

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

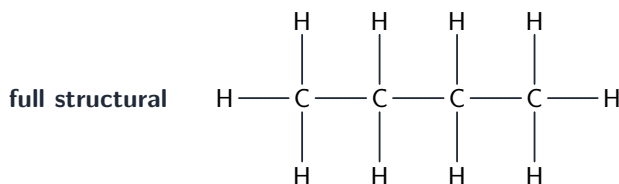
■ Same formula, different substances

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 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$



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, CH ₃ COCH ₃
carboxylic acid	-COOH (carboxyl)	-oic acid	ethanoic acid, CH ₃ COOH
ether	C-O-C (ether)	alkoxy-	methoxymethane, CH ₃ OCH ₃
ester	-COO- (ester)	-yl -oate	methyl ethanoate, CH ₃ COOCH ₃
amine	-NH ₂ (amino)	-amine	ethylamine, CH ₃ CH ₂ NH ₂
amide	-CONH ₂ (amido)	-amide	ethanamide, CH ₃ CONH ₂

Class	Functional group	Suffix or prefix	Example
nitrile	-C≡N	-nitrile	ethanenitrile, CH ₃ CN

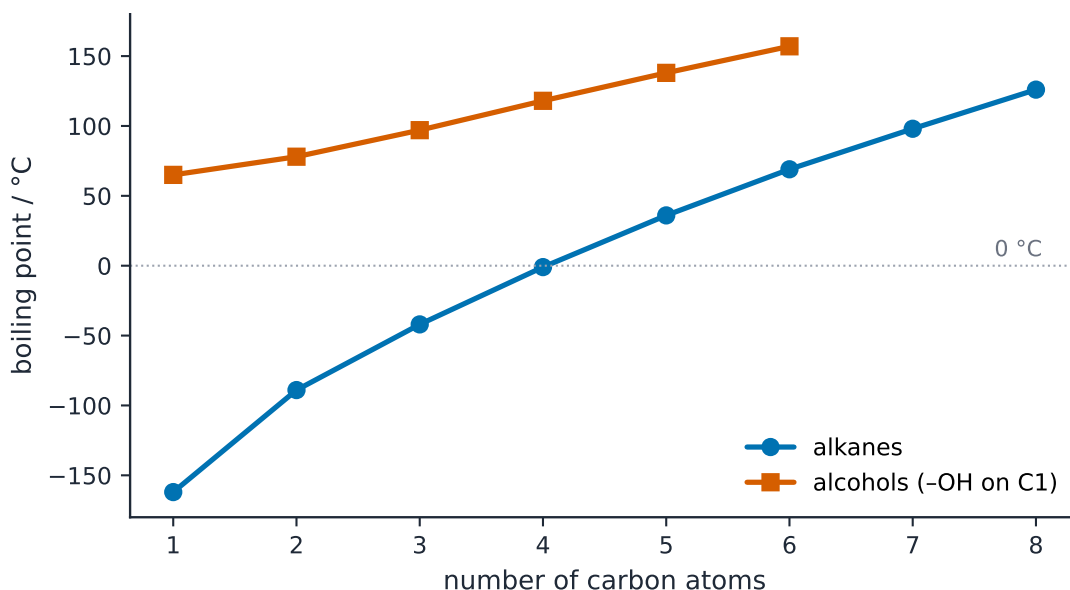
■ Homologous series

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 _n H _{2n+2}
alkenes	C _n H _{2n}
alcohols	C _n H _{2n+1} OH
carboxylic acids	C _n H _{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.

1. 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-

1. Add the suffix of the main functional group (-ene, -ol, -al, -one, -oic acid).
2. 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.
3. Name side chains (methyl-, ethyl-) and halogens (chloro-, bromo-) as prefixes with their position numbers, in alphabetical order.
4. 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**.

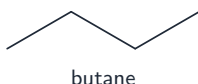
An aldehyde or carboxylic acid group is always on carbon 1, so it needs no number.

Structural isomers

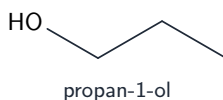
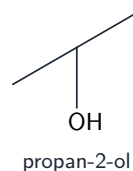
■ Same molecular formula, different structure

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

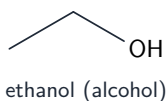
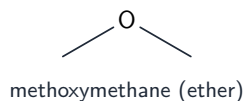
chain



positional



functional



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

Type	What changes	Example, C _n ...
chain	the carbon skeleton is branched differently	butane and 2-methylpropane, C ₄ H ₁₀
position	the functional group sits on a different carbon	propan-1-ol and propan-2-ol, C ₃ H ₈ O
functional group	the atoms form a different functional group	ethanol and methoxymethane, C ₂ H ₆ O

Alcohols are classified by the carbon that holds the –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

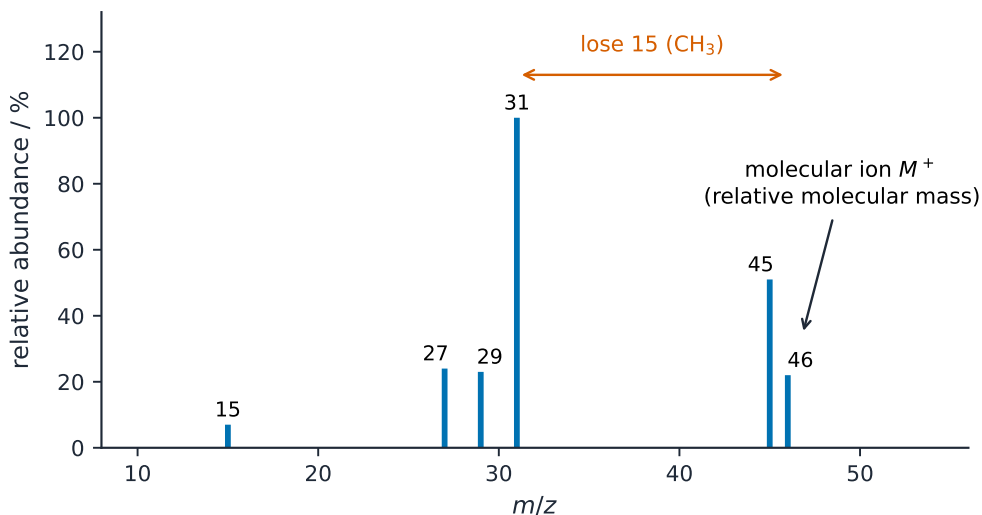
The **index of hydrogen deficiency** (IHD) counts how many rings and π bonds a molecule has. Each ring or double bond counts 1; a triple bond counts 2. For a compound C_cH_hN_nO_oX_x (X = halogen):

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

Oxygen does not affect the IHD. For C₃H₆O: $(6 + 2 - 6)/2 = 1$, so one C=C, one C=O or one ring. Benzene, C₆H₆: $(12 + 2 - 6)/2 = 4$ (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 .



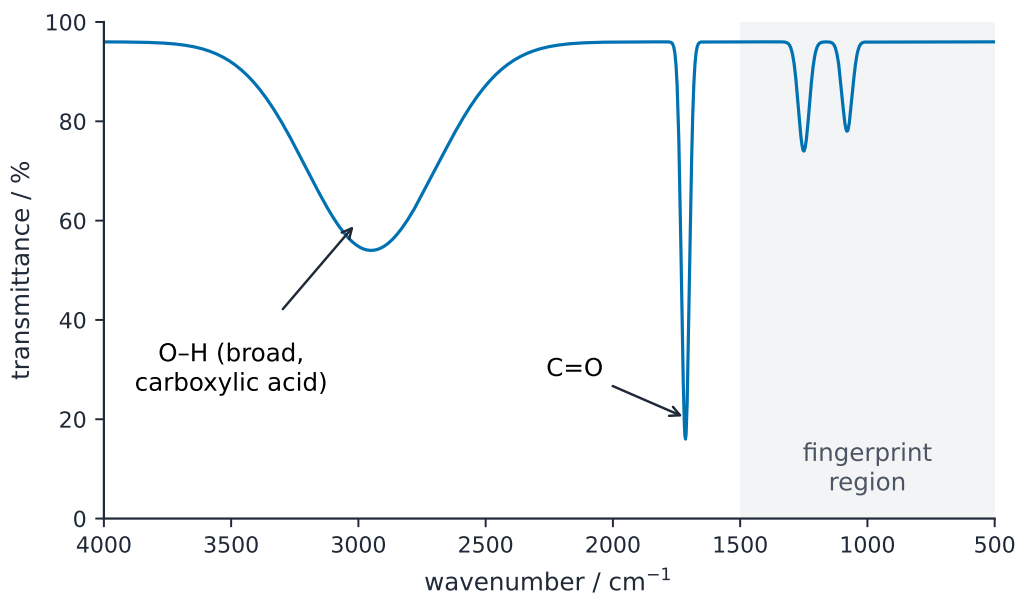
$$M^+ \text{ (highest } m/z) \approx M_r \cdot \text{gaps} = \text{masses lost}$$

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

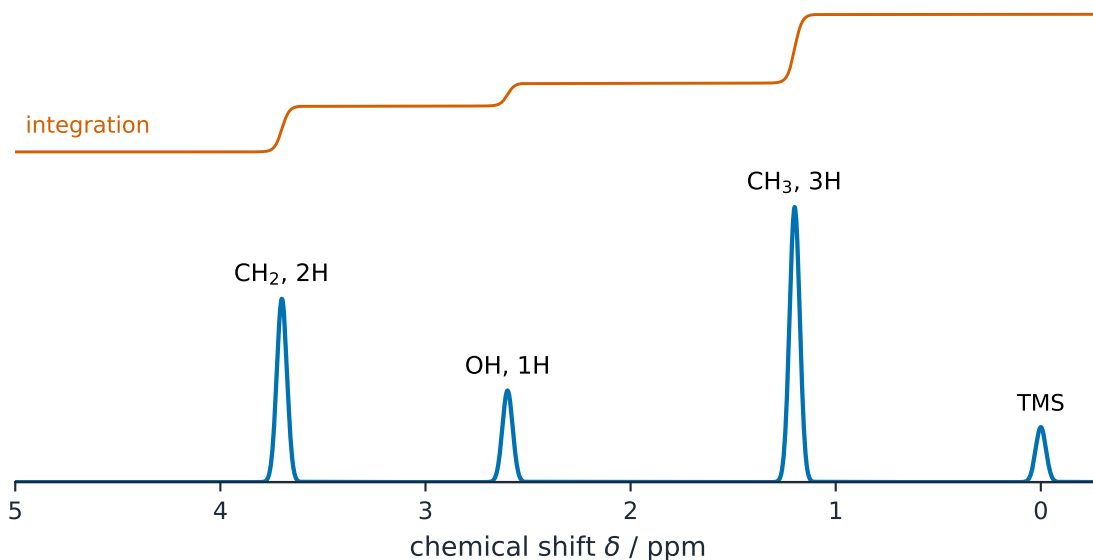
Bond	Wavenumber / cm^{-1} (data booklet)	Look
O–H in alcohols	3200–3600	broad
O–H in carboxylic acids	2500–3000	very broad
N–H	3300–3500	medium
C–H	2850–3090	strong, in most organic molecules
C=O	1700–1750	strong, sharp
C=C	1620–1680	medium
C–O	1050–1410	strong

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)
$\text{R}-\text{CH}_3$	0.9–1.0
CH next to $\text{C}=\text{O}$ ($-\text{CH}_2-\text{CO}-$)	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
$\text{R}-\text{OH}$	1.0–6.0
on a benzene ring	6.9–9.0
$-\text{CHO}$	9.4–10.0
$-\text{COOH}$	9.0–13.0

■ Worked example: using several techniques

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

- $\text{IHD} = (6 + 2 - 6)/2 = 1$: one $\text{C}=\text{O}$ (or $\text{C}=\text{C}$ or ring).
- IR: strong peak at 1740 cm^{-1} ($\text{C}=\text{O}$), 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 $\text{C}=\text{O}$.

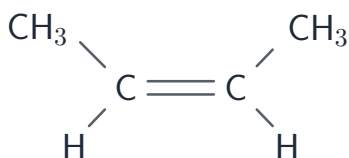
The compound is methyl propanoate, $\text{CH}_3\text{CH}_2\text{COOCH}_3$.

AHL: Stereoisomers

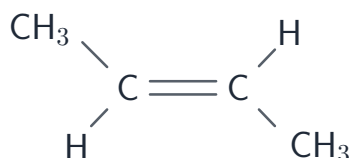
■ What stereoisomers are

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



cis: both CH_3 on the same side

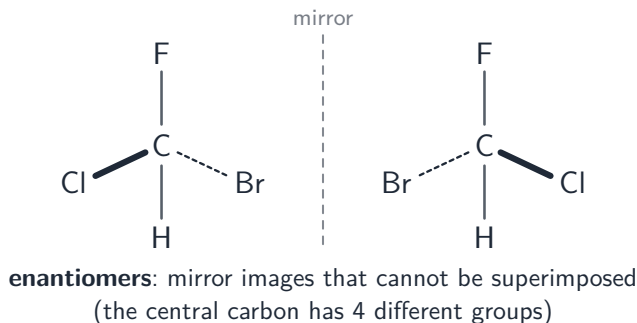


trans: CH_3 on opposite sides

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 $4\text{ }^\circ\text{C}$ and trans-but-2-ene at $1\text{ }^\circ\text{C}$.

■ Optical isomers



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

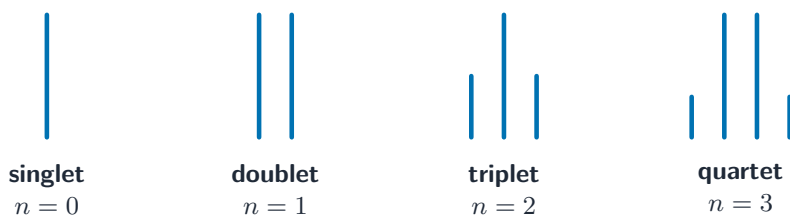
- A **chiral** carbon atom (a stereocentre) has four different atoms or groups attached.
- A molecule with one chiral carbon exists as two **enantiomers** : mirror images that cannot be superimposed, like a left and a right hand.
- Enantiomers have the same physical properties and the same chemical reactions, 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).



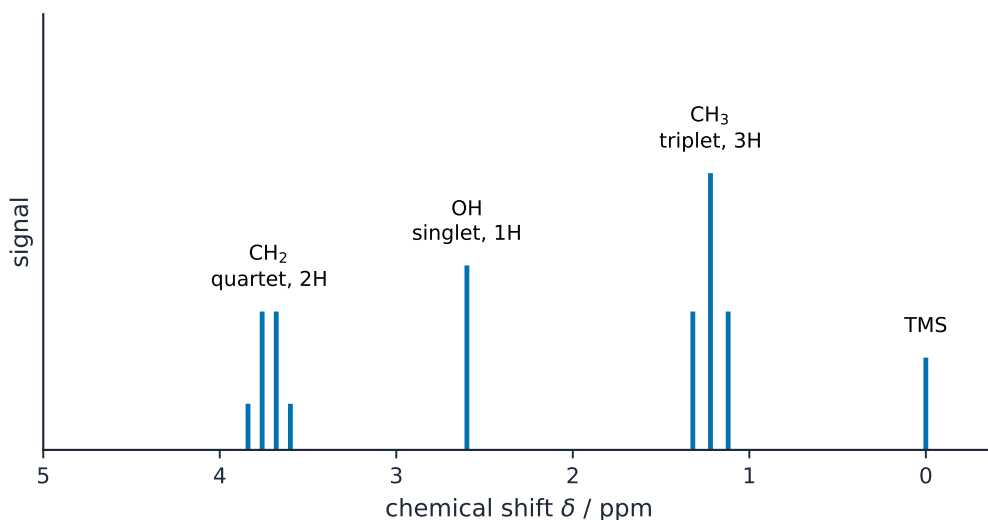
n equivalent neighbours split a peak into $n + 1$ lines

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, CH₃ has 2 neighbouring H (on CH₂), so it is a triplet; CH₂ has 3 neighbouring H (on CH₃), 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 O-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. O–H of an alcohol is present (broad, $3200\text{--}3600\text{ cm}^{-1}$); C=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 C=O (no neighbouring H), the quartet at 4.1 is O– 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.