

DP IB Chemistry: SL



10.1 Fundamentals of Organic Chemistry

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10.1.1 Homologous Series

Your notes

Homologous Series

- Organic chemistry is the chemistry of carbon compounds
- Carbon forms a vast number of compounds because it can form strong covalent bonds with itself
- This enables it to form long chains of carbon atoms, and hence an almost infinite variety of carbon compounds are known
- The tendency of identical atoms to form covalent bonds with each other and hence form chains is known as **catenation**

Catenation in carbon allows an almost infinite variety of chains, branches and rings

- Carbon always forms four covalent bonds which can be single, double or triple bonds
- A **functional group** is a specific atom or group of atoms which confer certain physical and chemical properties onto the molecule
- Organic molecules are classified by the dominant **functional group** on the molecule
- Organic compounds with the same functional group, but a different number of carbon atoms, are said to belong to the same **homologous series**
- Every time a carbon atom is added to the chain, two hydrogen atoms are also added

Homologous Series of Alkanes Table



Name of alkane	Number of carbons	Chemical formula	Boiling point in °C	State at room temperature	Melting point in °C
Methane	1	CH₄	-162	gas	-182
Ethane	2	C ₂ H ₆	-89	gas	-183
Propane	3	C ₃ H ₈	-42	gas	-188
Butane	4	C ₄ H ₁₀	-1	gas	-138
Pentane	5	C ₅ H ₁₂	36	liquid	-130

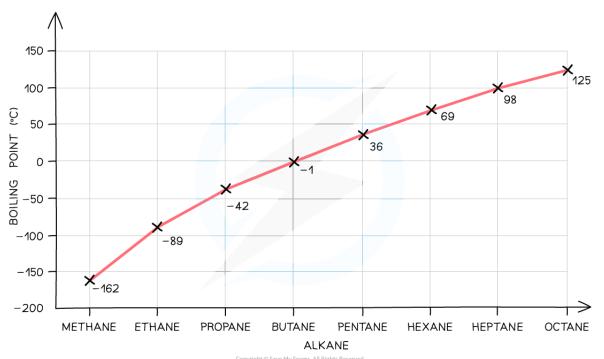


- Things we can say about a **homologous series**:
 - each member has the same **functional group**
 - each member has the same **general formula**
 - each member has similar chemical properties
 - each member differs by -CH₂-
 - members have gradually changing physical properties, for example, boiling point, melting point and density
- As a homologous series is ascended, the size of the molecule increases
- This has an effect on the physical properties, such as boiling point and density



Boiling Point Trends

• A graph of boiling point for the first eight alkanes looks like this:



- The broad trend is that **boiling point increases** with increased molecular size
- Each additional -CH₂ (called the **homologous increment**) adds 8 more electrons to the molecule
- This increases the strength of the **London Dispersion Forces**
- Stronger LDF leads to a higher boiling point
- These trends are followed in other homologous series





10.1.2 Understanding Organic Molecules

Your notes

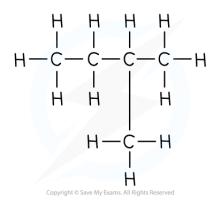
Representing Formulae

- Organic compounds can be represented in a number of ways:
 - Empirical Formulae
 - Molecular Formulae
 - Structural Formulae
 - Condensed Structural Formulae
- The **empirical formula** shows the **simplest possible ratio** of the atoms in a molecule
- For example:
 - Hydrogen peroxide is H_2O_2 but the empirical formula is HO
- The molecular formula shows the actual number of atoms in a molecule
- For example:

The molecular formulae of butane and butene

- The structural formula shows the spatial arrangement of all the atoms and bonds in a molecule
- This is also known as the **displayed formula** or **graphical formula**.
- For example:

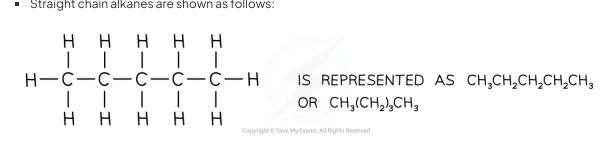






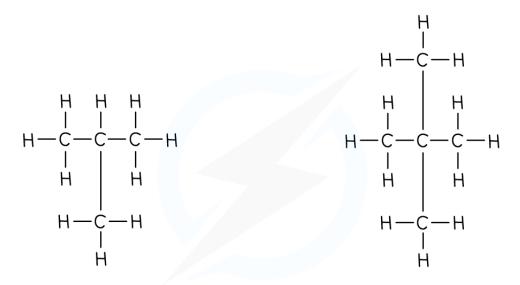
The structural formula of 2-methylbutane

- In a condensed structural formulae enough information is shown to make the structure clear, but most of the actual covalent bonds are omitted
- Only important bonds are always shown, such as double and triple bonds
- Identical groups can be bracketed together
- Side groups are also shown using brackets
- Straight chain alkanes are shown as follows:



Representing condensed structural formulae of straight chains

Branched alkanes are shown as follows:





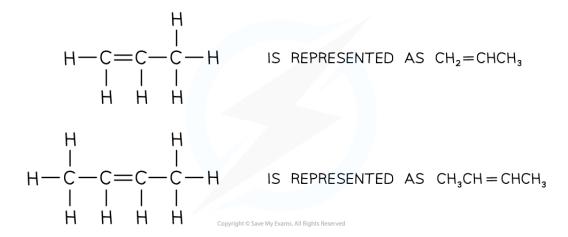
IS REPRESENTED AS $CH_3CH(CH_3)CH_3$ OR $CH_3CH(CH_3)_2$

IS REPRESENTED AS $CH_3C(CH_3)_2CH_3$ OR $CH_3C(CH_3)_3$ OR $C(CH_3)_4$

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Representing condensed structural formulae of branched alkanes

Alkenes are shown as follows:

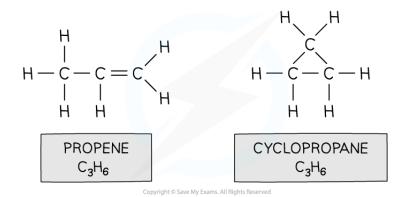


Representing condensed structural formulae of alkenes

Isomers

- Structural isomers are compounds that have the same molecular formula but different structural formulae
 - Eg. propene and cyclopropane





Both propene and cyclopropane are made up of 3 carbon and 6 hydrogen atoms but the structure of the two molecules differs

- There are three different types of structural isomerism:
 - Branch-Chain isomerism
 - Positional isomerism
 - Functional group isomerism

Branch-Chain isomerism

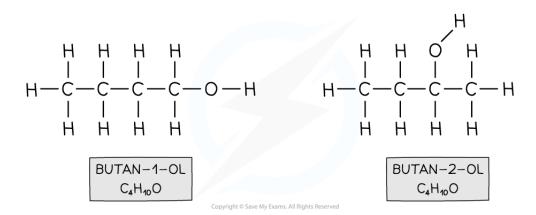
- **Branch-Chain isomerism** is when compounds have the same molecular formula, but their longest hydrocarbon chain is not the same
- This is caused by branching
 - Eg. pentane and 2,2-dimethylpropane



Both compounds are made up of the same atoms however the longest carbon chain in pentane is 5 and in 2,2-dimethylpropane it is 3 (with two methyl branches)

Positional isomerism

- Positional isomers arise from differences in the position of a functional group in each isomer
 - The functional group can be located on different carbons
 - For example, butan-1-ol and butan-2-ol



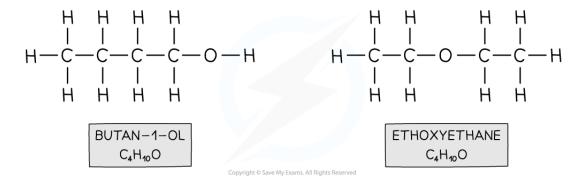
Both compounds have an alcohol group and are made up of 4 carbon, 10 hydrogen and one oxygen atom however in butan-1-ol the functional group is located on the first carbon and in butan-2-ol on the second carbon



Functional group isomerism

- When different functional groups result in the same molecular formula, functional group isomers arise
- The isomers have very different chemical properties as they have different functional groups
 - For example, butanol and ethoxyethane





Both compounds have the same molecular formula however butan-1-ol contains an alcohol functional group and ethoxyethane an ether functional group

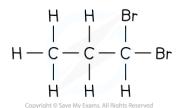
 You should be able to deduce all possible isomers for organic compounds knowing their molecular formula

Worked example

How many isomers are there of, $C_3H_6Br_2$?

Answer:

Step 1: Draw the structural formula of the compound



Step 2: Determine whether there is functional group, branch-chain or positional isomerism

• Functional group? No, as Br is the only functional group possible

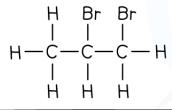
- Branch-chain? No, as the longest chain can only be 3
- Positional? Yes, as the two bromine atoms can be bonded to different carbon atoms



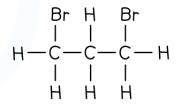
AND

1,1-DIBROMOPROPANE

2,2-DIBROMOPROPANE



1,2-DIBROMOPROPANE



1,3-DIBROMOPROPANE

C₃H₆Br₂ THEREFORE HAS 4 STRUCTURAL ISOMERS
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AND



Worked example

How many isomers are there of the compound with molecular formula C_4H_{10} ?

Answer:

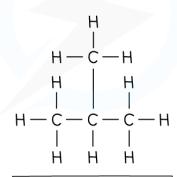
Step 1: Draw the structural formula of the compound





Step 2: Determine whether it is a functional group, chain or positional isomerism

- Functional group? No, as there are no functional groups
- Positional? No, as there are no functional groups which can be positioned on different carbon atoms
- Chain? yes!



2-METHYLPROPANE

C4H10 THEREFORE HAS 2 STRUCTURAL ISOMERS

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Examiner Tip

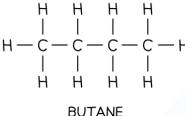
Don't be fooled by molecules by bending and turning through 90 degrees - that does not make them isomers. The best test is to try and name them - isomers will have a different name.



Saturated & Unsaturated

Saturated & unsaturated hydrocarbons

- Saturated hydrocarbons are hydrocarbons which contain single bonds only resulting in the maximum number of hydrogen atoms in the molecule
- Unsaturated hydrocarbons are hydrocarbons which contain carbon-carbon double or triple bonds



BUTENE

SATURATED HYDROCARBON

AS THERE'RE ONLY SINGLE C-H BONDS AND EVERY CARBON IS BONDED TO THE MAXIMUM NUMBER OF HYDROGEN ATOMS

UNSATURATED HYDROCARBON

THE HYDROCARBON CONTAINS A DOUBLE BOND AND NOT ALL CARBON ATOMS ARE BONDED TO THE MAXIMUM NUMBER OF HYDROGEN ATOMS (FIRST CARBON CAN BOND 3 H-ATOMS, BUT IT'S ONLY BONDED TO 2)

The diagram shows saturated hydrocarbons which contain single bonds only and unsaturated hydrocarbons which contain double/triple bonds as well



10.1.3 Nomenclature

Your notes

Nomenclature

- **Systematic nomenclature** can be used to name organic compounds and therefore make it easier to refer to them
- The **alkanes** provide the basis of the naming system and the **stem** of each name indicates how many carbon atoms are in the **longest chain** in one molecule of the compound

Nomenclature of Organic Compounds Table



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Number of C atoms	Molecular formula of straight-chain alkane	Name of alkane	Stem used in naming
1	CH₄	methane	meth-
2	C ₂ H ₆	ethane	eth-
3	C ₃ H ₈	propane	prop-
4	C ₄ H ₁₀	butane	but-
5	C ₅ H ₁₂	pentane	pent-
6	C ₆ H ₁₄	hexane	hex-
7	C ₇ H ₁₆	heptane	hept-
8	C ₈ H ₁₈	octane	oct-
9	C ₉ H ₂₀	nondne	non-
10	C ₁₀ H ₂₂	decane	dec-

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Although the table shows up to 10 carbons for reference, in your IB Chemistry exam you are only required to name molecules with up to 6 carbons



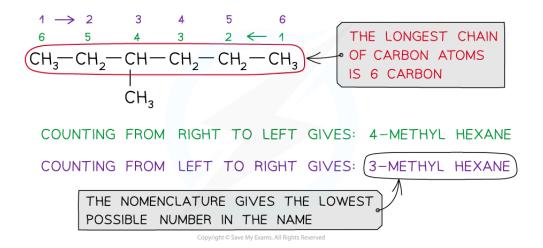


Chains & Branches

- If there are any side-chains or functional groups present, then the position of these groups are indicated by numbering the carbon atoms in the longest chain starting at the end that gives the lowest possible numbers in the name
- The hydrocarbon **side-chain** is shown in **brackets** in the structural formula

CH₃CH(CH₃)CH₂CH₃

- The side-chain is named by adding '-yl' to the normal alkane **stem**
- This type of group is called an **alkyl** group

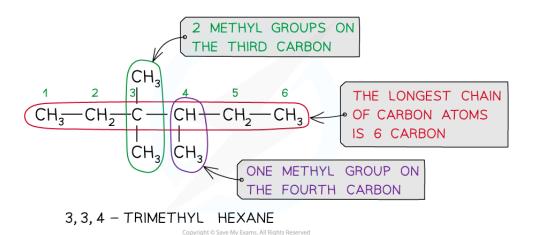


Naming Side Chains

- If there are more than one of the same alkyl side-chain or functional groups, **di-** (for two), **tri-** (for three) or **tetra-** (for four) is added in front of its name
- The adjacent **numbers** have a comma between them
- Numbers are separated from words by a hyphen

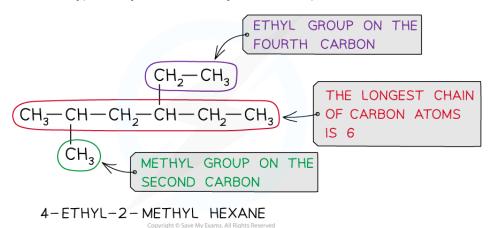






Naming Multiple Side Chains

• If there is more than one type of alkyl side-chain, they are listed in alphabetic order



Naming Side Chains in Alphabetical Order



An **aliphatic** compound is **straight** or **branched-chain** and also includes **cyclic** organic compounds that do not contain a **benzene** ring



10.1.4 Organic Families - Hydrocarbons

Your notes

Alkanes

- **Hydrocarbons** are compounds containing hydrogen and carbon only
- There are four families of hydrocarbons you should know: alkanes, alkenes, alkynes and arenes
- Alkanes have the general molecular formula C_nH_{2n+2} . They contain only single bonds and are said to be saturated
- Alkanes are named using the nomenclature rule alk + ane
- The **alk** depends on the number of carbons as outlined in the previous Section 10.1.2

Structural Formula	Name	Molecular Formula
H H—C—H H	methane	CH₄
H H I I H—C—C—H I I H H	ethane	C₂H ₆
H H H I I I H—C—C——H I I I H H H H Copyright © Save My Exams. All Rights Reserved	propane	C₃H ₈



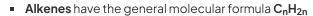
H H H H 	butane	C₄H ₁₀
H H H H 	pentane	C₅H ₁₂
H H H H H H H H H H H H H H H H H H H	hexane	C ₆ H₁₄



The first six members of the alkane family



Alkenes



- They are said to be **unsaturated**
- Alkenes are named using the nomenclature rule **alk + ene**
- In molecules with a straight chain of 4 or more carbon atoms, the position of the C=C double bond must be specified
- The carbon atoms on the straight chain must be numbered, starting with the end closest to the double
- The lowest-numbered carbon atom participating in the double bond is indicated just before the -ene:

Structural Formula	Name	Molecular Formula
H $C = C$ H	ethene	C₂H₄
C = C - C - H H H H H H H H	propene	C₃H ₆
C = C - C - C - H H H H H H H H H H	but-1-ene	C₄H ₈





$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	pent-1-ene	C₅H ₄₀
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	hex-1-ene	C ₆ H₁₂



The first five members of the alkene family

- There is a distinction to be made between the name of the **functional group** and the name of the **family**
- The name of the family is **alkene**, but the name of the functional group is **alkenyl**



Alkynes

- Alkynes have the general molecular formula C_nH_{2n-2}
- The triple bond makes them **unsaturated** molecules
- Alkynes are named using the nomenclature rule alk + yne
- As with alkenes, in molecules with a straight chain of 4 or more carbon atoms, the position of the triple bond must be specified
- The carbon atoms on the straight chain must be numbered, starting with the end closest to the triple
- The lowest-numbered carbon atom participating in the triple bond is indicated just before the -yne:

Structural Formula	Name	Molecular Formula
H—C≡C—H	ethyne	C₂H₂
H—C≡C—C—H 	propyne	C₃H₄
H H H I I I I I I I I I I I I I I I I I	but-1-yne	C₄H ₆



H H H		
H H H H	hex-1-yne	C _e H ₁₀

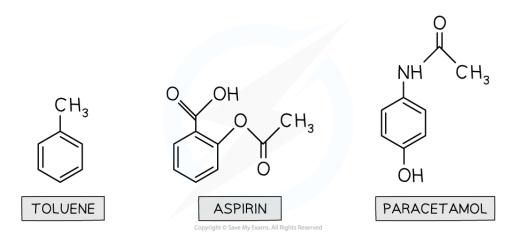


The first five members of the alkyne family

• The name of the functional group is **alkynyl**

Arenes

- Arene is the collective name given to compounds with one or more rings with pi electrons that are delocalised throughout the ring(s)
- Compounds with this feature are said to be **aromatic**
- This doesn't mean they are necessarily smelly, although a lot of naturally occurring arenes do have distinctive smells!



Arenes are present in many everyday chemicals and pharmaceuticals

- Benzene, C₆H₆, is the only aromatic hydrocarbon that is covered in IB Chemistry and is dealt with in Section 10.1.12
- The functional group in **benzene** is known as a **phenyl group** when attached to other molecules



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10.1.5 Organic Families - Halogenoalkanes

Your notes

Halogenoalkanes

- Halogenoalkanes or Haloalkanes have the general molecular formula, C_nH_{2n+1}X, where X represents a halogen
- Haloalkanes are named using the prefix chloro-, bromo- or iodo-, with the ending -ane
- In molecules with a straight chain of three or more carbon atoms, the position of the halogen atom must also be specified
- The carbon atoms on the straight chain must be numbered, starting with the end closest to the halogen atom
- The number of the carbon atom attached to the halogen is indicated before the prefix:

Haloalkanes Examples Table

Structural Formula	Name	Molecular Formula
H H H—C—C—Cl H H	chloroethane	C₂H₅Cl
H Br H H—C—C—C—H H H H	2-bromopropane	C₃H ₇ Br
H H H H H	1—iodopentane	C ₅ H ₁₁ I







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- The position of all halogens in dihaloalkanes except those with one carbon atom must be specified.
- If there is more than one of the same type of halogen atom on the molecule, the di (two), tri (three) or tetra (four) prefixes must also be used

Dihaloalkanes Examples Table

Structural Formula	Name	Molecular Formula
H H H-C-C-Cl H Cl	1,1-dichloroethane	C₂H₄Cl₂
H H H-C-C-Cl Cl H	1,2-dichloroethane	C₂H₄Cl₂
H H H Br—C—C—C—H H Cl H	1-bromo-2-chloropropane	C₃H ₆ BrCl

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10.1.6 Organic Families - Alcohols & Ethers

Your notes

Alcohols & Ethers

Alcohols

- Alcohols are a family of molecules that contain the hydroxyl functional group, -OH
- Their general formula is C_nH_{2n+1}OH
- The nomenclature of alcohols follows the pattern **alkan + ol**
- If there are two **-OH** groups present the molecule is called a **diol**

The first four Alcohols and their Structures Table

ALCOHOL	STRUCTURAL FORMULA	DISPLAYED FORMULA
METHANOL	CH ₃ OH	H-C-H H-C-H
ETHANOL	CH ₃ CH ₂ OH	H H-O-H H-O-H H-O-H
PROPANOL	CH ₃ CH ₂ CH ₂ OH	H H H H - C - C - C - H H H H H H H H H
BUTANOL	CH ₃ CH ₂ CH ₂ CH ₂ OH	H - C - H - H - C - H - H - C - H - H -

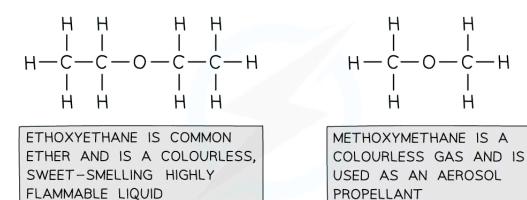
Classification of alcohols

- Alcohols are classified as primary, secondary or tertiary depending on the number of carbons attached to the functional group carbon
- This is covered in detail in Section 10.1.11



Ethers

- Ethers are a family of molecules that contain the ether functional group, R-O-R, where R is an alkyl group
- Their general formula is C_nH_{2n+2}O
- The nomenclature of ether follows the pattern alkoxy + alkane
- Sometimes you will see an older nomenclature for **ethers** where each **R** group is given an **alkyl** name
 - For Example: CH₃OCH₃ is dimethyl ether and C₂H₅OCH₃ is ethyl methyl ether
- Ethers are functional group isomers of alcohols



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Ethers are useful substances





10.1.7 Organic Families - Carbonyls

Your notes

Carbonyls

- Carbonyl is the collective name for compounds containing the functional group C=O
- The general formula of a carbonyl is $C_nH_{2n}O$
- The two sub-families of carbonyls are aldehyde and ketone (known in some countries as alkanals and alkanones)

Aldehydes

- If the carbonyl group is on the end of a chain then it is an aldehyde and has the functional group formula, RCHO
 - the H is written before the O so as not to confuse it with an alcohol
- The nomenclature of **carbonyls** follows the pattern **alkan + al**
- There is no need to use numbers in the name as aldehyde will always be on the number 1 carbon atom

Ketones

- Ketones have a minimum of three carbons and have the general functional group formula, RCOR
- The nomenclature of **ketones** follows the pattern **alkan + one**
- After butanone, the carbonyl group can have positional isomers, so numbering must be used
 - For example pentan-2-one and pentan-3-one

Aldehyde and Ketone Examples Table

Your notes

Structural Formula	Name	Molecular Formula
О H—С—Н	methanal (also known as formaldehyde)	CH₂O
H O H—C—C—H H	ethanal	C ₂ H ₄ O
H H O I H—C—C—C—H I H H Copyright © Save My Exams. All Rights F	propanal	C₃H ₆ O
h ö h	propanone	C ₃ H ₆ O

H O H 	propanone (also known as acetone)	C₃H ₆ O
H O H H H H-C-C-C-C-H H H H	pentan-2-one	C₅H₁₀O

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- As they have a very similar functional group arrangement, **aldehydes** and **ketones** show similar chemical reactions
- Differences in their chemistry are due to the reactions that involve the Hon the **aldehyde** or the nature of the R group
- The difference in **electronegativity** between oxygen and carbon means the C=O is polar, leading to dipole-dipole attractions between the molecules which results in:
 - higher than expected boiling points for small molecules



- solubility in water for the lower members of the families
- Aldehydes and ketones with the same number of carbons are functional group isomers



10.1.8 Organic Families - Carboxylic Acids & Esters

Your notes

Carboxylic Acids & Esters

Carboxylic acids

- Carboxylic acids is the name given to compounds containing the functional group carboxyl, -COOH
- The general formula of a carboxylic acid is C_nH_{2n+1}COOH which can be shortened to just RCOOH
 - (In some countries the family is called alkanoic acid)
- The nomenclature of carboxylic acid follows the pattern alkan + oic acid
- There is no need to use numbers in the name as the carboxyl group will always be on the number 1 carbon atom

Carboxylic Acids Examples Table

Structural Formula	Name	Molecular Formula
0 H—C—O— H	methanoic acid (also known as formic acid)	HCO₂H
H O H-C-C-O-H H	ethanoic acid (also known as acetic acid)	CH₃CO₂H
H H O H-C-C-C-O-H H H	propanoic acid	C₂H₅CO₂H

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Esters

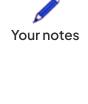
Esters are functional group isomers of carboxylic acids and contain the functional group,
 carboxylate, -COOR



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- The general formula of an ester is usually represented as **RCOOR** where **R** can be the same or different on either side of the carboxylate group
- The nomenclature of **esters** follows the pattern **alkyl + alkanoate**
- The alkyl group in the name is the **R** group attached to the oxygen

Esters Examples Table



Structural Formula	Name	Molecular Formula
0 H H - C - O - H H - H	methyl methanoate	HCO₂CH₃
H O H I I H - C - C - O - C - H I H	methyl ethanoate	CH ₃ CO ₂ CH ₃
H O H H 	ethyl ethanoate	C ₂ H ₅ CO ₂ C ₂ H ₅

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- Carboxylic acids and esters contain few similarities in their chemical and physical properties
- **H-bonds** are present between **carboxylic acid** molecules and not between **esters**, so this affects the melting point, boiling point and solubility:
 - Smaller chain **carboxylic acids** are soluble in water and have higher boiling points than expected (e.g. ethanoic acid is 117 °C)
 - Esters are insoluble in water and have lower boiling points than their isomeric carboxylic acids (e.g. methyl methanoate is 31 °C)





Examiner Tip

The C in RCOOR is included in the name of the first R group, so $C_3H_7COOCH_3$ is methyl butanoate not methyl propanoate. Don't be fooled by the order of the atoms in the linear formula: $CH_3OC(O)C_3H_7$ is also an acceptable way to write the formula of methyl butanoate!





10.1.9 Organic Families - Organic Nitrogen Compounds

Your notes

Organic Nitrogen Compounds

Amines

- There are three organic nitrogen families that you need to know: amines, amides and nitriles
- Amine is the name given to compounds containing the functional group amino, -NH₂
- Amines are derived from ammonia where one H in ammonia (NH₃)has been replaced by an R (alkyl) aroup
- The general formula of an amine is C_nH_{2n+1}NH₂ which can be shortened to just RNH₂

Amides

- Amide is the name given to compounds containing the functional group carboxamide, -CONH₂
- Amides are a combination of amino and carbonyl groups
- The general formula of an **amide** is C_nH_{2n+1}CONH₂ which can be shortened to just **RCONH**₂

Nitriles

- Nitriles are compounds containing the functional group nitrile, -CN
- This is the same CN group that is called a cyanide group as an ion, just as hydroxyl group, OH is called hydroxide in inorganic chemistry
- The general formula of an **nitrile** is $C_nH_{2n+1}CN$ which can be shortened to just RCN

Organic Nitrogen Compounds Examples

Your notes	

Structural Formula	Name	Molecular Formula
H 	methylamine or aminomethane	CH₃NH₂
H O H-C-C-N-H H H	ethanamide	CH₃CONH₂
H H—C—C≡Ñ H	ethanenitrile	CH ₃ CN

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Examiner Tip

Be careful about counting all the carbons when naming a nitrile. For example C_3H_7CN is butanenitrile not propanenitrile as the longest chain is 4 carbons.

You are not required to know the nomenclature of these nitrogen compounds, but you are expected to identify the functional groups in molecules.

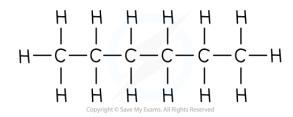


10.1.10 3-D modelling

Your notes

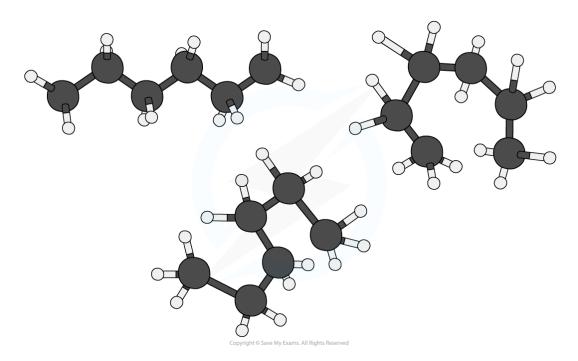
3-D Modelling

- Representing 3-D molecules on a 2D surface is not easy and the best way to understand 3-D structures is to use modelling kits or 3-D modelling software, such as ACD Labs ChemSketch
- For simplification, complex organic molecules are shown with 90° bond angles that give the minimum information of which atoms are connected together as in this representation of hexane, C_6H_{14}



A simplified displayed structure for hexane

- The true structure of hexane looks very different when viewed in 3-D modelling software
- Free rotation of the single bonds gives rise to structures that look different on paper:



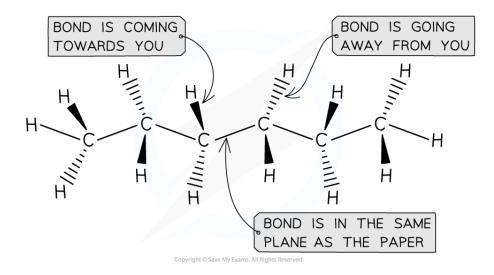
Different 3-D structures for hexane



- By convention, when showing using 3-D models or drawings, carbon is black, hydrogen is white and oxygen is red
- These structures may not contain accurate atomic radii, bond angles or bond lengths (modelling software usually allows you to manipulate these), but they convey information about the orientation of atoms that is very important in stereochemistry
- Stereochemistry is the study of the relative spatial arrangements of atoms in molecules

Stereochemical drawings

- To simplify 3-D drawings, chemists use a convention of drawing 'wedge' bonds to show bonds coming
 out of the plane of the paper or receding away from the plane
 - A single solid line indicates the bond is in the same plane as the paper
 - The solid wedge shows the bond is coming towards you and the hatched or partial wedge bond is going away from you
- The stereochemical drawing for hexane is shown below:



A stereochemical drawing for hexane

 Stereochemical drawings are particularly useful for representing isomers and complex biomolecules such as carbohydrates and proteins

Examiner Tip

You are not expected to be able to draw 3-D molecules, but in an exam you may be presented with 3-D drawings from which you have to extract information such as the molecular formula or functional group



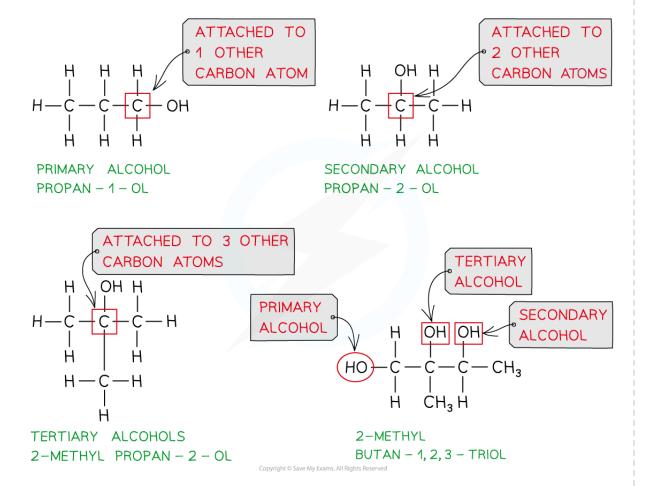
10.1.11 Primary, Secondary & Tertiary atoms

Your notes

Primary, Secondary & Tertiary Atoms

Alcohols and halogenoalkanes

- **Primary alcohols** and **halogenoalkanes** are those in which the carbon atom bonded to the functional group is attached to **one** other carbon atom (or alkyl group)
- In secondary alcohols and halogenoalkanes the functional group carbon atom is attached to two other carbon atoms (or alkyl groups)
- In tertiary alcohols and halogenoalkanes the functional group carbon atom is attached to three other carbon atoms (or alkyl groups)

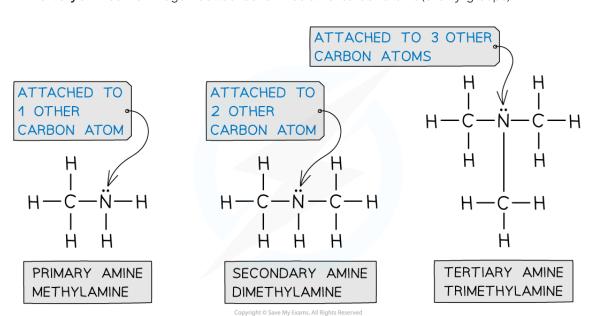


Classifying primary, secondary and tertiary alcohols and alcohols with more than one alcohol group

Amines



- Amines follow a slightly different classification system, although the terms primary, secondary and tertiary are still used
- The classification is based on the number of alkyl groups attached to the nitrogen in the amine
- Primary amines are those in which the nitrogen is attached to one other carbon atom (or alkyl group)
- In secondary amines the nitrogen atom is attached to two other carbon atoms (or alkyl groups)
- In **tertiary amines** the nitrogen is attached to **three** other carbon atoms (or alkyl groups)



Primary, secondary and tertiary Amines





10.1.12 Benzene

Your notes

Benzene

Kekulé structure for benzene

- Kekulé suggested that benzene was a **hexagon** with three double bonds
- It was therefore equivalent to three ethene molecules

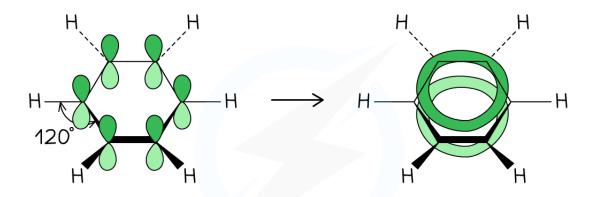
Problems with Kekulé's structure for benzene

- Since benzene has three double bonds, it should have similar reactivity to ethene
- However, this turned out not to be the case
 - Ethene undergoes addition reactions whereas benzene rarely does (only under very harsh conditions) and instead undergoes substitution reactions
- The presence of three double bonds also suggested that benzene had shorter double and longer single bonds
 - In fact, the bond lengths in benzene were **exactly** the same
 - They were found to be an **intermediate** between single and double bonds
- The benzene is also much more stable than Kekulé's suggested structure for benzene
 - Less energy was required to hydrogenate a benzene molecule compared to the hydrogenation of three ethene molecules
 - This means that the bonds broken in benzene are stronger than the double bonds in ethene
- The increase in stability of benzene is known as the delocalisation energy and is caused by the delocalised electrons in the benzene structure
- The C-C in benzene are an intermediate between single and double bonds which is a result of these
 delocalised electrons

Shape of benzene

- Benzene is a planar regular hexagon with bond angles of 120°
 - All the bonds are identical due to the delocalization of electrons
- Each sp² hybridised carbon atom in benzene forms:
 - A σ bond with two other carbons
 - A σ bond with one hydrogen atom
- The remaining p orbital is **overlapping** with the p orbitals on both sides of it
 - To achieve maximum overlap, the benzene ring must be planar
- This results in the formation of a system of π bonds spread out over the whole ring
- Due to this, the electrons are not bound to specific atoms but can instead freely move around the structure and are said to be **delocalised**







OVERLAP OF P ORBITALS PRODUCES A RING OF DELOCALISED ELECTRONS ABOVE AND BELOW THE PLANE OF BENZENE'S CARBON ATOMS

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Benzene has a π system of delocalised electrons with carbon atoms that have bond angles of 120°