An introduction to AS Level organic chemistry

A-Level Chemistry

Formulas, functional groups and naming

Crude oil is a complex mixture of hydrocarbons — the feedstock for organic chemistry.

A **hydrocarbon** 碳氢化合物 is a compound of only carbon and hydrogen. **Alkanes** 烷烃 are the simplest hydrocarbons and have no functional group.

A **functional group** 官能团 is the reactive part of a molecule. It decides the physical and chemical properties of the compound, so molecules with the same functional group behave alike (for example the –OH group in alcohols).

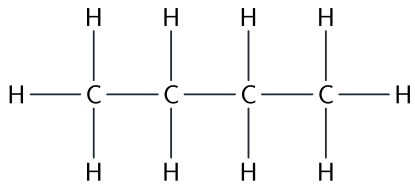
Types of formula

Formula	What it shows
general formula 通式	the pattern for a whole family, e.g. alkanes are C_nH_{2n+2}
molecular formula 分子式	the actual number of each atom, e.g. C_4H_{10}
structural formula 结构式	the groups in order, e.g. $CH_3CH_2CH_2CH_3$
displayed formula 展开式	every atom and every bond drawn out
skeletal formula 骨架式	lines for bonds; carbons at corners, hydrogens on carbon not shown

molecular C_4H_{10}

structural $CH_3CH_2CH_2CH_3$

displayed



skeletal

The same molecule (butane) shown four ways — molecular, structural, displayed and skeletal — each hiding more detail than the last

You can read off the **empirical formula** 实验式 (simplest ratio) from any of these.

Naming

Use systematic **nomenclature** 命名法: a stem for the number of carbons (meth-, eth-, prop-, but-, pent-, hex- for 1 to 6), an ending for the functional group, and numbers to show where groups are.

Characteristic organic reactions

Some key terms

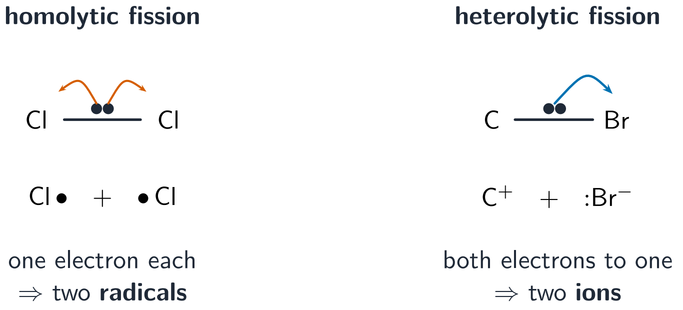
- a **homologous series** 同系列 is a family of compounds with the same functional group and general formula, where each member differs by CH_2.

- a **saturated** 饱和 compound has only single C–C bonds; an **unsaturated** 不饱和 compound has a C=C double bond (or a triple bond).

Breaking bonds

A covalent bond can break in two ways:

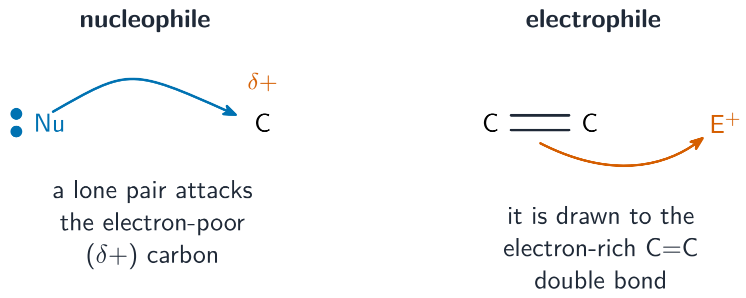
- **homolytic fission** 均裂: the bond splits evenly, one electron to each atom. This makes two **free radicals** 自由基 (species with an unpaired electron).
- **heterolytic fission** 异裂: the bond splits unevenly, both electrons going to one atom. This makes two ions.



Homolytic fission gives one electron to each atom (two radicals); heterolytic fission gives both electrons to one atom (two ions)

Attacking species

- a **nucleophile** 亲核试剂 is a species with a lone pair that is attracted to a positive (electron-poor) centre.
- an **electrophile** 亲电试剂 is a species attracted to a negative (electron-rich) centre, such as a C=C double bond.



A nucleophile uses its lone pair to attack an electron-poor centre; an electrophile is drawn to an electron-rich one such as a C=C bond

Types of reaction

Reaction	What happens
addition 加成	two molecules join to make one
substitution 取代	one atom or group is swapped for another
elimination 消去	a small molecule is removed, making a double bond
hydrolysis 水解	a molecule is split apart by water
condensation 缩合	two molecules join and a small molecule (such as water) is lost

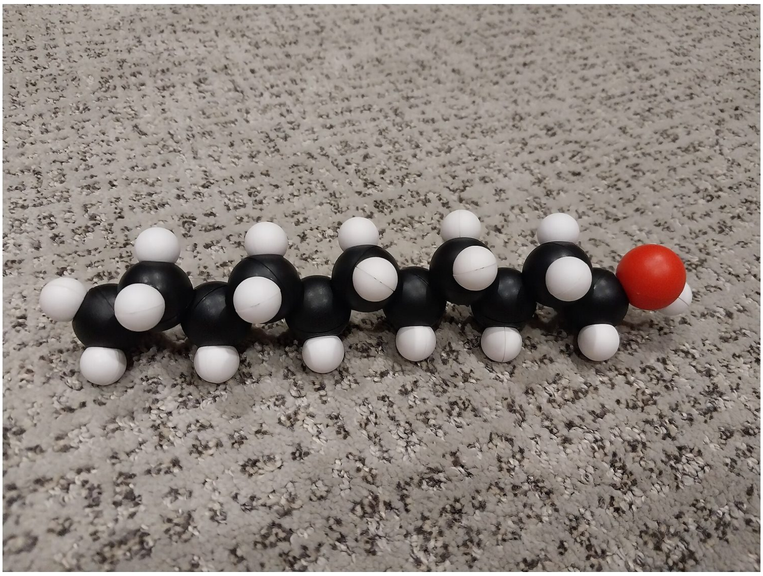
For organic redox, the symbol [O] stands for one oxygen atom from an oxidising agent, and [H] for one hydrogen atom from a reducing agent.

Types of mechanism

A free-radical reaction happens in three steps: **initiation** 引发 (radicals are made), **propagation** 增长 (radicals react and make new radicals), and **termination** 终止 (two radicals join and stop the chain).

The main mechanisms you meet are **free-radical substitution** 自由基取代 (alkanes), **electrophilic addition** 亲电加成 (alkenes), **nucleophilic substitution** 亲核取代 (halogenoalkanes) and **nucleophilic addition** 亲核加成 (carbonyls). In mechanisms, a **curly arrow** 弯箭头 shows a pair of electrons moving; it starts at a bond or a **lone pair** 孤对电子.

Shapes of organic molecules



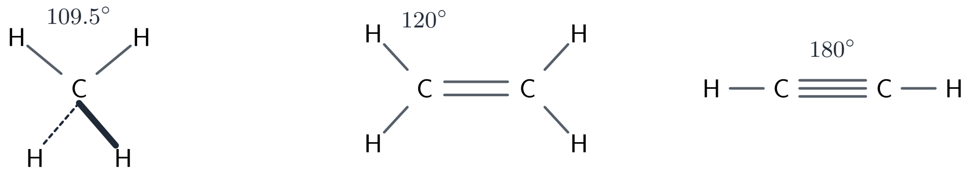
Organic molecules have definite three-dimensional shapes.

Organic molecules can be straight-chained, branched or **cyclic** 环状 (in a ring).

The shape around a carbon depends on its **hybridisation** 杂化:

Hybridisation	Bonds	Shape	Angle
sp^3	4 single	tetrahedral	109.5°
sp^2	1 double + 2 single	**planar** 平面 (flat)	120°
sp	1 triple (or 2 doubles)	linear	180°

Every single bond is a **sigma bond** σ 键, made by direct overlap. A double bond is one sigma bond plus one **pi bond** π 键, made by sideways overlap of p orbitals. Ethene is planar because of its sp^2 carbons.



sp^3: 4 single bonds
tetrahedral

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

sp: 1 triple bond
linear

The shape at a carbon follows from its hybridisation: sp^3 is tetrahedral (109.5°), sp^2 is planar (120°), sp is linear (180°)

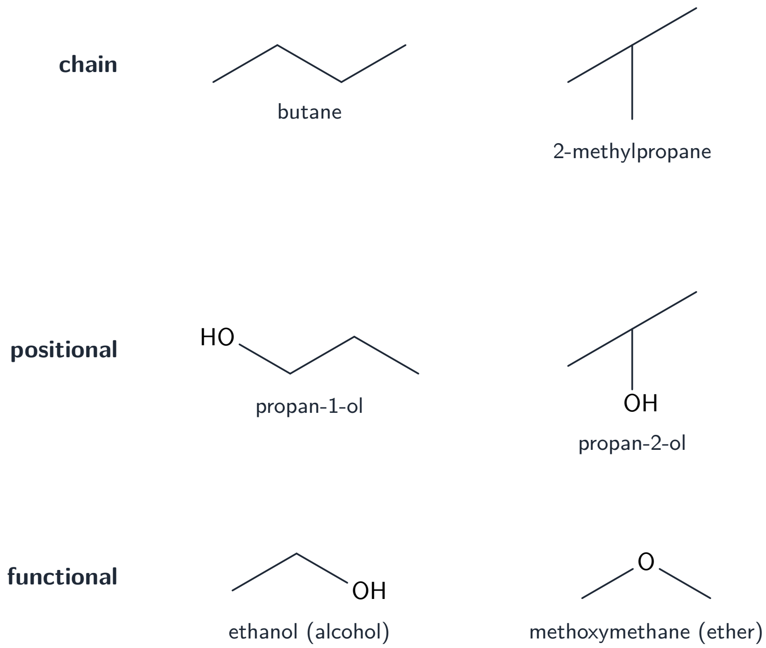
Isomerism

Isomers are compounds with the same molecular formula but a different arrangement of atoms. This is called **isomerism** 异构.

Structural isomerism

In **structural isomerism** 结构异构 the atoms are joined in a different order. There are three kinds:

- **chain isomerism** 链异构: the carbon chain is branched in different ways.
- **positional isomerism** 位置异构: the functional group is on a different carbon.
- **functional group isomerism** 官能团异构: the atoms form a different functional group (for example an alcohol and an ether).

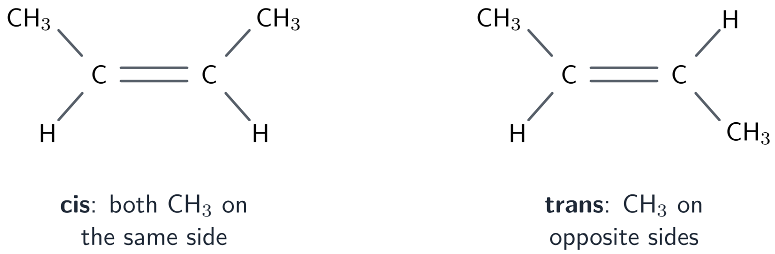


The three kinds of structural isomerism — chain, positional and functional-group — each pair sharing the same molecular formula

Stereoisomerism

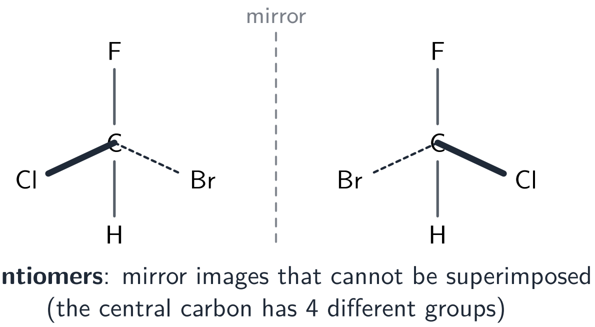
In **stereoisomerism** 立体异构 the atoms are joined in the same order but point in different directions in space.

- **geometrical isomerism** 几何异构 (cis/trans) happens at a C=C double bond. The pi bond stops the two carbons rotating (**restricted rotation** 受限旋转), so groups are fixed on the same side (**cis** 顺式) or opposite sides (**trans** 反式).



Cis–trans isomerism at a C=C bond: the methyl groups are fixed on the same side (cis) or opposite sides (trans) because the bond cannot rotate

- **optical isomerism** 旋光异构 happens at a **chiral** 手性 carbon — a **chiral centre** 手性中心 is a carbon with four different groups attached. Such a carbon gives two mirror-image forms called **enantiomers** 对映体. A molecule may have more than one chiral centre.



Optical isomerism: a carbon with four different groups gives two mirror-image forms (enantiomers) that cannot be superimposed

From a molecular formula you can deduce the possible isomers by trying different chains, positions and functional groups.

Worked example. Explain why but-2-ene shows **cis-trans** (E/Z) isomerism but but-1-ene does not. Stereoisomerism at a C=C needs two things: restricted rotation about the double bond (both alkenes have that), **and** two **different** groups on **each**

of the two double-bond carbons. In but-2-ene, $CH_3CH{=}CHCH_3$, each double-bond carbon carries an H and a CH_3 - different, so the methyl groups can sit on the same side (**cis** / **Z**) or on opposite sides (**trans** / **E**). In but-1-ene, $CH_2{=}CHCH_2CH_3$, the first carbon carries **two hydrogens** - identical, so swapping them changes nothing and only one form exists. Test **each** double-bond carbon separately: two identical groups on **either** carbon kills the isomerism, however different the other carbon may be.

Exam tips

- Know the difference between **general, molecular, structural, displayed and skeletal** formulas — questions ask for a specific one.
- Name systematically: longest chain, lowest locants, substituents alphabetical; a wrong locant loses the mark.
- Classify each reaction by **type and reagent** (addition, substitution, elimination, oxidation).
- **E/Z isomerism** needs restricted rotation about a $C = C$ **and** two different groups on each carbon.