

Functional groups: classification of organic compounds

International Baccalaureate · IB Diploma · Chemistry · HL

Scope and prerequisites

This handout teaches Structure 3.2, Functional groups: classification of organic compounds, for the course first assessed in 2025. Sections marked **AHL** are for Higher Level only.

Prerequisites: covalent bonding and molecular shapes from Structure 2.2, intermolecular forces and hydrogen bonding, and the mole and empirical formulae from Structure 1.4. Use the data booklet for infrared and ^1H NMR data.

Representing organic molecules

■ Same formula, different substances

Ethanol and methoxymethane both have the formula $\text{C}_2\text{H}_6\text{O}$. Ethanol is the liquid in alcoholic drinks and boils at $78\text{ }^\circ\text{C}$; methoxymethane is a gas used in aerosol sprays and boils at $-24\text{ }^\circ\text{C}$. The atoms are the same, but they are joined in a different order. In organic chemistry the formula alone is not enough: you need to show the structure.

■ Types of formula

molecular	C_4H_{10}
condensed	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$
full structural	<pre> H H H H H — C — C — C — C — H H H H H</pre>
skeletal	

Each type of formula shows less detail than the one above it

Formula	What it shows	Butan-1-ol
molecular	the number of atoms of each element	$\text{C}_4\text{H}_{10}\text{O}$
empirical	the simplest whole-number ratio	$\text{C}_4\text{H}_{10}\text{O}$
condensed structural	the atoms on each carbon, in order	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$
full structural	every atom and every bond	all 15 atoms and 14 bonds drawn
skeletal	carbon chain as a zigzag; C and H on carbon left out	a zigzag of 4 corners with OH at one end

In a **skeletal formula** each corner and each line end is a carbon atom, and each carbon has enough hydrogen atoms to make four bonds. Atoms other than C and H (and H atoms on them, as in OH) are always written.

A benzene ring, C_6H_6 , is drawn as a hexagon with a circle inside, which shows the delocalized electrons. A benzene ring attached to a chain is a **phenyl** group, C_6H_5- .

Functional groups and homologous series

■ Functional groups

A **functional group** is the atom or group of atoms that gives a compound its typical reactions. Compounds with the same functional group react in similar ways.

Class	Functional group	Suffix or prefix	Example
alkane	C–C only	-ane	propane, $\text{CH}_3\text{CH}_2\text{CH}_3$
alkene	C=C	-ene	propene, $\text{CH}_2=\text{CHCH}_3$
alkyne	$\text{C}\equiv\text{C}$	-yne	ethyne, $\text{HC}\equiv\text{CH}$
halogenoalkane	–X (F, Cl, Br, I)	fluoro-, chloro-, bromo-, iodo-	bromoethane, $\text{CH}_3\text{CH}_2\text{Br}$
alcohol	–OH (hydroxyl)	-ol	ethanol, $\text{CH}_3\text{CH}_2\text{OH}$
aldehyde	–CHO (carbonyl at the chain end)	-al	ethanal, CH_3CHO

Class	Functional group	Suffix or prefix	Example
ketone	C=O inside the chain (carbonyl)	-one	propanone, <chem>CH3COCH3</chem>
carboxylic acid	-COOH (carboxyl)	-oic acid	ethanoic acid, <chem>CH3COOH</chem>
ether	C-O-C (ether)	alkoxy-	methoxymethane, <chem>CH3OCH3</chem>
ester	-COO- (ester)	-yl -oate	methyl ethanoate, <chem>CH3COOCH3</chem>
amine	-NH ₂ (amino)	-amine	ethylamine, <chem>CH3CH2NH2</chem>
amide	-CONH ₂ (amido)	-amide	ethanamide, <chem>CH3CONH2</chem>

Class	Functional group	Suffix or prefix	Example
nitrile	-C≡N	-nitrile	ethanenitrile, <chem>CH3CN</chem>

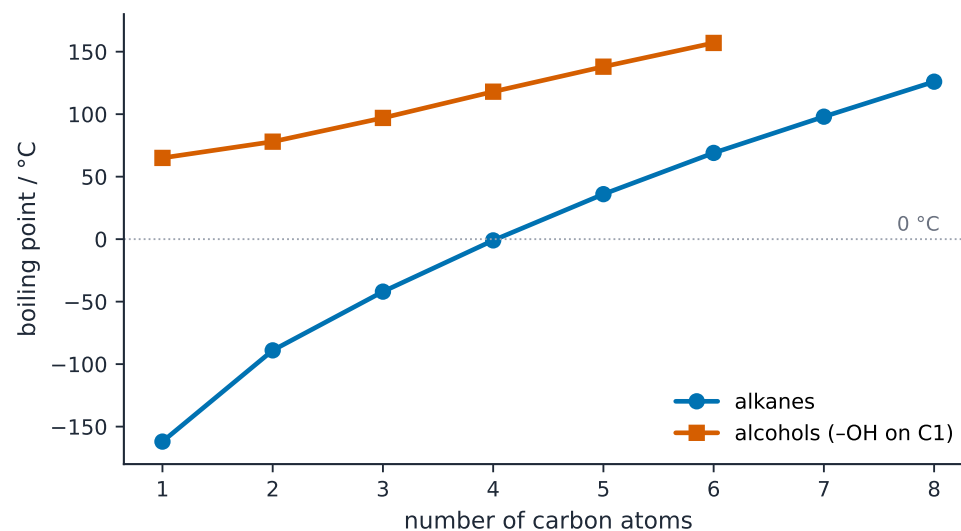
Homologous series

A **homologous series** is a family of compounds with the same functional group and the same general formula.

- Each member differs from the next by CH₂.
- They have similar chemical properties.
- Physical properties, such as boiling point, change gradually along the series.

Series	General formula
alkanes	C_nH_{2n+2}
alkenes	C_nH_{2n}
alcohols	$C_nH_{2n+1}OH$
carboxylic acids	$C_nH_{2n+1}COOH$

Trends in boiling point



Each extra CH₂ raises the boiling point; hydrogen bonding lifts the whole alcohol series

- Each extra CH₂ adds electrons and surface area, so London forces between molecules get stronger and the boiling point rises.
- Branched isomers have lower boiling points than straight chains: the molecules touch over a smaller area.
- Alcohols and carboxylic acids boil much higher than alkanes of similar mass because their molecules form hydrogen bonds.

Naming organic compounds

The IUPAC rules

The IUPAC system gives each compound one name built from three parts: prefix, stem and suffix.

- Find the longest carbon chain that contains the functional group. Its length gives the stem.

Carbons	1	2	3	4	5	6
Stem	meth-	eth-	prop-	but-	pent-	hex-

- Add the suffix of the main functional group (-ene, -ol, -al, -one, -oic acid).
- Number the chain from the end that gives the functional group the lowest number. Put the number before the suffix: but-1-ene, propan-2-ol.
- Name side chains (methyl-, ethyl-) and halogens (chloro-, bromo-) as prefixes with their position numbers, in alphabetical order.
- Use di-, tri- for repeated groups: 2,2-dimethylpropane.

■ Worked examples

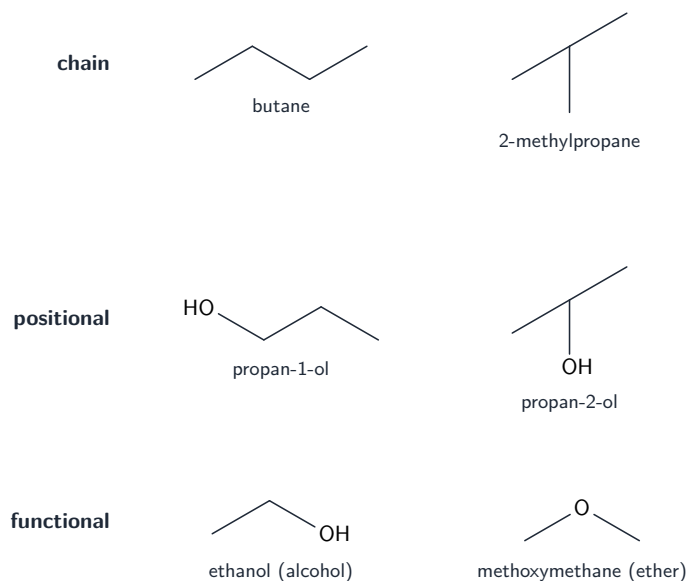
- $\text{CH}_3\text{CH}(\text{OH})\text{CH}_3$: 3 carbons, $-\text{OH}$ on carbon 2 $\rightarrow$ **propan-2-ol**.
- $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$: longest chain 4 carbons, methyl on carbon 2 $\rightarrow$ **2-methylbutane** (not 3-methylbutane).
- $\text{CH}_2=\text{CHCH}_2\text{CH}_3$: 4 carbons, $\text{C}=\text{C}$ starting at carbon 1 $\rightarrow$ **but-1-ene**.
- $\text{CH}_3\text{CHBrCH}_3$: **2-bromopropane**.
- $\text{CH}_3\text{CH}_2\text{COOH}$: 3 carbons including the COOH carbon $\rightarrow$ **propanoic acid**.

An aldehyde or carboxylic acid group is always on carbon 1, so it needs no number.

Structural isomers

■ Same molecular formula, different structure

Structural isomers have the same molecular formula but a different structural formula: the atoms are joined in a different order.



Structural isomers differ in their chain, in the position of a group, or in the functional group itself

Type	What changes	Example, $\text{C}_n\text{...}$
chain	the carbon skeleton is branched differently	butane and 2-methylpropane, C_4H_{10}
position	the functional group sits on a different carbon	propan-1-ol and propan-2-ol, $\text{C}_3\text{H}_8\text{O}$
functional group	the atoms form a different functional group	ethanol and methoxymethane, $\text{C}_2\text{H}_6\text{O}$

Alcohols are classified by the carbon that holds the $-\text{OH}$: **primary** (that carbon has one other carbon attached), **secondary** (two) or **tertiary** (three). Propan-1-ol is primary; propan-2-ol is secondary; 2-methylpropan-2-ol is tertiary. Halogenoalkanes are classified the same way.

Identifying compounds

■ Index of hydrogen deficiency

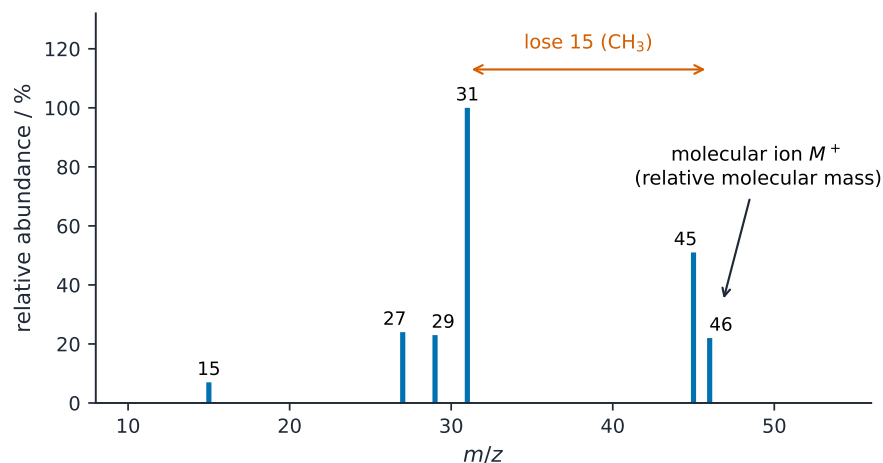
The **index of hydrogen deficiency** (IHD) counts how many rings and π bonds a molecule has. Each ring or double bond counts 1; a triple bond counts 2. For a compound $\text{C}_c\text{H}_h\text{N}_n\text{O}_o\text{X}_x$ (X = halogen):

$$\text{IHD} = \frac{2c + 2 + n - h - x}{2}$$

Oxygen does not affect the IHD. For $\text{C}_3\text{H}_6\text{O}$: $(6 + 2 - 6)/2 = 1$, so one $\text{C}=\text{C}$, one $\text{C}=\text{O}$ or one ring. Benzene, C_6H_6 : $(12 + 2 - 6)/2 = 4$ (one ring and three double bonds).

■ Mass spectrometry

In a **mass spectrometer** molecules are ionized and break into fragments. The spectrum shows each ion's mass-to-charge ratio, m/z .



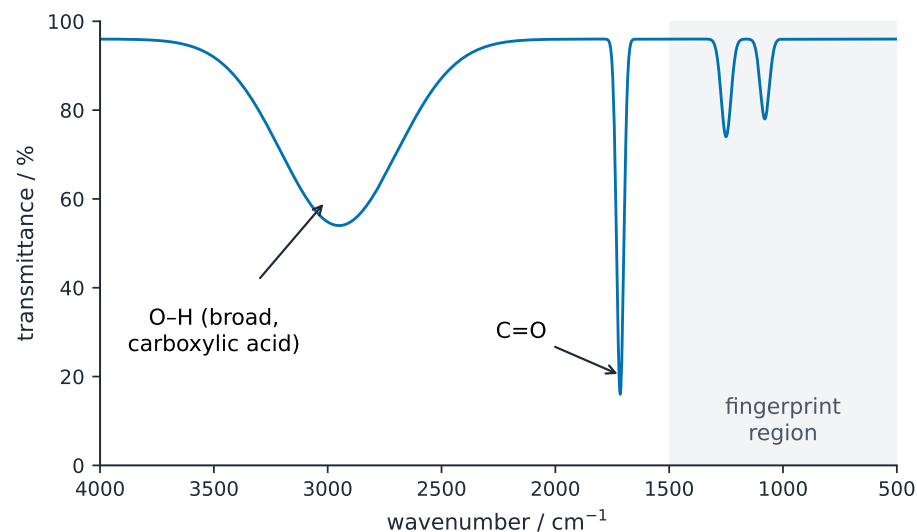
M^+ (highest m/z) $\approx M_r$ · gaps = masses lost

The molecular ion gives M_r ; the gaps between peaks show which pieces broke off

- The **molecular ion** peak, at the highest m/z , gives the relative molecular mass: 46 for ethanol.
- Fragment peaks show what was lost. Common losses: 15 (CH_3), 17 (OH), 29 (C_2H_5 or CHO), 31 (CH_3O), 45 (COOH).
- For ethanol, 31 is CH_2OH^+ : the molecule lost CH_3 ($46 - 15$).

■ Infrared spectroscopy

Bonds absorb infrared radiation at frequencies that make them vibrate. Each type of bond absorbs in its own range, so an IR spectrum shows which **bonds**, and so which functional groups, are present. The x-axis is the **wavenumber** in cm^{-1} ; absorptions appear as dips in transmittance.



A broad O-H band and a strong C=O band together mean a carboxylic acid

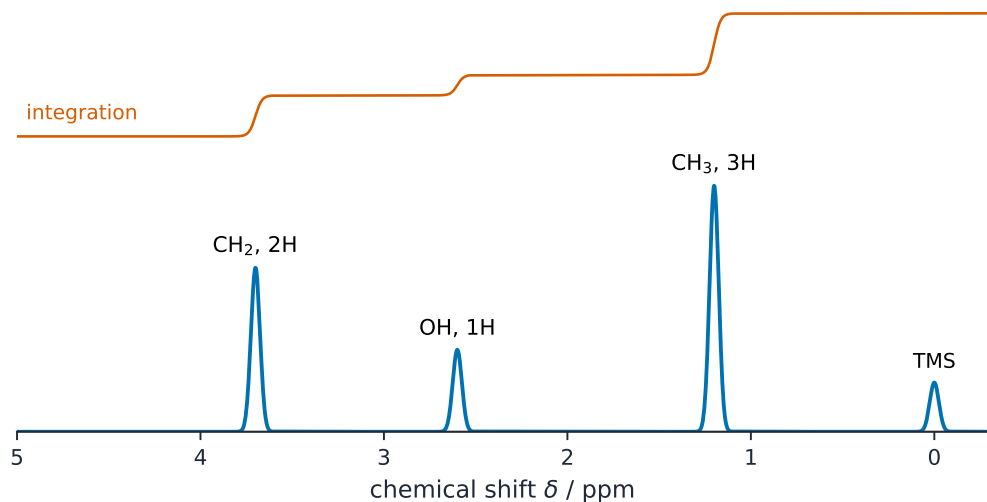
Bond	Wavenumber / cm^{-1} (data booklet)	Look
O-H in alcohols	3200–3600	broad
O-H in carboxylic acids	2500–3000	very broad
N-H	3300–3500	medium
C-H	2850–3090	strong, in most organic molecules
C=O	1700–1750	strong, sharp
C=C	1620–1680	medium
C-O	1050–1410	strong

Below about 1500 cm^{-1} lies the **fingerprint region**: a complex pattern that is unique to each compound and can be matched to a database.

^1H NMR spectroscopy

■ What the spectrum shows

In ^1H **nuclear magnetic resonance** (NMR) spectroscopy, hydrogen nuclei in a strong magnetic field absorb radio waves. Hydrogen atoms in different surroundings absorb at slightly different frequencies.



Three peaks for three hydrogen environments; the integration gives their ratio

- **Number of peaks** = the number of different hydrogen environments. Ethanol, $\text{CH}_3\text{CH}_2\text{OH}$, has three.
- **Chemical shift**, δ in ppm, tells you what each hydrogen is near. Electronegative atoms nearby move the peak to a higher shift.
- **Integration**: the area under each peak is proportional to the number of hydrogen atoms in that environment: 2 : 1 : 3 for ethanol.
- **TMS**, tetramethylsilane, $\text{Si}(\text{CH}_3)_4$, is the reference at $\delta = 0$. It gives one strong peak away from most others, and it is inert.

Hydrogen type	δ / ppm (data booklet)
R- CH_3	0.9–1.0
CH next to C=O ($-\text{CH}_2-\text{CO}-$)	2.2–2.7
CH next to O ($-\text{O}-\text{CH}_2-$)	3.3–3.7
CH next to the O of an ester ($-\text{COO}-\text{CH}_2-$)	3.7–4.8
R-OH	1.0–6.0
on a benzene ring	6.9–9.0
-CHO	9.4–10.0
-COOH	9.0–13.0

■ Worked example: using several techniques

A compound has molecular formula $\text{C}_3\text{H}_6\text{O}_2$.

- IHD = $(6 + 2 - 6)/2 = 1$: one C=O (or C=C or ring).
- IR: strong peak at 1740 cm^{-1} (C=O), no broad band at $2500\text{--}3600\text{ cm}^{-1}$, so no O-H: not an acid. An ester is likely.
- MS: molecular ion at m/z 74, which matches M_r for $\text{C}_3\text{H}_6\text{O}_2$.
- ^1H NMR: three peaks at 3.7 (3H), 2.3 (2H) and 1.1 (3H). The 3.7 peak is CH_3 next to O; the 2.3 peak is CH_2 next to C=O.

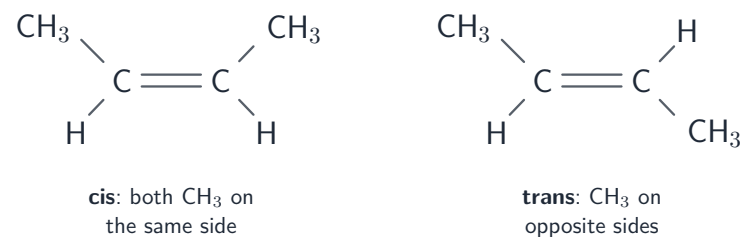
The compound is methyl propanoate, $\text{CH}_3\text{CH}_2\text{COOCH}_3$.

AHL: Stereoisomers

■ What stereoisomers are

Stereoisomers have the same structural formula (the same atoms joined in the same order) but a different arrangement of the atoms in space.

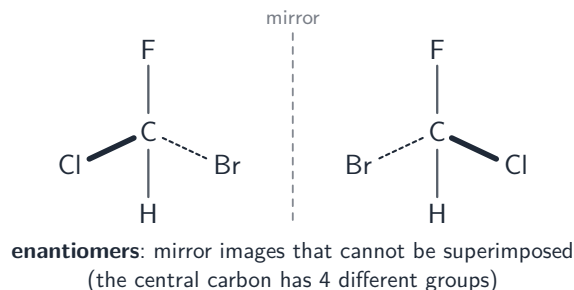
■ Cis-trans isomers



Rotation about $\text{C}=\text{C}$ is restricted, so the two forms do not interconvert

- A $\text{C}=\text{C}$ double bond cannot rotate, because rotation would break the π bond.
- **Cis-trans isomers** form when each carbon of the $\text{C}=\text{C}$ has two different groups.
- **Cis:** the same groups on the same side. **Trans:** on opposite sides.
- Ring compounds can show the same isomerism, because a ring also stops rotation: cis- and trans-1,2-dichlorocyclopropane.
- Cis and trans isomers often have different physical properties. Cis-but-2-ene boils at 4°C and trans-but-2-ene at 1°C .

■ Optical isomers



A carbon with four different groups has two mirror-image forms

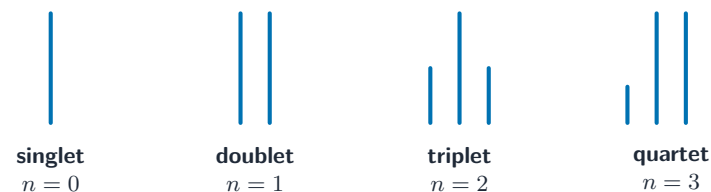
- A **chiral** carbon atom (a stereocentre) has four different atoms or groups attached.
- A molecule with one chiral carbon exists as two **enantiomers** : mirror images that cannot be superimposed, like a left and a right hand.
- Enantiomers have the same physical properties and the same chemical reactions, except with other chiral substances.
- Enantiomers rotate **plane-polarized light** by the same angle in opposite directions. A polarimeter measures this rotation.
- A **racemic mixture** has equal amounts of the two enantiomers. Their rotations cancel, so it does not rotate the light.

Example: butan-2-ol, $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$. Carbon 2 carries H, OH, CH_3 and C_2H_5 , four different groups, so it is chiral. Many drugs are chiral, and the two enantiomers can act very differently in the body.

AHL: Splitting in ^1H NMR

■ The $n + 1$ rule

In a high-resolution spectrum each peak can be split into several lines. The splitting comes from hydrogen atoms on the **neighbouring** carbon atoms (spin-spin coupling).



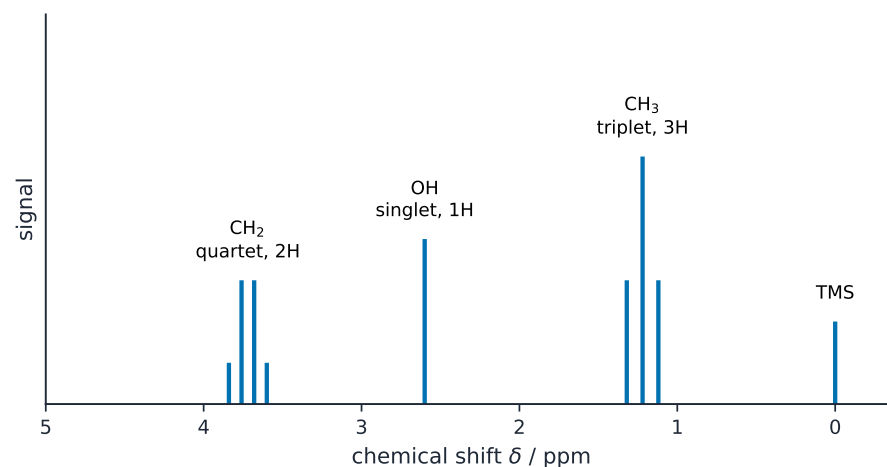
n equivalent neighbours split a peak into $n + 1$ lines

A peak with n equivalent neighbouring H atoms splits into $n + 1$ lines

Neighbouring H	Lines	Name	Line heights
0	1	singlet	1
1	2	doublet	1 : 1
2	3	triplet	1 : 2 : 1
3	4	quartet	1 : 3 : 3 : 1

- Hydrogen atoms in the same environment do not split each other.
- The O–H hydrogen usually appears as a singlet: it exchanges quickly between molecules and does not couple.

■ Reading a high-resolution spectrum



$n+1$ rule · integration 3 : 2 : 1 · TMS = 0 ppm

CH₃ next to CH₂ gives a triplet; CH₂ next to CH₃ gives a quartet

In ethanol, CH_3 has 2 neighbouring H (on CH_2), so it is a triplet; CH_2 has 3 neighbouring H (on CH_3), so it is a quartet. A triplet with a quartet is the sign of an ethyl

group, CH_3CH_2- .

In methyl propanoate from the worked example, the 3.7 peak ($\text{O}-\text{CH}_3$) is a singlet, because its carbon is joined to O, which carries no H; the CH_2 is a quartet and the CH_3 at 1.1 is a triplet.

Practice

1. Draw the skeletal formula of pentan-2-ol and write its condensed structural formula.
2. Name: (a) $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$, (b) $\text{CH}_3\text{COCH}_2\text{CH}_3$, (c) $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3$, (d) $(\text{CH}_3)_3\text{CBr}$.
3. Give the general formula of the alkenes and the formula of the alkene with 5 carbon atoms.
4. Explain why butan-1-ol (117°C) boils at a much higher temperature than pentane (36°C), although their M_r values are similar.
5. Draw and name the structural isomers of $\text{C}_4\text{H}_{10}\text{O}$ that are alcohols, and classify each as primary, secondary or tertiary.
6. Calculate the IHD of $\text{C}_4\text{H}_8\text{O}_2$ and of $\text{C}_6\text{H}_5\text{Cl}$.
7. A mass spectrum has peaks at m/z 58 (molecular ion) and 43. Suggest the ion at 43 and what was lost, for propanone.
8. An IR spectrum has a broad band at 3350 cm^{-1} and no absorption at $1700\text{--}1750\text{ cm}^{-1}$. Which functional group is present, and which is absent?
9. How many peaks, and in what ratio, are in the ^1H NMR spectrum of (a) propanone, (b) propan-1-ol, (c) methyl ethanoate?
10. Explain why TMS is used as the reference in ^1H NMR.
11. **AHL.** Explain why but-2-ene shows cis–trans isomerism but but-1-ene does not.
12. **AHL.** Identify the chiral carbon in 2-chlorobutane and describe how its two enantiomers could be told apart.
13. **AHL.** Predict the splitting of each peak in the ^1H NMR spectrum of chloroethane, $\text{CH}_3\text{CH}_2\text{Cl}$.
14. **AHL.** $\text{C}_4\text{H}_8\text{O}_2$ shows IR absorptions at 1740 cm^{-1} and no $\text{O}-\text{H}$ band. Its ^1H NMR spectrum has a singlet (3H) at 2.0, a quartet (2H) at 4.1 and a triplet (3H) at 1.3. Identify the compound.

Answers.

1. Zigzag of 5 carbons with OH on the second carbon; $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_2\text{CH}_3$.
2. (a) butanal, (b) butanone, (c) ethyl propanoate, (d) 2-bromo-2-methylpropane.
3. C_nH_{2n} ; C_5H_{10} (for example pent-1-ene).
4. Both have London forces of similar strength, but butan-1-ol molecules also form hydrogen bonds through their $-\text{OH}$ groups. More energy is needed to separate them.

5. Butan-1-ol, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ (primary); butan-2-ol, $\text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$ (secondary); 2-methylpropan-1-ol, $(\text{CH}_3)_2\text{CHCH}_2\text{OH}$ (primary); 2-methylpropan-2-ol, $(\text{CH}_3)_3\text{COH}$ (tertiary).
6. $\text{C}_4\text{H}_8\text{O}_2$: $(8 + 2 - 8)/2 = 1$. $\text{C}_6\text{H}_5\text{Cl}$: $(12 + 2 - 5 - 1)/2 = 4$.
7. 43 is CH_3CO^+ ; a CH_3 group (15) was lost: $58 - 15 = 43$.
8. $\text{O}-\text{H}$ of an alcohol is present (broad, $3200\text{--}3600\text{ cm}^{-1}$); $\text{C}=\text{O}$ is absent.
9. (a) 1 peak. (b) 4 peaks, 3 : 2 : 2 : 1 (CH_3 , CH_2 , CH_2 , OH). (c) 2 peaks, 3 : 3.
10. TMS gives one strong peak (12 equivalent H) at a shift away from most organic signals; it is inert and volatile, so it is easy to remove.
11. **AHL.** In but-2-ene each C of the $\text{C}=\text{C}$ carries two different groups (H and CH_3), and the $\text{C}=\text{C}$ cannot rotate. In but-1-ene one carbon of the $\text{C}=\text{C}$ carries two H atoms, so the two “isomers” would be identical.
12. **AHL.** Carbon 2 (bonded to H, Cl, CH_3 and C_2H_5). The enantiomers rotate plane-polarized light by the same angle in opposite directions, measured with a polarimeter.
13. **AHL.** CH_3 : triplet (2 neighbouring H); CH_2 : quartet (3 neighbouring H), at a higher shift because it is next to Cl.
14. **AHL.** Ethyl ethanoate, $\text{CH}_3\text{COOCH}_2\text{CH}_3$: the singlet at 2.0 is CH_3 next to $\text{C}=\text{O}$ (no neighbouring H), the quartet at 4.1 is $\text{O}-\text{CH}_2$ next to CH_3 , the triplet at 1.3 is the CH_3 of the ethyl group.

Exam tips

- Write the IUPAC name with numbers and hyphens exactly: propan-2-ol, not 2-propanol.
- Choose the longest chain that includes the functional group, and number from the end nearer to it.
- In IR, quote the bond and its wavenumber range from the data booklet, not just the functional group.
- In ^1H NMR, the number of peaks is the number of environments; the integration ratio is not the splitting pattern.
- **AHL.** For cis–trans isomerism, check that both carbons of the $\text{C}=\text{C}$ carry two different groups.
- **AHL.** Splitting counts the H atoms on the next carbon, not on the carbon itself.