

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.

Image: Glasbruch2007, CC BY-SA 3.0 (commons.wikimedia.org)

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.

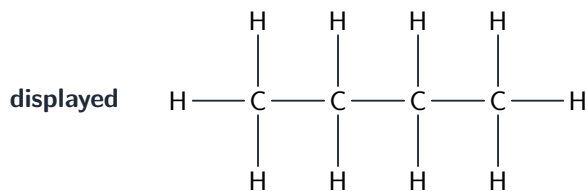
A **functional group** 官能团 is the reactive part of a molecule. It decides the physical and chemical properties of the compound, so molecules with the same functional group behave alike (for example the -OH group in alcohols).

Types of formula

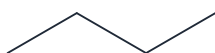
Formula	What it shows
general formula 通式	the pattern for a whole family, e.g. alkanes are $\text{C}_n\text{H}_{2n+2}$
molecular formula 分子式	the actual number of each atom, e.g. C_4H_{10}
structural formula 结构式	the groups in order, e.g. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$
displayed formula 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 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$



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



one electron each
 $\Rightarrow$ two **radicals**

heterolytic fission



both electrons to one
 $\Rightarrow$ 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 $\text{C}=\text{C}$ double bond.

nucleophile



a lone pair attacks
the electron-poor
($\delta+$) carbon

electrophile



it is drawn to the
electron-rich $\text{C}=\text{C}$
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 $\text{C}=\text{C}$ 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 $[\text{O}]$ stands for one oxygen atom from an oxidising agent, and $[\text{H}]$ 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.

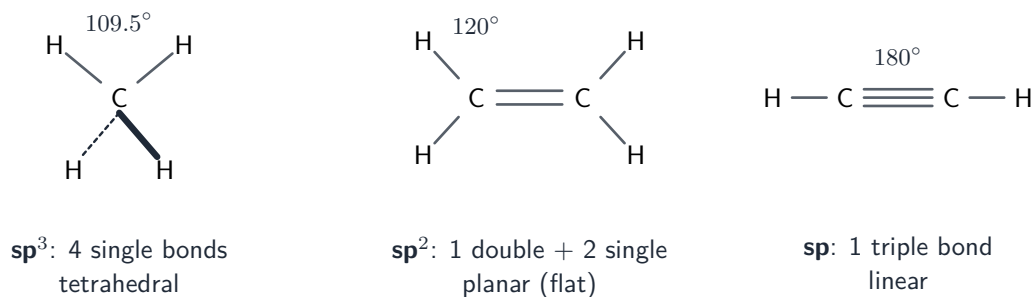
Image: 山本海行, CC BY-SA 4.0 (commons.wikimedia.org)

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.



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

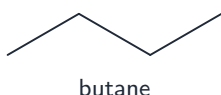
Isomers are compounds with the same molecular formula but a different arrangement of atoms. This is called **isomerism** 异构.

Structural isomerism

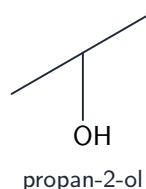
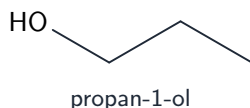
In **structural isomerism** 结构异构 the atoms are joined in a different order. There are three kinds:

- **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).

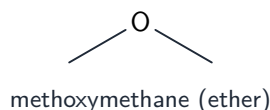
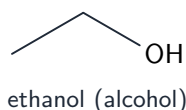
chain



positional



functional

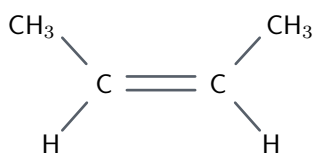


The three kinds of structural isomerism —chain, positional and functional-group —each pair sharing the same molecular formula

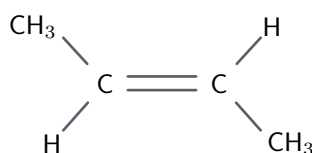
Stereoisomerism

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).



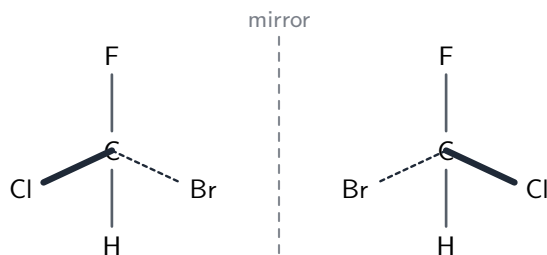
cis: both CH₃ on the same side



trans: CH₃ on opposite sides

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.



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

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, $\text{CH}_3\text{CH}=\text{CHCH}_3$, 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, $\text{CH}_2=\text{CHCH}_2\text{CH}_3$, 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.