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Premium IB tuition — Physics, Chemistry, Maths

IB DIPLOMA CHEMISTRY · FIRST ASSESSMENT 2025

Structure 3.2
Nomenclature & Structural Isomers

Booklet 5 · Understandings 3.2.5 – 3.2.6

How to give every organic compound one unambiguous IUPAC name, how to draw a structure from its name, and how the same molecular formula can describe several different compounds

Complete revision notes & memory points · Standard Level & Higher Level

How the level tags work in this booklet

SL + HL **Core material.** Understandings 3.2.5 (IUPAC nomenclature) and 3.2.6 (structural isomers) are common to both levels. Every student must know them, and must practise them: naming is a skill learned by doing, so this booklet contains over a hundred naming and isomer exercises with full answers.

HL Higher level only: the isomers of disubstituted benzene compounds and what they tell us about the structure of benzene (section 6.6). SL students can skip this section and the questions marked HL.

Inside this booklet

1. What the syllabus actually asks of you
2. 3.2.5 — The IUPAC system
3. 3.2.5 — Naming hydrocarbons
4. 3.2.5 — Naming compounds with a functional group
5. 3.2.5 — Esters, ethers and everyday names
6. 3.2.6 — Structural isomers
7. Key points to memorise
8. Check yourself
9. Answers

1 What the syllabus actually asks of you

Booklet 4 sorted organic compounds into classes by their functional groups. This booklet gives each compound its own **name**, and then shows why names matter: the same molecular formula can belong to several different compounds, called **structural isomers**, and only a systematic name (or a structural formula) tells them apart. The rules come from the **International Union of Pure and Applied Chemistry (IUPAC)**, and their aim is simple: one structure, one name, and every name leads back to exactly one structure.

Understanding	What it says	What you must be able to do	Level
3.2.5 IUPAC nomenclature	'IUPAC nomenclature' refers to a set of rules used by the International Union of Pure and Applied Chemistry to apply systematic names to organic and inorganic compounds.	Apply IUPAC nomenclature to **saturated or mono-unsaturated** compounds that have **up to six carbon atoms in the parent chain** and contain **one type** of the following functional groups: **halogeno, hydroxyl, carbonyl, carboxyl**. Include straight-chain and branched-chain isomers.	SL + HL
3.2.6 Structural isomers	Structural isomers are molecules that have the same molecular formula but different connectivities.	Recognize isomers, including **branched, straight-chain, position and functional group** isomers. **Primary, secondary and tertiary** alcohols, halogenoalkanes and amines should be included.	SL + HL

Reading the syllabus closely

- 'Up to six carbons in the **parent chain**': the whole molecule can be bigger (3-ethyl-2-methylhexane has nine carbons) but the longest chain has at most six. The stems you need are **meth- to hex-**.
- 'Saturated or mono-unsaturated': alkanes, plus compounds with **one** C=C or C≡C.
- 'One type of functional group': for example two –OH groups (a diol) or two different halogens, but not an –OH and a C=O together.
- The names of **amines, amides, esters and ethers** are not assessed under 3.2.5, but you meet them constantly in Reactivity 3.4, so section 5 shows how they work. The classification of amines as primary, secondary or tertiary **is** required by 3.2.6.

Linking questions and connections for 3.2.5 – 3.2.6

- **Booklet 4 (3.2.2 – 3.2.3):** functional groups and homologous series give the suffixes and the stems. → section 2
- **Structure 3.2.4 and 2.2:** branched isomers have lower boiling points (weaker London dispersion forces). → section 6.2
- **Reactivity 3.2 – 3.4:** primary, secondary and tertiary alcohols oxidize differently; halogenoalkanes react by different mechanisms. → section 6.4
- HL **Structure 2.2:** how does the fact that there are only three isomers of dibromobenzene support the current model of benzene's structure? → section 6.6
- **Booklet 6 (HL 3.2.7):** stereoisomers have the same connectivity, so they need prefixes such as *cis* and *trans* on top of the IUPAC name.

> **What the data booklet gives you — and what it does not**
>
> Nothing on nomenclature. The stems, the suffixes and prefixes, the numbering rules and the meaning of primary, secondary and tertiary must all be learned, and the only reliable way to learn them is practice.

2 Structure 3.2.5 — The IUPAC system SL + HL

2.1 The three parts of a name

Every systematic name is built from up to three parts, written together as one word: a **prefix** for the side chains and other substituents, a **stem** for the number of carbons in the longest chain, and a **suffix** for the class of compound.

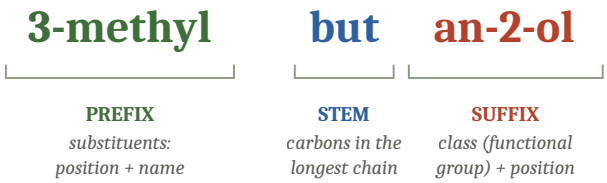


Figure 1 — The anatomy of a name. 3-Methylbutan-2-ol has a four-carbon chain (but), an –OH on carbon 2 (-2-ol) and a methyl branch on carbon 3 (3-methyl).

C atoms in chain	Stem	Alkane
1	meth-	methane, CH_4
2	eth-	ethane, C_2H_6
3	prop-	propane, C_3H_8
4	but-	butane, C_4H_{10}
5	pent-	pentane, C_5H_{12}
6	hex-	hexane, C_6H_{14}

Alkyl group	Formula	Prefix
from methane	$-CH_3$	methyl
from ethane	$-CH_2CH_3$ ($-C_2H_5$)	ethyl
from propane	$-CH_2CH_2CH_3$	propyl
from butane	$-C_4H_9$	butyl

Learn the stems in order with a mnemonic such as **M**onkeys **E**at **P**eeled **B**ananas. 'Straight chain' means **unbranched**, not straight in the sense of 180°: the chain can be drawn bent or zig-zagging round corners and is still the same chain.

2.2 Suffixes and prefixes for each class

The functional group decides the ending. Some groups, the halogens and alkyl branches, are only ever shown as prefixes. The groups marked * always contain carbon 1 of the chain, so their position never needs a number.

Class	Functional group	Suffix (ending)	Example	Notes
alkane	C–C only	**-ane**	propane	
alkene	C=C	**-ene**	but-2-ene, $CH_3CH{=}CHCH_3$	number = lower-numbered carbon of the C=C
alkyne	C≡C	**-yne**	pent-2-yne, $CH_3C{\equiv}CCH_2CH_3$	as for alkenes
halogenoalkane	–F, –Cl, –Br, –I	prefix **fluoro-, chloro-, bromo-, iodo-**	2-bromopropane	halogens are always prefixes
alcohol	–OH	**-ol**	propan-2-ol, $CH_3CH(OH)CH_3$	prefix hydroxy- if not the main group
aldehyde *	–CHO	**-al**	propanal, CH_3CH_2CHO	C=O carbon is C1: no number
ketone	C–CO–C	**-one**	pentan-2-one, $CH_3COCH_2CH_2CH_3$	number needed from pentan-on
carboxylic acid *	–COOH	**-oic acid**	propanoic acid, CH_3CH_2COOH	–COOH carbon is C1: no number
ester	–COO–	alkyl **-oate**	methyl propanoate	two words; see section 5
ether	–O–	prefix **alkoxy-**	methoxyethane	not assessed; see section 5
amine, amide	$-NH_2$, $-CONH_2$	**-amine, -amide**	ethanamine, ethanamide	recognize only; naming not assessed

2.3 The method

Method — naming a compound from its structure

1. **Find the longest carbon chain that contains the functional group** (for alkenes and alkynes, the chain must contain the C=C or C≡C). Look round corners and into branches: the longest chain is often not the one drawn horizontally. This gives the **stem**.
2. **Identify the functional group** and so the **suffix**. Drop the final 'e' of the alkane name before a suffix that starts with a vowel: propane + ol → propan**ol**, but ethane + diol → ethane**diol**.
3. **Number the chain** from the end that gives the **functional group** the lowest number. If that does not decide it (or there is no suffix group), number to give the **substituents** the lowest set of numbers.
4. **Name the substituents** (alkyl groups, halogens) with the number of the carbon each is on. Use di-, tri-, tetra- for two, three, four of the same kind, and give every one a number: 2,2-dimethyl, not 2-dimethyl.
5. **Assemble the name**: substituents in **alphabetical order** (ignoring di-, tri-, tetra-), then the stem, then the suffix with its number.

Punctuation rules

- **Commas** between numbers: 2,3-dimethylbutane. **Hyphens** between numbers and letters: but-2-ene, 2-chloropropane.
- No spaces in a name, except in two-part names such as carboxylic acids (ethanoic acid) and esters (ethyl ethanoate).
- The number of a suffix group goes immediately before the suffix: but-**2**-ene, pentan-**3**-ol. Older styles such as 2-butene or 3-pentanol are still seen, but the IUPAC form is preferred.
- Leave out numbers only where there is no possible alternative: propanal, propanone, butanone, methylpropene. An unnecessary number such as propan-2-one is usually accepted; a missing necessary one is not.

The six commonest naming errors

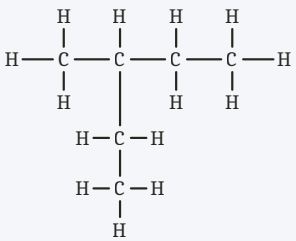
- **Missing the longest chain**: 2-ethylbutane is really 3-methylpentane, because the ethyl group extends the chain.
- **A methyl or ethyl on the end carbon**: 1-methylbutane is pentane. An alkyl group on C1 (or an ethyl on C2) always means you have not found the longest chain.
- **Numbering from the wrong end**: butan-3-ol is butan-2-ol; 3-methylbutane is 2-methylbutane.
- **Substituents in numerical, not alphabetical, order**: 2-methyl-3-ethylpentane should be 3-ethyl-2-methylpentane.
- **Forgetting di-** or a number: 2-methyl-2-methylbutane and 2-dimethylbutane are both wrong; write 2,2-dimethylbutane.
- **Spelling the ending wrongly**: propanal (aldehyde) and propanol (alcohol) differ by one letter.

3 Structure 3.2.5 — Naming hydrocarbons SL + HL

3.1 Alkanes: straight and branched chains

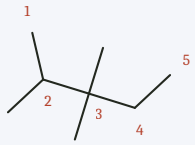
For an alkane there is no functional group, so the longest chain gives the stem, and the chain is numbered to give the branches the lowest numbers.

Worked example 1 — the longest chain is not always horizontal



- The horizontal chain has four carbons, but turning down into the ethyl group gives a chain of **five**: the stem is **pent**-, and this is a **pentane**.
- The five-carbon chain carries a single CH_3 branch. Numbered from either end it is on carbon 3.
- Name: **3-methylpentane**, $CH_3CH_2CH(CH_3)CH_2CH_3$. Writing '2-ethylbutane' is the classic error.

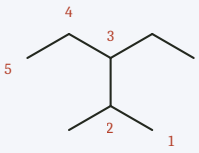
Worked example 2 — several branches



- Longest chain: five carbons, so **pentane**.
- Numbered from the left, the methyl groups are on 2, 3 and 3: the set {2, 3, 3}. From the right they would be on 3, 3 and 4. The first point of difference is 2 against 3, so number from the left.
- Three methyl groups: **tri**methyl, with three numbers.

Name: **2,3,3-trimethylpentane**, $CH_3CH(CH_3)C(CH_3)_2CH_2CH_3$.

Worked example 3 — different branches go in alphabetical order

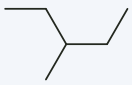
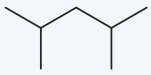
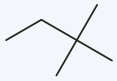
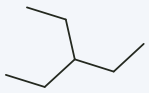


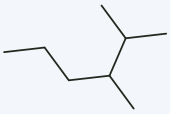
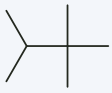
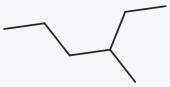
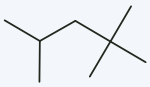
- Longest chain: five carbons (pentane). There are two choices of five-carbon chain here; both carry the same two branches, so either gives the same name.
- Numbering from the right gives {2, 3}; from the left {3, 4}. Number from the right: methyl on C2, ethyl on C3.
- **E**thyl comes before **m**ethyl in the alphabet.

Name: **3-ethyl-2-methylpentane**, $CH_3CH(CH_3)CH(C_2H_5)CH_2CH_3$.

Practice A **Name these alkanes**

Give the IUPAC name of each alkane. Check every answer: the longest chain, then the numbering, then the alphabetical order.

(a)  **(b)**  **(c)**  **(d)** 

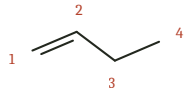
(e)  **(f)**  **(g)**  **(h)** 

(i) $CH_3CH(CH_3)CH_2CH_2CH_3$ **(j)** $(CH_3)_3CCH_2CH_3$

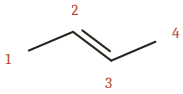
(k) $CH_3CH_2CH(CH_3)CH(CH_3)CH_3$ **(l)** $CH_3CH_2C(CH_3)_2CH_2CH_3$

3.2 Alkenes and alkynes

The C=C (or C≡C) is the functional group. The longest chain must **contain** the multiple bond, even if a longer chain exists elsewhere, and it is numbered to give the multiple bond the lowest number. The number given is that of the **first** carbon of the double bond: in $CH_3CH{=}CHCH_2CH_3$ the C=C joins carbons 2 and 3, so the name is pent-2-ene. Alkenes with four or more carbons need a number; ethene and propene do not, because there is only one possible position.



but-1-ene



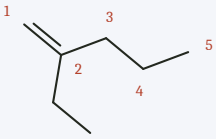
but-2-ene


methylpropene
(2-methylprop-1-ene)


pent-2-yne

Figure 2 — Alkenes and an alkyne. 'But-3-ene' does not exist: numbered from the other end it is but-1-ene.

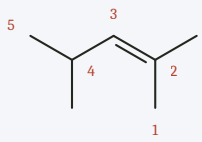
Worked example 4 — the chain must include the C=C



- The longest chain containing the C=C runs from the $=CH_2$ through C2 to the end of the propyl group: five carbons, a **pentene**. (The ethyl branch could also be followed, but that chain has only four carbons.)
- Number from the $=CH_2$ end: the double bond starts at C1, **pent-1-ene**.
- An ethyl branch on C2: **2-ethyl**.

Name: **2-ethylpent-1-ene**, $CH_2{=}C(C_2H_5)CH_2CH_2CH_3$.

Worked example 5 — the double bond decides the numbering, not the branches

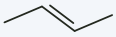


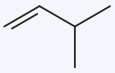
- Five-carbon chain containing the C=C: **pentene**.
- From the right the C=C starts at C2; from the left at C3. Number from the right: **pent-2-ene**.
- Methyl groups on C2 and C4: **2,4-dimethyl**.

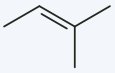
Name: **2,4-dimethylpent-2-ene**, $(CH_3)_2C{=}CHCH(CH_3)CH_3$.

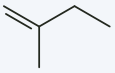
Practice B — Name these alkenes and alkynes

Give the IUPAC name of each compound. Remember that the chain must contain the multiple bond.

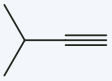
(a) 

(b) 

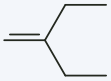
(c) 

(d) 

(e)

(f) 

(g) 

(h) 

(i) $CH_2{=}CHCH_2CH_2CH_2CH_3$

(j) $CH_3CH{=}CHCH(CH_3)CH_3$

(k) $CH_3C{\equiv}CCH_2CH_2CH_3$

(l) $(CH_3)_2C{=}C(CH_3)_2$

Practice C — Draw these hydrocarbons

Draw the skeletal formula of each compound, then write its condensed structural formula.

(a) 2-methylbutane **(b)** 3,3-dimethylpentane **(c)** 2,3,4-trimethylpentane **(d)** 3-ethyl-3-methylhexane

(e) pent-1-ene **(f)** 4-methylpent-2-ene **(g)** hex-2-yne **(h)** 2,3-dimethylbut-2-ene

4 Structure 3.2.5 — Naming compounds with a functional group SL + HL

4.1 Halogenoalkanes

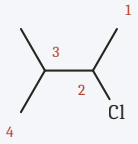
Halogen atoms are always named as **prefixes**: fluoro-, chloro-, bromo-, iodo-. The parent name is the alkane. Halogens and alkyl branches are treated in exactly the same way: number the chain to give the lowest set of numbers to **all** the substituents together, then list them alphabetically.



2-bromopropane | 1,2-dichloropropane | 2-bromo-2-chloropropane | 1-chloro-2-methylpropane

Figure 3 — Halogenoalkanes. In 2-bromo-2-chloropropane both halogens are on C2; bromo is listed before chloro alphabetically.

Worked example 6 — when both directions give the same numbers

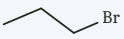


- Four-carbon chain: **butane**, with a Cl and a CH_3 as substituents.
- From the left: chloro on 2, methyl on 3, the set {2, 3}. From the right: methyl on 2, chloro on 3, also {2, 3}. A tie.
- Tie-break rule: give the lower number to the substituent that comes **first in the alphabet**. **C**hloro before **m**ethyl, so chloro gets 2.

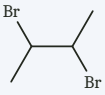
Name: **2-chloro-3-methylbutane**, $CH_3CHClCH(CH_3)CH_3$.

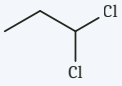
Practice D Name these halogenoalkanes

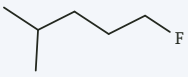
Give the IUPAC name of each compound.

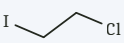
(a) 

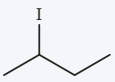
(b) 

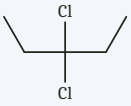
(c) 

(d) 

(e) 

(f) 

(g) 

(h) 

(i) $CH_3CHBrCH_2CH_3$

(j) $CH_2ClCHClCH_2Cl$

(k) $CH_3CH_2C(CH_3)BrCH_3$

(l) CHF_2CF_3

4.2 Alcohols

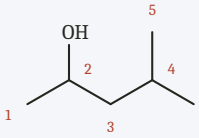
The –OH group is shown by the suffix **-ol**, with a number for its position from propanol upwards. The chain is numbered to give the –OH the lowest number, **even if the branches then get higher numbers**, because the functional group takes priority over alkyl groups and halogens. Two –OH groups make a **diol**, and the 'e' of the alkane is kept because 'diol' starts with a consonant.



propan-1-ol | propan-2-ol | 2-methylpropan-2-ol | ethane-1,2-diol

Figure 4 — Alcohols. Ethane-1,2-diol is the antifreeze used in car engines.

Worked example 7 — the –OH outranks the methyl group

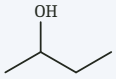


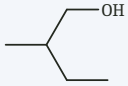
- Five-carbon chain with the –OH: **pentanol**.
- Number from the end nearer the –OH: the OH is on C2 (from the other end it would be C4). So **pentan-2-ol**.
- The methyl group is then on C4. It gets the higher number, but that does not matter: the functional group has priority.

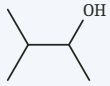
Name: **4-methylpentan-2-ol**, $CH_3CH(OH)CH_2CH(CH_3)CH_3$. The common wrong answer, '2-methylpentan-4-ol', numbers to suit the branch.

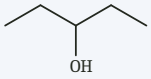
Practice E — Name these alcohols

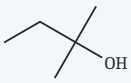
Give the IUPAC name of each alcohol.

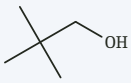
(a) 

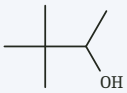
(b) 

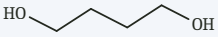
(c) 

(d) 

(e) 

(f) 

(g) 

(h) 

(i) $CH_3CH_2CH_2CH_2CH_2OH$

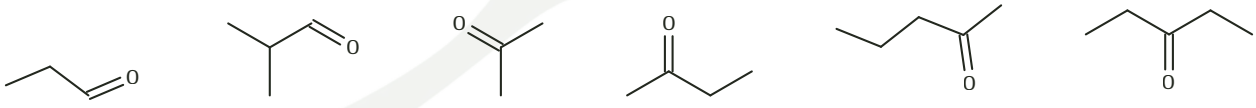
(j) $CH_3CH(OH)CH(CH_3)CH_2CH_3$

(k) $(CH_3)_2C(OH)CH(CH_3)_2$

(l) $CH_2(OH)CH(OH)CH_2OH$

4.3 Aldehydes and ketones

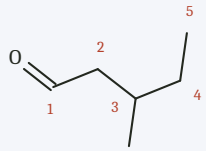
Both contain the carbonyl group, C=O. In an **aldehyde** the C=O is at the **end** of the chain (–CHO); its carbon is always C1, so no number is used: the suffix is **-al**. In a **ketone** the C=O is **inside** the chain, joined to two other carbons; the suffix is **-one**, and from five carbons upwards a number shows its position.



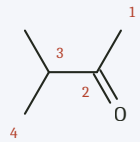
propanal | 2-methylpropanal | propanone | butanone | pentan-2-one | pentan-3-one

Figure 5 — Aldehydes and ketones. Propanone and butanone need no number: a C=O on C1 would make an aldehyde, so the ketone C=O can only be on C2.

Worked example 8 — numbering a branched aldehyde and ketone



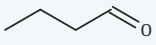
Aldehyde. The –CHO carbon is C1, so numbering starts there. The chain has five carbons and a methyl branch on C3: **3-methylpentanal**, $CH_3CH_2CH(CH_3)CH_2CHO$.

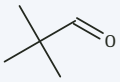


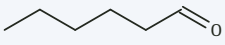
Ketone. Four-carbon chain with the C=O: butanone. Numbering from the left puts the C=O on C2 and the methyl on C3: **3-methylbutan-2-one**, $CH_3COCH(CH_3)CH_3$. (Here the 2 is needed, because the methyl group must be located.)

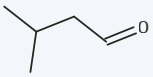
Practice F **Name these aldehydes and ketones**

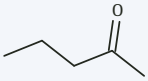
Give the IUPAC name of each compound, and say whether it is an aldehyde or a ketone.

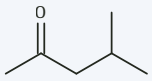
(a) 

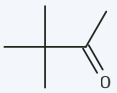
(b) 

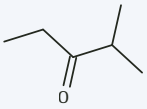
(c) 

(d) 

(e) 

(f) 

(g) 

(h) 

(i) $CH_3CH_2CH_2CH_2CHO$

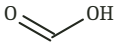
(j) $CH_3CH_2COCH_2CH_2CH_3$

(k) $(CH_3)_2CHCH_2CH_2CHO$

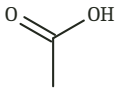
(l) $HCHO$

4.4 Carboxylic acids

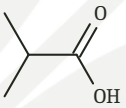
The –COOH group is always at the end of the chain and its carbon is C1, so it never needs a number. The name is the stem + **-oic acid**, and the carbon of the –COOH group is **counted** in the stem: CH_3COOH has two carbons, so it is **ethanoic acid**, not methanoic acid.



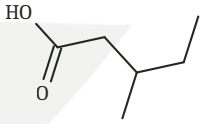
methanoic acid



ethanoic acid



2-methylpropanoic acid



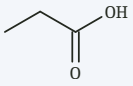
3-methylpentanoic acid

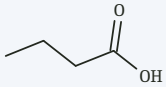
Figure 6 — Carboxylic acids. Count from the –COOH carbon.

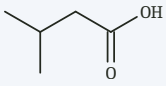
Salts of carboxylic acids are named like inorganic salts: metal first, then the stem + **-oate**. CH_3COONa is sodium ethanoate; $(HCOO)_2Ca$ is calcium methanoate.

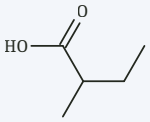
Practice G **Name these carboxylic acids**

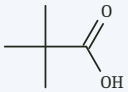
Give the IUPAC name of each acid.

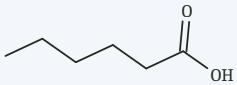
(a) 

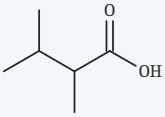
(b) 

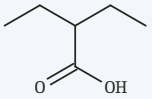
(c) 

(d) 

(e) 

(f) 

(g) 

(h) 

(i) HCOOH

(j) $CH_3CH_2CH(CH_3)CH_2COOH$

(k) CH_3COOK

(l) $(CH_3CH_2COO)_2Mg$

Examiner traps in naming compounds with a functional group

- Number the chain from the end nearer the **functional group** (–OH, C=O, –COOH, C=C), not the end nearer a branch or halogen.
- Never give a number to –CHO or –COOH: 'propan-1-al' and 'butan-1-oic acid' are not used.
- Include the C of –CHO or –COOH when counting the chain: CH_3CH_2COOH is propanoic acid.
- Halogens are prefixes, never suffixes: 2-chloropropane, not propan-2-chloride.
- -al (aldehyde), -ol (alcohol), -one (ketone): check the ending against the structure every time.
- A ketone needs at least three carbons; '2-methylpropanone' cannot exist, because a methyl on C2 of propanone makes the chain longer (it is butanone).

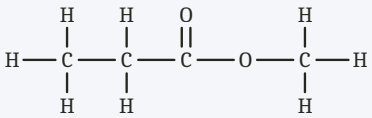
5 Structure 3.2.5 — Esters, ethers and everyday names SL + HL

These classes are not in the list for 3.2.5, so their names will not be assessed in this topic. You need ester names in Reactivity 3.4 (esterification), though, and they follow neatly from the acid names, so learn them now.

5.1 Esters

An ester forms when the alkyl group of an alcohol replaces the H of a carboxylic acid: R–COOH + R′–OH → R–COO–R′ + H_2O. Like a salt, it has a two-word name: the **alkyl group from the alcohol** first, then the **-oate** from the acid.

Worked example 9 — naming an ester from its structure



1. Find the C=O. The carbon of the C=O and everything on **its** side of the single-bonded O comes from the acid: here three carbons, so **propanoate**.
2. The group attached to the other side of that O comes from the alcohol: one carbon, so **methyl**.
3. Write the alkyl group first: **methyl propanoate**, $CH_3CH_2COOCH_3$.

Condensed formulas of esters are written acid part first, so read $CH_3COOCH_2CH_3$ as CH_3COO | CH_2CH_3: ethyl ethanoate. Be careful with $HCOOCH_3$ (methyl methanoate) and CH_3OOCCH_3, which is written the other way round and is methyl ethanoate.

5.2 Ethers

In an ether, R–O–R′, the **longer** alkyl chain is the parent alkane and the shorter chain with the O is an **alkoxy** prefix (methoxy, ethoxy, propoxy). $CH_3OCH_2CH_3$ is methoxyethane; $CH_3CH_2OCH_2CH_3$ is ethoxyethane (traditionally 'diethyl ether', the first surgical anaesthetic); $CH_3OCH_2CH_2CH_3$ is 1-methoxypropane (often written methoxypropane).

5.3 Traditional names

Many compounds also have older, traditional names, which you will still see on labels and in everyday use. They are accepted in some contexts, but in an exam the IUPAC name is expected.

Traditional name	IUPAC name	Formula	Everyday use
acetone	propanone	CH_3COCH_3	nail-varnish remover, solvent
acetic acid	ethanoic acid	CH_3COOH	vinegar (about 5% solution)
formaldehyde	methanal	$HCHO$	preserving biological specimens
formic acid	methanoic acid	$HCOOH$	ant and nettle stings
isopropyl alcohol	propan-2-ol	$CH_3CH(OH)CH_3$	hand sanitizer, cleaning electronics
ethyl alcohol	ethanol	C_2H_5OH	alcoholic drinks, fuel
ethylene glycol	ethane-1,2-diol	$HOCH_2CH_2OH$	antifreeze
glycerol	propane-1,2,3-triol	$HOCH_2CH(OH)CH_2OH$	soaps, cosmetics

Nature of Science and TOK — the limits of a naming system

The IUPAC system gives clear, logical names to the small molecules in this course, which is why chemists in every country accept it. For large molecules it becomes unwieldy: the systematic name of ordinary table sugar, sucrose, runs to more than a hundred characters. Biochemists therefore keep using short traditional names, and IUPAC itself regularly adds new rules as new kinds of structure are discovered. A classification system is a human construct, judged by how well it helps people communicate. Is a name that is perfectly precise but that nobody uses a better name than one that everybody uses?

Practice H **Esters, ethers and salts**

Name each compound.

(a)	CH_3COOCH_3	**(b)**	$HCOOCH_2CH_3$	**(c)**	$CH_3CH_2COOCH_2CH_3$	**(d)**	$CH_3CH_2CH_2COOCH_3$
(e)	CH_3OCH_3	**(f)**	$CH_3CH_2OCH_2CH_3$	**(g)**	CH_3COONa	**(h)**	$CH_3CH_2CH_2OCH_3$

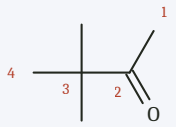
5.4 From a name to a structure

Drawing a structure from a name is the same process in reverse, and it is the best way to check a name you have written yourself: if your name leads to a different structure, the name is wrong.

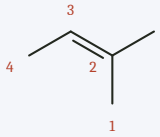
Method — drawing a structure from its name

1. Find the **stem** and draw that many carbons in a zig-zag. Number them from one end.
2. Read the **suffix** and put the functional group on the carbon with that number (for -al and -oic acid, on C1).
3. Read the **prefixes** and attach each substituent to its numbered carbon.
4. Add H atoms so every carbon has four bonds (for a full or condensed formula), then check the molecular formula.

Worked example 10 — 3,3-dimethylbutan-2-one and 2-methylbut-2-ene



3,3-dimethylbutan-2-one. But- = four carbons; -2-one = C=O on C2; 3,3-dimethyl = two methyl groups on C3. Condensed: $CH_3COC(CH_3)_3$; molecular formula $C_6H_{12}O$.



2-methylbut-2-ene. Four carbons; the C=C starts at C2, so it joins C2 and C3; a methyl group on C2. Condensed: $(CH_3)_2C{=}CHCH_3$; C_5H_{10}.

Practice I **Draw these compounds**

Draw a skeletal formula for each compound and give its molecular formula.

(a)	2-bromo-3-methylbutane	**(b)**	3-methylbutan-1-ol	**(c)**	2-methylpentan-3-one	**(d)**	3-ethylpentanal
(e)	2,2-dimethylbutanoic acid	**(f)**	1,1,2-trichloroethane	**(g)**	hex-3-ene	**(h)**	3-methylbutan-2-ol

Practice J **What's wrong with these names?**

Each name describes a real structure but breaks a rule. Draw the structure and give the correct name.

(a)	2-ethylpentane	**(b)**	1-methylbutane	**(c)**	3-methylbutane	**(d)**	butan-3-ol
(e)	2-methylpentan-4-ol	**(f)**	pent-4-ene	**(g)**	2-methylbutan-3-one	**(h)**	3-chloro-2-methylbutane
(i)	2-methyl-3-ethylpentane	**(j)**	2,2-methylpropane	**(k)**	1-propanal	**(l)**	2-ethylpropan-1-ol

6 Structure 3.2.6 — Structural isomers SL + HL

6.1 Same formula, different connectivity

Definition to learn

Structural isomers are compounds with the **same molecular formula** but **different connectivities** (their atoms are joined together in a different order). Each isomer is a different compound, with its own physical and chemical properties and its own IUPAC name.

There are three kinds of structural isomer, and one molecular formula can show all three at once:

Type	What differs	Example
chain (branched) isomers	the carbon skeleton: straight chain or branched	butane and 2-methylpropane, C_4H_{10}
position isomers	the position of the functional group on the same skeleton	propan-1-ol and propan-2-ol, C_3H_8O
functional group isomers	the functional group itself, so they belong to different classes	propanal and propanone, C_3H_6O

Method — finding all the structural isomers of a formula

1. Use the general formula to decide which classes are possible (e.g. $C_4H_{10}O$ fits $C_nH_{2n+2}O$: alcohols and ethers).
2. Start with the **longest chain**. Place the functional group in every **distinct** position.
3. Shorten the chain by one carbon, add a methyl branch in every distinct position, and place the functional group again. Continue until no shorter chain is possible.
4. **Name every structure.** Two drawings with the same name are the same compound, however different they look, so count each name once only.

6.2 Chain isomers

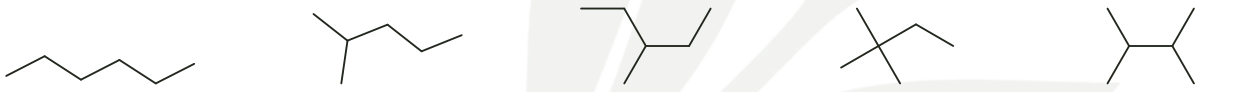
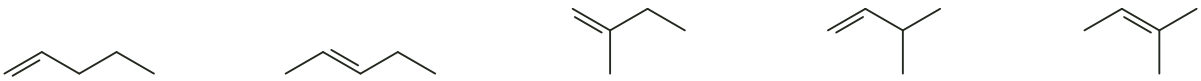


Figure 7 — The five structural isomers of hexane, C_6H_{14}: one with a six-carbon chain, two with a five-carbon chain and two with a four-carbon chain. Any other drawing turns out to be one of these five.

The number of isomers grows rapidly with chain length: C_4H_{10} has 2, C_5H_{12} 3, C_6H_{14} 5, C_7H_{16} 9 and $C_{10}H_{22}$ 75. This is one reason why carbon forms so many compounds. Branched isomers have lower boiling points than their straight-chain isomers because they have less surface contact and weaker London dispersion forces (pentane 36 °C, 2-methylbutane 28 °C, 2,2-dimethylpropane 10 °C; Booklet 4, section 5.5). Branched alkanes also burn more smoothly in car engines, which is why petrol rich in branched alkanes has a higher 'octane number'.

6.3 Position isomers

Position isomers have the same carbon skeleton and the same functional group, but the group is in a different place. Alkenes, alcohols, halogenoalkanes and ketones all show position isomerism.



pent-1-ene | pent-2-ene | 2-methylbut-1-ene | 3-methylbut-1-ene | 2-methylbut-2-ene

Figure 8 — The five non-cyclic alkene isomers of C_5H_{10}. Pent-1-ene and pent-2-ene are position isomers; the others add chain isomerism. (Pent-2-ene also has *cis* and *trans* forms, which are stereoisomers: HL Booklet 6.)

6.4 Primary, secondary and tertiary compounds

Position isomers of alcohols and halogenoalkanes are classified by the carbon atom that carries the functional group. The classification matters because it changes their chemistry: primary, secondary and tertiary alcohols give different products on oxidation (Reactivity 3.2), and halogenoalkanes react by different mechanisms (Reactivity 3.4).

Definitions to learn

- A **primary** (1°) alcohol or halogenoalkane: the carbon carrying the –OH or –X is bonded to **one** other carbon atom (it has two H atoms). Methanol and the halogenomethanes, with no other carbon, are also counted as primary.
- A **secondary** (2°) compound: that carbon is bonded to **two** other carbon atoms (one H atom).
- A **tertiary** (3°) compound: that carbon is bonded to **three** other carbon atoms (no H atoms).
- **Amines** are classified by the **nitrogen** atom instead: a primary amine has **one** carbon bonded to the N ($R–NH_2$), a secondary amine two (R_2NH) and a tertiary amine three (R_3N).



butan-1-ol **primary** | butan-2-ol **secondary** | 2-methylpropan-1-ol **primary** | 2-methylpropan-2-ol **tertiary**

Figure 9 — The four alcohol isomers of C_4H_9OH. Count the carbons bonded to the carbon carrying the –OH.



methylamine (methanamine) **primary** | dimethylamine **secondary** | trimethylamine **tertiary**

Figure 10 — Amines are classified by the number of carbon atoms bonded to the nitrogen (red). You need to classify amines, but not name them.

Worked example 11 — the eight alcohols with the formula $C_5H_{11}OH$

Work systematically: five-carbon chain first, then four-carbon chain with a methyl branch, then three-carbon chain with two methyl branches.

Chain	Isomer	Class
5 carbons	pentan-1-ol; pentan-2-ol; pentan-3-ol	1°; 2°; 2°
4 carbons + methyl	2-methylbutan-1-ol; 3-methylbutan-1-ol; 2-methylbutan-2-ol; 3-methylbutan-2-ol	1°; 1°; 3°; 2°
3 carbons + 2 methyl	2,2-dimethylpropan-1-ol	1°

Notice that 'pentan-4-ol' is pentan-2-ol and '2-methylbutan-4-ol' is 3-methylbutan-1-ol: naming each structure stops you counting the same isomer twice.

6.5 Functional group isomers

Classes that share a general formula (Booklet 4, section 4.2) are functional group isomers of each other. They have different functional groups, so their chemical **and** physical properties differ greatly: ethanol is a liquid that boils at 78 °C, while its isomer methoxymethane is a gas (−24 °C) used as an aerosol propellant.

General formula	Classes	Example: isomers of the same formula
$C_nH_{2n+2}O$	alcohols and ethers	C_2H_6O: ethanol CH_3CH_2OH and methoxymethane CH_3OCH_3
$C_nH_{2n}O$	aldehydes and ketones	C_3H_6O: propanal CH_3CH_2CHO and propanone CH_3COCH_3
$C_nH_{2n}O_2$	carboxylic acids and esters	$C_3H_6O_2$: propanoic acid CH_3CH_2COOH, methyl ethanoate CH_3COOCH_3 and ethyl methanoate $HCOOCH_2CH_3$
C_nH_{2n}	alkenes and cycloalkanes	C_3H_6: propene $CH_2{=}CHCH_3$ and cyclopropane

Model answer: "Draw and name the structural isomers of C_4H_9Br and classify each as primary, secondary or tertiary." (4 marks)

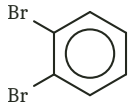
1-bromobutane, $CH_3CH_2CH_2CH_2Br$, primary **[1]**; 2-bromobutane, $CH_3CH_2CHBrCH_3$, secondary **[1]**; 1-bromo-2-methylpropane, $(CH_3)_2CHCH_2Br$, primary **[1]**; 2-bromo-2-methylpropane, $(CH_3)_3CBr$, tertiary **[1]**. (Structures may be drawn as full, condensed or skeletal formulas unless the question says otherwise.)

Model answer: "Explain why butan-1-ol and 2-methylpropan-2-ol are described as structural isomers." (2 marks)

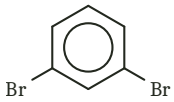
They have the same molecular formula, $C_4H_{10}O$ / C_4H_9OH **[1]**, but different structural formulas: the atoms are joined in a different order (a straight chain with the OH on C1, compared with a branched chain with the OH on the central carbon) **[1]**.

6.6 Disubstituted benzene compounds HL

When one H atom of benzene is replaced, for example by Cl, NH_2 or NO_2, only one compound can form: all six positions on the ring are identical. Chlorobenzene, phenylamine and nitrobenzene each have no position isomers. When **two** H atoms are replaced, there are exactly **three** isomers, because the second group can be next to the first, one carbon further round, or opposite it. The ring is numbered to give the lowest possible numbers.



1,2-dibromobenzene



1,3-dibromobenzene



1,4-dibromobenzene

Figure 11 — The three isomers of dibromobenzene, $C_6H_4Br_2$. '1,5-' and '1,6-' are just 1,3- and 1,2- numbered the other way round the ring.

HL Linking question — what do the three isomers tell us about benzene?

If benzene were cyclohexa-1,3,5-triene, with fixed alternating single and double bonds (one Kekulé structure), the two Br atoms in a 1,2-isomer could be joined by a C=C or by a C–C. These would be two different compounds, so there would be **four** dibromobenzenes, not three. Only **one** 1,2-isomer has ever been found.

This supports the modern model: the six C–C bonds in benzene are **identical**, with the π electrons **delocalized** around the ring, so every pair of neighbouring positions is equivalent. The same conclusion follows from the equal C–C bond lengths (140 pm) and the unusual stability of benzene (Structure 2.2, HL).

Practice K Structural isomers

Draw (skeletal formulas are fine) and name, where asked, every structural isomer in each part.

1. The three isomers of C_5H_{12}.
2. The three non-cyclic isomers of C_4H_8 (one of them has two stereoisomers, which you can ignore here).
3. The two isomers of C_3H_7Cl. Classify each as primary or secondary.
4. The three isomers of C_3H_8O. Identify the two position isomers and the functional group isomer.
5. The three isomers of C_4H_8O that are aldehydes or ketones. Name them.
6. Four isomers of $C_4H_8O_2$: two carboxylic acids and two esters. Name the acids.
7. The two alkynes with the formula C_4H_6. What kind of isomers are they?
8. The four amines with the formula C_3H_9N. Classify each as primary, secondary or tertiary (no names needed).
9. HL The three isomers of dimethylbenzene, $C_6H_4(CH_3)_2$. Suggest which has the highest melting point, and why.
10. HL How many isomers of trichlorobenzene, $C_6H_3Cl_3$, exist? Name them using ring numbers.

Examiner traps in 3.2.6

- Structural isomers have the **same molecular formula**. Count the atoms in every structure you draw.
- Do not draw the same isomer twice in a different orientation. Naming each structure is the best check.
- Primary, secondary and tertiary for alcohols and halogenoalkanes depend on the **carbon** that carries the group; for amines they depend on the **nitrogen**. 2-Methylpropan-1-ol is primary, even though the molecule is branched.
- Different classes with the same formula are functional group isomers, so they have **different chemical properties**. Chain and position isomers in the same class usually have similar chemistry but different physical properties.
- *cis* and *trans* isomers are **not** structural isomers: they have the same connectivity (Booklet 6).

7 Key points to memorise

Everything below is either wording that examiners look for, or knowledge you must carry into the exam yourself.

A The naming method

- Prefix (substituents) + stem (longest chain containing the functional group) + suffix (class).
- Stems: meth, eth, prop, but, pent, hex. Alkyl groups: methyl, ethyl, propyl.
- Number from the end giving the functional group (–OH, C=O, C=C) the lowest number; then the lowest set of numbers for substituents; then, in a tie, the lower number to the substituent first in the alphabet.
- Substituents alphabetical, ignoring di-/tri-/tetra-. Every substituent needs a number. Commas between numbers, hyphens between numbers and letters.
- Drop the alkane's final 'e' before a vowel (propanol), keep it before a consonant (ethanediol).

B Endings to know

- -ane alkane · -ene alkene · -yne alkyne · fluoro/chloro/bromo/iodo- halogenoalkane · -ol alcohol
- -al aldehyde (C1, no number) · -one ketone · -oic acid carboxylic acid (C1, no number)
- alkyl alkanoate ester · alkoxyalkane ether · metal alkanoate salt (esters, ethers: not assessed in 3.2.5)

C Structural isomers

- **Structural isomers:** same molecular formula, different connectivity (different structural formula).
- Types: chain (branched/straight), position, functional group. C_4H_{10} 2, C_5H_{12} 3, C_6H_{14} 5 isomers.
- 1°, 2°, 3° alcohols and halogenoalkanes: the C bearing the group is bonded to 1, 2, 3 other C atoms. Amines: 1, 2, 3 C atoms bonded to the N.
- Shared general formulas: alcohols/ethers, aldehydes/ketones, acids/esters, alkenes/cycloalkanes.
- HL Disubstituted benzenes: exactly three isomers (1,2-, 1,3-, 1,4-), evidence for six identical delocalized C–C bonds.

D Command terms — what each one is actually asking for

- **State the name / Name** — the full IUPAC name, correctly spelled and punctuated.
- **Draw** (a structure) — full structural formula if asked for; otherwise condensed or skeletal is usually accepted. Make the connectivity unambiguous.
- **Deduce** (the isomers) — work them out systematically and show each one.
- **Identify / Classify** (as 1°, 2°, 3°) — give the class; no explanation unless asked.
- **Explain** (why compounds are isomers) — same molecular formula + different structural formula / connectivity.

8 Check yourself

These questions mix everything in the booklet, in the style of exam questions. Cover the answers. Questions marked HL are for Higher Level students.

1. What is the IUPAC name of $CH_3CH(CH_3)CH(CH_3)CH_2CH_3$?

   A 2-methyl-3-methylpentane
   B 2,3-dimethylpentane
   C 3,4-dimethylpentane
   D 1,2-dimethylbutane

2. What is the IUPAC name of $(CH_3)_2CHCH_2CHO$?

   A 2-methylbutanal
   B 3-methylbutanal
   C 3-methylbutan-1-one
   D 2-methylbutan-4-al

3. Which name is correct?

   A butan-3-ol
   B 2-ethylbutane
   C pent-3-ene
   D 3-methylpentan-2-one

4. Which compound is a tertiary alcohol?

   A $(CH_3)_3COH$
   B $(CH_3)_2CHOH$
   C $(CH_3)_2CHCH_2OH$
   D $CH_3CH_2CH(OH)CH_3$

5. How many structural isomers have the formula C_6H_{14}?

   A 3 B 4 C 5 D 6

6. Which pair are functional group isomers?

   A propan-1-ol and propan-2-ol
   B butane and 2-methylpropane
   C propanal and propanone
   D but-1-ene and but-2-ene

7. Which compound is a secondary halogenoalkane?

   A $CH_3CH_2CH_2CH_2Cl$
   B $(CH_3)_2CHCH_2Cl$
   C $CH_3CH_2CHClCH_3$
   D $(CH_3)_3CCl$

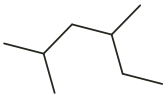
8. What is the name of the ester $CH_3CH_2COOCH_2CH_3$?

   A ethyl propanoate
   B propyl ethanoate
   C ethyl ethanoate
   D propyl propanoate

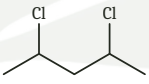
9. Name the following compounds. (a) $CH_3CH_2CH_2CH(CH_3)_2$ (b) $CH_3CH{=}C(CH_3)CH_3$ (c) $CH_3CHBrCHBrCH_3$ (d) $CH_3CH_2CH(OH)CH(CH_3)_2$ (e) $CH_3CH_2CH(CH_3)CHO$ (f) $CH_3COCH_2CH(CH_3)_2$ (g) $(CH_3)_3CCOOH$ (h) $CH_3C{\equiv}CCH(CH_3)_2$. **[8]**

10. Name the compounds shown. **[6]**

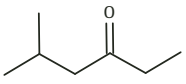
(a)



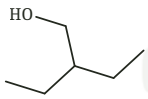
(b)



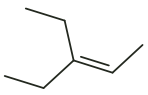
(c)



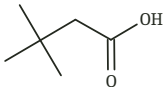
(d)



(e)



(f)



11. Draw a skeletal formula for each compound. (a) 2,3-dimethylbutan-2-ol (b) 4-methylpent-1-ene (c) 3-ethylhexane (d) 2-methylbutanoic acid (e) 1,2-dichloro-2-methylpropane (f) hexan-3-one. **[6]**

12. A student names a compound '2-ethyl-3-methylbutane'. Draw the structure the student intended and give its correct IUPAC name. **[2]**

13. Explain why 'propan-2-al' cannot be the name of a compound. **[1]**

14. State the meaning of the term *structural isomers*. **[1]**

15. Draw and name all the non-cyclic structural isomers of C_5H_{10}. **[5]**

16. Deduce the structures of the four isomers of C_4H_9OH, name them and classify each as primary, secondary or tertiary. **[4]**

17. Draw and name two functional group isomers for each formula: (a) C_3H_8O (b) C_3H_6O (c) $C_3H_6O_2$. **[6]**

18. Classify each amine as primary, secondary or tertiary: (a) $CH_3CH_2NH_2$ (b) $(CH_3)_2NCH_2CH_3$ (c) $CH_3NHCH_2CH_3$ (d) $(CH_3)_3CNH_2$. **[4]**

19. Explain, with reference to intermolecular forces, why 2,2-dimethylpropane has a lower boiling point than its isomer pentane. **[2]**

20. Pentan-2-one and pentan-3-one are isomers. (a) State the type of structural isomerism shown. (b) Draw and name a third ketone with the formula $C_5H_{10}O$. (c) Name an aldehyde with the same formula. **[3]**

21. Which of these is **not** an isomer of hexane?

A 2-methylpentane
B 2,2-dimethylbutane
C 3-ethylpentane
D 2,3-dimethylbutane

22. Ethanol and methoxymethane both have the formula C_2H_6O. Explain why ethanol is a liquid at room temperature but methoxymethane is a gas. **[3]**

23. HL Draw and name the three isomers of dichlorobenzene. **[3]**

24. HL Explain how the number of isomers of $C_6H_4Br_2$ supports the delocalized model of benzene. **[2]**

9 Answers

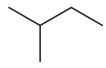
Practice A — alkanes

(a) 3-methylpentane
(b) 2,4-dimethylpentane
(c) 2,2-dimethylbutane
(d) 3-ethylpentane
(e) 2,3-dimethylhexane
(f) 2,2,3-trimethylbutane
(g) 3-methylhexane
(h) 2,2,4-trimethylpentane
(i) 2-methylpentane
(j) 2,2-dimethylbutane
(k) 2,3-dimethylpentane
(l) 3,3-dimethylpentane

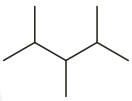
Practice B — alkenes and alkynes

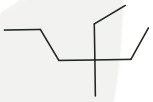
(a) but-2-ene
(b) 3-methylbut-1-ene
(c) 2-methylbut-2-ene
(d) 2-methylbut-1-ene
(e) but-2-yne
(f) 3-methylbut-1-yne
(g) hex-3-ene
(h) 2-ethylbut-1-ene (the chain must contain the C=C)
(i) hex-1-ene
(j) 4-methylpent-2-ene
(k) hex-2-yne
(l) 2,3-dimethylbut-2-ene

Practice C — drawing hydrocarbons

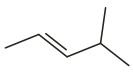
(a) 
$CH_3CH(CH_3)CH_2CH_3$

(b) 
$CH_3CH_2C(CH_3)_2CH_2CH_3$

(c) 
$CH_3CH(CH_3)CH(CH_3)CH(CH_3)CH_3$

(d) 
$CH_3CH_2C(CH_3)(C_2H_5)CH_2CH_2CH_3$

(e) 
$CH_2{=}CHCH_2CH_2CH_3$

(f) 
$CH_3CH{=}CHCH(CH_3)CH_3$

(g) 
$CH_3C{\equiv}CCH_2CH_2CH_3$

(h) 
$(CH_3)_2C{=}C(CH_3)_2$

Practice D — halogenoalkanes

(a) 1-bromopropane
(b) 2-chloro-2-methylpropane
(c) 2,3-dibromobutane
(d) 1,1-dichloropropane
(e) 1-fluoro-4-methylpentane (lowest set {1,4}, not {2,5})
(f) 1-chloro-2-iodoethane (tie: chloro first alphabetically)
(g) 2-iodobutane
(h) 3,3-dichloropentane
(i) 2-bromobutane
(j) 1,2,3-trichloropropane
(k) 2-bromo-2-methylbutane
(l) 1,1,1,2,2-pentafluoroethane

Practice E — alcohols

(a) butan-2-ol
(b) 2-methylbutan-1-ol
(c) 3-methylbutan-2-ol
(d) pentan-3-ol
(e) 2-methylbutan-2-ol
(f) 2,2-dimethylpropan-1-ol
(g) 3,3-dimethylbutan-2-ol
(h) butane-1,4-diol
(i) pentan-1-ol
(j) 3-methylpentan-2-ol
(k) 2,3-dimethylbutan-2-ol
(l) propane-1,2,3-triol

Practice F — aldehydes and ketones

(a) butanal (aldehyde)
(b) 2,2-dimethylpropanal (aldehyde)
(c) hexanal (aldehyde)
(d) 3-methylbutanal (aldehyde)
(e) pentan-2-one (ketone)
(f) 4-methylpentan-2-one (ketone)

(g) 3,3-dimethylbutan-2-one (ketone)
(h) 2-methylpentan-3-one (ketone)
(i) pentanal (aldehyde)
(j) hexan-3-one (ketone)
(k) 4-methylpentanal (aldehyde)
(l) methanal (aldehyde)

Practice G — carboxylic acids

(a) propanoic acid
(b) butanoic acid
(c) 3-methylbutanoic acid
(d) 2-methylbutanoic acid
(e) 2,2-dimethylpropanoic acid
(f) hexanoic acid
(g) 2,3-dimethylbutanoic acid
(h) 2-ethylbutanoic acid
(i) methanoic acid
(j) 3-methylpentanoic acid
(k) potassium ethanoate
(l) magnesium propanoate

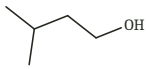
Practice H — esters, ethers and salts

(a) methyl ethanoate
(b) ethyl methanoate
(c) ethyl propanoate
(d) methyl butanoate
(e) methoxymethane
(f) ethoxyethane
(g) sodium ethanoate
(h) 1-methoxypropane (methoxypropane)

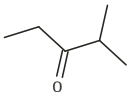
Practice I — drawing compounds

(a) 

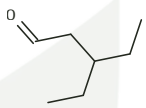
$C_5H_{11}Br$

(b) 

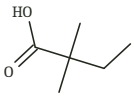
$C_5H_{12}O$

(c) 

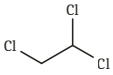
$C_6H_{12}O$

(d) 

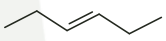
$C_7H_{14}O$

(e) 

$C_6H_{12}O_2$

(f) 

$C_2H_3Cl_3$

(g) 
C_6H_{12}

(h) 

$C_5H_{12}O$

Practice J — corrected names

(a) 3-methylhexane (the ethyl extends the chain)
(b) pentane
(c) 2-methylbutane (number from the other end)
(d) butan-2-ol
(e) 4-methylpentan-2-ol (the –OH takes the low number)
(f) pent-1-ene
(g) 3-methylbutan-2-one
(h) 2-chloro-3-methylbutane (tie: chloro first alphabetically)
(i) 3-ethyl-2-methylpentane (alphabetical order)
(j) 2,2-dimethylpropane (di- is needed)
(k) propanal (an aldehyde needs no number)
(l) 2-methylbutan-1-ol (the ethyl extends the chain)

Practice K — structural isomers

1. pentane, 2-methylbutane, 2,2-dimethylpropane.
2. but-1-ene, but-2-ene, methylpropene ($CH_2{=}C(CH_3)_2$).
3. 1-chloropropane, $CH_3CH_2CH_2Cl$ (primary); 2-chloropropane, $CH_3CHClCH_3$ (secondary).
4. propan-1-ol and propan-2-ol are position isomers; methoxyethane, $CH_3OCH_2CH_3$, is a functional group isomer of both.
5. butanal $CH_3CH_2CH_2CHO$; 2-methylpropanal $(CH_3)_2CHCHO$; butanone $CH_3COCH_2CH_3$.
6. Acids: butanoic acid $CH_3CH_2CH_2COOH$ and 2-methylpropanoic acid $(CH_3)_2CHCOOH$. Esters: any two of methyl propanoate $CH_3CH_2COOCH_3$, ethyl ethanoate $CH_3COOCH_2CH_3$, propyl methanoate $HCOOCH_2CH_2CH_3$, $HCOOCH(CH_3)_2$.
7. but-1-yne $HC{\equiv}CCH_2CH_3$ and but-2-yne $CH_3C{\equiv}CCH_3$: position isomers.
8. $CH_3CH_2CH_2NH_2$ and $(CH_3)_2CHNH_2$ (both primary: one C on the N); $CH_3NHCH_2CH_3$ (secondary); $(CH_3)_3N$ (tertiary).

9. 1,2-, 1,3- and 1,4-dimethylbenzene. 1,4-Dimethylbenzene has the highest melting point (13 °C, against about −25 °C and −48 °C): it is the most symmetrical, so its molecules pack most efficiently in the solid lattice.
10. Three: 1,2,3-, 1,2,4- and 1,3,5-trichlorobenzene.

Check yourself

1. **B.** Methyl groups on C2 and C3 of a pentane chain.
2. **B.** The –CHO carbon is C1; the methyl is on C3.
3. **D.** A should be butan-2-ol, B 3-methylpentane, C pent-2-ene.
4. **A.** The C–OH carbon is bonded to three other carbons.
5. **C.** Hexane, 2-methylpentane, 3-methylpentane, 2,2-dimethylbutane, 2,3-dimethylbutane.
6. **C.** Aldehyde and ketone; A and D are position isomers, B chain isomers.
7. **C.** The C–Cl carbon is bonded to two other carbons.
8. **A.** Acid part CH_3CH_2COO (propanoate); alcohol part CH_2CH_3 (ethyl).
9. (a) 2-methylpentane (b) 2-methylbut-2-ene (c) 2,3-dibromobutane (d) 2-methylpentan-3-ol (e) 2-methylbutanal (f) 4-methylpentan-2-one (g) 2,2-dimethylpropanoic acid (h) 4-methylpent-2-yne **[1]** each.
10. (a) 2,4-dimethylhexane (b) 2,4-dichloropentane (c) 5-methylhexan-3-one (d) 2-ethylbutan-1-ol (e) 3-ethylpent-2-ene (f) 3,3-dimethylbutanoic acid **[1]** each.
11. (a) $(CH_3)_2C(OH)CH(CH_3)_2$ (b) $CH_2{=}CHCH_2CH(CH_3)_2$ (c) $CH_3CH_2CH(C_2H_5)CH_2CH_2CH_3$ (d) $CH_3CH_2CH(CH_3)COOH$ (e) $CH_2ClCCl(CH_3)_2$ (f) $CH_3CH_2COCH_2CH_2CH_3$, each drawn as a skeletal formula **[1]** each.
12. The structure is $CH_3CH_2CH(CH_3)CH(CH_3)CH_3$ **[1]**, whose longest chain has five carbons: 2,3-dimethylpentane **[1]**.
13. An aldehyde C=O must be on C1 (the end of the chain); a C=O on C2 of propane is a ketone, propanone **[1]**.
14. Compounds with the same molecular formula but different structural formulas / connectivities **[1]**.
15. pent-1-ene, pent-2-ene, 2-methylbut-1-ene, 3-methylbut-1-ene, 2-methylbut-2-ene **[1]** each.
16. butan-1-ol (primary), butan-2-ol (secondary), 2-methylpropan-1-ol (primary), 2-methylpropan-2-ol (tertiary) **[1]** each, for structure, name and class.
17. (a) propan-1-ol or propan-2-ol, and methoxyethane (b) propanal and propanone (c) propanoic acid, and methyl ethanoate or ethyl methanoate **[1]** for each structure with its name.
18. (a) primary (b) tertiary (c) secondary (d) primary (one carbon bonded to the N) **[1]** each.
19. 2,2-Dimethylpropane is more branched and nearly spherical, so there is less surface contact between molecules **[1]**; its London dispersion forces are weaker, so less energy is needed to separate the molecules **[1]**.
20. (a) position isomers **[1]** (b) 3-methylbutan-2-one, $CH_3COCH(CH_3)_2$ **[1]** (c) any of pentanal, 2-methylbutanal, 3-methylbutanal, 2,2-dimethylpropanal **[1]**.
21. **C.** 3-Ethylpentane is C_7H_{16}, an isomer of heptane.
22. Ethanol has an O–H group, so hydrogen bonds form between its molecules **[1]**; methoxymethane has no H bonded to O, so it has only dipole–dipole and London dispersion forces **[1]**. More energy is needed to separate ethanol molecules, so its boiling point is much higher **[1]**.
23. 1,2-dichlorobenzene, 1,3-dichlorobenzene, 1,4-dichlorobenzene **[1]** each.
24. Only three isomers exist, and only one 1,2-isomer **[1]**. With fixed alternating single and double bonds there would be two different 1,2-isomers (Cl–C=C–Cl and Cl–C–C–Cl), so all six C–C bonds must be identical, with delocalized π electrons **[1]**.

Where this fits in Structure 3.2

- **Booklet 4** — 3.2.1 to 3.2.4: formulas, functional groups and classes, homologous series and physical trends.
- **Booklet 5** (this booklet) — 3.2.5 and 3.2.6: IUPAC nomenclature and structural isomers.
- **Booklet 6** (HL) — 3.2.7: stereoisomers, *cis–trans* isomerism and optical isomerism.
- **Next** — HL 3.2.8 and 3.2.9: identifying organic compounds from mass spectra, IR and ^{1}H NMR spectra.
- Links forward: **Reactivity 3.2** (oxidation of 1°, 2° and 3° alcohols), **Reactivity 3.4** (esterification, substitution of halogenoalkanes), **Reactivity 3.3** (reactions of alkenes).

These notes are a free resource, shared for any IB student who finds them useful.

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