Functional groups: classification of organic compounds

Structure 3.2 · SL

Same formula, different connections

> Molecular formula alone does not determine structure or properties.

- Ethanol and methoxymethane share C_2H_6O.
- An O–H donor changes interactions between pure molecules.

Interconvert formula types

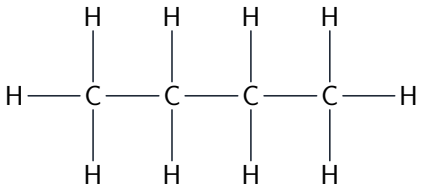
molecular

C_4H_{10}

condensed

$CH_3CH_2CH_2CH_3$

full structural



skeletal



Count carbon corners and ends; retain heteroatoms and their attached H.

Build a three-dimensional carbon model

A flat connectivity drawing need not show the actual bond angles.

- An sp^3 carbon has four approximately tetrahedral bond directions.
- C=C centres are approximately planar; a C≡C region is linear.

Recognize whole functional groups

Connection	**Class**
R–OH	alcohol
R–CHO / R–C(=O)–R	aldehyde / ketone
R–COOH / R–COOR	acid / ester
R–O–R / R–C(=O)–NH_2	ether / **primary** amide

Distinguish addition and substitution

Addition

$\mathrm{CH_2{=}CH_2 + H_2 \rightarrow CH_3CH_3}$

Ni catalyst and heat: C=C becomes C–C; two C–H bonds form.

Substitution

$\mathrm{C_2H_5Br + OH^- \rightarrow C_2H_5OH + Br^-}$

Aqueous hydroxide and heat: C–Br is replaced by C–O.

Distinguish oxidation and polymerization

Oxidation

$\mathrm{CH_3CH_2OH + [O] \rightarrow CH_3CHO + H_2O}$

Acidified dichromate; distil ethanal. Carbon loses C–H and gains a second bond to O.

Addition polymerization

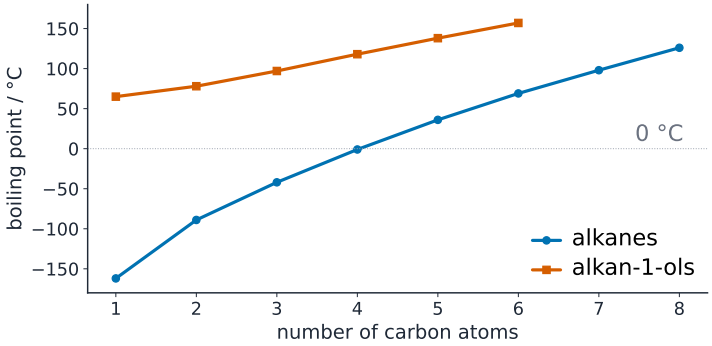
$\mathrm{n CH_2{=}CH_2 \rightarrow [-CH_2 - CH_2-]_n}$

Suitable initiator/catalyst: C=C opens; new C–C links join monomers without a small product.

Use a general formula with its conditions

Simple acyclic series	**General formula**
alkanes	C_nH_{2n+2}
monoalkenes	C_nH_{2n}
monohydric alcohols	$C_nH_{2n+1}OH$
monocarboxylic acids	$C_nH_{2n}O_2$

Explain the normal boiling-point trend



Comparable longer chains have stronger dispersion; alcohols also hydrogen-bond.

Melting requires a packing explanation

> Do not transfer an exact boiling-point order to melting points.

- Crystal packing and symmetry affect the solid.
- Branching can change packing as well as intermolecular contact.

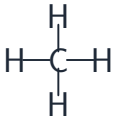
Name a branched parent chain

1. **Structure.** $CH_3CH_2CH(CH_3)CH_3$.
2. **Parent.** Four-carbon chain: butane.
3. **Locant.** Number from the nearer branch: 2-methylbutane.

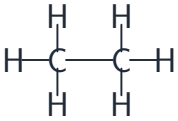
Decision

Include the characteristic group in the parent and apply its locant priority.

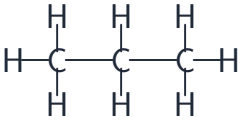
A homologous series



methane
CH_4



ethane
C_2H_6



propane
C_3H_8

each step adds a CH_2 unit

general formula C_nH_{2n+2}

The same general formula, C_nH_{2n+2}

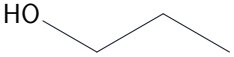
Distinguish structural isomer types

chain



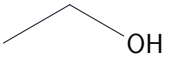
butane

position

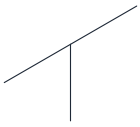


propan-1-ol

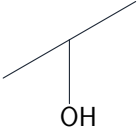
functional group



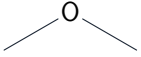
ethanol



2-methylpropane



propan-2-ol



methoxymethane

Same formula; different connectivity.

Classify at the correct atom

Alcohol and halogenoalkane

Propan-2-ol: the OH carbon has two carbon neighbours.

2-Bromopropane: the Br carbon also has two.

Amine

CH_3NH_2 **primary**; $(CH_3)_2NH$ **secondary**.

$(CH_3)_3N$ is **tertiary** despite having no N–H bond.

Check a full structural drawing

1. **Formula.** Butan-1-ol: $C_4H_{10}O$.
2. **Atoms.** $4 + 10 + 1 = 15$ atoms.
3. **Bonds.** A connected acyclic all-single-bond drawing has 14 bonds.

Decision

Its four-carbon skeletal chain has two corners and two ends.

Exam tips

> Check structure and atom counts before interpreting a property.

- Count corners and ends, complete valences and classify at the correct atom.
- Use a parent, locants and explicit reaction or measurement conditions.

Check yourself

Apply the model

Give all four alcohol constitutional isomers of $C_4H_{10}O$.

Compare amine and alcohol classification; explain an ether's hydrogen-bond acceptor role.

Explain why a general formula cannot alone distinguish an alkene from a cycloalkane.