Introduction to Organic Chemistry

A-Level Chemistry ▪ Topic 13

A-Level Chemistry

What we will cover

1. Types of formula
2. Bond fission
3. Nucleophiles & electrophiles
4. Mechanisms
5. Hybridisation & shapes
6. Isomerism

the feedstock of organics

1 Formulas and reactions

Types of formula

empirical

CH_2 – simplest ratio

molecular

C_2H_4 – actual numbers

structural

$CH_2{=}CH_2$ – how they join

displayed

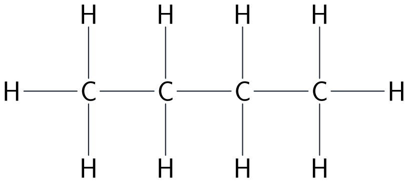
every bond drawn

Types of formula, in detail

molecular C_4H_{10}

structural $CH_3CH_2CH_2CH_3$

displayed



skeletal

> The same molecule (butane) shown four ways – molecular, structural, displayed and skeletal – eac

The formula types, and the reaction types

empirical formula 实验式	the simplest whole-number ratio of atoms
molecular formula	the actual number of each atom in one molecule
displayed formula 结构式	every atom and every bond drawn out
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
organic redox	[O] stands for one oxygen atom from an oxidising agent, and [H] for one hydrogen from a reducing agent

> [O] and [H] are a shorthand that keeps organic equations balanced without writing out the whole oxidising agent. Use them – the mark scheme does.

Five ways to write the same compound

General formula	The pattern for a whole family: alkanes are C_nH_{2n+2}.
Molecular formula	The actual number of each atom: C_4H_{10}.
Structural formula	The groups in order: $CH_3CH_2CH_2CH_3$.
Displayed formula	Every atom and every bond drawn out – what a mechanism question needs.
Skeletal formula	Lines for bonds, carbons at the corners, hydrogens on carbon not shown.

A **homologous series** 同系列 is a family sharing one functional group and one general formula, each member differing by CH_2.

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.

Bond fission

- **homolytic fission** 均裂 – one electron each → two **free radicals** 自由基
- **heterolytic fission** 异裂 – both electrons to one atom → two ions

homolytic fission

$$\mathrm{Cl} \overset{\bullet\bullet}{\text{———}} \mathrm{Cl}$$

$$\mathrm{Cl}\bullet \quad + \quad \bullet\mathrm{Cl}$$

one electron each

$\Rightarrow$ two **radicals**

heterolytic fission

$$\mathrm{C} \overset{\bullet\bullet}{\text{———}} \mathrm{Br}$$

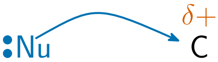
$$\mathrm{C}^{+} \quad + \quad :\mathrm{Br}^{-}$$

both electrons to one

$\Rightarrow$ two **ions**

Nucleophiles and electrophiles

nucleophile



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

electrophile

it is drawn to the electron-rich C=C double bond

- a **nucleophile** 亲核试剂 (lone pair) attacks an electron-poor centre
- an **electrophile** 亲电试剂 is drawn to an electron-rich centre (C=C)

Reaction types: **addition** 加成, **substitution** 取代, **elimination** 消去, **hydrolysis** 水解.

Mechanisms

free-radical substitution 自由基取代 – alkanes

electrophilic addition 亲电加成 – alkenes

nucleophilic substitution 亲核取代 – halogenoalkanes

nucleophilic addition 亲核加成 – carbonyls

Free-radical steps: **initiation** 引发 → **propagation** 增长 → **termination** 终止. A **curly arrow** 弯箭头 shows a pair of electrons moving.

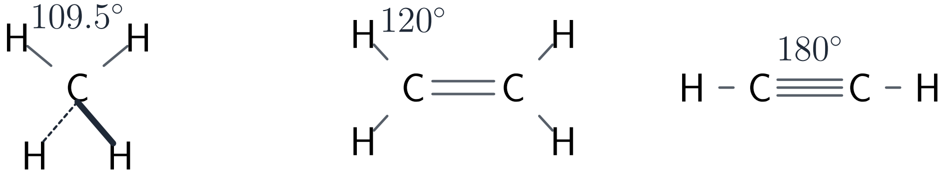
2 Shape and isomerism

Hybridisation and shapes

- sp^3 – tetrahedral, $109.5°$
- sp^2 – planar, $120°$ (ethene)
- sp – linear, $180°$

Single $= \sigma$; double $= \sigma + \pi$.

Hybridisation and shapes, in detail



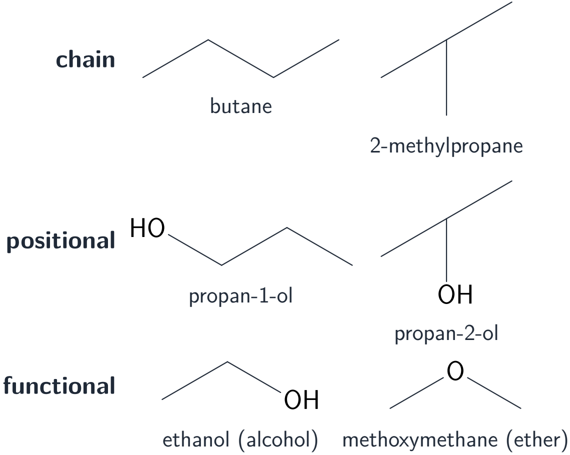
sp^3: 4 single bonds
tetrahedral

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 ($180°$)

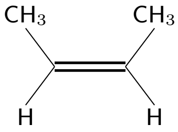
Structural isomerism



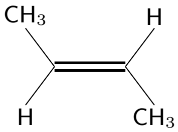
Same molecular formula, atoms joined differently:

- **chain** 链异构
- **positional** 位置异构
- **functional group** 官能团异构

Stereoisomerism

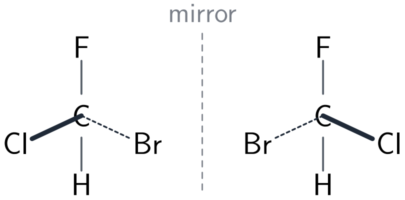


cis
both CH_3
same side

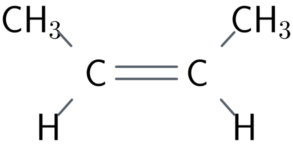


trans
CH_3
opposite sides

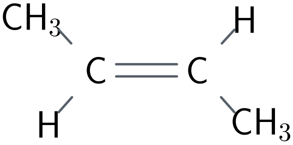
cis vs trans at C=C



Stereoisomerism, continued



cis: both CH_3 on the same side



trans: CH_3 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

Isomerism, and where stereoisomerism comes from

structural isomerism	the atoms are joined in a different order
chain, position, functional group 官能团	the three kinds – a different skeleton, a different position, or a different group entirely
stereoisomerism 立体异构	the atoms are joined in the same order but point in different directions in space
cis–trans	restricted rotation about a C=C double bond, or around a ring (**cyclic** 环状)
optical isomerism	a **chiral centre** 手性中心: a carbon with four different groups
the test	a chiral molecule is non-superimposable on its mirror image, and rotates plane-polarised light

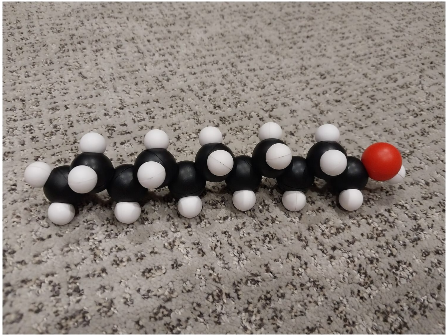
> Look for the C=C or the four-different-groups carbon. Those two features are what *make* a molecule capable of stereoisomerism at all.

The kinds of isomerism

Chain isomerism	Structural: the carbon skeleton is branched differently.
Positional isomerism	**Positional isomerism 位置异构**: the same functional group sits on a different carbon.
Functional group isomerism	**Functional group isomerism 官能团异构**: the same atoms form a *different* functional group – an alcohol and an ether.
Geometrical isomerism	Stereo: **geometrical isomerism 几何异构** (cis/trans) at a C=C double bond, because the double bond cannot rotate.
Optical isomerism	Stereo: a carbon with four different groups gives two non-superimposable mirror images.

A **saturated** 饱和 compound has only single C–C bonds; an **unsaturated** 不饱和 one has a double or triple bond – and that is exactly what makes geometrical isomerism possible.

Shapes of organic molecules



Organic molecules have definite three-dimensional shapes.

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.

3 Recap

Worked example – structural isomers

Draw and name the structural isomers of C_4H_{10}, and state the type of isomerism.

- Straight chain: $CH_3CH_2CH_2CH_3$ – **butane**.
- Branched: $(CH_3)_3CH$ – **2-methylpropane**.
- There are only two: a 3-carbon chain cannot take a CH_3 anywhere else.
- Same molecular formula, different skeleton $\Rightarrow$ chain isomerism.

Isomers share a molecular formula. **Chain** = different skeleton; **position** = group moved; **functional group** = a different group entirely.

Topic 13 – key takeaways

1 Functional group

the reactive part sets the properties

2 Bond fission

homolytic (radicals) vs heterolytic (ions)

3 Shapes

sp^3/sp^2/sp give tetrahedral/planar/linear

4 Isomerism

structural; cis/trans; optical (chiral)

Breaking bonds

- **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.

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.

Check yourself

1. Homolytic fission makes two of what?
2. A nucleophile attacks an electron-rich or electron-poor centre?
3. What is the shape at an sp^2 carbon?
4. A chiral carbon has how many different groups?

Answers **1.** free radicals **2.** electron-poor **3.** planar $(120°)$ **4.** four