **AHL.** For $A(g) \rightleftharpoons 2B(g)$, $K_c = 1.6 \times 10^{-5}$. The initial [A] is 0.10 mol dm^{-3}. Use an approximation to find [B] at equilibrium, and state the assumption.
13. **AHL.** Calculate K at 298 K for a reaction with $\Delta G^\ominus = -11.4$ kJ mol^{-1}.

Answers.

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1. The forward and reverse rates are equal; the concentrations stay constant (both reactions still happen). It needs a closed system.
2. CO_2 gas escapes, so the reverse reaction $CaO + CO_2 \rightarrow CaCO_3$ cannot keep pace. The system is not closed.
3. $K_c = \dfrac{[NO]^4[H_2O]^6}{[NH_3]^4[O_2]^5}$
4. $K_c = \dfrac{0.020 \times 0.080}{0.040} = 0.040.$
5. K_c is extremely small, so the mixture is almost all reactants; hardly any product forms.
6. (a) Yield increases: 3 gas molecules on the left, 1 on the right, so the equilibrium shifts to the right. (b) Yield decreases: the forward reaction is exothermic, so the equilibrium shifts left (endothermic direction) and K falls. (c) No change in yield; equilibrium is reached faster.
7. It turns darker brown. The forward reaction $N_2O_4 \rightarrow 2NO_2$ is endothermic, so a higher temperature shifts the equilibrium to the right, making more brown NO_2.
8. A lower temperature would give a higher equilibrium yield (exothermic forward reaction) but the rate would be too slow. 450 °C gives a reasonable yield at a reasonable rate: a compromise.
9. **AHL.** $Q = 0.60^2/(0.050 \times 0.050) = 0.36/0.0025 = 144$. $Q > K$, so the mixture reacts backwards: [HI] falls, $[H_2]$ and $[I_2]$ rise.
10. **AHL.** Change: SO_3 +1.60, SO_2 −1.60, O_2 −0.80. Equilibrium: SO_2 0.40, O_2 0.20, SO_3 1.60 mol dm^{-3}. $K_c = 1.60^2/(0.40^2 \times 0.20) = 2.56/0.032 = 80$.
11. **AHL.** $4.0 = x^2/(1.00 - x)^2$, so $2.0 = x/(1.00 - x)$, $x = 2.0 - 2.0x$, $x = 0.67$ mol of ester.
12. **AHL.** Assume [A] stays 0.10. $[B]^2 = 1.6 \times 10^{-5} \times 0.10 = 1.6 \times 10^{-6}$, $[B] = 1.3 \times 10^{-3}$ mol dm^{-3}. Assumption: so little A reacts (6×10^{-4} mol dm^{-3}, under 1%) that [A] at equilibrium equals its initial value.
13. **AHL.** $\ln K = 11\,400/(8.31 \times 298) = 4.60$; $K = e^{4.60} = 99$, or 1.0×10^2 to 2 significant figures.

Exam tips

- "Dynamic" means both reactions continue; "equilibrium" means the rates are equal. Never write that the concentrations are equal.
- Write K_c with products over reactants and coefficients as powers; use equilibrium concentrations only.
- Only temperature changes K. Concentration and pressure change the position; a catalyst changes neither.
- For a temperature question, state the sign of ΔH first; for a pressure question, count the gas molecules on each side.

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- **AHL.** Compare Q with K before saying which way a mixture reacts.
- **AHL.** In an ICE table the changes follow the mole ratio; convert moles to concentrations unless the volume cancels.
- **AHL.** In $\Delta G^{\ominus} = -RT\ln K$, convert kJ to J.

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Reactivity 3.1 · Proton transfer reactions

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 3.1, Proton transfer reactions, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: amount of substance and concentration from Structure 1.4, equilibrium and K from Reactivity 2.3, and logarithms to base 10. You will use K_w and K_a or pK_a values from the data booklet.

Brønsted–Lowry acids and bases

What do vinegar, stomach acid and cleaning ammonia have in common?

Vinegar and stomach acid both turn blue litmus red, and ammonia solution turns red litmus blue. One idea explains all three: in every acid–base reaction a **proton** , an H^+ ion, moves from one particle to another.

Acids donate, bases accept

- A **Brønsted–Lowry acid** - is a proton donor.
- A **Brønsted–Lowry base** - is a proton acceptor. A base must have a lone pair to accept the proton.

In water a proton never exists on its own: it bonds to a water molecule to form the oxonium ion, H_3O^+. Writing $H^+(aq)$ is a short form for $H_3O^+(aq)$.

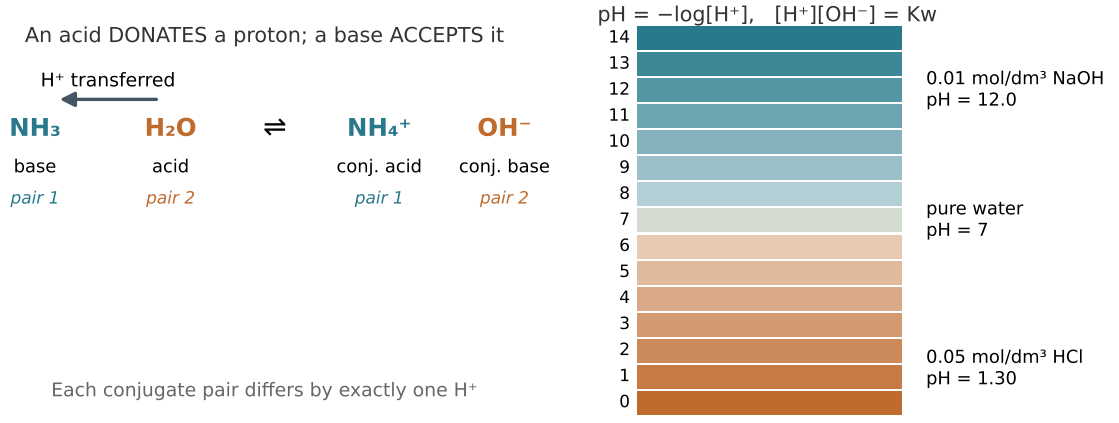
$$HCl(aq) + H_2O(l) \rightarrow H_3O^+(aq) + Cl^-(aq)$$

Conjugate acid–base pairs

When an acid donates a proton, what is left can accept a proton back: it is a base. A **conjugate acid–base pair** is two species that differ by one proton.

$$NH_3(aq) + H_2O(l) \rightleftharpoons NH_4^+(aq) + OH^-(aq)$$

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A Brønsted–Lowry acid donates H^+ and a base accepts it; pH = –log[H^+]

Here NH_3 (base) and NH_4^+ (its conjugate acid) are one pair; H_2O (acid) and OH^- (its conjugate base) are the other.

Water acts as a base with HCl and as an acid with NH_3. A species that can both donate and accept a proton is **amphiprotic** . Other examples are HCO_3^-, HSO_4^- and $H_2PO_4^-$.

pH and the ionic product of water

The pH scale

The concentration of H^+ in solutions ranges from about 1 to 10^{-14} mol dm^{-3}. The **pH** scale turns this into simple numbers:

$$\text{pH} = -\log_{10}[\text{H}^+] \qquad [\text{H}^+] = 10^{-\text{pH}}$$

- A decrease of one pH unit means $[H^+]$ is **ten times** larger.
- pH has no units. Give it to the same number of decimal places as the significant figures in $[H^+]$.

Worked example: $[H^+] = 0.050$ mol dm^{-3} gives $\text{pH} = -\log(0.050) = 1.30$. A solution of pH 3.40 has $[H^+] = 10^{-3.40} = 4.0 \times 10^{-4}$ mol dm^{-3}.

Water ionizes a little

Pure water contains a tiny amount of ions:

$$\text{H}_2\text{O(l)} \rightleftharpoons \text{H}^+\text{(aq)} + \text{OH}^-\text{(aq)}$$

The **ionic product of water** , K_w, is

$$K_w = [\text{H}^+][\text{OH}^-] = 1.00 \times 10^{-14} \text{ at } 298 \text{ K}$$

In pure water $[H^+] = [OH^-] = 1.00 \times 10^{-7}$, so the pH is 7.00. A solution is **neutral** when $[H^+] = [OH^-]$, acidic when $[H^+] > [OH^-]$ and alkaline when $[H^+] < [OH^-]$.

The ionization of water is endothermic, so K_w increases with temperature. At 50 °C pure water has a pH of about 6.6, but it is still neutral, because $[H^+]$ and $[OH^-]$ are still equal.

■ pH of strong acids and bases

A strong acid or strong alkali is fully ionized, so the concentration of ions comes straight from the concentration of the solution.

- 0.020 mol dm^{-3} HCl: $[H^+] = 0.020$, pH = 1.70.
- 0.010 mol dm^{-3} NaOH: $[OH^-] = 0.010$, so $[H^+] = K_w/0.010 = 1.0 \times 10^{-12}$, pH = 12.00.

Strong and weak acids and bases

■ Full and partial ionization

- A **strong acid** ionizes completely in water: HCl, HNO_3, H_2SO_4 (first proton). A **strong base** ionizes or dissociates completely: group 1 hydroxides and $Ba(OH)_2$.
- A **weak acid** ionizes only partly; the equilibrium lies to the left: ethanoic acid and other carboxylic acids, carbonic acid. A **weak base** accepts protons only partly: ammonia and amines.

$$CH_3COOH(aq) + H_2O(l) \rightleftharpoons CH_3COO^-(aq) + H_3O^+(aq)$$

In 0.10 mol dm^{-3} ethanoic acid only about 1 molecule in 80 is ionized at any moment.

Do not confuse **strong** with **concentrated**. Strength is about how far the acid ionizes; concentration is how much acid is dissolved in each dm^3. A dilute solution of a strong acid can have a higher pH than a concentrated solution of a weak acid.

The stronger an acid, the weaker its conjugate base: Cl^- has almost no tendency to accept a proton, while CH_3COO^- accepts one easily.

■ Telling them apart

Compare solutions of the **same concentration** at the same temperature:

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Test	0.10 **mol dm^{-3} HCl (strong)**	0.10 **mol dm^{-3} CH_3COOH (weak)**
pH	1.0	about 2.9
electrical conductivity	high (many ions)	low (few ions)
rate with magnesium or $CaCO_3$	fast bubbling	slow bubbling

The total volume of gas, and the amount of alkali needed to neutralize each solution, are the **same**: as the weak acid reacts, its equilibrium shifts and more molecules ionize.

Neutralization and pH curves

Neutralization

An acid and a base react to form a salt and water. For any strong acid and strong base the reaction is the same:

$$H^+(aq) + OH^-(aq) \rightarrow H_2O(l) \qquad \Delta H \approx -57 \text{ kJ mol}^{-1}$$

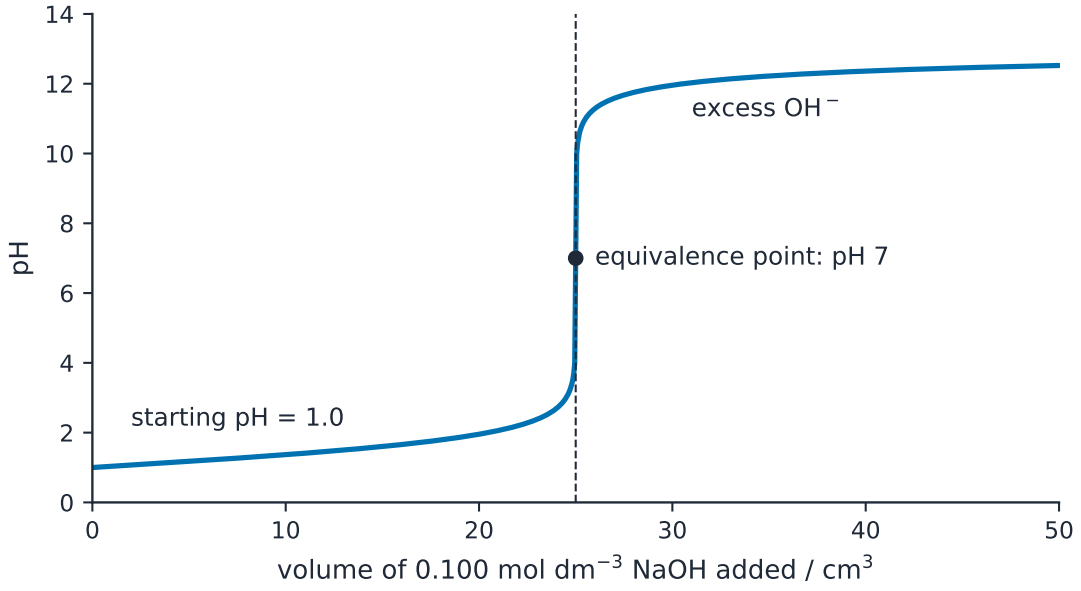
Neutralization is exothermic. Other reactions of acids:

- with a metal carbonate or hydrogencarbonate: salt, water and carbon dioxide;
- with a reactive metal: salt and hydrogen;
- with a metal oxide or hydroxide: salt and water.

The pH curve of a strong acid and a strong base

A **pH curve** shows how the pH changes as one solution is added to another in a titration.

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The pH changes very little until almost all the acid is used up, then jumps by several units

- The **equivalence point** is where the amounts of acid and base match the equation. For a strong acid and strong base it is at pH 7.
- Near the equivalence point one drop of alkali changes the pH by several units. This steep section is why an indicator can show the end point sharply.
- The starting pH comes from the acid concentration, and the final pH approaches the pH of the alkali.

AHL: pOH, K_a and K_b

pOH

The same logarithm works for hydroxide ions:

$$\text{pOH} = -\log_{10}[\text{OH}^-] \qquad \text{pH} + \text{pOH} = 14.00 \text{ at } 298 \text{ K}$$

So for 0.010 mol dm^{-3} NaOH, pOH = 2.00 and pH = 12.00.

Acid and base dissociation constants

The extent of ionization of a weak acid is measured by its **acid dissociation constant**, K_a:

$$\text{HA} \rightleftharpoons \text{H}^+ + \text{A}^- \qquad K_a = \frac{[\text{H}^+][\text{A}^-]}{[\text{HA}]}$$

For a weak base, $\text{B} + \text{H}_2\text{O} \rightleftharpoons \text{BH}^+ + \text{OH}^-$:

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$$K_b = \frac{[\mathrm{BH^+}][\mathrm{OH^-}]}{[\mathrm{B}]}$$

As with pH, $\mathrm{p}K_a = -\log K_a$ and $\mathrm{p}K_b = -\log K_b$. A **larger** K_a (smaller $\mathrm{p}K_a$) means a **stronger** acid.

For a conjugate pair, $K_a \times K_b = K_w$, so $\mathrm{p}K_a + \mathrm{p}K_b = 14.00$ at 298 K. Ethanoic acid has $\mathrm{p}K_a = 4.76$, so the ethanoate ion has $\mathrm{p}K_b = 9.24$.

■ pH of a weak acid

Assume that only a little of the acid ionizes, so [HA] at equilibrium is about the starting concentration, and that $[\mathrm{H^+}] = [\mathrm{A^-}]$.

Worked example: the pH of 0.100 mol $\mathrm{dm^{-3}}$ ethanoic acid, $K_a = 1.74 \times 10^{-5}$.

- $K_a = \dfrac{x^2}{0.100}$, so $x^2 = 1.74 \times 10^{-6}$.
- $x = [\mathrm{H^+}] = 1.32 \times 10^{-3}$ mol $\mathrm{dm^{-3}}$.
- $\mathrm{pH} = -\log(1.32 \times 10^{-3}) = 2.88$.

The assumption holds because only 1.3% of the acid has ionized. The same method gives $[\mathrm{OH^-}]$ for a weak base from K_b.

■ Working backwards to K_a

A 0.0500 mol $\mathrm{dm^{-3}}$ solution of a weak acid has pH 3.10. Then $[\mathrm{H^+}] = 10^{-3.10} = 7.94 \times 10^{-4}$, and

$$K_a = \frac{(7.94 \times 10^{-4})^2}{0.0500} = 1.26 \times 10^{-5}, \qquad \mathrm{p}K_a = 4.90$$

AHL: Salts, pH curves and indicators

■ The pH of salt solutions

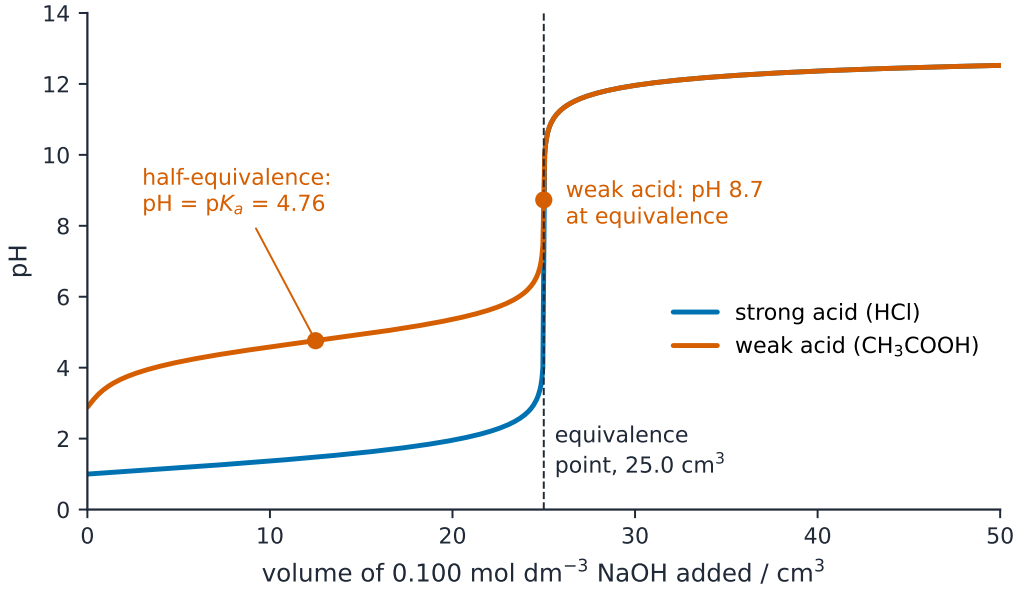
A salt solution is not always neutral. The ion from the weak partner reacts with water.

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Salt made from	Example	Solution
strong acid + strong base	NaCl	neutral, pH 7
weak acid + strong base	CH_3COONa	alkaline: $CH_3COO^- + H_2O \rightleftharpoons CH_3COOH + OH^-$
strong acid + weak base	NH_4Cl	acidic: $NH_4^+ \rightleftharpoons NH_3 + H^+$

Highly charged small metal ions also give acidic solutions. In $[Fe(H_2O)_6]^{3+}$ the Fe^{3+} ion pulls electron density from the water ligands, so a proton is released: iron(III) and aluminium salts are acidic.

■ pH curves with weak acids and bases



For a weak acid, pH = pKa exactly halfway to equivalence

Points to read from a pH curve:

- The **starting pH** is higher for a weak acid of the same concentration.

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- The **equivalence point** is above 7 for a weak acid with a strong base (the salt is alkaline), below 7 for a strong acid with a weak base, and at 7 only for strong with strong. A weak acid with a weak base has no sharp jump.
- At the **half-equivalence point** half the acid has become A^-, so $[HA] = [A^-]$ and $K_a = [H^+]$: $\mathbf{pH} = \mathbf{p}K_a$. This is how K_a is measured.
- The gently sloping region before equivalence is a buffer region.

Choosing an indicator

An acid–base **indicator** is a weak acid, HIn, whose molecule and conjugate base have different colours:

$$HIn(aq) \rightleftharpoons H^+(aq) + In^-(aq)$$

The colour changes over about two pH units centred on its pK_a (the end point is where $[HIn] = [In^-]$). Choose an indicator whose range lies **within the steep part** of the pH curve.

Indicator	pK_a	Colour change (acid → alkali)	Range	Use for
methyl orange	3.7	red → yellow	3.1–4.4	strong acid + weak base
bromothymol blue	7.0	yellow → blue	6.0–7.6	strong acid + strong base
phenolphthalein	9.6	colourless → pink	8.3–10.0	weak acid + strong base

For strong acid and strong base the jump is so long (pH 3 to 11) that any of the three works.

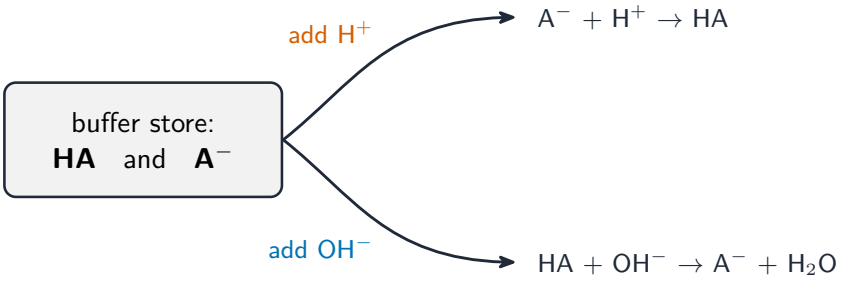
AHL: Buffer solutions

What a buffer does

A **buffer solution** resists a change in pH when small amounts of acid or alkali are added. Blood is buffered at pH 7.4; a change of only 0.3 units can be fatal.

A buffer contains a weak acid and its conjugate base (or a weak base and its conjugate acid), both in large amounts. For example: ethanoic acid with sodium ethanoate, or ammonia with ammonium chloride.

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either way, the pH barely changes

The large reserves of HA and A^- remove added H^+ or OH^-

- Add a little acid: $CH_3COO^- + H^+ \rightarrow CH_3COOH$.
- Add a little alkali: $CH_3COOH + OH^- \rightarrow CH_3COO^- + H_2O$.

Because both reserves are large, the ratio $[A^-]/[HA]$ hardly changes, and so the pH hardly changes.

A buffer can also be made by part-neutralizing a weak acid with a strong base: adding 12.5 cm^3 of NaOH to 25.0 cm^3 of ethanoic acid in the pH curve above gives equal amounts of HA and A^-.

The pH of a buffer

Rearranging K_a and taking logarithms:

$$\text{pH} = \text{p}K_a + \log_{10}\frac{[A^-]}{[HA]}$$

- When $[A^-] = [HA]$, $\text{pH} = \text{p}K_a$.
- To make a buffer of a chosen pH, pick an acid with $\text{p}K_a$ close to that pH and adjust the ratio.
- **Diluting** a buffer with water does not change its pH, because the ratio stays the same; it does reduce the **buffer capacity**, the amount of acid or alkali it can absorb.

Worked example: a buffer contains 0.20 mol dm^{-3} CH_3COOH and 0.10 mol dm^{-3} CH_3COONa ($\text{p}K_a = 4.76$).

$$\text{pH} = 4.76 + \log\frac{0.10}{0.20} = 4.76 - 0.30 = 4.46$$

Practice

1. Identify the two conjugate acid–base pairs in $HNO_3 + H_2O \rightarrow NO_3^- + H_3O^+$.
2. Write equations to show that HCO_3^- is amphiprotic.
3. Calculate the pH of: (a) 0.0025 mol dm^{-3} HCl, (b) 0.050 mol dm^{-3} KOH.
4. A solution has pH 4.70. Calculate $[H^+]$ and $[OH^-]$.
5. Describe two experiments that distinguish 0.10 mol dm^{-3} solutions of a strong and a weak acid, with the expected results.
6. Explain why pure water at 60 °C has a pH below 7 but is still neutral.
7. Sketch the pH curve when 0.100 mol dm^{-3} NaOH is added to 20.0 cm^3 of 0.100 mol dm^{-3} HCl, marking the start pH and the equivalence point.
8. **AHL.** Calculate the pH of 0.050 mol dm^{-3} methanoic acid, p$K_a = 3.75$.
9. **AHL.** The pK_b of ammonia is 4.75. Calculate pK_a of the ammonium ion, and the pH of 0.10 mol dm^{-3} ammonia.
10. **AHL.** Predict whether solutions of (a) KNO_3, (b) Na_2CO_3, (c) NH_4NO_3 are acidic, neutral or alkaline, and explain one of them with an equation.
11. **AHL.** Choose an indicator for titrating ethanoic acid with sodium hydroxide, and explain your choice.
12. **AHL.** Calculate the pH of a buffer made from 0.050 mol NH_3 and 0.10 mol NH_4Cl in 1.0 dm^3 of solution (pK_a of $NH_4^+ = 9.25$). Explain how it resists a small addition of acid.

Answers.

1. HNO_3 (acid) and NO_3^- (conjugate base); H_3O^+ (acid) and H_2O (conjugate base).
2. As an acid: $HCO_3^- + H_2O \rightleftharpoons CO_3^{2-} + H_3O^+$. As a base: $HCO_3^- + H_3O^+ \rightleftharpoons H_2CO_3 + H_2O$.
3. (a) pH $= -\log(0.0025) = 2.60$. (b) $[H^+] = 1.00 \times 10^{-14}/0.050 = 2.0 \times 10^{-13}$, pH $= 12.70$.
4. $[H^+] = 10^{-4.70} = 2.0 \times 10^{-5}$ mol dm^{-3}; $[OH^-] = 1.00 \times 10^{-14}/2.0 \times 10^{-5} = 5.0 \times 10^{-10}$ mol dm^{-3}.
5. Any two: measure the pH (strong about 1, weak about 3); measure the conductivity (strong much higher); add magnesium ribbon or calcium carbonate (strong bubbles faster). Use the same concentration, volume and temperature.
6. Ionization of water is endothermic, so at higher temperature the equilibrium shifts right and $[H^+]$ rises above 10^{-7}, giving pH below 7. But $[H^+] = [OH^-]$ still, so the water is neutral.
7. Start at pH 1.0; slow rise; vertical jump from about pH 3 to 11 at 20.0 cm^3 with the equivalence point at pH 7; then levelling off near pH 12–13.
8. **AHL.** $K_a = 10^{-3.75} = 1.78 \times 10^{-4}$. $x^2 = 1.78 \times 10^{-4} \times 0.050 = 8.9 \times 10^{-6}$, $x = 2.98 \times 10^{-3}$, pH $= 2.53$.

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9. **AHL.** $pK_a = 14.00 - 4.75 = 9.25$. $K_b = 10^{-4.75} = 1.78 \times 10^{-5}$; $[OH^-]^2 = 1.78 \times 10^{-6}$, $[OH^-] = 1.33 \times 10^{-3}$, pOH = 2.88, pH = 11.12.
10. **AHL.** (a) neutral (strong acid, strong base). (b) alkaline: $CO_3^{2-} + H_2O \rightleftharpoons HCO_3^- + OH^-$. (c) acidic: $NH_4^+ \rightleftharpoons NH_3 + H^+$.
11. **AHL.** Phenolphthalein. The equivalence point is about pH 8.7 and the steep section runs from about pH 7 to 11; phenolphthalein changes colour between 8.3 and 10.0, inside this range. Methyl orange would change far too early.
12. **AHL.** $pH = 9.25 + \log(0.050/0.10) = 9.25 - 0.30 = 8.95$. Added H^+ reacts with the large reserve of ammonia, $NH_3 + H^+ \rightarrow NH_4^+$, so the ratio $[NH_3]/[NH_4^+]$ and the pH change very little.

Exam tips

- Define acids and bases as proton **donors** and **acceptors**; a base needs a **lone pair**.
- Conjugate pairs differ by exactly **one** H^+; always pair each acid with its own conjugate base.
- Give pH to as many **decimal places** as $[H^+]$ has significant figures.
- Compare strong and weak acids at the **same concentration**; never use "strong" to mean "concentrated".
- Neutral means $[H^+] = [OH^-]$, which is pH 7 only at 298 K.
- **AHL.** For a weak acid, state the assumptions: $[H^+] = [A^-]$ and [HA] is about the starting concentration.
- **AHL.** At half-equivalence, $pH = pK_a$. Choose an indicator whose range lies within the **steep** part of the curve.
- **AHL.** Explain buffer action with an **equation** for each addition, and say that the ratio of the reserves barely changes.

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Electron transfer reactions

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 3.2, Electron transfer reactions, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: ions and ionic formulas from Structure 2.1, alcohols and other functional groups from Structure 3.2, and amounts in moles from Structure 1.4. At Higher Level you will also use Gibbs energy from Reactivity 1.4 and data booklet values of $E^{\ominus}$.

Oxidation and reduction

What do rusting, batteries and breathalysers share?

An iron nail rusts, a phone battery powers a screen, and a breath test turns orange dichromate green. Each one moves electrons from one substance to another. These are **redox** reactions: **red**uction and **ox**idation always happen together.

Electrons and oxidation states

- **Oxidation** is loss of electrons, or an increase in oxidation state.
- **Reduction** is gain of electrons, or a decrease in oxidation state.

A memory aid: OIL RIG, "oxidation is loss, reduction is gain" of electrons.

The **oxidation state** of an atom is the charge it would have if all its bonds were ionic. Use these rules in order:

1. An element on its own is 0 (Fe, O_2, Cl_2).
2. A simple ion has its charge (Na^+ is $+1$, O^{2-} is -2).
3. The oxidation states in a compound add up to 0; in an ion they add up to the charge.
4. F is always -1. O is usually -2 (but -1 in peroxides). H is usually $+1$ (but -1 in metal hydrides such as NaH).

Worked example. Find the oxidation state of Mn in MnO_4^- and of Cr in $Cr_2O_7^{2-}$.

- MnO_4^-: $x + 4(-2) = -1$, so $x = +7$.
- $Cr_2O_7^{2-}$: $2x + 7(-2) = -2$, so $2x = +12$ and $x = +6$.

Oxidation states are written with the sign first (+7), and they appear in names as Roman numerals: manganate(VII), dichromate(VI), iron(III) chloride.

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Oxidizing and reducing agents

- An **oxidizing agent** oxidizes another substance, so it is itself reduced. It gains electrons.
- A **reducing agent** reduces another substance, so it is itself oxidized. It loses electrons.

In $Zn + Cu^{2+} \rightarrow Zn^{2+} + Cu$, zinc is oxidized (0 to +2) and is the reducing agent; Cu^{2+} is reduced (+2 to 0) and is the oxidizing agent.

Half-equations

Splitting a redox reaction

A **half-equation** shows the oxidation or the reduction on its own, with the electrons written in.

$$Zn \rightarrow Zn^{2+} + 2e^- \qquad \text{(oxidation)}$$

$$Cu^{2+} + 2e^- \rightarrow Cu \qquad \text{(reduction)}$$

Balancing half-equations in acid

For ions such as MnO_4^-, balance in this order:

1. Balance the atoms other than O and H.
2. Add H_2O to balance O.
3. Add H^+ to balance H.
4. Add electrons to balance the charge.

Worked example. MnO_4^- is reduced to Mn^{2+} in acid.

1. Mn is balanced.
2. Four O on the left, so add $4H_2O$ on the right.
3. Eight H on the right, so add $8H^+$ on the left.
4. Charge on the left: $-1 + 8 = +7$. On the right: +2. Add $5e^-$ on the left.

$$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$$

Combining half-equations

Multiply the half-equations so the electrons lost equal the electrons gained, then add them and cancel. With iron(II), $Fe^{2+} \rightarrow Fe^{3+} + e^-$, multiply by 5:

$$MnO_4^- + 8H^+ + 5Fe^{2+} \rightarrow Mn^{2+} + 5Fe^{3+} + 4H_2O$$

Check: the charges are equal on both sides (+17 and +17).

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The activity series

Which metal gives up electrons more easily?

Metals react by losing electrons, so a more reactive metal is a stronger reducing agent. The **activity series** lists metals in order:

K > Na > Li > Ca > Mg > Al > Zn > Fe > Pb > (H) > Cu > Ag > Au

A metal displaces a less active metal from a solution of its ions. In this **displacement** reaction the more active metal is oxidized:

$$Zn(s) + CuSO_4(aq) \rightarrow ZnSO_4(aq) + Cu(s)$$

The blue colour fades and a brown-pink coating of copper forms on the zinc. Copper does not react with zinc sulfate solution.

Halogens

Halogens react by gaining electrons, so they are oxidizing agents. Their strength falls down the group: $Cl_2 > Br_2 > I_2$. A halogen displaces a less reactive halogen from its halide ions:

$$Cl_2(aq) + 2Br^-(aq) \rightarrow 2Cl^-(aq) + Br_2(aq)$$

The colourless solution turns orange-yellow.

Metals and acids

Metals above hydrogen in the series react with dilute acids to give a salt and hydrogen. The metal is oxidized and H^+ is reduced:

$$Mg(s) + 2H^+(aq) \rightarrow Mg^{2+}(aq) + H_2(g)$$

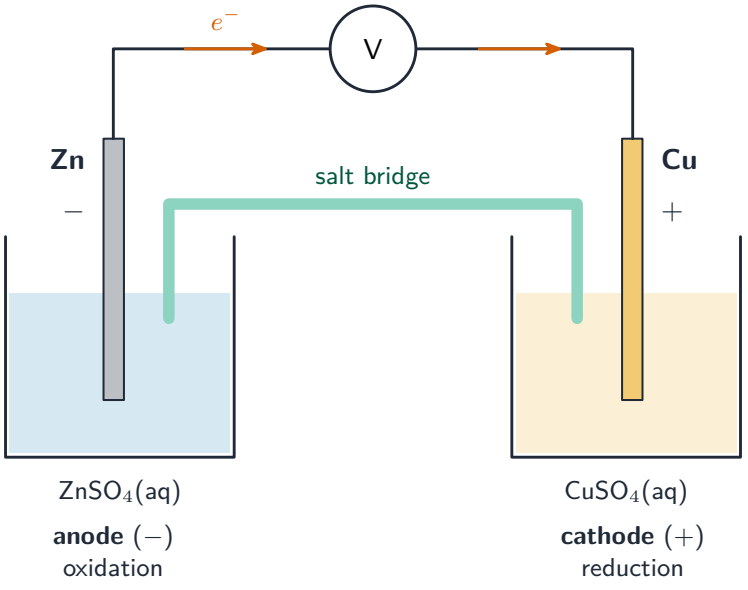
Metals below hydrogen, such as copper and silver, do not react with dilute HCl or H_2SO_4.

Primary and secondary cells

Turning a redox reaction into a current

If zinc sits in copper(II) sulfate solution, electrons pass straight from Zn to Cu^{2+} and the energy is lost as heat. A **primary cell** (also called a voltaic cell) keeps the two half-reactions apart, so the electrons must flow through a wire. Chemical energy becomes electrical energy.

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Electrons flow through the wire from the anode to the cathode

- At the **anode**, oxidation happens: $Zn \rightarrow Zn^{2+} + 2e^-$. In a primary cell the anode is the negative electrode.
- At the **cathode**, reduction happens: $Cu^{2+} + 2e^- \rightarrow Cu$. In a primary cell the cathode is the positive electrode.
- Electrons flow through the external wire from anode to cathode.
- The **salt bridge**, for example filter paper soaked in $KNO_3(aq)$, lets ions move between the solutions. Without it, charge builds up and the current stops. Negative ions move towards the anode and positive ions towards the cathode.

The more active metal is always the anode. A larger gap in the activity series gives a larger voltage.

Secondary cells

A **secondary cell** is rechargeable. When it discharges, it works as a primary cell. To recharge it, an external supply pushes current the other way and reverses the reactions.

Cell	Used in	Note
lead–acid	cars	heavy; lead and sulfuric acid are toxic
lithium-ion	phones, laptops, electric cars	light, stores a lot of energy; Li^+ ions move between the electrodes
nickel–metal hydride	rechargeable AA cells	less energy than lithium-ion, but safer

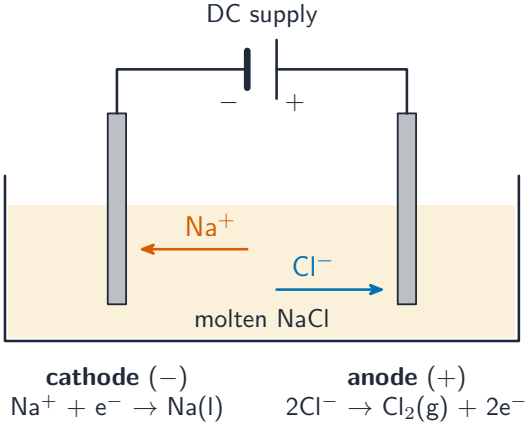
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A **fuel cell** is different: it is fed continuously with fuel (such as hydrogen) and oxygen, so it is not recharged. Its only product with hydrogen is water.

Electrolytic cells

Using electricity to force a reaction

An **electrolytic cell** uses electrical energy to drive a redox reaction that would not happen on its own. This is **electrolysis**. The **electrolyte** must be molten or dissolved, so its ions can move.



In electrolysis the cathode is negative and the anode positive

The names follow the same rule as in every cell: oxidation at the anode, reduction at the cathode. But the signs are reversed: in an electrolytic cell the cathode is negative because the power supply pushes electrons onto it.

For molten sodium chloride:

$$\text{cathode } (-): \quad \mathrm{Na^+ + e^- \rightarrow Na(l)}$$

$$\text{anode } (+): \quad \mathrm{2Cl^- \rightarrow Cl_2(g) + 2e^-}$$

Molten lead(II) bromide gives lead at the cathode and brown bromine vapour at the anode.

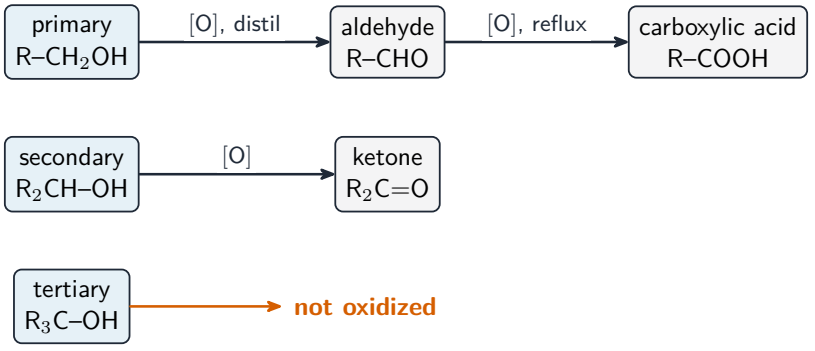
	Primary cell	**Electrolytic cell**
Energy change	chemical → electrical	electrical → chemical
Reaction	spontaneous	not spontaneous
Anode	negative, oxidation	positive, oxidation
Cathode	positive, reduction	negative, reduction

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Redox in organic chemistry

Oxidation of alcohols

The usual oxidizing agent is acidified potassium dichromate(VI). It changes from orange ($Cr_2O_7^{2-}$) to green (Cr^{3+}) as it oxidizes the alcohol. In equations we write [O] for the oxygen it supplies.



What an alcohol oxidizes to depends on its class

- A primary alcohol gives an aldehyde. To stop there, **distillation** removes the aldehyde as soon as it forms: $CH_3CH_2OH + [O] \rightarrow CH_3CHO + H_2O$.
- Heating under **reflux** keeps the aldehyde in the flask, so it is oxidized further to a carboxylic acid: $CH_3CH_2OH + 2[O] \rightarrow CH_3COOH + H_2O$.
- A secondary alcohol gives a ketone: propan-2-ol gives propanone.
- A tertiary alcohol has no H atom on the C–OH carbon, so it is not oxidized. The dichromate stays orange.

Reduction of carbonyl compounds

Reducing agents add hydrogen, written [H]:

- A carboxylic acid is reduced to a primary alcohol by lithium aluminium hydride, $LiAlH_4$, in dry ether. The aldehyde forms on the way but cannot be isolated.
- An aldehyde is reduced to a primary alcohol, and a ketone to a secondary alcohol, by sodium borohydride, $NaBH_4$, or by $LiAlH_4$.

$$CH_3COCH_3 + 2[H] \rightarrow CH_3CH(OH)CH_3$$

Hydrogenation

Hydrogenation adds hydrogen across a C=C or C≡C bond, with a nickel catalyst at about 150 °C (or Pt or Pd at room temperature). An alkyne gives an alkene and then an alkane:

$$C_2H_2 + H_2 \rightarrow C_2H_4 \qquad C_2H_4 + H_2 \rightarrow C_2H_6$$

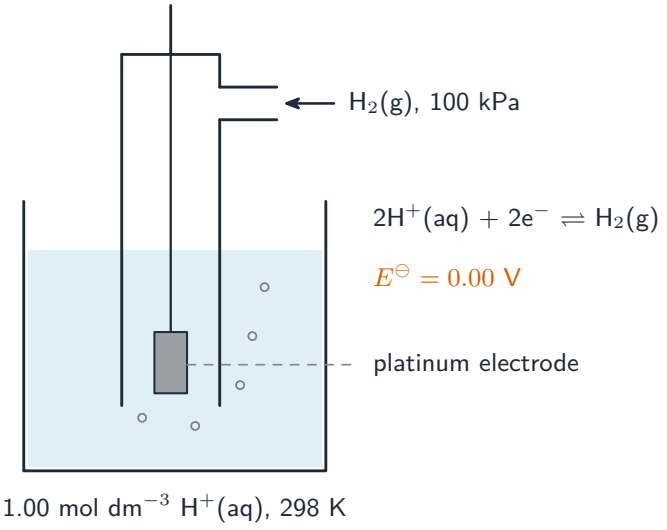
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Hydrogenation of vegetable oils makes them more saturated and harder, for margarine.

AHL: Electrode potentials

The standard hydrogen electrode

We cannot measure the potential of one half-cell on its own, only the difference between two. So every half-cell is measured against one reference: the **standard hydrogen electrode** , which is defined as 0.00 V.

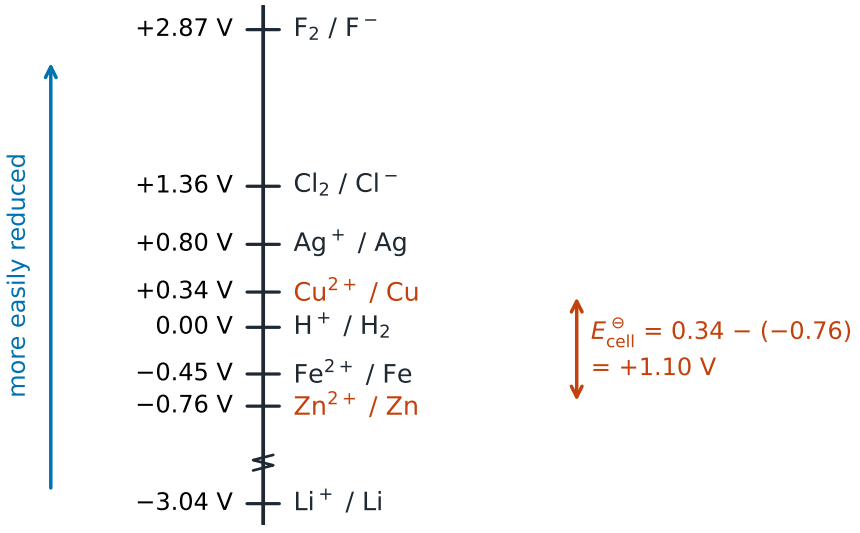


The reference half-cell: hydrogen gas over platinum in 1.00 mol dm^{-3} acid

The **standard electrode potential** , $E^\ominus$, of a half-cell is the voltage it gives when joined to the standard hydrogen electrode under standard conditions: 298 K, 100 kPa and 1.00 mol dm^{-3} for every solution. Values are listed as reductions, in the data booklet.

Reading the series

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The more positive $E^\ominus$, the more easily the oxidized form is reduced

- A more positive $E^\ominus$ means the oxidized form (left side) gains electrons more easily: it is a stronger oxidizing agent. F_2 is the strongest.
- A more negative $E^\ominus$ means the reduced form (right side) loses electrons more easily: it is a stronger reducing agent. Li is the strongest.

Cell potentials

In a cell, the half-cell with the more positive $E^\ominus$ is reduced (the cathode). The **cell potential** is:

$$E^\ominus_{\text{cell}} = E^\ominus_{\text{cathode}} - E^\ominus_{\text{anode}}$$

For the Zn/Cu cell: $E^\ominus_{\text{cell}} = +0.34 - (-0.76) = +1.10$ V.

A reaction is **spontaneous** under standard conditions if $E^\ominus_{\text{cell}}$ is positive. Do not multiply $E^\ominus$ values when you multiply a half-equation: they do not depend on the amount.

> **Worked example.** Will Cl_2 oxidize Fe^{2+} to Fe^{3+}? $E^\ominus(Cl_2/Cl^-) = +1.36$ V and $E^\ominus(Fe^{3+}/Fe^{2+}) = +0.77$ V.

1. Cl_2 is reduced (cathode), Fe^{2+} is oxidized (anode).
2. $E^\ominus_{\text{cell}} = 1.36 - 0.77 = +0.59$ V.
3. Positive, so yes: $Cl_2 + 2Fe^{2+} \rightarrow 2Cl^- + 2Fe^{3+}$.

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Linking $E^\ominus$ and $\Delta G^\ominus$

$$\Delta G^\ominus = -nFE^\ominus_{\text{cell}}$$

Here n is the number of moles of electrons transferred in the equation and F is the **Faraday constant**, 9.65×10^4 C mol^{-1}. A positive $E^\ominus_{\text{cell}}$ gives a negative $\Delta G^\ominus$: both mean the reaction is spontaneous.

For the Zn/Cu cell, $n = 2$: $\Delta G^\ominus = -2 \times 96\,500 \times 1.10 = -2.12 \times 10^5$ J mol^{-1} $= -212$ kJ mol^{-1}.

AHL: Electrolysis of aqueous solutions

Water competes

In an aqueous solution, water can also be oxidized or reduced:

$$\text{cathode: } 2H_2O + 2e^- \rightarrow H_2 + 2OH^- \qquad E^\ominus = -0.83 \text{ V}$$

$$\text{anode: } 2H_2O \rightarrow O_2 + 4H^+ + 4e^- \qquad E^\ominus = +1.23 \text{ V (for the reduction)}$$

- At the cathode, the species with the more positive $E^\ominus$ is reduced. Cu^{2+} (+0.34 V) and Ag^+ (+0.80 V) are reduced to metal. Na^+ (−2.71 V) and K^+ are not: hydrogen forms instead.
- At the anode, water usually gives oxygen. But a concentrated chloride solution gives chlorine, because a high $[Cl^-]$ makes its oxidation easier.

Electrolyte (inert electrodes)	Cathode	Anode
concentrated NaCl(aq)	H_2	Cl_2
dilute NaCl(aq)	H_2	mainly O_2
$CuSO_4$(aq)	Cu	O_2
dilute H_2SO_4(aq)	H_2	O_2

An **inert electrode**, such as platinum or graphite, does not take part in the reaction.

Electroplating

In **electroplating** a thin layer of metal is put on an object by electrolysis.

- The object is the cathode: $Cu^{2+} + 2e^- \rightarrow Cu$.
- The anode is the plating metal, which dissolves: $Cu \rightarrow Cu^{2+} + 2e^-$.
- The electrolyte contains ions of the plating metal, such as $CuSO_4$(aq). Copper ions are made at the anode as fast as they are used at the cathode, so the blue colour stays the same.

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Practice

1. Give the oxidation state of: (a) S in H_2SO_4 (b) N in NH_4^+ (c) Cl in ClO_3^- (d) O in H_2O_2.
2. In $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$, identify the oxidizing agent and the reducing agent, with oxidation states.
3. Balance the half-equation for $Cr_2O_7^{2-}$ being reduced to Cr^{3+} in acid.
4. Combine your answer to 3 with $Fe^{2+} \rightarrow Fe^{3+} + e^-$ to give the overall equation.
5. Predict whether a reaction happens, and write an ionic equation if it does: (a) Mg + $FeSO_4$(aq) (b) Cu + $ZnSO_4$(aq) (c) Br_2(aq) + KI(aq).
6. A cell is made from Mg in $MgSO_4$(aq) and Cu in $CuSO_4$(aq). Identify the anode and the cathode, write the half-equations and state the direction of electron flow.
7. Explain the role of the salt bridge.
8. Compare the electrolysis of molten $PbBr_2$ with the cell in question 6: the energy change, and the signs of the electrodes.
9. Name the product when each is heated with acidified $K_2Cr_2O_7$: (a) propan-1-ol, distilled (b) propan-1-ol, under reflux (c) butan-2-ol (d) 2-methylpropan-2-ol.
10. State the reducing agent and the product when propanone is reduced.
11. **AHL.** Calculate $E^{\ominus}_{\text{cell}}$ for a cell made from Ag^+/Ag (+0.80 V) and Zn^{2+}/Zn (−0.76 V). Write the overall equation.
12. **AHL.** Calculate $\Delta G^{\ominus}$ for the cell in question 11.
13. **AHL.** Use $E^{\ominus}$ values to decide whether I_2 (+0.54 V) can oxidize Fe^{2+} to Fe^{3+} (+0.77 V).
14. **AHL.** Predict the products at each electrode in the electrolysis of (a) concentrated KCl(aq) (b) $AgNO_3$(aq), with inert electrodes.
15. **AHL.** Describe how to silver-plate a spoon.

Answers.

1. (a) +6 (b) −3 (c) +5 (d) −1.
2. Fe goes from +3 to 0, so Fe_2O_3 is reduced: it is the oxidizing agent. C goes from +2 to +4, so CO is oxidized: it is the reducing agent.
3. $Cr_2O_7^{2-} + 14H^+ + 6e^- \rightarrow 2Cr^{3+} + 7H_2O$.
4. $Cr_2O_7^{2-} + 14H^+ + 6Fe^{2+} \rightarrow 2Cr^{3+} + 6Fe^{3+} + 7H_2O$.
5. (a) Yes: $Mg + Fe^{2+} \rightarrow Mg^{2+} + Fe$. (b) No: Cu is less active than Zn. (c) Yes: $Br_2 + 2I^- \rightarrow 2Br^- + I_2$.
6. Mg is the anode: $Mg \rightarrow Mg^{2+} + 2e^-$. Cu is the cathode: $Cu^{2+} + 2e^- \rightarrow Cu$. Electrons flow through the wire from Mg to Cu.
7. It lets ions move between the half-cells, which keeps each solution neutral and completes the circuit.

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8. Electrolysis turns electrical energy into chemical energy and is not spontaneous; its cathode is negative and its anode positive. The cell in 6 turns chemical energy into electrical energy; its anode is negative and its cathode positive.
9. (a) propanal (b) propanoic acid (c) butanone (d) no reaction.
10. $NaBH_4$ (or $LiAlH_4$); propan-2-ol.
11. **AHL.** $E^{\ominus}_{\text{cell}} = 0.80 - (-0.76) = +1.56$ V. $Zn + 2Ag^+ \rightarrow Zn^{2+} + 2Ag$.
12. **AHL.** $n = 2$: $\Delta G^{\ominus} = -2 \times 96\,500 \times 1.56 = -3.01 \times 10^5$ J mol^{-1} $= -301$ kJ mol^{-1}.
13. **AHL.** I_2 would be reduced: $E^{\ominus}_{\text{cell}} = 0.54 - 0.77 = -0.23$ V. Negative, so no reaction. (The reverse, Fe^{3+} oxidizing I^-, is spontaneous.)
14. **AHL.** (a) H_2 at the cathode, Cl_2 at the anode. (b) Ag at the cathode, O_2 at the anode.
15. **AHL.** Make the spoon the cathode and a piece of silver the anode, in a solution of a silver salt such as $AgNO_3$(aq), and pass a direct current.

Exam tips

- Oxidation is loss of electrons; the oxidizing agent is the one that is reduced.
- Balance half-equations in the order: other atoms, O with H_2O, H with H^+, charge with e^-. Check that the charges balance.
- Oxidation is always at the anode. Only the signs change between primary and electrolytic cells.
- Say "distil" for an aldehyde and "reflux" for a carboxylic acid; name the colour change, orange to green.
- **AHL.** $E^{\ominus}_{\text{cell}} = E^{\ominus}_{\text{cathode}} - E^{\ominus}_{\text{anode}}$; never multiply $E^{\ominus}$ by the coefficients.
- **AHL.** In $\Delta G^{\ominus} = -nFE^{\ominus}$ the answer is in J mol^{-1}; divide by 1000 for kJ.

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Reactivity 3.3 · Electron sharing reactions

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 3.3, Electron sharing reactions, for the course first assessed in 2025. This topic is the same at Standard Level and Higher Level.

Prerequisites: covalent bonds and electronegativity from Structure 2.2, alkanes and structural formulas from Structure 3.2, and bond enthalpies from Reactivity 1.2. You will use bond enthalpy values from the data booklet.

Radicals

Why does sunlight matter?

Methane and chlorine can be mixed in the dark and nothing happens. Put the same mixture in sunlight and it reacts at once. The product is never pure chloromethane: it always contains CH_2Cl_2, $CHCl_3$ and CCl_4 as well. One kind of particle explains all of this: the radical.

What a radical is

- A **free radical** , usually just called a radical, is a particle with an **unpaired electron** .
- We show the unpaired electron with a single dot: Cl•, Br•, •CH_3, •OH.
- A radical can be a single atom, such as Cl•, or a group of atoms, such as the methyl radical •CH_3.

Radicals are very reactive. The unpaired electron "wants" a partner, so a radical reacts with almost any molecule it hits to make a new bond.

Do not confuse a radical with an ion. Cl• has 17 electrons and no charge; the chloride ion Cl^- has 18 electrons and a full outer shell, so it is not a radical.

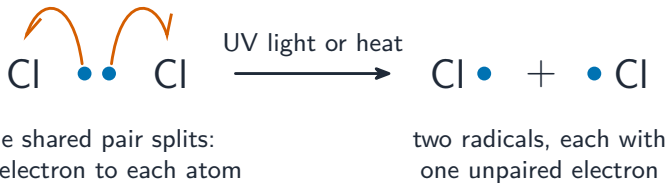
Homolytic fission

Breaking a bond evenly

A covalent bond is a shared pair of electrons. When the bond breaks so that each atom keeps one electron of the pair, the break is called **homolytic fission** . It always makes two radicals.

$$Cl_2 \rightarrow Cl\bullet + Cl\bullet$$

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In homolytic fission each atom takes one electron of the shared pair

A **single-barbed arrow** (also called a fishhook arrow) shows the movement of ONE electron. A normal double-barbed arrow shows a PAIR of electrons; you will use it in Reactivity 3.4.

■ What supplies the energy?

Breaking a bond is endothermic, so homolytic fission needs energy from **ultraviolet light** or from heat. The halogens split most easily because their bonds are weak:

Bond	Bond enthalpy / kJ mol^{-1}
Br–Br	193
Cl–Cl	242
C–C	346
C–H	414

In a mixture of methane and chlorine, UV light breaks Cl–Cl, not C–H, because Cl–Cl is the weaker bond.

Alkanes and radical substitution

■ Why alkanes are unreactive

Alkanes such as methane do not react with acids, alkalis or most other polar reagents. There are two reasons:

1. **Strong bonds.** C–C (346 kJ mol^{-1}) and C–H (414 kJ mol^{-1}) need a lot of energy to break.
2. **Almost no polarity.** The electronegativities of C (2.6) and H (2.2) are close, so C–H bonds are almost **non-polar** . No part of the molecule attracts a charged reagent.

Alkanes do react in two ways: they burn, and they react with radicals.

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The chain reaction

Methane and chlorine react in UV light by **radical substitution** : a chlorine atom takes the place of a hydrogen atom. It is a **chain reaction** with three stages.

1. initiation $Cl_2 \xrightarrow{UV} 2\,Cl^{\bullet}$

UV light splits the weakest bond, Cl–Cl, into two radicals

2. propagation $CH_4 + Cl^{\bullet} \longrightarrow CH_3^{\bullet} + HCl$

$CH_3^{\bullet} + Cl_2 \longrightarrow CH_3Cl + Cl^{\bullet}$

each step uses a radical and makes a new one, so the chain continues

3. termination $Cl^{\bullet} + Cl^{\bullet} \longrightarrow Cl_2$ $CH_3^{\bullet} + Cl^{\bullet} \longrightarrow CH_3Cl$ $CH_3^{\bullet} + CH_3^{\bullet} \longrightarrow C_2H_6$

two radicals join, so the chain ends

Initiation makes radicals, propagation passes them on, termination removes them

1. **Initiation** : UV light splits chlorine molecules into radicals.

$$Cl_2 \rightarrow 2Cl\bullet$$

2. **Propagation** : each step uses one radical and makes another, so the chain keeps going.

$$CH_4 + Cl\bullet \rightarrow \bullet CH_3 + HCl$$

$$\bullet CH_3 + Cl_2 \rightarrow CH_3Cl + Cl\bullet$$

The Cl• made in the second step starts the first step again. One initiation can lead to thousands of propagation cycles.

3. **Termination** : two radicals join, so the chain stops.

$$Cl\bullet + Cl\bullet \rightarrow Cl_2 \qquad \bullet CH_3 + Cl\bullet \rightarrow CH_3Cl \qquad \bullet CH_3 + \bullet CH_3 \rightarrow C_2H_6$$

The overall equation is the sum of the two propagation steps:

$$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$$

Note that a hydrogen atom, not •H, is taken by the chlorine radical in the first propagation step. The products of propagation are HCl and $\bullet CH_3$, never CH_3Cl and •H.

Counting steps from equations

To decide which stage an equation is:

Radicals on the left	Radicals on the right	Stage
0	2	initiation
1	1	propagation
2	0	termination

A mixture of products

Further substitution

Chloromethane still has C–H bonds, so a Cl• radical can attack it too:

$$CH_3Cl + Cl\bullet \rightarrow \bullet CH_2Cl + HCl$$

$$\bullet CH_2Cl + Cl_2 \rightarrow CH_2Cl_2 + Cl\bullet$$

The same can happen again to give $CHCl_3$ and finally CCl_4. Termination also adds products such as ethane. So radical substitution always gives a **product mixture** (several products together), which must be separated, for example by fractional distillation.

To get more of...	Use...
CH_3Cl	a large excess of methane, so Cl• usually meets CH_4
CCl_4	a large excess of chlorine

Evidence for the chain model

- Nothing happens in the dark, but the reaction starts at once in UV light: radicals must be made first.
- A short burst of light causes a lot of reaction: each radical is passed on many times.
- Traces of ethane appear even though no C–C bond was in the reactants: two $\bullet CH_3$ radicals must have joined.

Larger alkanes

Ethane reacts in the same way:

$$C_2H_6 + Cl\bullet \rightarrow \bullet C_2H_5 + HCl \qquad \bullet C_2H_5 + Cl_2 \rightarrow C_2H_5Cl + Cl\bullet$$

In propane, a chlorine radical can remove a hydrogen atom from an end carbon or from the middle carbon, so two different monochloro products form: 1-chloropropane and 2-chloropropane.

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Bromine reacts in the same way, but more slowly, because the first propagation step is endothermic for bromine.

Energy changes in the chain

Use bond enthalpies to see why the propagation steps run so easily with chlorine.

Bond	C–H	Cl–Cl	H–Cl	C–Cl	H–Br
Bond enthalpy / kJ mol^{-1}	414	242	431	324	366

Worked example. Find ΔH for each propagation step of the chlorination of methane.

1. $CH_4 + Cl\bullet \rightarrow \bullet CH_3 + HCl$: break C–H, form H–Cl. $\Delta H = 414 - 431 = -17$ kJ mol^{-1}.
2. $\bullet CH_3 + Cl_2 \rightarrow CH_3Cl + Cl\bullet$: break Cl–Cl, form C–Cl. $\Delta H = 242 - 324 = -82$ kJ mol^{-1}.
3. Add the two steps: $\Delta H = -99$ kJ mol^{-1} for $CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$.

Both propagation steps are exothermic, so once a few radicals are made the chain runs quickly.

For bromine the first step is $414 - 366 = +48$ kJ mol^{-1}. It is endothermic, so bromination is slower than chlorination.

Radicals in the atmosphere

How CFCs destroy ozone

Chlorofluorocarbons (CFCs), such as CCl_2F_2, were used in fridges and spray cans. They are unreactive near the ground, so they drift up into the **stratosphere** . There, strong UV light breaks the C–Cl bond (324 kJ mol^{-1}), which is weaker than the C–F bond (492 kJ mol^{-1}):

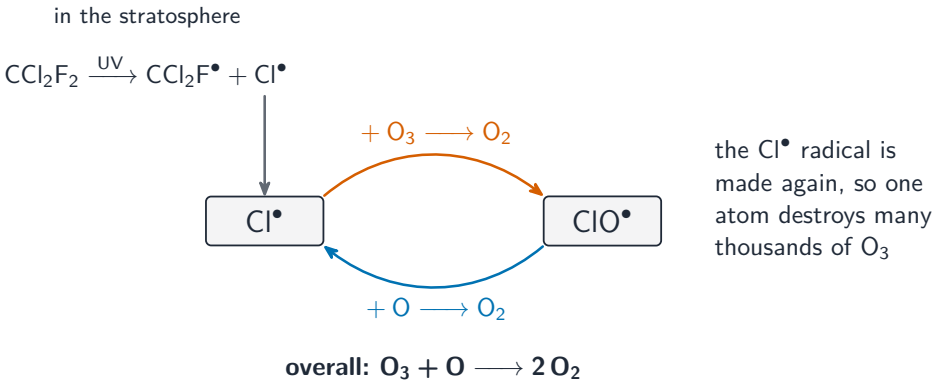
$$CCl_2F_2 \rightarrow \bullet CCl_2F + Cl\bullet$$

The chlorine radical then destroys **ozone** in two propagation steps:

$$Cl\bullet + O_3 \rightarrow ClO\bullet + O_2$$

$$ClO\bullet + O \rightarrow Cl\bullet + O_2$$

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The chlorine radical is made again at the end of each cycle

Overall: $O_3 + O \rightarrow 2O_2$. The chlorine radical is made again, so one Cl atom can destroy many thousands of ozone molecules before a termination step removes it. This is why CFCs were banned by the Montreal Protocol (1987).

Practice

1. Which of these are radicals: Cl^-, Cl•, •CH_3, CH_4, •OH, OH^-? Explain your choice.
2. Write an equation for the homolytic fission of bromine. State the condition needed.
3. Draw single-barbed arrows to show the homolytic fission of the C–Cl bond in CH_3Cl.
4. Give two reasons why alkanes are unreactive with acids and alkalis.
5. Ethane reacts with chlorine in UV light. Write equations for the initiation step, the two propagation steps and a termination step that forms butane.
6. State whether each step is initiation, propagation or termination: (a) •CH_3+Cl• → CH_3Cl (b) $CH_3Cl + Cl\bullet \rightarrow \bullet CH_2Cl + HCl$ (c) $Br_2 \rightarrow 2Br\bullet$.
7. Explain why the reaction of methane with chlorine gives a mixture of products. Suggest how to make chloromethane the main product.
8. Use bond enthalpies (C–H 414, H–Br 366, Br–Br 193, C–Br 285 kJ mol^{-1}) to find ΔH for each propagation step in the bromination of methane, and for the overall reaction.
9. How many different monochloro products form when propane reacts with chlorine in UV light? Name them.
10. Explain, with equations, how one chlorine atom from a CFC can destroy many ozone molecules.

Answers.

1. Cl•, •CH_3 and •OH: each has an unpaired electron. Cl^-, OH^- and CH_4 have all electrons paired.

2. $Br_2 \rightarrow 2Br\bullet$, in UV light (or heat).
3. One single-barbed arrow from the bond to C and one from the bond to Cl, giving $\bullet CH_3 + Cl\bullet$.
4. C–C and C–H bonds are strong; the bonds are almost non-polar, so nothing attracts a charged or polar reagent.
5. $Cl_2 \rightarrow 2Cl\bullet$; $C_2H_6 + Cl\bullet \rightarrow \bullet C_2H_5 + HCl$; $\bullet C_2H_5 + Cl_2 \rightarrow C_2H_5Cl + Cl\bullet$; $2\bullet C_2H_5 \rightarrow C_4H_{10}$.
6. (a) termination (b) propagation (c) initiation.
7. Chloromethane still has C–H bonds, so Cl• substitutes it further to CH_2Cl_2, $CHCl_3$ and CCl_4; termination adds ethane. Use a large excess of methane.
8. Step 1: $414 - 366 = +48$ kJ mol^{-1}. Step 2: $193 - 285 = -92$ kJ mol^{-1}. Overall: -44 kJ mol^{-1}.
9. Two: 1-chloropropane and 2-chloropropane.
10. UV gives Cl• from the CFC; $Cl\bullet + O_3 \rightarrow ClO\bullet + O_2$; $ClO\bullet + O \rightarrow Cl\bullet + O_2$. The Cl• is made again, so the cycle repeats thousands of times until termination.

Exam tips

- Always draw the dot on a radical, and put it on the atom that has the unpaired electron: $\bullet CH_3$, not CH_3.
- In the first propagation step the products are $\bullet CH_3$ and HCl. Writing •H loses the mark.
- A single-barbed arrow moves one electron; a double-barbed arrow moves a pair.
- Termination steps have two radicals on the left and none on the right.
- "Mixture of products" needs a reason: the product still has C–H bonds, and termination joins radicals.

Reactivity 3.4 · Electron-pair sharing reactions

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Reactivity 3.4, Electron-pair sharing reactions, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: covalent and coordination bonds and electronegativity from Structure 2.2, functional groups and classes of compounds from Structure 3.2, and homolytic fission and radicals from Reactivity 3.3. At Higher Level you will also use rate expressions from Reactivity 2.2.

Nucleophiles and electrophiles

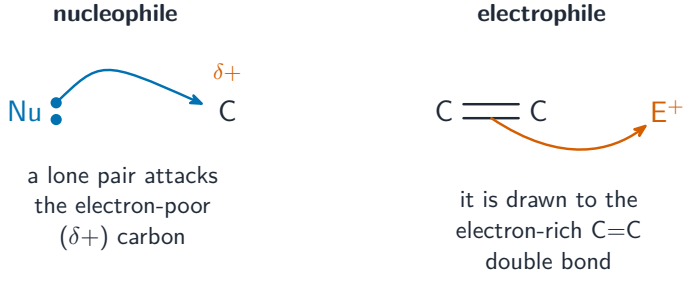
Why does bromoethane react with alkali, but ethane does not?

Shake bromoethane with warm sodium hydroxide solution and ethanol forms. Do the same with ethane and nothing happens. The difference is one polar bond. In Reactivity 3.3 a bond broke so that each atom took one electron. In this unit a whole electron pair moves, and a new bond forms from a pair that one particle gives to another.

Two kinds of reagent

- A **nucleophile** is a reactant that forms a new bond by giving both electrons of the bond. It has a lone pair, and it is neutral or negative: OH^-, H_2O, NH_3, CN^-, Cl^-.
- An **electrophile** is a reactant that forms a new bond by accepting both electrons of the bond. It is positive or has a partial positive charge: H^+, NO_2^+, Br_2 near a C=C bond, the H of HBr.

"Nucleophile" means "nucleus-loving": it is attracted to a positive centre. "Electrophile" means "electron-loving": it is attracted to a region of high electron density.



A nucleophile gives an electron pair; an electrophile takes one

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Heterolytic fission and curly arrows

Breaking a bond unevenly

When a covalent bond breaks and **both** bonding electrons go to one atom, the break is **heterolytic fission** . The atom that takes the pair is usually the more electronegative one. Heterolytic fission makes ions, not radicals.

$$CH_3Br \rightarrow CH_3^+ + Br^-$$

heterolytic fission



both electrons go to Br: a cation and an anion form

homolytic fission



one electron to each atom: two radicals form

A curly arrow moves an electron pair; a single-barbed arrow moves one electron

Drawing curly arrows

A **curly arrow** (with a full, double-barbed head) shows the movement of an electron PAIR.

- The tail starts where the pair is now: a lone pair, a bond, or a negative charge.
- The head points to where the pair goes: an atom (to form a new bond) or an atom that leaves with the pair.
- Every curly arrow must start at electrons. An arrow that starts at a nucleus or a positive charge loses the mark.

Nucleophilic substitution

Halogenoalkanes have a polar bond

In a **halogenoalkane** , such as bromoethane, the halogen is more electronegative than carbon (Br 3.0, C 2.6). The C–Br bond is polar, so the carbon is $\delta+$. A nucleophile attacks this $\delta+$ carbon.

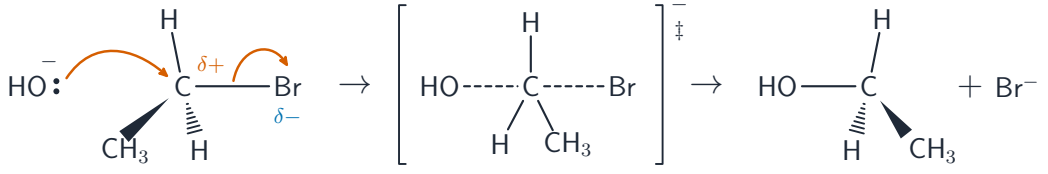
The reaction

In **nucleophilic substitution** , a nucleophile gives an electron pair to form a new bond as another bond breaks. The group that leaves with the old bonding pair is the **leaving group** .

$$CH_3CH_2Br + OH^- \rightarrow CH_3CH_2OH + Br^-$$

Here OH^- is the nucleophile and Br^- is the leaving group. Conditions: warm, with aqueous sodium hydroxide.

S_N2 (primary, e.g. bromoethane): one step



lone pair on O attacks the $\delta+$ C from the side away from Br

transition state: O–C half-formed, C–Br half-broken

ethanol + bromide ion; the three groups have flipped

One curly arrow makes the new O–C bond; a second breaks C–Br

Two curly arrows describe the change:

1. From a lone pair on the O of OH^- to the $\delta+$ carbon: the new C–O bond forms.
2. From the C–Br bond to Br: the bonding pair leaves with Br as Br^-.

Other nucleophiles give other products: water gives an alcohol slowly, and ammonia gives an amine.

Electrophilic addition to alkenes

Why alkenes attract electrophiles

The C=C double bond in an alkene has four electrons between two carbon atoms: a region of high electron density. Electrophiles are attracted to it. In **electrophilic addition** the double bond opens and two new single bonds form, so one molecule adds across the C=C.

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Three additions to learn

Reagent	Conditions	Example with ethene	Product
halogen, Br_2	room temperature	$C_2H_4 + Br_2 \rightarrow CH_2BrCH_2Br$	1,2-dibromoethane
hydrogen halide, HBr	room temperature	$C_2H_4 + HBr \rightarrow CH_3CH_2Br$	bromoethane
water (steam)	H_3PO_4 catalyst, about 300 °C	$C_2H_4 + H_2O \rightarrow CH_3CH_2OH$	ethanol

The reaction with bromine is the test for an alkene: orange bromine water turns colourless. An alkane gives no colour change in the dark.

The addition of steam to ethene is how ethanol is made in industry.

AHL: Lewis acids and bases

A wider definition

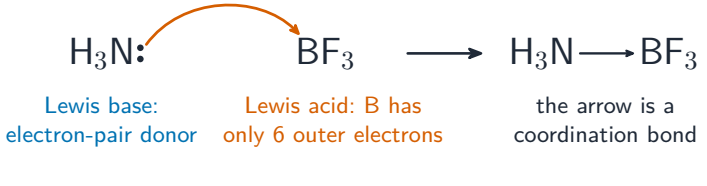
- A **Lewis acid** is an electron-pair acceptor.
- A **Lewis base** is an electron-pair donor.

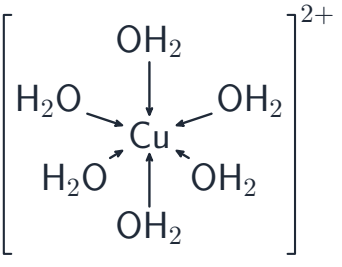
Every Brønsted–Lowry base is a Lewis base: to accept a proton, it gives its lone pair to H^+. But the Lewis definition also covers reactions with no proton at all.

When a Lewis base reacts with a Lewis acid, the bond that forms is a **coordination bond** : both shared electrons come from the same atom.

$$NH_3 + BF_3 \rightarrow H_3N{\rightarrow}BF_3$$

Boron in BF_3 has only six outer electrons, so it can accept a pair.





A Lewis base gives a lone pair; a Lewis acid accepts it

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Complex ions

Transition element ions are Lewis acids. Molecules or ions with a lone pair, called **ligands**, form coordination bonds to the metal ion and give a **complex ion**:

$$Cu^{2+} + 6H_2O \rightarrow [Cu(H_2O)_6]^{2+}$$

Water, ammonia, Cl^- and CN^- are common ligands. The number of coordination bonds to the metal ion is its **coordination number**; it is 6 here.

Linking the ideas

Nucleophiles are Lewis bases: they give an electron pair. Electrophiles are Lewis acids: they accept one. So all of this unit's mechanisms are Lewis acid–base reactions.

AHL: S_N1 and S_N2 mechanisms

Two routes for nucleophilic substitution

How the halogenoalkane reacts depends on how many carbon atoms are bonded to the carbon that carries the halogen.

Halogenoalkane	Example	Main mechanism
primary: one alkyl group on the C–X carbon	bromoethane	S_N2
secondary: two alkyl groups	2-bromopropane	both
tertiary: three alkyl groups	2-bromo-2-methylpropane	S_N1

S_N2: one step

S_N2 means substitution, nucleophilic, bimolecular. The nucleophile attacks the carbon from the side opposite the halogen while the C–X bond breaks, all in one step (see the bromoethane figure above).

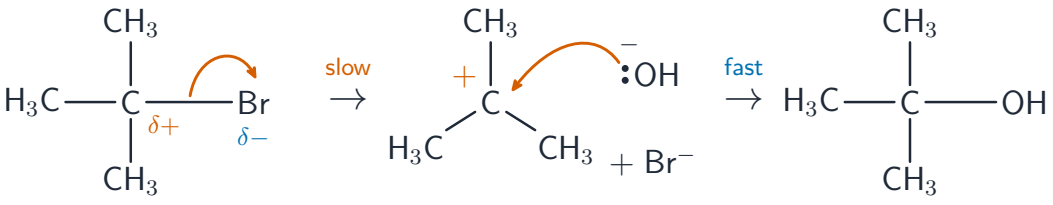
- In the **transition state** the O–C bond is half made and the C–Br bond half broken; the negative charge is spread over both.
- Two particles are in the only step, so rate = $k[RBr][OH^-]$.
- The other three groups flip over, like an umbrella in the wind. If the carbon is a chiral centre, one enantiomer gives the other: S_N2 is **stereospecific**, with **inversion of configuration**.
- Primary halogenoalkanes react this way because the back of the carbon is open to attack.

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S_N1: two steps

S_N1 means substitution, nucleophilic, unimolecular.

S_N1 (tertiary, e.g. 2-bromo-2-methylpropane): two steps



the C–Br bond breaks: both electrons go to Br

tertiary carbocation: three alkyl groups push electrons in and stabilize it

2-methylpropan-2-ol

The slow first step makes a carbocation; the nucleophile then attacks fast

1. Slow: the C–Br bond breaks heterolytically to give a **carbocation** and Br^-.
2. Fast: the nucleophile attacks the positive carbon.

- The slow first step is the **rate-determining step** . Only the halogenoalkane is in it, so rate = k[RBr].
- The carbocation is planar, so the nucleophile can attack from either side. A chiral reactant gives a mixture of both enantiomers.
- Tertiary halogenoalkanes react this way because three alkyl groups push electrons towards the positive carbon and make the carbocation stable enough to form. The bulky groups also block back attack.

The solvent

S_N1 is faster in protic solvents such as water, which have O–H bonds and surround and stabilize both ions formed in step 1. S_N2 is faster in polar aprotic solvents such as propanone, which do not surround the nucleophile so tightly, so it stays reactive.

The leaving group

The rate of substitution depends on the halogen. Iodoalkanes react fastest:

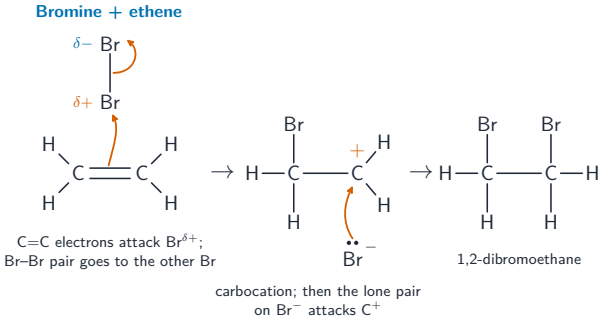
Bond	**C–Cl**	**C–Br**	**C–I**
Bond enthalpy / kJ mol^{-1}	324	285	228
Relative rate	slowest		fastest

C–I is the least polar of the three, so polarity cannot explain the order. Bond strength does: the weakest bond, C–I, breaks most easily, so I^- is the best leaving group.

AHL: Electrophilic addition mechanisms

Bromine and ethene

A Br_2 molecule is non-polar, but the electron-rich C=C bond repels the electrons in Br–Br as it gets close. This induces a dipole: the near Br becomes $\delta+$.



The C=C electrons attack the electrophile; the anion then attacks the carbocation

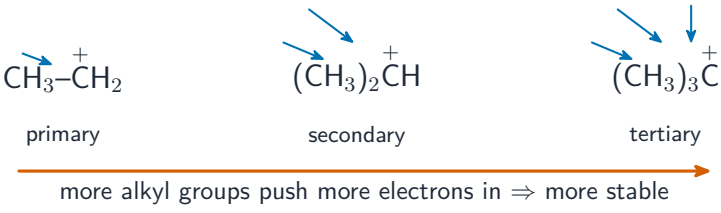
1. A curly arrow from the C=C bond to the $\delta+$ Br; a second from the Br–Br bond to the far Br.
2. A carbocation and Br^- form.
3. A curly arrow from a lone pair on Br^- to the positive carbon gives 1,2-dibromoethane.

HBr reacts in the same way, but it is already polar, with H as $\delta+$.

Unsymmetric alkenes: Markovnikov's rule

When HBr adds to propene, two products are possible: 1-bromopropane and 2-bromopropane. The major product is 2-bromopropane.

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Markovnikov: HBr adds so the *more stable* carbocation forms

More alkyl groups on C^+ make the carbocation more stable

- The H adds to the end carbon so the positive charge is on the middle carbon. That is a secondary carbocation, which is more stable than the primary one.
- Alkyl groups push electron density towards the positive carbon, which spreads out the charge. Stability: tertiary > secondary > primary.
- The more stable carbocation forms faster, so its product is the major product.

Markovnikov's rule says this in short form: the H atom adds to the carbon of the C=C that already has more H atoms.

AHL: Electrophilic substitution of benzene

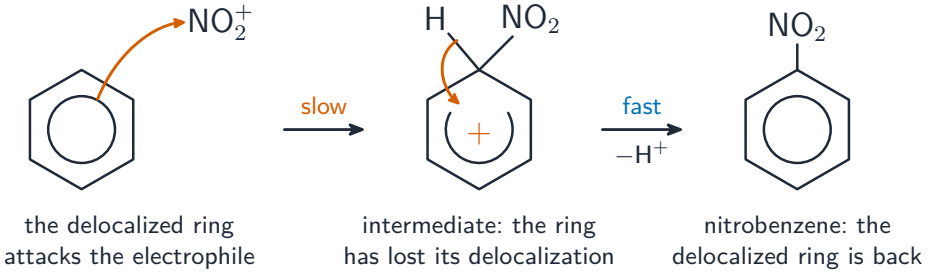
Why benzene substitutes instead of adding

Benzene has six **delocalized** π electrons in a ring above and below the plane. Delocalization makes benzene extra stable. Addition would destroy the ring of delocalized electrons, so benzene reacts by **electrophilic substitution**: an electrophile replaces an H atom and the delocalized ring is kept.

Nitration

Benzene is warmed to about 50 °C with a mixture of concentrated nitric and sulfuric acids. The acids form the electrophile, the **nitronium ion**:

$$HNO_3 + H_2SO_4 \rightarrow NO_2^+ + HSO_4^- + H_2O$$



The ring attacks NO_2^+, then loses H^+ to get its delocalization back

1. A curly arrow from the delocalized ring to the N of NO_2^+. This is slow: the intermediate has lost its delocalization and carries a positive charge, shown by a broken ring (horseshoe) with + inside.
2. A curly arrow from the C–H bond into the ring. H^+ leaves and the delocalized ring is restored. HSO_4^- takes the H^+, so H_2SO_4 is a catalyst.

Overall: $C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$.

Practice

1. Classify each species as a nucleophile or an electrophile: OH^-, NO_2^+, NH_3, H^+, CN^-.
2. Explain the difference between heterolytic and homolytic fission, and say what kind of arrow each uses.
3. Write an equation for the reaction of 1-bromopropane with aqueous sodium hydroxide. Identify the nucleophile and the leaving group.
4. Explain why the carbon atom in the C–Br bond of a halogenoalkane is attacked by nucleophiles.
5. Write equations for the reactions of propene with (a) bromine, (b) steam. Name the organic products.
6. Describe a test to tell cyclohexene from cyclohexane, with the result for each.
7. **AHL.** Explain why BF_3 is a Lewis acid but not a Brønsted–Lowry acid.
8. **AHL.** For $[Fe(H_2O)_6]^{3+}$, identify the ligand, the type of bond to the metal ion and the coordination number.
9. **AHL.** 2-bromo-2-methylpropane reacts with hydroxide ions. Name the mechanism, write the rate expression and explain why this mechanism is preferred.
10. **AHL.** A single enantiomer of 2-bromobutane reacts with OH^- by S_N2. Describe the product.
11. **AHL.** Explain why 1-iodobutane is hydrolysed faster than 1-chlorobutane.
12. **AHL.** Explain why the major product of HBr + propene is 2-bromopropane.
13. **AHL.** Write the equation for the formation of the electrophile in the nitration of benzene, and explain why benzene undergoes substitution rather than addition.

Answers.

1. Nucleophiles: OH^-, NH_3, CN^-. Electrophiles: NO_2^+, H^+.
2. Heterolytic: both bonding electrons go to one atom, giving ions; one curly arrow (double-barbed). Homolytic: one electron to each atom, giving radicals; two single-barbed arrows.
3. $CH_3CH_2CH_2Br + OH^- \rightarrow CH_3CH_2CH_2OH + Br^-$. Nucleophile OH^-; leaving group Br^-.
4. Br is more electronegative than C, so the C–Br bond is polar and C is $\delta+$; the lone pair of a nucleophile is attracted to it.

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5. (a) $CH_3CH{=}CH_2 + Br_2 \rightarrow CH_3CHBrCH_2Br$, 1,2-dibromopropane. (b) $CH_3CH{=}CH_2 + H_2O \rightarrow CH_3CH(OH)CH_3$, propan-2-ol (major; some propan-1-ol).
6. Add bromine water and shake: cyclohexene turns it from orange to colourless; with cyclohexane it stays orange.
7. **AHL.** B in BF_3 has only six outer electrons, so it can accept an electron pair (Lewis acid); it has no H to donate as a proton.
8. **AHL.** Ligand H_2O; coordination bonds from O lone pairs to Fe^{3+}; coordination number 6.
9. **AHL.** S_N1; rate = $k[(CH_3)_3CBr]$. It is tertiary: three alkyl groups stabilize the carbocation, and the bulky groups block back attack.
10. **AHL.** The other enantiomer of butan-2-ol: the nucleophile attacks from the back, so the configuration is inverted.
11. **AHL.** C–I (228 kJ mol^{-1}) is weaker than C–Cl (324 kJ mol^{-1}), so it breaks more easily; I^- is a better leaving group.
12. **AHL.** H adds to the end CH_2 carbon, giving a secondary carbocation, which is more stable than the primary one because two alkyl groups push electrons towards C^+. It forms faster, so 2-bromopropane is the major product.
13. **AHL.** $HNO_3 + H_2SO_4 \rightarrow NO_2^+ + HSO_4^- + H_2O$. Substitution keeps the delocalized π ring and its extra stability; addition would destroy it.

Exam tips

- Every curly arrow starts at a lone pair, a bond or a negative charge, never at an atom's nucleus or a positive charge.
- Show the lone pair on the nucleophile and the $\delta+/\delta-$ on the C–X bond.
- Bromine water decolourized means C=C; say "colourless", not "clear".
- **AHL.** Primary S_N2, rate = $k[RX][Nu^-]$; tertiary S_N1, rate = $k[RX]$.
- **AHL.** The leaving-group order is set by bond strength (C–I weakest), not by polarity.
- **AHL.** In nitration, draw the intermediate with a horseshoe and +, and show H^+ leaving.

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Experimental programme

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches experimental planning, chemical measurement, uncertainty, graph interpretation and evaluation for the IB Chemistry experimental programme. Use these methods throughout supervised practical work. Sections marked **AHL** are for Higher Level only.

Prerequisites: mole and concentration calculations, balanced equations and straight-line graphs. All numerical datasets and investigations below are original, invented teaching examples. They illustrate methods rather than reporting real measurements.

Design a question that measurements can answer

A useful research question specifies the independent variable, dependent variable and chemical system. "How does temperature affect chemistry?" is too broad. "How does initial temperature affect the time for a specified magnesium strip to produce 20 cm^3 of hydrogen in hydrochloric acid of fixed concentration?" identifies quantities that can be measured. Temperature is the independent variable; elapsed time is the dependent variable. For the same collected volume, $1/t$ can compare average rates, but it is not automatically an initial rate.

Identify control variables and explain their effects: acid concentration and volume, magnesium mass and exposed area, apparatus geometry and mixing. "Keep everything the same" gives neither a method nor a reason. Select a range wide enough to reveal a trend while keeping the process measurable and the apparatus within approved limits. A pilot trial can reveal a reaction too fast to time or gas leakage before the full investigation.

Use repeated trials at each condition to estimate scatter and judge reliability. Randomizing the order of conditions can reduce the influence of drift, such as gradual room-temperature change. Repeats at one concentration do not replace a range of concentrations. Continuous variables can take intermediate values; a discrete variable such as the number of identical pieces takes separate countable values.

A risk assessment connects a hazard, exposure route and control: acid splashes → eye/skin exposure → appropriate eye protection and controlled handling; flammable solvent → ignition → suitable heating and removal of flames. Follow the teacher's apparatus limits and disposal instructions. Plan waste minimization and any environmental or ethical issues before collecting data.

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Choose and use measuring equipment

Choose the instrument for the quantity and required precision, not merely the nearest container.

- **Mass:** tare a stable balance; keep the vessel dry and record its displayed precision. Weighing by difference subtracts the final container mass from its initial mass.
- **Volume:** a volumetric pipette delivers one specified volume; a burette delivers a variable volume by subtracting readings; a volumetric flask contains a specified total volume at its mark. A beaker is normally unsuitable for precise concentration preparation.
- **Time, temperature and length:** define the start/finish event, immerse a temperature probe consistently without touching the vessel, and avoid parallax when reading a scale. A fast sensor can still have a calibration offset or response lag.
- **pH:** calibrate an appropriate probe using suitable buffers, rinse between samples and allow stabilization. A pH reading is not a direct measurement of acid concentration for every chemical system.
- **Electrical quantities:** an ammeter measures current in series; a voltmeter measures potential difference in parallel. Choose a suitable range and account for electrode/contact conditions when comparing cells.

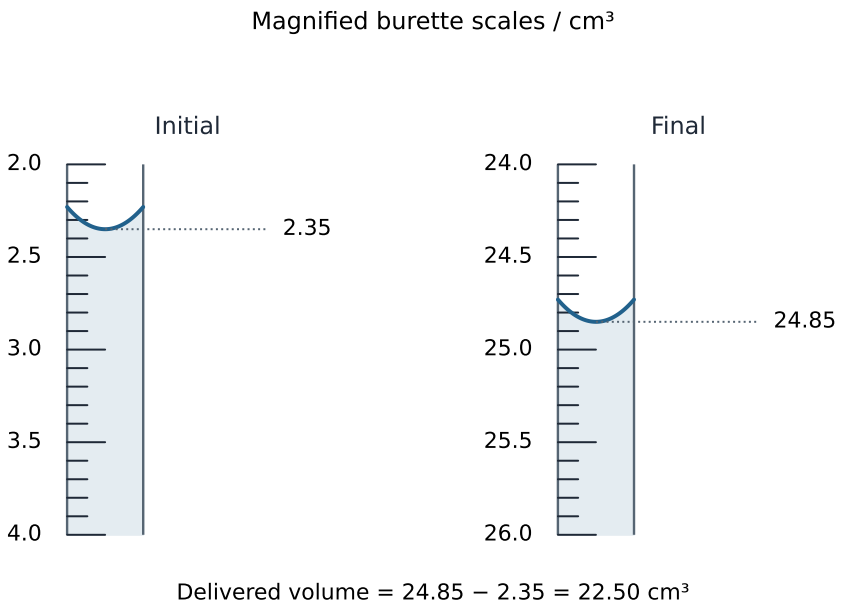
A **systematic error** shifts measurements consistently, for example a calibration offset. Random error produces unpredictable scatter. Repetition can reduce uncertainty in a mean caused by random variation, but it does not remove a shared offset. A gas leak or heat loss may create a directional bias without being a simple constant zero error.

Accuracy concerns agreement with the appropriate reference; precision concerns the spread or resolution of measurements. Closely agreeing repeats can all be inaccurate. A reference comparison must use matching conditions and a trustworthy reference value.

■ Read a burette as a difference

For a clear aqueous solution with a concave meniscus, read the bottom at eye level. Burette values increase downwards. Record initial and final readings to the precision supported by the scale and stated method; do not assume the initial reading is zero. Check that the tip is filled and free of air bubbles before starting.

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Delivered volume = final reading minus initial reading; read the meniscus consistently at eye level.

For the invented readings 2.35 ± 0.05 and 24.85 ± 0.05 cm^3,

$$V = 24.85 - 2.35 = 22.50 \text{ cm}^3,$$

$$u_V = 0.05 + 0.05 = 0.10 \text{ cm}^3.$$

The conservative result is 22.50 ± 0.10 cm^3. The uncertainty values are given for this example; consult the apparatus specification and method rather than assuming every burette has this uncertainty.

Chemical techniques: purpose and critical detail

■ Make a known concentration

A **standard solution** has a reliably known concentration. Calculate the solute amount and mass using $n = cV$ and $m = nM$. Dissolve the solid, transfer it quantitatively into a suitable volumetric flask, rinse the original vessel into the flask, then add solvent to the mark and mix thoroughly. Make the final adjustment at the appropriate temperature. Purity, hydration and the suitability of the solute as a standard matter; an accurately weighed impure or water-absorbing sample does not automatically give an accurate concentration.

For dilution, use $c_1V_1 = c_2V_2$ because solute amount is conserved, provided there is no reaction or loss. Transfer the aliquot with a pipette and dilute **to** the final flask volume, not by adding that entire volume of solvent. Never pipette by mouth.

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In a titration, rinse a burette with its titrant and a pipette with the solution it will deliver; use a clean conical flask, normally rinsed with deionized water. Swirl, approach the endpoint dropwise and choose an indicator whose change occurs in the appropriate steep region. The observed endpoint is not the definition of the stoichiometric equivalence point. Acid–base and redox titrations both require a balanced equation; some redox systems are self-indicating. Keep a rough titre separate from the carefully obtained concordant trials and state the selection rule.

Separate, purify and characterize

- **Filtration** separates an insoluble solid from a liquid; it does not remove dissolved salt. A separating funnel separates suitable immiscible liquid layers.
- **Recrystallization** uses a suitable solvent in which the product is much more soluble hot than cold. Cool to crystallize, collect and wash with a little cold solvent; too much solvent can reduce recovery.
- **Drying to constant mass** means repeating a suitable heat–cool–weigh cycle until successive masses agree within the stated criterion. Cool before weighing; constant mass does not prove chemical purity or justify heating a decomposing compound more strongly.
- **Distillation** vaporizes and condenses a component for collection, using volatility differences. **Reflux** returns condensed vapour to the reaction vessel, allowing prolonged heating with less volatile material lost. Neither setup should be sealed during ordinary atmospheric heating.
- **Paper/TLC chromatography** compares movement of substances under specified conditions. Keep the sample above the initial solvent level; mark the solvent front promptly. R_f is distance moved by the spot from the baseline divided by distance moved by the solvent front from the same baseline. Matching R_f alone does not prove identity.
- **Melting-point determination** can support a purity assessment: impurities often depress and broaden a melting range, but comparison requires suitable heating and a relevant reference. A single melting point is not a complete structural identification.

Measure chemical behaviour

- **Calorimetry:** measure temperature change and the mass being heated; use insulation and account for apparatus heat capacity and heat exchange where relevant. The reaction and surroundings have opposite heat signs.
- **Electrochemical cells:** keep electrode surfaces, electrolyte conditions and temperature consistent; a high-resistance voltmeter reduces current drawn during a potential-difference measurement.

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- **Colorimetry/spectrophotometry:** choose a suitable wavelength, use a blank and consistent clean cuvettes, and build a calibration using known concentrations. A calibration range must be justified; extrapolation outside it can fail if the relationship ceases to be linear.
- **Physical/digital molecular models:** use them to investigate connectivity and geometry, stating model assumptions and limitations. A ball-and-stick bond is a representation, not a rigid stick physically joining atoms.

Record raw data and propagate uncertainty

Keep original readings, units, apparatus uncertainties and qualitative observations. Put units and common uncertainties in column headings; use consistent decimal places for an instrument. Record unexpected changes and failed trials honestly. Preserve raw data before calculations or spreadsheet transformations. For database work, retain the source, conditions, units and any filtering choices; for sensors, record calibration and sampling settings.

An **uncertainty** quantifies a limitation on the result. Absolute uncertainty has the measured quantity's unit; fractional uncertainty is $u_x/|x|$, and percentage uncertainty is that fraction multiplied by 100. These are not the same as percentage disagreement with a reference.

For the conservative maximum-uncertainty method used here:

- In addition or subtraction, add absolute uncertainties: $u_{a\pm b} = u_a + u_b$.
- In multiplication or division, add fractional uncertainties: $u_y/|y| \approx u_a/|a| + u_b/|b|$ for $y = ab$ or a/b.
- A defined exact conversion or stoichiometric coefficient adds no measurement uncertainty. Multiplying a measured value by an exact coefficient scales its absolute uncertainty by the same factor, leaving its percentage uncertainty unchanged.

These are conservative first-order estimates for small uncertainties, not a claim that every error reaches its maximum simultaneously. Statistical combination of independent random standard uncertainties can instead use quadrature; do not switch between conventions halfway through an answer. Shared/correlated errors need separate treatment. Subtracting two readings from the same instrument can cancel a truly constant zero offset, even though the conservative reading-uncertainty sum is still used when requested.

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■ **Worked example: titration concentration**

Use 25.00 ± 0.03 cm^3 of NaOH and a titre of 22.50 ± 0.10 cm^3 of HCl of concentration 0.1000 mol dm^{-3} with 0.20% uncertainty. The balanced reaction is 1:1.

$$c_{\mathrm{NaOH}} = \frac{c_{\mathrm{HCl}} V_{\mathrm{HCl}}}{V_{\mathrm{NaOH}}} = \frac{0.1000 \times 22.50}{25.00} = 0.09000 \text{ mol dm}^{-3}.$$

Volumes share the same units, so their ratio is dimensionless. Maximum percentage uncertainty is

$$100\frac{u_c}{c} = 0.20 + 100\frac{0.10}{22.50} + 100\frac{0.03}{25.00} \approx 0.76\%.$$

$$u_c = 0.09000 \times 0.00764 \approx 0.00069 \text{ mol dm}^{-3}.$$

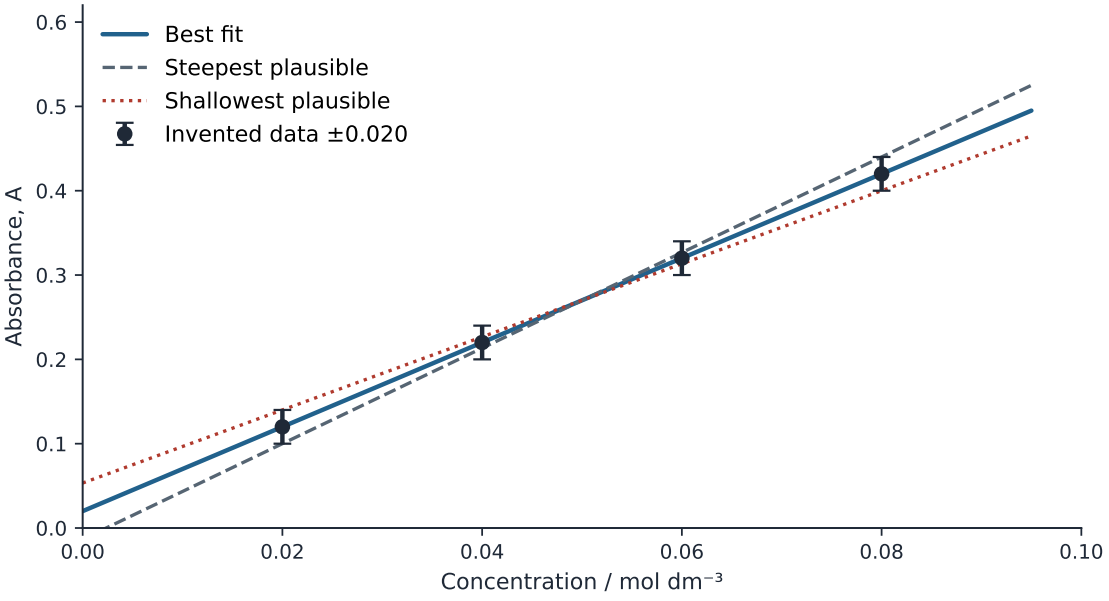
A suitably rounded result is 0.0900 ± 0.0007 mol dm^{-3}. Keep guard digits until this final rounding; quote the value and absolute uncertainty to the same decimal place.

Graphs, gradients and model testing

Put the independent variable on the horizontal axis and the dependent variable on the vertical axis, with quantities and units. Use a readable scale covering the useful data range; a plotted axis need not always start at zero. A qualitative sketch has labelled but unscaled axes. Scatter plots suit paired continuous measurements; bar charts compare categories, and histograms describe a continuous distribution grouped into intervals.

Plot justified uncertainty bars and a best-fit line or curve. Do not join every noisy point with straight segments and call the changing slopes a physical model. A gradient is $\Delta y/\Delta x$ using two widely separated points on the fitted line, not necessarily two measured points. Its unit is vertical-axis unit divided by horizontal-axis unit. A tangent gives an instantaneous gradient; a chord gives an average gradient.

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Treat the full set of uncertainty bars as constraints; endpoint choices alone do not guarantee a plausible line.

In the invented calibration, concentrations 0.020, 0.040, 0.060 and 0.080 mol dm^{-3} give absorbances 0.120, 0.220, 0.320 and 0.420, each with ±0.020 uncertainty; horizontal uncertainty is neglected. The best line is $A = 5.00c + 0.020$.

The steepest allowed line goes through $(0.020, 0.100)$ and $(0.080, 0.440)$; the shallowest through $(0.020, 0.140)$ and $(0.080, 0.400)$. Both also intersect the intervening bars:

$$m_{\max} = \frac{0.440 - 0.100}{0.080 - 0.020} = 5.67\ \mathrm{dm}^3\,\mathrm{mol}^{-1},$$

$$m_{\min} = \frac{0.400 - 0.140}{0.080 - 0.020} = 4.33\ \mathrm{dm}^3\,\mathrm{mol}^{-1}.$$

A symmetric gradient estimate is $m \approx (m_{\max} + m_{\min})/2 = 5.00$, with $u_m \approx (m_{\max} - m_{\min})/2 = 0.67\ \mathrm{dm}^3\,\mathrm{mol}^{-1}$. This graphical range describes the stated bars and straight-line model, not a formal statistical confidence interval.

A nonzero intercept may suggest a blank offset, a background signal or an incomplete model. Investigate it; do not automatically force the graph through the origin. An excellent R^2 describes how well a fitted model accounts for variation in the chosen response data; it does not prove accuracy, causation or the absence of systematic error. Even an exact line can contain a shared calibration bias. Inspect residuals, the data range and the chemistry too. Interpolation stays within the measured range; extrapolation extends beyond it and needs additional justification.

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AHL: Powers and exponential models

For $y = x^n$ with an exact exponent and small uncertainty,

$$\frac{u_y}{|y|} \approx |n| \frac{u_x}{|x|}.$$

The magnitude matters: for $y = 1/x^2$, a 2% uncertainty in x gives about 4% in y, not −4%. Constants known exactly do not contribute. This first-order approximation becomes unreliable for very large fractional uncertainties or values near singularities.

An exponential model can be linearized. If $c = c_0 e^{-kt}$, then $\ln(c/c_0) = -kt$. Plotting the dimensionless logarithm against time gives gradient $-k$. For an invented $k = 0.0200\ \text{s}^{-1}$ and $c_0 = 0.1000\ \text{mol dm}^{-3}$, at 30.0 s:

$$c = 0.1000 e^{-0.0200(30.0)} = 0.0549\ \text{mol dm}^{-3}.$$

The half-time satisfies $1/2 = e^{-kt}$, so $t = \ln 2/k = 34.7$ s. An approximately straight transformed plot supports the model over the tested range; it does not independently establish a chemical mechanism.

Conclude and evaluate

Answer the research question using processed data and uncertainty. Separate observations from explanations: "the temperature rose" is an observation; "the reaction transferred heat to the solution" is an interpretation supported by a model. Compare relevant references under matching conditions, and distinguish accuracy, precision, reliability and validity.

Do not delete a point because it weakens the trend. Inspect the raw record, repeat where appropriate and give a defensible reason for including or excluding an anomalous trial. Retain the original value and the decision. A spreadsheet trend line or simulation produces an output from inputs and assumptions; check units and formulae, preserve provenance and test whether the model represents the chemical system.

An evaluation should link a limitation to its likely effect and a feasible improvement. "Use better equipment" is incomplete. For a small titre, a suitable larger aliquot can reduce percentage reading uncertainty without changing chemical stoichiometry, provided apparatus and reagent limits allow it. For heat loss, better insulation or time-series correction addresses the bias; repeating the same poorly insulated method does not remove it.

Practice

Use conservative maximum uncertainty unless stated otherwise. All additional data are invented.

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1. Turn “Does acid concentration affect reaction speed?” into a measurable research question. Identify independent/dependent variables and two justified controls.
2. A balance reads 6.237 ± 0.001 g before transfer and 2.104 ± 0.001 g after transfer. Find the transferred mass and its uncertainty.
3. A burette gives 2.35 ± 0.05 cm^3 initially and 24.85 ± 0.05 cm^3 finally. Calculate titre and percentage uncertainty. Explain why using only one reading uncertainty is wrong.
4. A temperature rises from 20.0 ± 0.1 °C to 26.0 ± 0.1 °C. Find the rise and percentage uncertainty. Does adding 273 to both readings change the rise?
5. A 0.2000 mol dm^{-3} stock has 0.50% uncertainty. Dilute 25.00 ± 0.03 cm^3 to 250.0 ± 0.15 cm^3. Calculate concentration and its maximum percentage uncertainty.
6. Use the titration worked example to calculate the NaOH concentration and uncertainty. What happens to the calculated concentration if an air bubble initially in the burette tip fills with titrant during the titre?
7. Identify a suitable technique to obtain an insoluble solid, purify a soluble crystalline solid, collect a volatile liquid, and heat a reacting mixture while returning vapour. Give one important distinction for each pair.
8. A calibration is $A = 5.00c + 0.020$, with c in mol dm^{-3}. Find the concentration for $A = 0.270$. Explain why dividing absorbance by 5.00 without the intercept is wrong.
9. Recalculate the steepest and shallowest gradients in the calibration above and estimate the gradient uncertainty. Why must the lines be checked against intermediate bars too?
10. A chromatography spot moves 3.6 cm and the solvent front 6.0 cm from the baseline. Find R_f. Explain why a matching R_f under different conditions does not prove identity.
11. Three titres are 22.45, 22.50 and 22.55 cm^3. Find mean and range. Explain why close agreement and a high calibration R^2 do not prove accuracy, and give a justified approach to an anomalous fourth titre.
12. **AHL.** For a cube edge $x = 2.00 \pm 0.02$ cm, estimate volume and uncertainty using the small-uncertainty power rule. State its approximate nature.
13. **AHL.** For $c = c_0 e^{-kt}$ with $c_0 = 0.1000$ mol dm^{-3} and $k = 0.0200$ s^{-1}, calculate c at 30.0 s and the half-time. State the gradient and unit of a plot of $\ln(c/c_0)$ against time.

■ Worked answers

1. For example: how does HCl concentration over a specified safe range affect the time for a fixed magnesium strip to produce 20 cm^3 hydrogen at constant initial temperature? Independent: HCl concentration; dependent: elapsed time to that volume. Control magnesium mass/exposed area because reactive quantity and surface affect the rate; control temperature because it affects reaction rate. State

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acid volume and apparatus too.

2. $m = 6.237 - 2.104 = 4.133$ g; $u_m = 0.001 + 0.001 = 0.002$ g. Report 4.133 ± 0.002 g.
3. $V = 24.85 - 2.35 = 22.50$ cm^3; $u_V = 0.10$ cm^3. Percentage uncertainty $= 100(0.10/22.50) = 0.44\%$. Delivered volume depends on both readings, so both reading uncertainties enter the conservative difference estimate.
4. $\Delta T = 6.0 \pm 0.2$ K; percentage uncertainty $= 100(0.2/6.0) = 3.3\%$. Converting both readings by adding the same Celsius-to-kelvin offset leaves their difference unchanged.
5. $c_2 = c_1V_1/V_2 = 0.2000(25.00/250.0) = 0.02000$ mol dm^{-3}. Maximum percentage uncertainty $= 0.50 + 100(0.03/25.00) + 100(0.15/250.0) = 0.68\%$. Absolute uncertainty is $0.02000(0.0068) = 0.000136$ mol dm^{-3}; with two uncertainty digits, report 0.02000 ± 0.00014 mol dm^{-3}.
6. $c = 0.1000(22.50/25.00) = 0.09000$ mol dm^{-3}; maximum uncertainty $\approx 0.76\%$, giving 0.0900 ± 0.0007 mol dm^{-3}. Filling an initial tip bubble makes the indicated titre exceed liquid delivered into the flask; the calculated amount of acid and hence NaOH concentration is too high in this model.
7. Insoluble solid: filtration. Soluble crystalline product: recrystallization followed by collection/drying; filtration alone cannot remove dissolved impurities. Volatile liquid collection: distillation; prolonged reaction with condensate returned: reflux. Reflux does not collect the distillate as product outside the reaction vessel.
8. $c = (A - 0.020)/5.00 = (0.270 - 0.020)/5.00 = 0.0500$ mol dm^{-3}. Ignoring the intercept assigns background absorbance to the analyte and overestimates concentration.
9. $m_{\max} = 0.340/0.060 = 5.67$; $m_{\min} = 0.260/0.060 = 4.33$ dm^3 mol^{-1}. Midpoint 5.00 and half-range 0.67 dm^3 mol^{-1}. An endpoint-extreme line might miss other bars; it must remain plausible for the whole dataset and model.
10. $R_f = 3.6/6.0 = 0.60$, dimensionless. Solvent, stationary phase and other conditions affect movement; different substances can also share an R_f. Compare under matched conditions with additional evidence.
11. Mean $= (22.45 + 22.50 + 22.55)/3 = 22.50$ cm^3; range $= 22.55 - 22.45 = 0.10$ cm^3. A common calibration bias can preserve both precision and a strong linear fit. Inspect the fourth trial's raw observations and method, repeat if possible and justify any exclusion rather than deleting it because it weakens agreement.
12. **AHL.** $V = x^3 = 8.00$ cm^3; fractional uncertainty $u_V/V \approx 3(0.02/2.00) = 0.030$. Thus $u_V \approx 0.24$ cm^3, giving 8.00 ± 0.24 cm^3 with two uncertainty digits. This is a first-order estimate for small uncertainty, not exact evaluation of both cubed bounds.
13. **AHL.** $c = 0.1000e^{-0.0200(30.0)} = 0.0549$ mol dm^{-3}. $t_{1/2} = \ln 2/0.0200 = 34.7$ s. Since $\ln(c/c_0) = -kt$, gradient is -0.0200 s^{-1}.

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Exam tips

- Distinguish a reading from a difference and an absolute uncertainty from a percentage. State which uncertainty convention you use.
- Record original values and units, then keep guard digits until final rounding. Precision of repeats is not proof of accuracy.
- A gradient needs units and a model; an intercept, residual pattern or anomaly needs investigation, not automatic deletion.
- Link each evaluation point to a direction or consequence and a specific feasible improvement. Answer the research question within the supported range.
- **AHL.** Multiply fractional uncertainty by the magnitude of an exact exponent; check the axes and sign when linearizing an exponential model.

Reference: IB Chemistry guide: tools and inquiry skills.

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