

1 • Structure, Bonding and Introduction to Organic Chemistry

Pearson Edexcel • International A-Level • Chemistry

From particles to a chemical prediction

Why can a tiny mass of a gas fill a large flask? Why does solid sodium chloride not carry current, while its solution does? Unit 1 links particle counting, electronic structure and bonding to observable behaviour, then uses the same ideas to explain organic reactions.

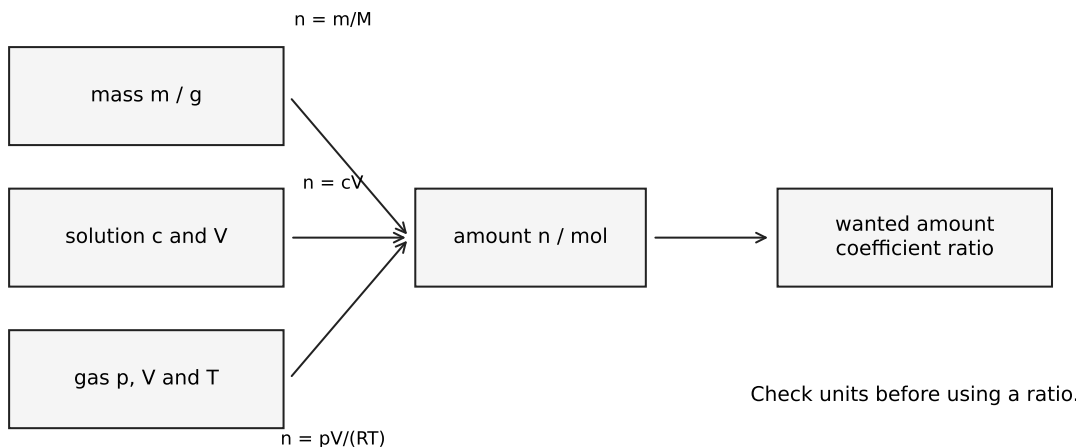
Use this reference with sheets 1.1–1.5 and their narrower skill companions. You need simple algebra, powers of ten and balanced equations. Topics 1–5 of the Pearson specification define this unit. Kinetics and equilibrium belong to Unit 2; they are not prerequisites for these sheets.

Count particles, then use the equation

An **atom** is one particle of an element . An element contains only one type of atom, defined by proton number. An **ion** has an electrical charge because its electron count differs from its proton count. A **molecule** is a discrete group of covalently bonded atoms. A compound contains different elements chemically combined. An empirical formula gives the simplest whole-number atom ratio; a molecular formula gives actual atom numbers in one molecule. Ionic lattices have formula units, not separate molecules.

The **mole** is the unit of amount of substance. The particle count is $N = nL$, where $L = 6.02 \times 10^{23} \text{ mol}^{-1}$. Thus one mole contains 6.02×10^{23} of the specified entities. Always say whether you count atoms, molecules, ions or formula units. A mole of methane molecules contains five moles of atoms.

Relative atomic mass , A_r , compares the abundance-weighted mean atom mass with one-twelfth of a carbon-12 atom's mass. Relative molecular mass , M_r , adds the relative atomic masses in a molecule. Relative formula mass applies the same sum to a formula unit, including giant structures. Both are ratios without units. **Molar mass** , M , is mass per mole, in g mol^{-1} .



Choose the route to amount.

Use $n = m/M$ for a mass, $n = cV$ for a solution with V in dm^3 , and $pV = nRT$ for a gas with pressure in Pa, volume in m^3 and temperature in K. A stated molar gas volume can replace the gas equation only under its stated conditions. At the usual classroom RTP approximation, use $24 \text{ dm}^3 \text{ mol}^{-1}$. Divide cm^3 by 1000 to obtain dm^3 .

Worked reacting-mass method. The equation is $\text{Mg} + 2\text{HCl} \rightarrow \text{MgCl}_2 + \text{H}_2$. There is excess acid and 0.480 g magnesium, with $M(\text{Mg}) = 24.0 \text{ g mol}^{-1}$.

$$n(\text{Mg}) = \frac{m}{M} = \frac{0.480 \text{ g}}{24.0 \text{ g mol}^{-1}} = 0.0200 \text{ mol}$$

The coefficient ratio is $\text{Mg}:\text{H}_2 = 1:1$, so $n(\text{H}_2) = 0.0200 \text{ mol}$. At the stated RTP approximation:

$$V = nV_m = 0.0200 \text{ mol} \times 24 \text{ dm}^3 \text{ mol}^{-1} = 0.48 \text{ dm}^3$$

If both reactant amounts are given, compare amount divided by coefficient. The smaller value identifies the **limiting reagent**. Do not compare masses alone.

Mass concentration is m/V in g dm^{-3} ; amount concentration is n/V in mol dm^{-3} . Divide mass concentration by molar mass to convert between them. Parts per million, ppm, is a fraction multiplied by 10^6 ; state whether it is a mass fraction or, for gases at the same temperature and pressure, a volume fraction.

Formulae and experimental checks

To find an **empirical formula**, divide each element's mass by its A_r and divide the resulting amounts by the smallest amount. Multiply the whole ratio if necessary to obtain integers. Do not round 1.5 to 2: multiply all ratios by 2. To find a molecular

formula, divide measured M_r by empirical-formula mass and multiply every subscript by this integer.

Worked check. A compound contains 2.40 g carbon and 0.600 g hydrogen. Carbon amount is $n = m/M = 2.40/12.0 = 0.200$ mol; hydrogen atom amount is $n = m/M = 0.600/1.00 = 0.600$ mol. C:H = 1:3, so the empirical formula is CH_3 . If $M_r = 30.0$, the factor is $30.0/15.0 = 2$, giving C_2H_6 . The element masses add to the sample mass, 3.00 g.

Balance full equations without changing substance formulae, and include states: (s), (l), (g), (aq). For a precipitation, $\text{Ag}^+(\text{aq}) + \text{Cl}^-(\text{aq}) \rightarrow \text{AgCl}(\text{s})$ omits spectator ions. For an acid and carbonate, $\text{CO}_3^{2-}(\text{aq}) + 2\text{H}^+(\text{aq}) \rightarrow \text{CO}_2(\text{g}) + \text{H}_2\text{O}(\text{l})$ conserves both atoms and charge. A precipitate or gas is an observation; an equation explains the change. Zinc in copper(II) sulfate gives a reddish copper deposit while the blue solution fades: $\text{Zn}(\text{s}) + \text{Cu}^{2+}(\text{aq}) \rightarrow \text{Zn}^{2+}(\text{aq}) + \text{Cu}(\text{s})$. Magnesium in dilute acid dissolves with hydrogen bubbles: $\text{Mg}(\text{s}) + 2\text{H}^+(\text{aq}) \rightarrow \text{Mg}^{2+}(\text{aq}) + \text{H}_2(\text{g})$. An acid with a soluble base can warm without gas or precipitate: $\text{H}^+(\text{aq}) + \text{OH}^-(\text{aq}) \rightarrow \text{H}_2\text{O}(\text{l})$. Match each equation to the actual observation rather than treating every acid reaction as gas formation.

Percentage yield compares actual with theoretical product amount. For a theoretical 4.00 g and actual isolated dry 3.20 g, $\text{yield} = 3.20/4.00 \times 100\% = 80.0\%$.

Atom economy compares the balanced desired-product mass with all balanced product masses. Include equation coefficients. A high atom economy does not guarantee a high experimental yield.

$$\text{yield} = \frac{\text{actual product mass}}{\text{theoretical product mass}} \times 100\%$$

$$\text{atom economy} = \frac{\text{desired product molar mass} \times \text{coefficient}}{\sum(\text{product molar mass} \times \text{coefficient})} \times 100\%$$

In the molar-gas-volume practical, use a known limiting amount and collect the gas under measured conditions. Account for leaks, gas dissolving, incomplete reaction and dead space. A leak lowers measured gas volume and therefore the calculated molar volume. To confirm a formula by reaction with oxygen, heat to constant mass, cool before weighing and explain how loss of solid or incomplete oxidation changes the inferred ratio. Practical reasoning remains part of this theory unit.

Electronic structure is evidence about the atom

Protons and neutrons are in the nucleus; electrons occupy orbitals around it. Relative particle masses are approximately 1, 1 and $1/1836$; charges are +1, 0 and -1. Atomic number Z counts protons; mass number A counts protons plus neutrons. Thus neutrons = $A - Z$. A positive ion has fewer electrons than protons.

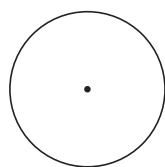
Isotopes have the same proton number but different neutron numbers.

A mass spectrometer forms gaseous positive ions, separates them by mass-to-charge ratio, m/z , and detects relative abundance, the proportion of the sample contributing each ion type. Vaporisation, ionisation, acceleration, separation and detection have distinct roles. In magnetic separation at a given accelerating potential, a lower m/z ion bends more; a higher charge lowers m/z , rather than making bending smaller. A doubly charged mass-40 ion appears at $m/z = 20$.

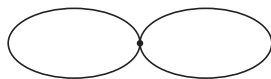
Worked isotope mean. For 60% mass-69 and 40% mass-71 gallium, $A_r = (69 \times 60 + 71 \times 40)/100 = 69.8$. The mean lies between the isotope masses, closer to the more abundant isotope. Molecular-ion peaks can identify M_r when charge is known. With chlorine isotope proportions 3:1, Cl_2 molecular-ion peaks at 70, 72 and 74 have probabilities 9/16, 6/16 and 1/16: the middle combination occurs in two orders.

An **orbital** holds at most two electrons with opposite spins. An s orbital is spherical; a p orbital has two lobes. There are 1, 3 and 5 orbitals in s, p and d subshells, holding at most 2, 6 and 10 electrons. Fill equal-energy orbitals singly before pairing. The first four quantum shells have maximum capacities 2, 8, 18 and 32 electrons. Their available subshells are 1s; 2s/2p; 3s/3p/3d; and 4s/4p/4d/4f. An f subshell has seven orbitals and holds fourteen electrons. The periodic table has s, p and d blocks according to the subshell receiving the differentiating electron. Write configurations through krypton, including the chromium and copper exceptions: Cr is $[\text{Ar}]3d^54s^1$ and Cu is $[\text{Ar}]3d^{10}4s^1$. For their positive ions, remove 4s electrons before 3d electrons. Electron-box notation must show both occupancy and spin.

P: $[\text{Ne}]3s^23p^3$



s orbital: spherical



one p orbital: two lobes



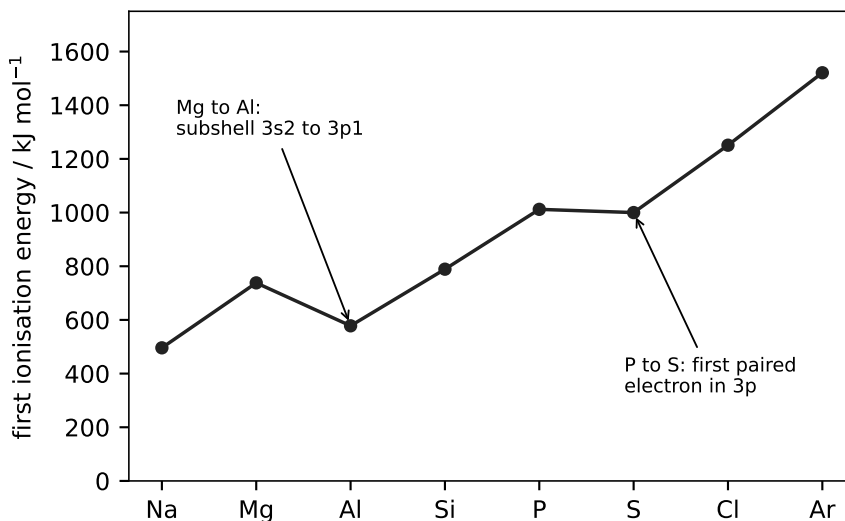
3s

three 3p orbitals

S adds $\downarrow$ to one 3p box.

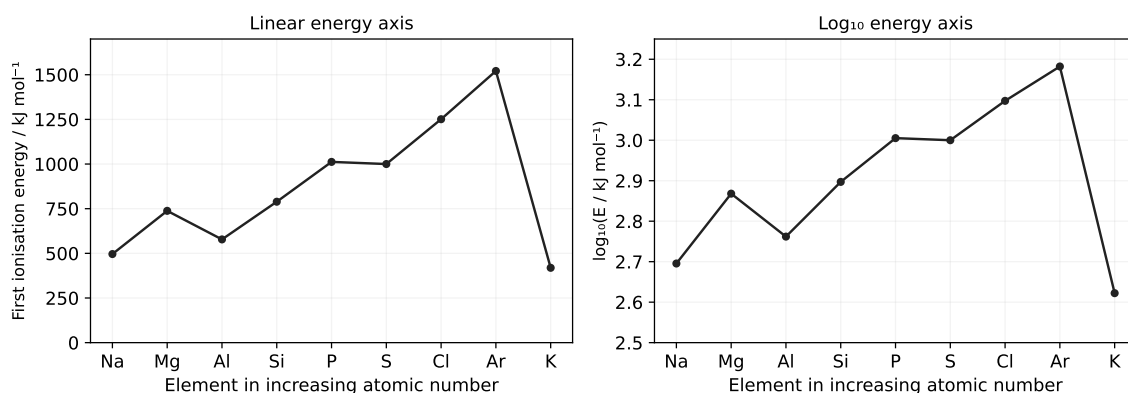
Orbital shapes and the singly occupied 3p orbitals in phosphorus.

First ionisation energy is the energy per mole for $\text{X}(\text{g}) \rightarrow \text{X}^+(\text{g}) + \text{e}^-$. Second ionisation removes an electron from $\text{X}^+(\text{g})$; third ionisation is $\text{X}^{2+}(\text{g}) \rightarrow \text{X}^{3+}(\text{g}) + \text{e}^-$. All ionisation steps are endothermic. Greater nuclear charge strengthens attraction; more shielding and greater electron distance weaken it. A large successive-energy jump reveals that all outer-shell electrons have been removed. This identifies the main-group outer electron count but does not alone count every occupied shell.



First ionisation energies across Period 3 with the magnesium-to-aluminium subshell drop and the phosphorus-to-sulfur pairing dip annotated.

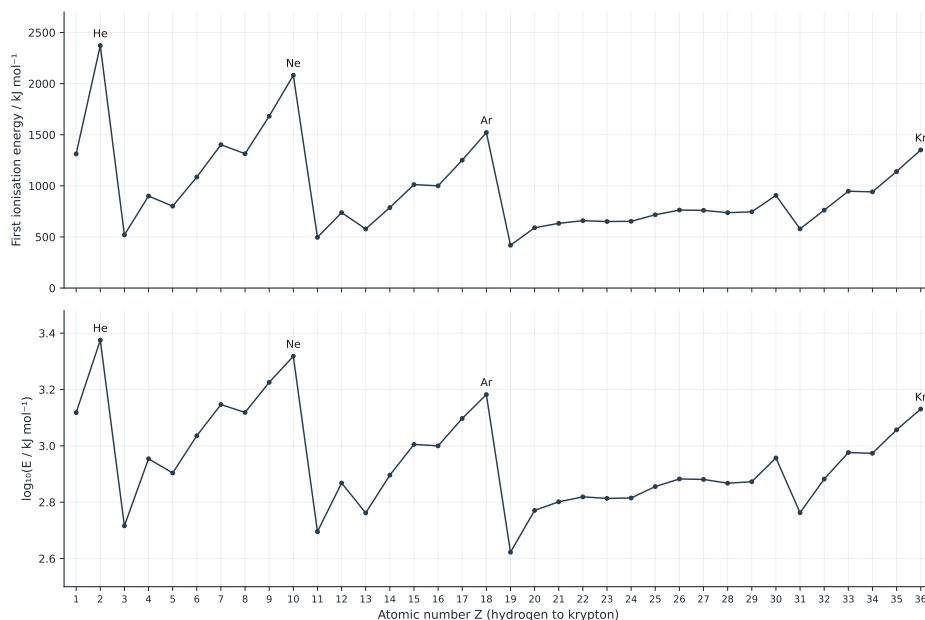
Across Period 3, nuclear charge rises while inner-shell shielding changes little, giving a broad first-ionisation increase. Al loses a higher-energy 3p electron more easily than Mg loses a 3s electron. S has a paired 3p electron with greater repulsion than the singly occupied 3p orbitals in P. Down a group, increased distance and shielding outweigh increased nuclear charge. Recurring trends across periods are **periodicity**; use labelled axes, and interpret a logarithmic axis as ratios rather than equal energy increments.



The same ionisation data on linear and logarithmic axes; potassium starts the next period.

The supplied first-36-element graphing task on sheet 1.2.2 tests both ordinary and logarithmic axes. Noble-gas peaks are followed by decreases when a new outer shell starts; subshell and pairing effects produce additional dips within a period. The transition series does not form one perfectly smooth rising line. Helium belongs to

the s block by $1s^2$ despite its noble-gas column.



First ionisation energies through krypton on linear and logarithmic axes.

Bonding, shape and bulk properties

An **ionic bond** is the net electrostatic attraction between oppositely charged ions throughout a giant lattice. Electron transfer forms ions; the attraction is the bond. Conductivity when molten or dissolved, ion migration and electron-density evidence support the ionic model. Coloured cations move toward the negative electrode in solution. Electron-density maps show electron distribution around nuclei; compare the distribution with the ion model, rather than assuming a contour directly records the history of electron transfer. Ionic solids lack mobile ions. Smaller ions and higher charges usually strengthen lattice attraction. In an isoelectronic series, greater proton number pulls the same electron population closer: the radius decreases from N^{3-} toward Al^{3+} . Down a group, extra occupied shells increase radius.

A **covalent bond** is attraction between two nuclei and a shared electron pair. Dot-and-cross diagrams identify electron origin. Include lone pairs and brackets/charge for ions. A coordinate bond uses a shared pair initially supplied by one atom, as when NH_3 donates a pair to H^+ to form NH_4^+ . Aluminium chloride can form Al_2Cl_6 with two chloride bridges and coordinate bonding; electron diagrams must account for every outer electron.



NaCl: bracketed ions; only each ion's outer shell shown.

CO₂: dots from C; crosses from O



Two shared pairs per C–O bond; two lone pairs per O.

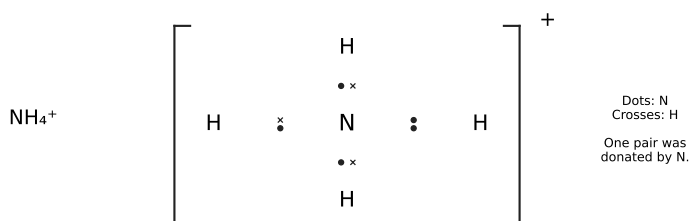
Ionic and multiple-bond outer-electron diagrams.

N₂: dots from left N; crosses from right N

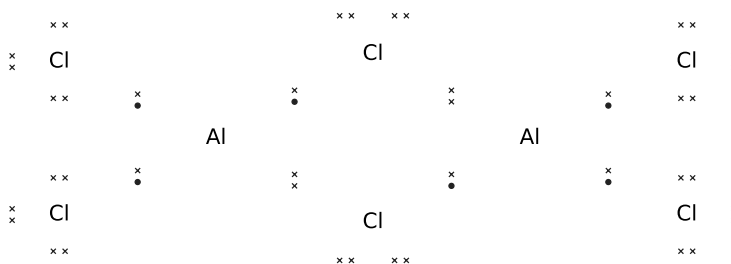


Three shared pairs and one lone pair per atom: ten outer electrons.

A triple bond and two lone pairs account for every outer electron of nitrogen.



Al_2Cl_6 : dots from Al; crosses from Cl



Each bridging Cl donates a pair to the other Al. All 48 outer electrons are shown.

Complete donor-pair diagrams for ammonium and aluminium chloride dimer.

Dots: central atom Crosses: outer atoms
Flat electron diagrams do not show the 3D shape.



NH_3 : 3 bond pairs + 1 lone pair

BF_3 : 3 bond pairs; B has 6 outer electrons

Completed outer-electron diagrams.

Electron pairs around a central atom repel and arrange apart. Lone pairs repel more strongly than bonding pairs, but there is no universal fixed angle reduction per lone pair. Count regions around the central atom; a multiple bond occupies one region. Bond length is the distance between nuclei; bond angle is the angle between adjacent bonds.

Regions	Example	Shape and typical angle
2	BeCl ₂ , CO ₂	linear, 180°
3	BCl ₃	trigonal planar, 120°
4	CH ₄ , NH ₄ ⁺	tetrahedral, 109.5°
3 bonds + lone pair	NH ₃	pyramidal, about 107°
2 bonds + 2 lone pairs	H ₂ O	bent, about 104.5°
5	gaseous PCl ₅	trigonal bipyramidal, 90°/120°
6	SF ₆	octahedral, 90°

Each carbon in ethene has three regions and a planar arrangement, with angles about 120°. **Electronegativity** is attraction for a bonding electron pair. Different electronegativities produce polar bonds. A molecule is polar only if its bond dipoles do not cancel: CO₂ is non-polar; H₂O is polar. Ionic and covalent bonding are ends of a continuum. Polarising power describes a cation's ability to distort another ion's electron cloud; polarisability describes how readily that cloud is distorted. A small, highly charged cation strongly distorts an anion's electron cloud; large anions are easier to polarise. Do not use one melting point alone as proof of structure.

Small molecular substances usually melt or boil by overcoming intermolecular attractions rather than breaking bonds inside molecules. Diamond has four covalent bonds per atom in a giant network; graphite has three per atom in layers and mobile delocalised electrons; graphene is a single layer. Diamond is hard and insulating; graphite layers can slide and conduct along them; graphene combines strength and conductivity. Metals contain positive ions attracted to delocalised electrons, which carry current in solid and molten metal.

The Period 2/3 melting trend follows changing structures: metallic elements, then giant covalent carbon/silicon, then small molecular non-metals and monatomic noble gases. In Period 2, lithium and beryllium are metallic; boron and carbon form giant covalent structures, then nitrogen, oxygen and fluorine are molecular and neon is monatomic. Molecular electron count and attractions help explain differences among the non-metals. A smooth nuclear-charge explanation alone cannot explain the whole melting trend. Stronger metallic attraction, involving ionic charge, ion size and the number of delocalised electrons, usually raises melting temperature; the detailed metal structure also matters. Heating a metal to melt it does not remove all its electrons.

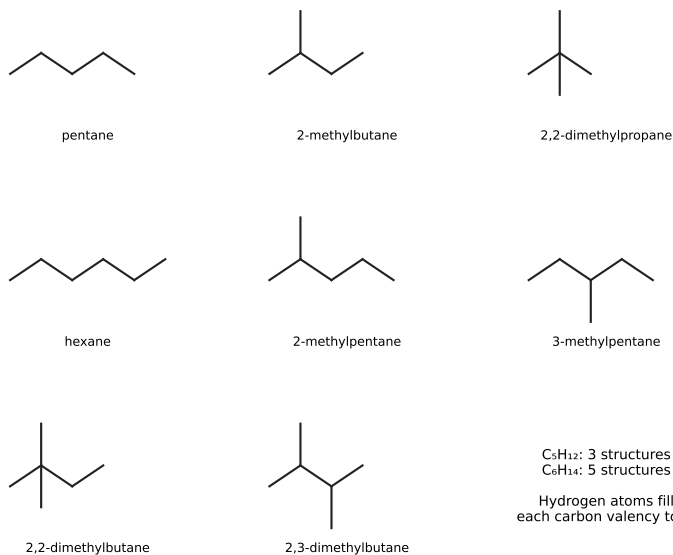
Organic formulae, fuels and radicals

A **functional group** gives characteristic reactions. A **homologous series** shares a functional group and general formula, with successive members differing by CH₂. Structural isomers have the same molecular formula but different atom connectivity. In displayed formulae show every atom and bond; in skeletal formulae each unlabelled end or corner is carbon, with enough implied H atoms for four bonds. Show heteroatoms and their attached hydrogen explicitly.

Use meth-, eth-, prop-, but-, pent-, hex-, hept-, oct-, non-, dec- for one to ten carbon

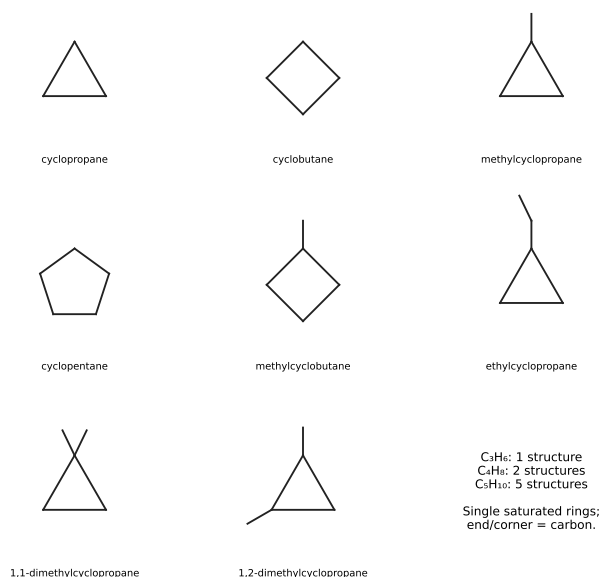
atoms. Choose a parent containing the relevant functional group and number to give its required lowest locant, then locate substituents. Acyclic alkanes have formula C_nH_{2n+2} ; single-ring cycloalkanes have C_nH_{2n} . Both are saturated: they contain only carbon-carbon single bonds. C_nH_{2n} alone does not prove an alkene because a cycloalkane can share it.

Generate structural isomers systematically: keep the formula fixed, change the longest chain or ring size, distribute the remaining carbon atoms, then remove rotated or renumbered duplicates. Pentane has three chain isomers; hexane has five. A different drawing direction alone does not make a new structure.

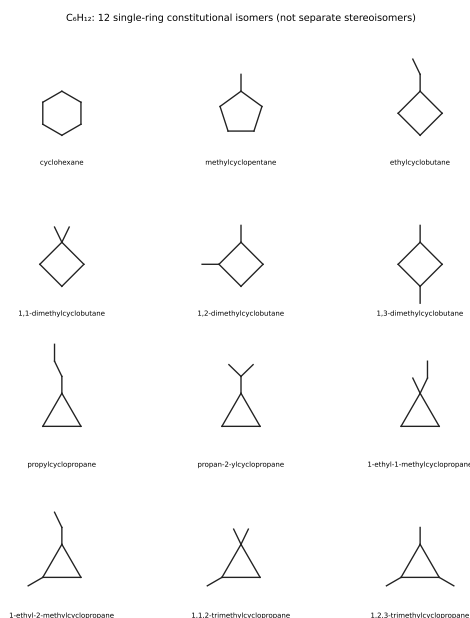


Complete chain-isomer formulae for pentane and hexane.

For saturated single rings, begin with the largest ring and shorten it while moving carbons into substituents. There is one C_3H_6 ring structure, two C_4H_8 and five C_5H_{10} structures. The C_6H_{12} set has twelve constitutional structures; distinct cis/trans forms are not counted again as structural isomers.



Complete single-ring structures for three, four and five total carbon atoms.



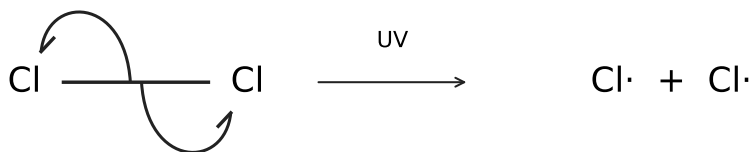
Complete single-ring structures for six total carbon atoms.

Fractional distillation separates crude oil into fractions with different boiling ranges. Cracking converts larger hydrocarbons to smaller products, including alkenes; reforming can change straight chains to branched or cyclic structures. Balance atoms in every proposed equation. Complete combustion of a hydrocarbon forms CO_2 and water. Incomplete combustion can form toxic CO or carbon particulates; CO reduces blood oxygen transport by binding haemoglobin. Fuel sulfur and high-temperature

nitrogen/oxygen reactions can produce acidic oxides. Carbon particulates harm air quality; unburned hydrocarbons can contribute to photochemical pollution. Removing fuel sulfur does not prevent nitrogen oxides formed from hot air. Carbon neutrality means no net carbon dioxide increase over the stated life-cycle boundary. Bioethanol's growth can take up CO₂, but processing and transport emissions prevent automatic carbon-neutral claims. Hydrogen makes water at use; its production method still matters.

A **hazard** is a potential source of harm; risk considers its likelihood and severity under actual conditions. Use the school's risk assessment, small quantities, ventilation and controls specific to flammability or toxicity. A safer alternative can reduce risk without pretending the original substance has no hazard.

A **free radical** has an unpaired electron. Homolytic fission gives one electron to each fragment; heterolytic fission gives both to one fragment, forming ions. UV light starts chlorine substitution by breaking Cl₂ homolytically: $\text{Cl}_2 \rightarrow 2\text{Cl}\cdot$. Use single-headed curly arrows for individual electrons.



Homolysis: one electron from the bond goes to each chlorine atom.
Each curly half-arrow tracks one electron.

UV initiation uses two single-electron half-arrows.

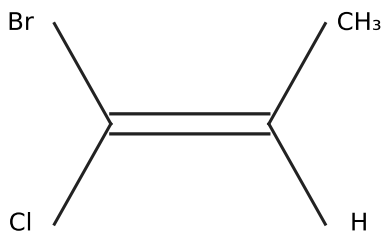
Propagation: $\text{Cl}\cdot + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3\cdot$, then $\text{CH}_3\cdot + \text{Cl}_2 \rightarrow \text{CH}_3\text{Cl} + \text{Cl}\cdot$. One radical is regenerated, so the chain continues. Termination joins two radicals, for example $2\text{CH}_3\cdot \rightarrow \text{C}_2\text{H}_6$. Further substitution and multiple possible positions produce mixtures, limiting the method's value for making one pure product.

Alkenes: follow the electron pair

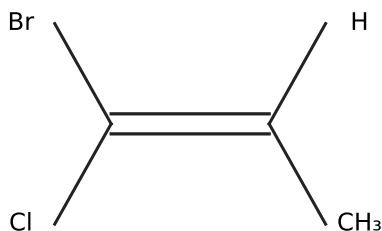
An acyclic alkene with one C=C has formula C_nH_{2n}. A cycloalkene with one ring and one double bond has C_nH_{2n-2}: the ring removes another two hydrogens. A double bond consists of a sigma bond σ from head-on orbital overlap and a pi bond π from sideways p-orbital overlap. Rotating one carbon would break pi overlap, so rotation is restricted. **E/Z isomerism** requires two different groups on each double-bond carbon. Rank the directly attached atoms by atomic number; if tied, compare the next atoms. Compare priorities separately on the two carbons. Higher-priority groups together give Z, opposite give E. Cis/trans is insufficient where

no suitable identical substituents can be compared.

Assign priority separately on each double-bond carbon.



A: Z (Br and CH₃ together)



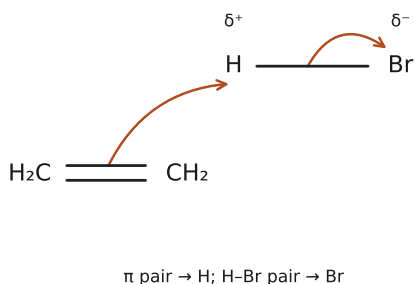
B: E (Br and CH₃ apart)

Assign E/Z from the priorities on each carbon.

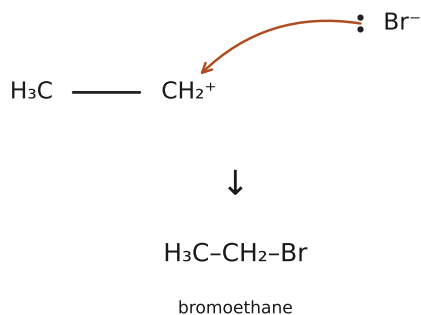
An **electrophile** accepts an electron pair. In HBr addition, a curly arrow begins at the pi bond and ends at H, while another begins at the H–Br bond and ends at Br. This forms a carbocation and Br[−]; a bromide lone pair then forms the new carbon–bromine bond. Propene mainly gives 2-bromopropane because its route forms a secondary rather than primary carbocation. Tertiary carbocations are generally more stable than secondary, which are more stable than primary, under these conditions.

For **ethene**, the two double-bond carbons are equivalent. Proton addition in either direction makes the same ethyl carbocation, CH₃CH₂⁺. Bromide donates a lone pair to its positive carbon, giving bromoethane; there are no two different constitutional products to choose between.

1 Form the ethyl carbocation



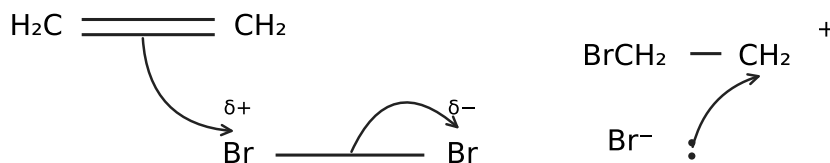
2 Bromide donates its lone pair



Complete electron-pair mechanism for ethene and hydrogen bromide.

Bromine is polarised by the electron-rich double bond and adds across it; ethene forms 1,2-dibromoethane. Bromine decolourisation supports unsaturation in an appropriate organic test but does not identify one unique alkene. Avoid unrequired claims about

stereochemical product mixtures.



Product: BrCH₂-CH₂Br

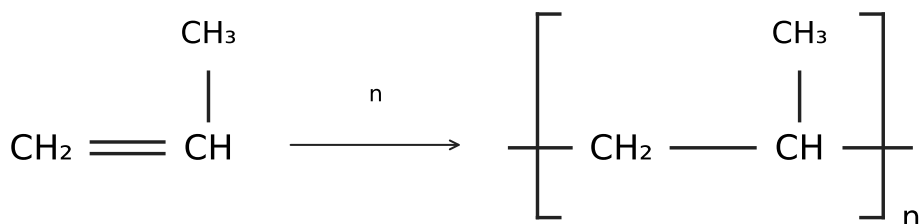
Simple electrophilic-addition model: π pair $\rightarrow$ Br δ^+ ; Br-Br pair $\rightarrow$ Br δ^- .
A bromide lone pair supplies the second C-Br bond.

Electron-pair arrows for bromine addition to ethene in the simple carbocation model.

Other additions: hydrogen with nickel gives an alkane; steam with an acid catalyst gives an alcohol; cold, dilute acidified manganate(VII) oxidises C=C to a diol. State reagents and conditions, not only product names. In **addition polymerisation**

, open each C=C into the polymer backbone, retain its side groups, and show brackets with bonds extending through them and n outside. A repeat unit

is the smallest backbone segment whose repetition describes the chain, including its side groups. No small molecule is eliminated. Polymer disposal needs evidence: sorting/recycling, persistence, biodegradable alternatives and removal of toxic incineration gases have different advantages and costs.



Propene $\rightarrow$ poly(propene); continuation bonds cross the brackets.
Side groups stay attached; no small molecule is eliminated.

Propene polymerisation preserves the methyl side group and shows continuation bonds.

Independent checks

1. A mass-40 ion gives $m/z = 20$. Explain its charge.
2. An element's first three ionisation energies are relatively close; the fourth is much greater. State what you can infer and what you cannot infer from this jump alone.
3. A gas occupies 0.240 dm^3 at a molar volume of $24.0 \text{ dm}^3 \text{ mol}^{-1}$. A 0.480 g sample made this gas in a 1:1 reaction. Find the sample's molar mass and state one reason the experimental value could be too high.
4. Why can the same molecular formula describe an alkene and a cycloalkane?
5. Predict the product when HBr adds to $\text{CH}_2=\text{C}(\text{CH}_3)_2$, and explain the preferred carbocation.

Answers. 1 A $2+$ ion has half the singly charged mass-to-charge ratio. 2 Three outer electrons, consistent with main Group 3/13; the jump alone does not establish period. 3 $n = V/V_m = 0.240/24.0 = 0.0100 \text{ mol}$; $M = m/n = 0.480/0.0100 = 48.0 \text{ g mol}^{-1}$. A leak lowers measured gas amount and raises inferred molar mass. 4 One ring or one double bond each reduces H count by two relative to an acyclic alkane. 5 2-bromo-2-methylpropane; H adds to CH_2 , forming a tertiary carbocation before Br^- supplies a pair to the positive carbon.