DP IB Chemistry: SL

Your notes

10.1 Fundamentals of Organic Chemistry

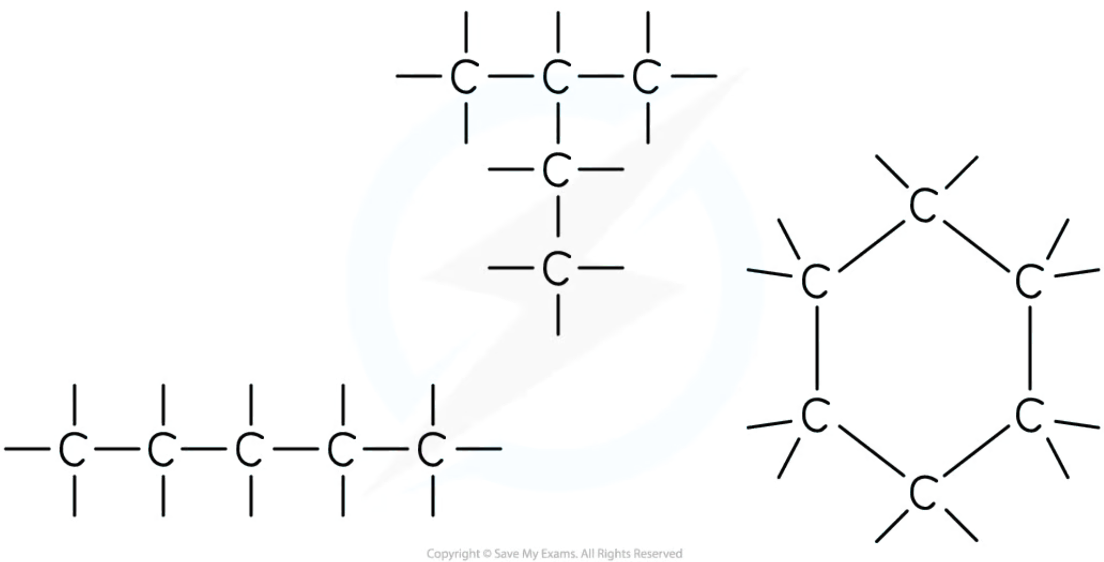
Contents

Your notes

10.1.1 Homologous Series

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

Your notes

Name of alkane	Number of carbons	Chemical formula	Boiling point in °C	State at room temperature	Melting point in °C
Methane	1	CH_4	−162	gas	−182
Ethane	2	C_2H_6	−89	gas	−183
Propane	3	C_3H_8	−42	gas	−188
Butane	4	C_4H_{10}	−1	gas	−138
Pentane	5	C_5H_{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 -CH_2-
  - 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

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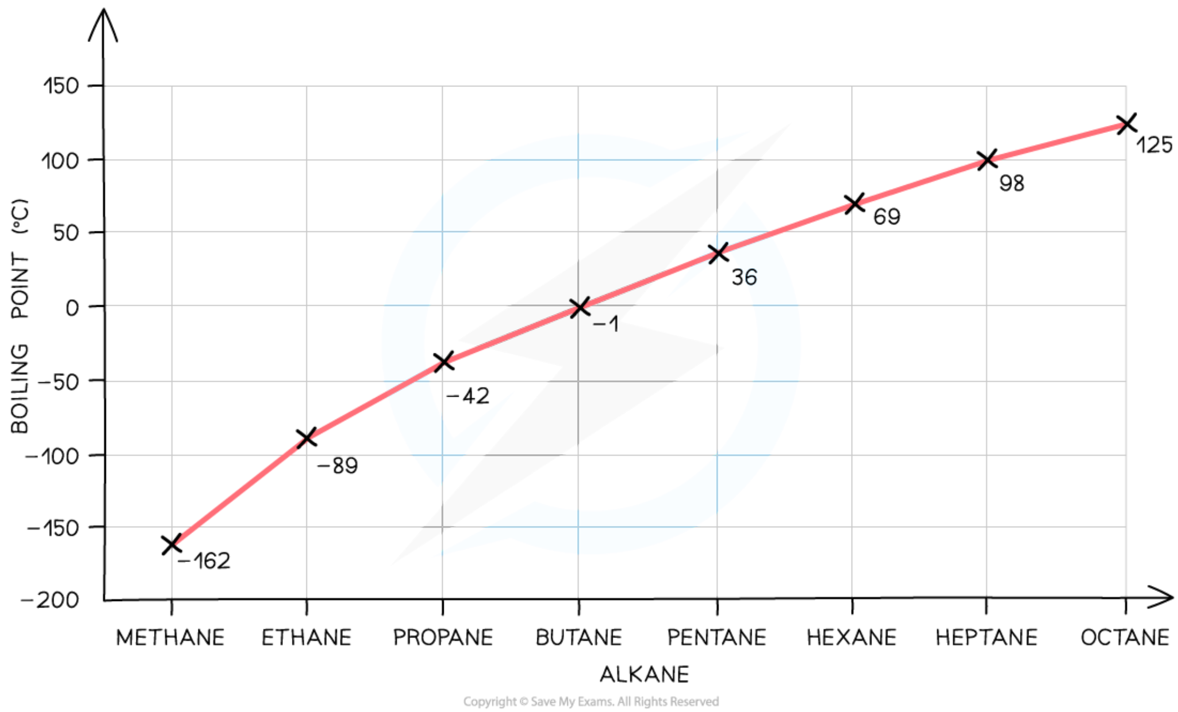
- A graph of boiling point for the first eight alkanes looks like this:



- The broad trend is that **boiling point increases** with increased molecular size
- Each additional -CH_2- (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**

Your notes

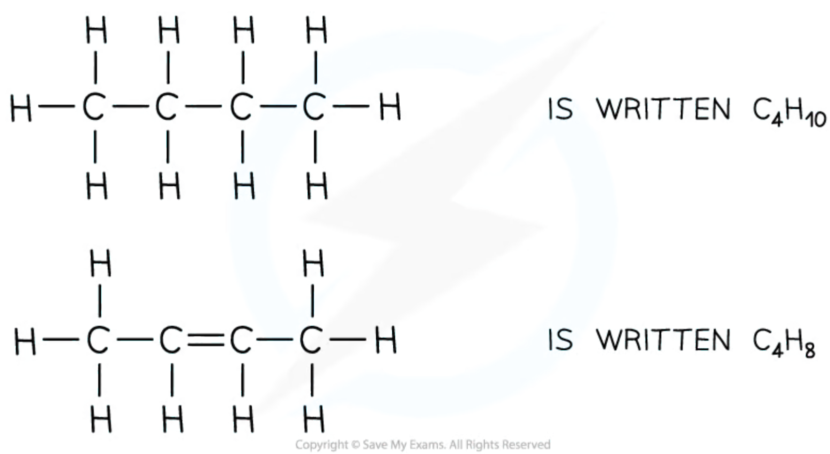
10.1.2 Understanding Organic Molecules

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:

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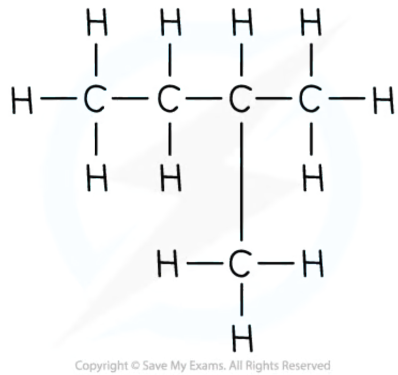
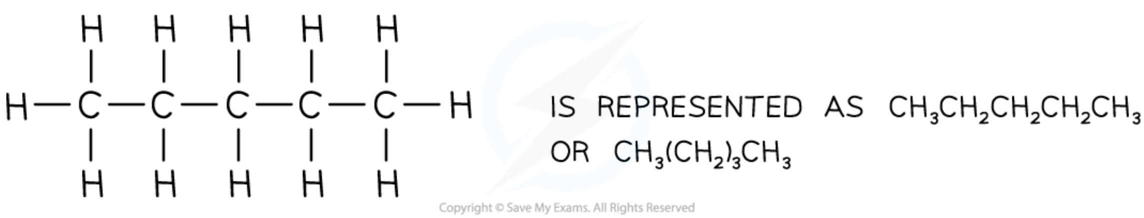


The structural formula of 2-methylbutane

- 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:

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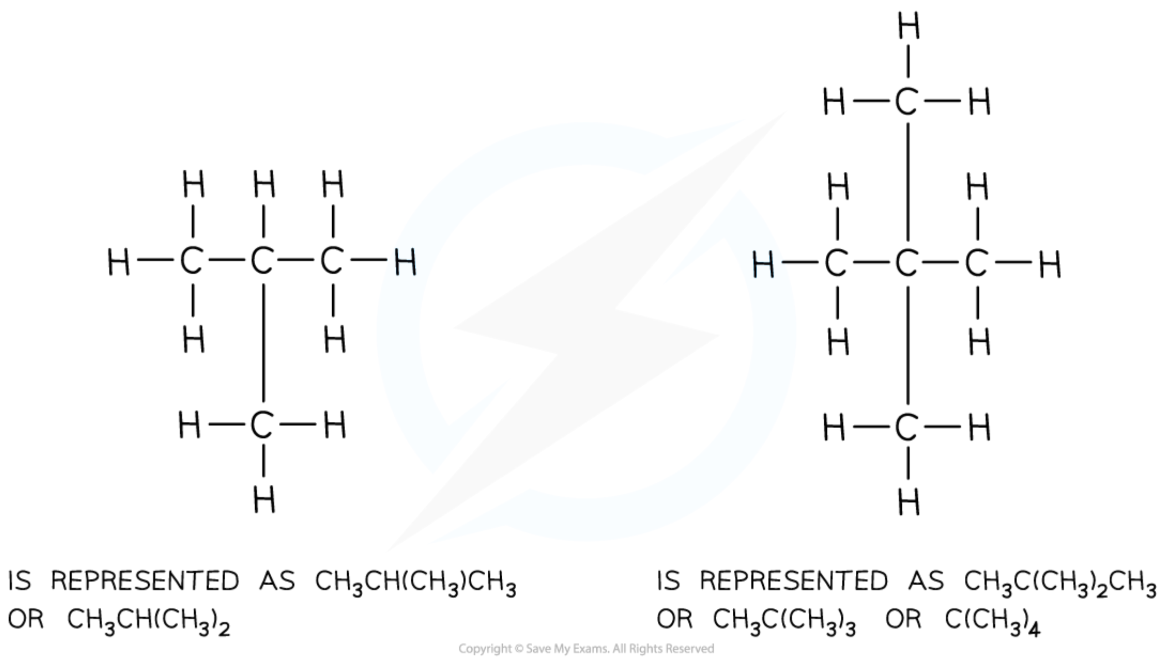
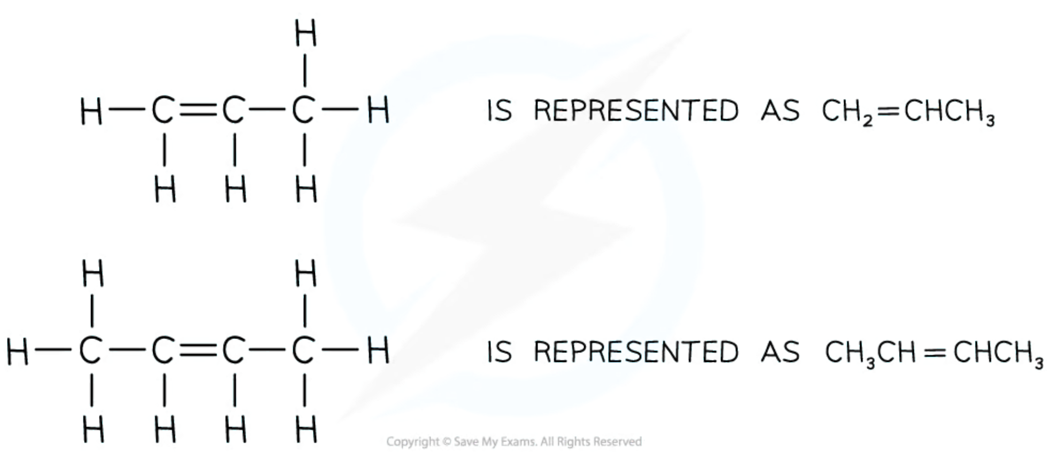


Representing condensed structural formulae of branched alkanes

- Alkenes are shown as follows:



Representing condensed structural formulae of alkenes

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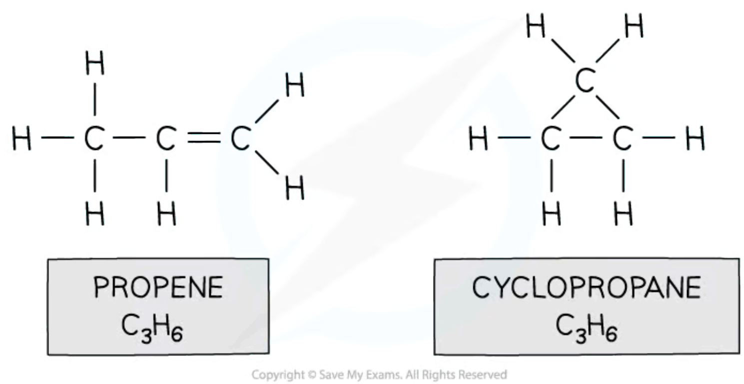
Isomers

- **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

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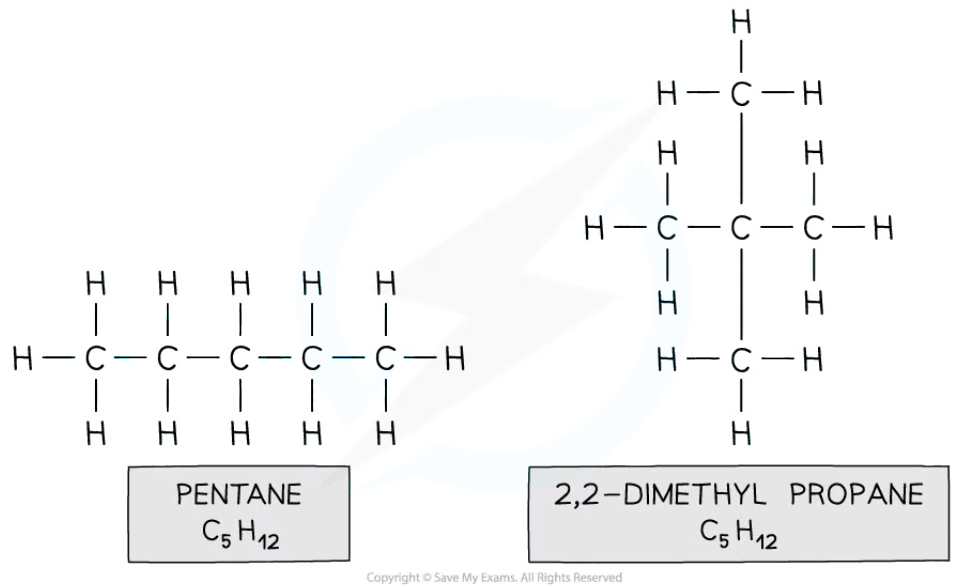
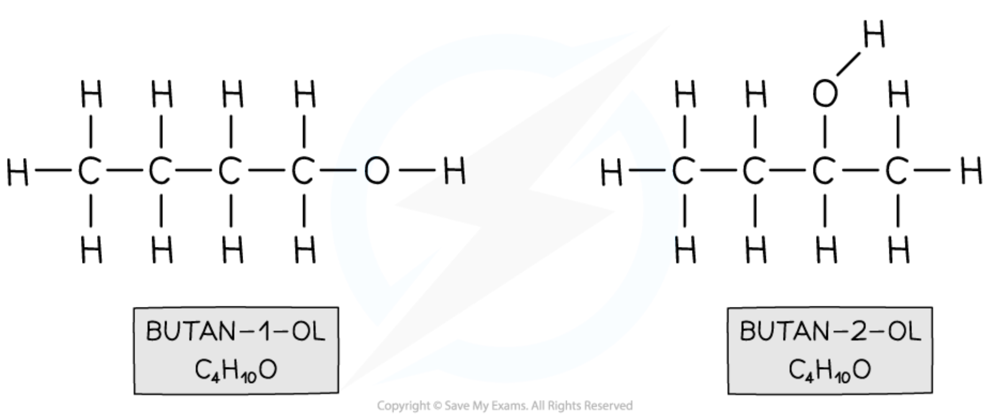


Both compounds are made up of the same atoms however the longest carbon chain in pentane is 5 and in 2,2-dimethylpropane it is 3 (with two methyl branches)

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



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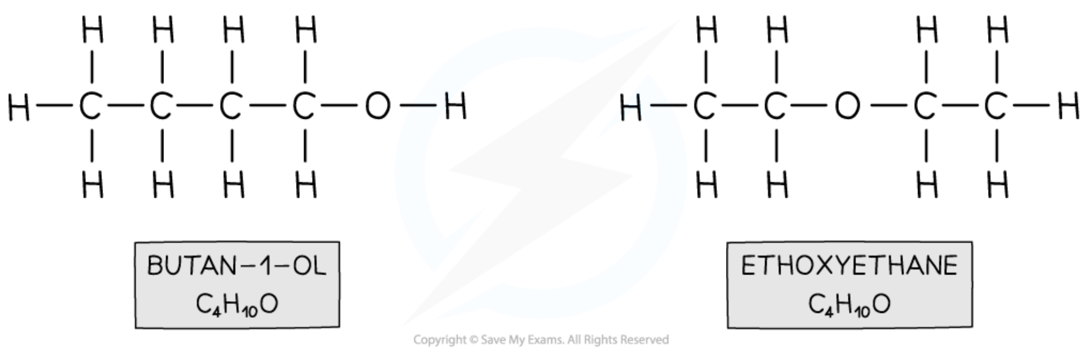
Both compounds have an alcohol group and are made up of 4 carbon, 10 hydrogen and one oxygen atom however in butan-1-ol the functional group is located on the first carbon and in butan-2-ol on the second carbon

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

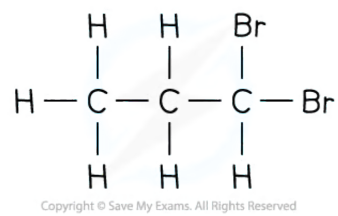
- You should be able to deduce all possible isomers for organic compounds knowing their molecular formula

Worked example

How many isomers are there of, $C_3H_6Br_2$?

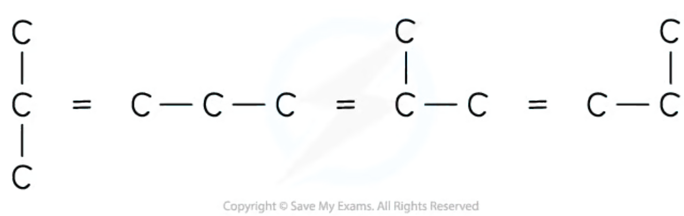
Answer:

Step 1: Draw the structural formula of the compound

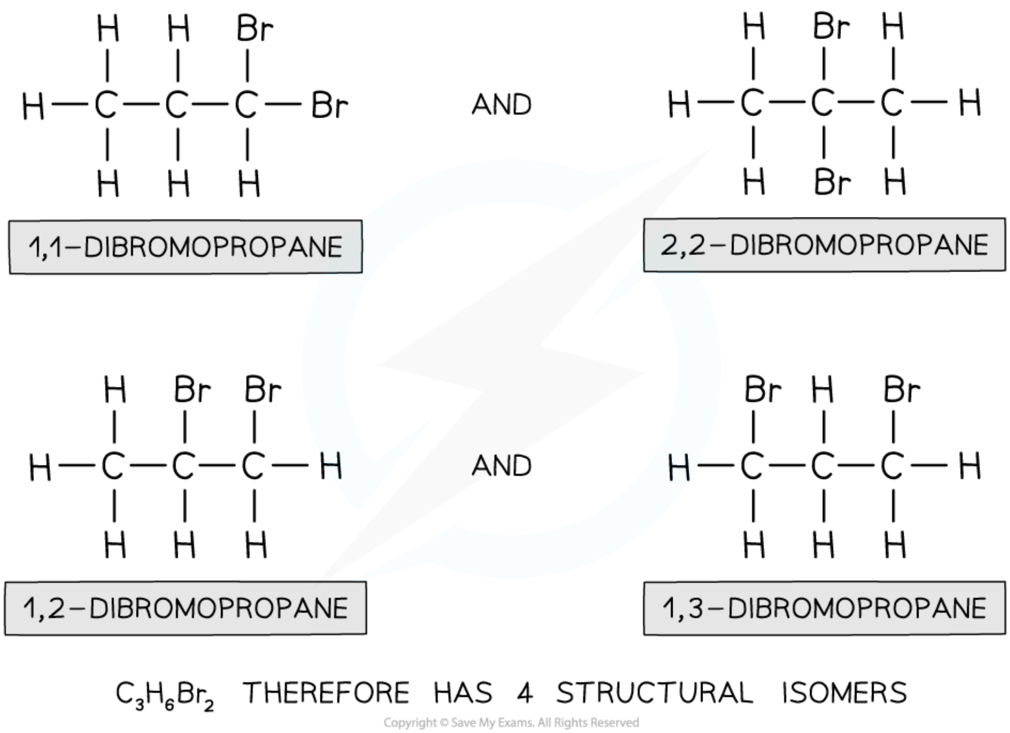


Step 2: Determine whether there is functional group, branch-chain or positional isomerism

- 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



Your notes

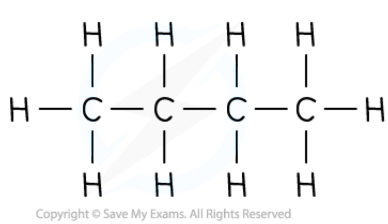


Worked example

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

Answer:

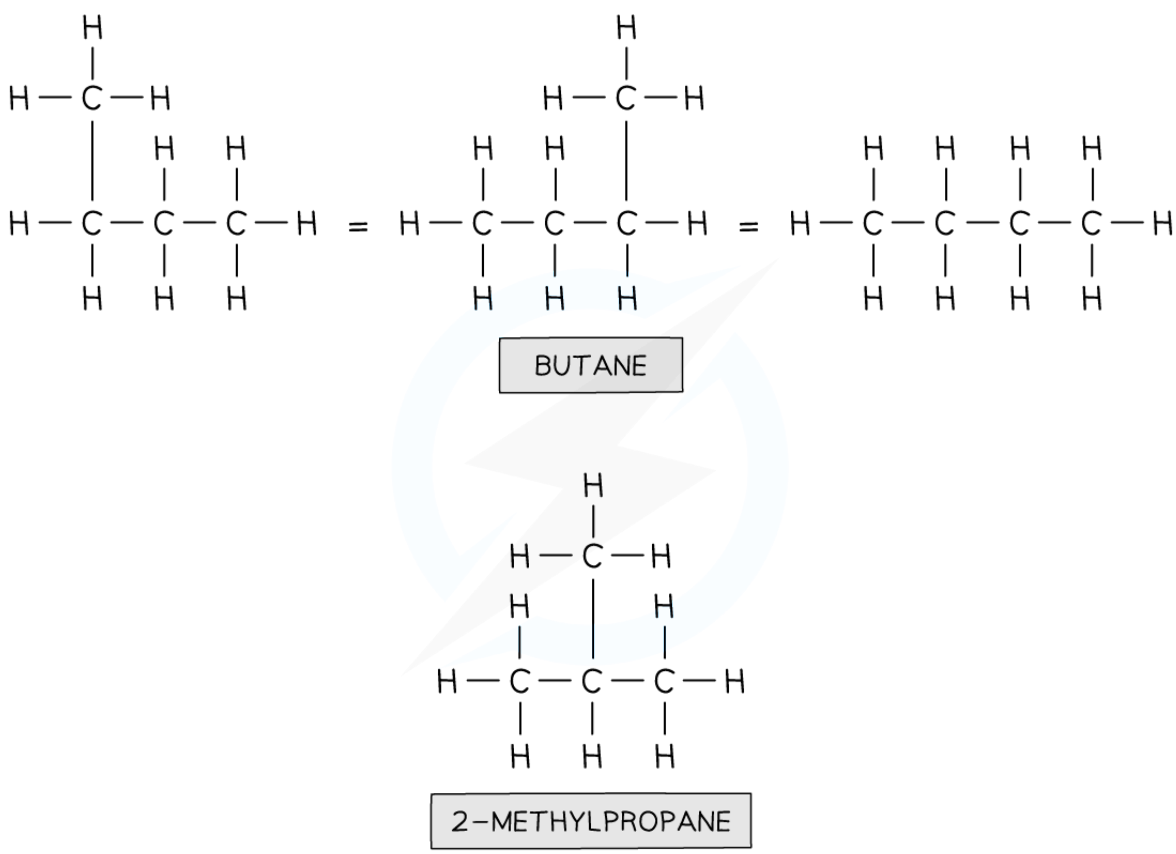
Step 1: Draw the structural formula of the compound



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!



C_4H_{10} THEREFORE HAS 2 STRUCTURAL ISOMERS

Your notes

Exam Tip

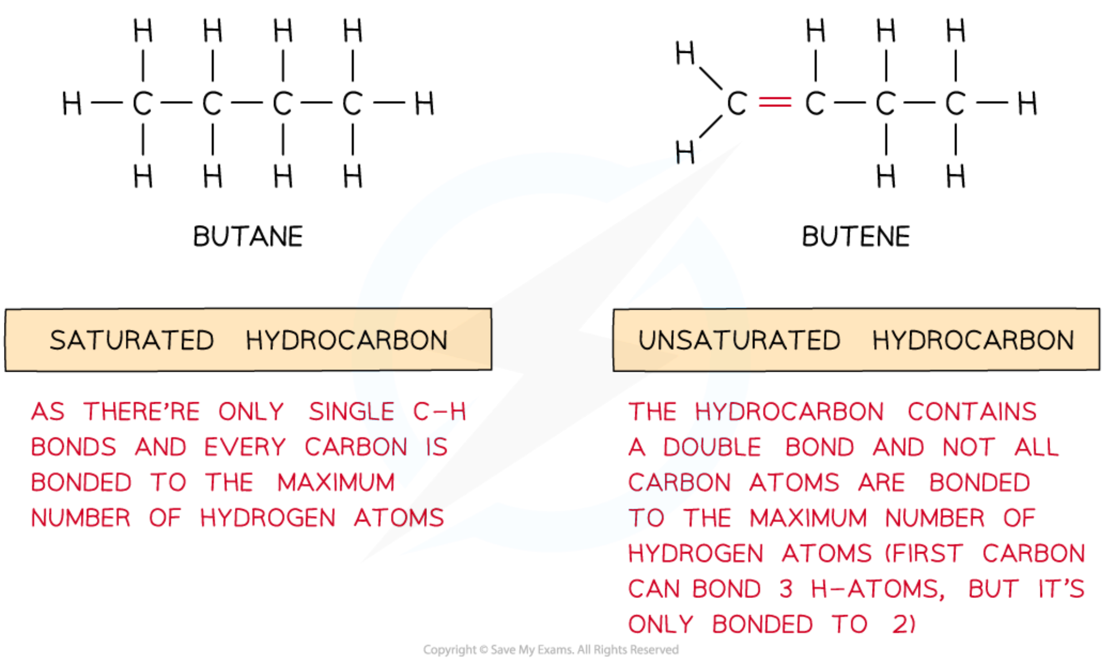
Don't be fooled by molecules by bending and turning through 90 degrees - that does not make them isomers. The best test is to try and name them - isomers will have a different name.

Your notes

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



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

Your notes

Number of C atoms	Molecular formula of straight-chain alkane	Name of alkane	Stem used in naming
1	CH_4	methane	meth-
2	C_2H_6	ethane	eth-
3	C_3H_8	propane	prop-
4	C_4H_{10}	butane	but-
5	C_5H_{12}	pentane	pent-
6	C_6H_{14}	hexane	hex-
7	C_7H_{16}	heptane	hept-
8	C_8H_{18}	octane	oct-
9	C_9H_{20}	nonane	non-
10	$C_{10}H_{22}$	decane	dec-

Exam Tip

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

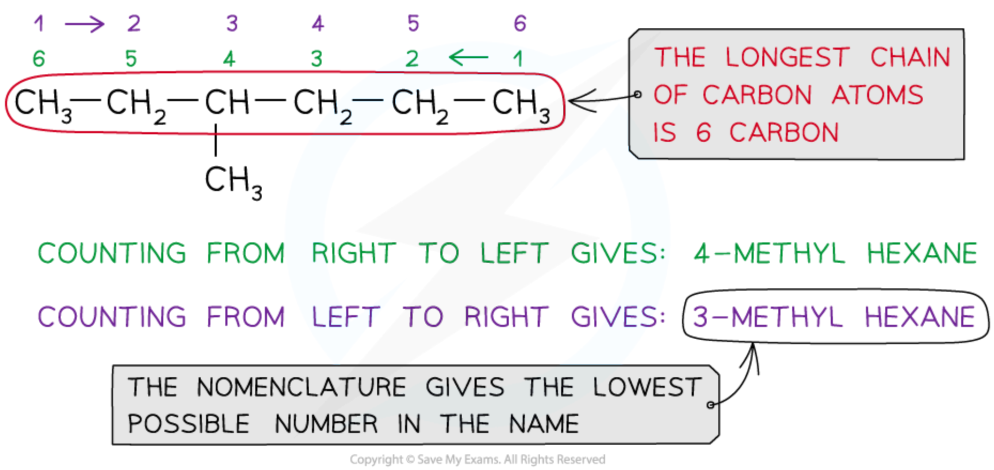
Chains & Branches

Your notes

- 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

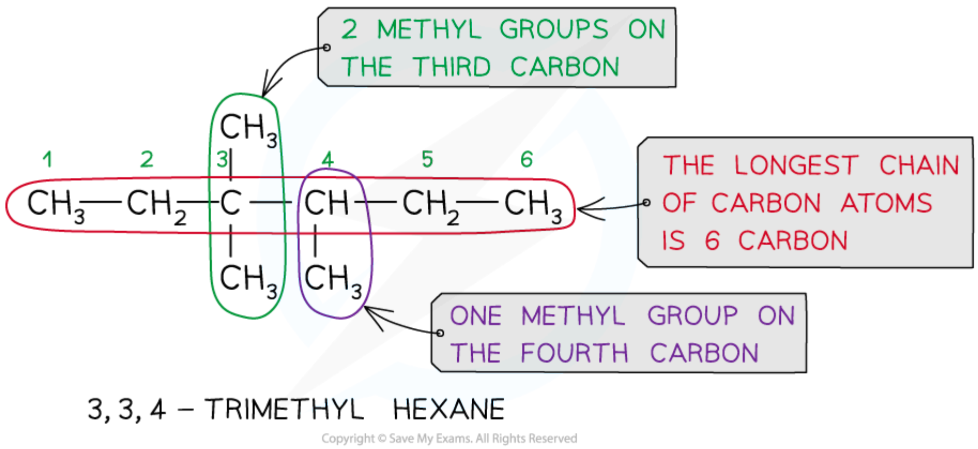
$CH_3CH\mathbf{(CH_3)}CH_2CH_3$

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



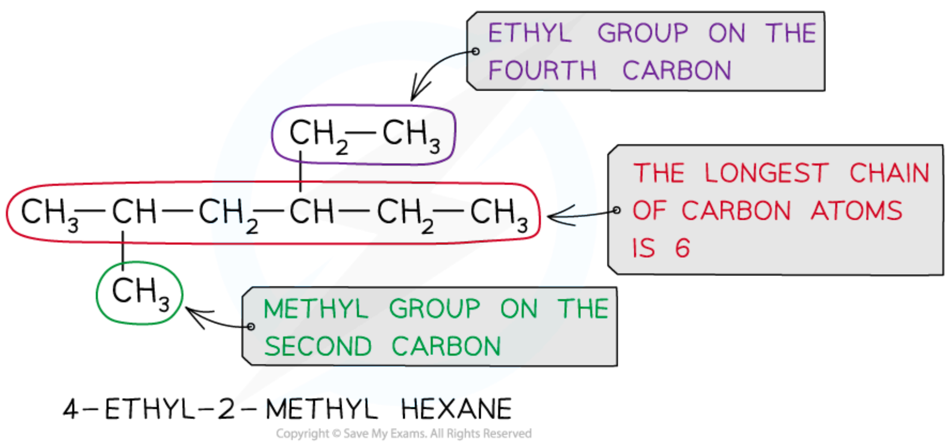
Naming Side Chains

- 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

Exam Tip

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

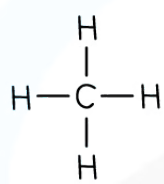
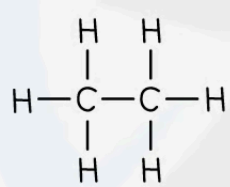
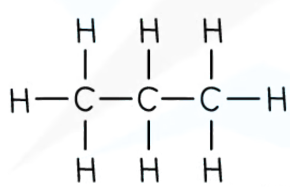
Your notes

10.1.4 Organic Families – Hydrocarbons

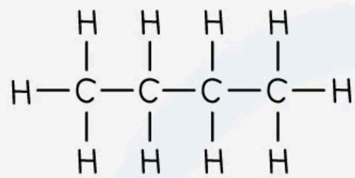
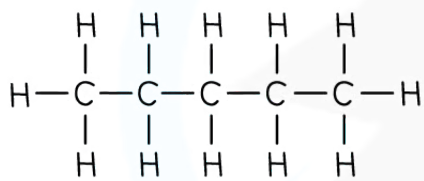
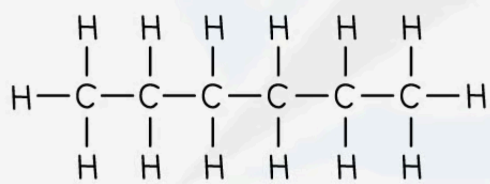
Your notes

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
	methane	CH_4
	ethane	C_2H_6
	propane	C_3H_8

Your notes

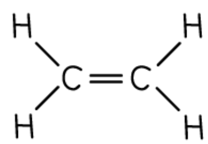
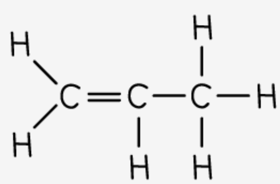
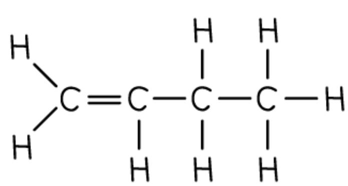
	butane	C_4H_{10}
	pentane	C_5H_{12}
	hexane	C_6H_{14}

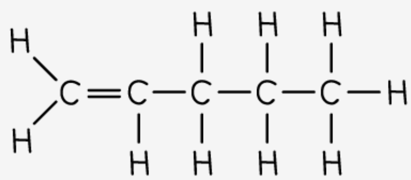
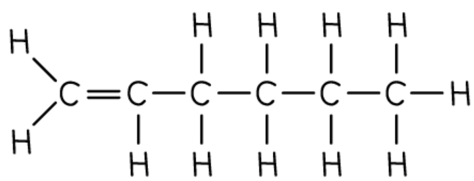
The first six members of the alkane family

Alkenes

Your notes

- **Alkenes** have the general molecular formula C_nH_{2n}
- 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 bond
- The lowest-numbered carbon atom participating in the double bond is indicated just before the -ene:

Structural Formula	Name	Molecular Formula
	ethene	C_2H_4
	propene	C_3H_6
	but-1-ene	C_4H_8

	pent−1−ene	C_5H_{10}
	hex−1−ene	C_6H_{12}

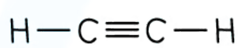
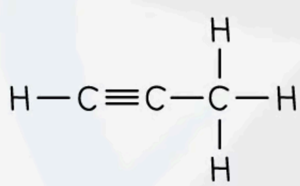
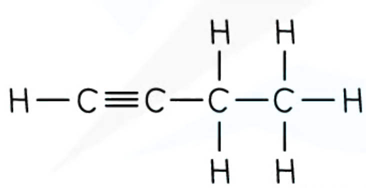
The first five members of the alkene family

- 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**

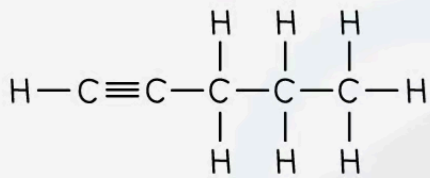
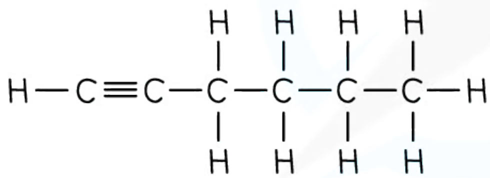
Your notes

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 bond
- The lowest-numbered carbon atom participating in the triple bond is indicated just before the -yne:

Structural Formula	Name	Molecular Formula
	ethyne	C_2H_2
	propyne	C_3H_4
	but-1-yne	C_4H_6

Your notes

	pent-1-yne	C_5H_8
	hex-1-yne	C_6H_{10}

The first five members of the alkyne family

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

Your notes

Your notes

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**, C_6H_6, 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

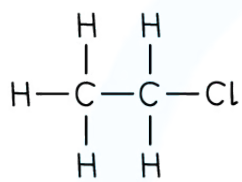
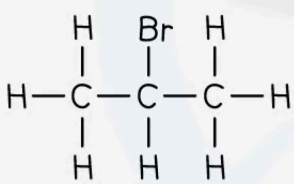
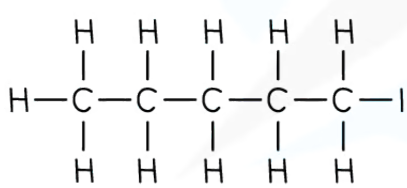
Your notes

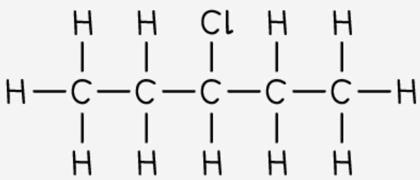
10.1.5 Organic Families - Halogenoalkanes

Halogenoalkanes

- **Halogenoalkanes** or **Haloalkanes** have the general molecular formula, $\mathbf{C_nH_{2n+1}X}$, 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:

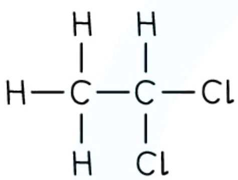
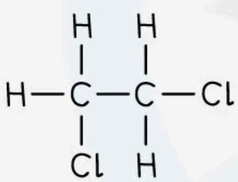
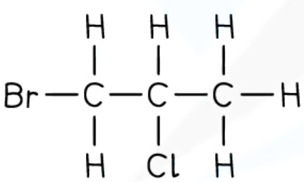
Haloalkanes Examples Table

Structural Formula	Name	Molecular Formula
	chloroethane	C_2H_5Cl
	2-bromopropane	C_3H_7Br
	1-iodopentane	$C_5H_{11}I$

	3-chloropentane	$C_5H_{11}Cl$

- 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
	1,1-dichloroethane	$C_2H_4Cl_2$
	1,2-dichloroethane	$C_2H_4Cl_2$
	1-bromo-2-chloropropane	C_3H_6BrCl

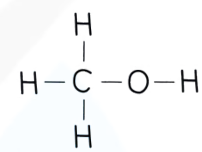
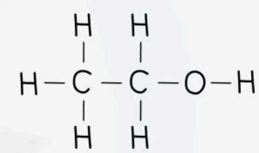
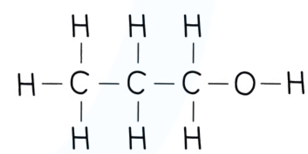
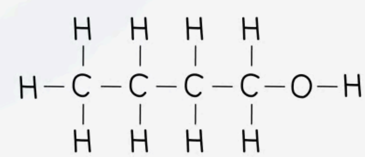
10.1.6 Organic Families - Alcohols & Ethers

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_3OH	
ETHANOL	CH_3CH_2OH	
PROPANOL	$CH_3CH_2CH_2OH$	
BUTANOL	$CH_3CH_2CH_2CH_2OH$	

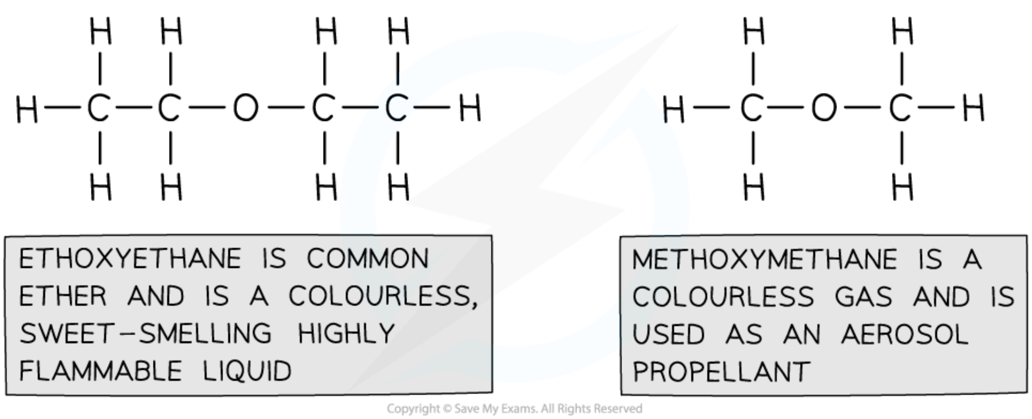
Classification of alcohols

- 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: CH_3OCH_3 is dimethyl ether and $C_2H_5OCH_3$ is ethyl methyl ether

- **Ethers** are **functional group isomers** of alcohols



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

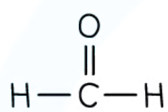
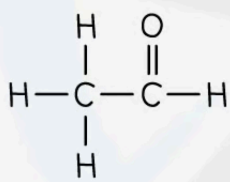
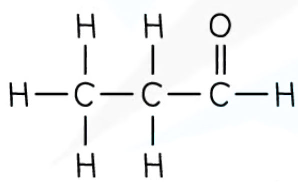
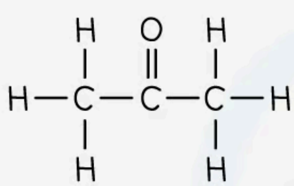
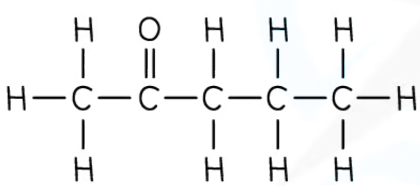
- If the carbonyl group is on the end of a chain then it is an **aldehyde** and has the functional group formula, **RCHO**
  - the H is written before the O so as not to confuse it with an alcohol
- The nomenclature of **carbonyls** follows the pattern **alkan + al**
- There is no need to use numbers 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
	methanal (also known as formaldehyde)	CH_2O
	ethanal	C_2H_4O
	propanal	C_3H_6O
	propanone (also known as acetone)	C_3H_6O
	pentan−2−one	$C_5H_{10}O$

- 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 H on 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**

Your notes

10.1.8 Organic Families – Carboxylic Acids & Esters

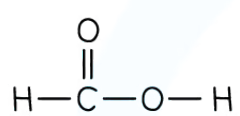
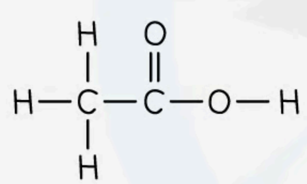
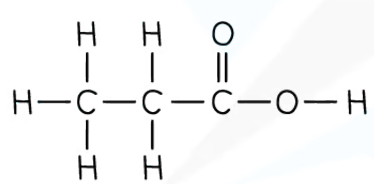
Your notes

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

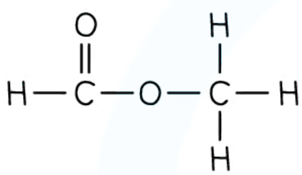
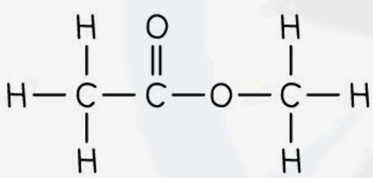
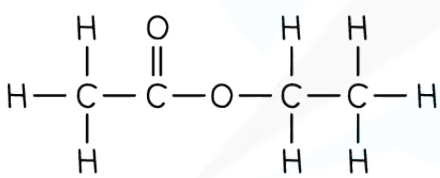
Structural Formula	Name	Molecular Formula
	methanoic acid (also known as formic acid)	HCO_2H
	ethanoic acid (also known as acetic acid)	CH_3CO_2H
	propanoic acid	$C_2H_5CO_2H$

Esters

Your notes

- **Esters** are **functional group isomers** of **carboxylic acids** and contain the functional group, **carboxylate**, **-COOR**
- 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
	methyl methanoate	HCO_2CH_3
	methyl ethanoate	$CH_3CO_2CH_3$
	ethyl ethanoate	$C_2H_5CO_2C_2H_5$

- **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)

Exam 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!

Your notes

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, -NH_2**
- **Amines** are derived from ammonia where one H in ammonia (NH_3)has been replaced by an R (alkyl) group
- The general formula of an amine is **$C_nH_{2n+1}NH_2$** which can be shortened to just **RNH_2**

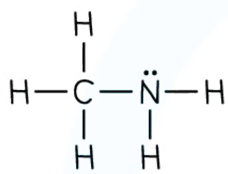
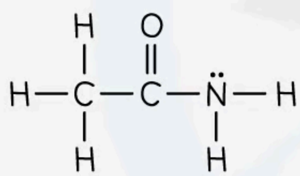
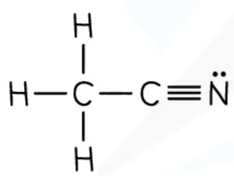
Amides

- **Amide** is the name given to compounds containing the functional group **carboxamide, -$CONH_2$**
- **Amides** are a combination of **amino** and **carbonyl** groups
- The general formula of an **amide** is **$C_nH_{2n+1}CONH_2$** 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

Structural Formula	Name	Molecular Formula
	methylamine or aminomethane	CH_3NH_2
	ethanamide	CH_3CONH_2
	ethanenitrile	CH_3CN

Exam 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.

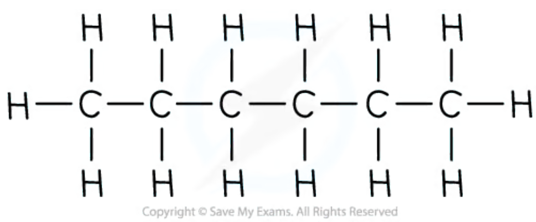
You are not required to know the nomenclature of these nitrogen compounds, but you are expected to identify the functional groups in molecules.

10.1.10 3-D modelling

Your notes

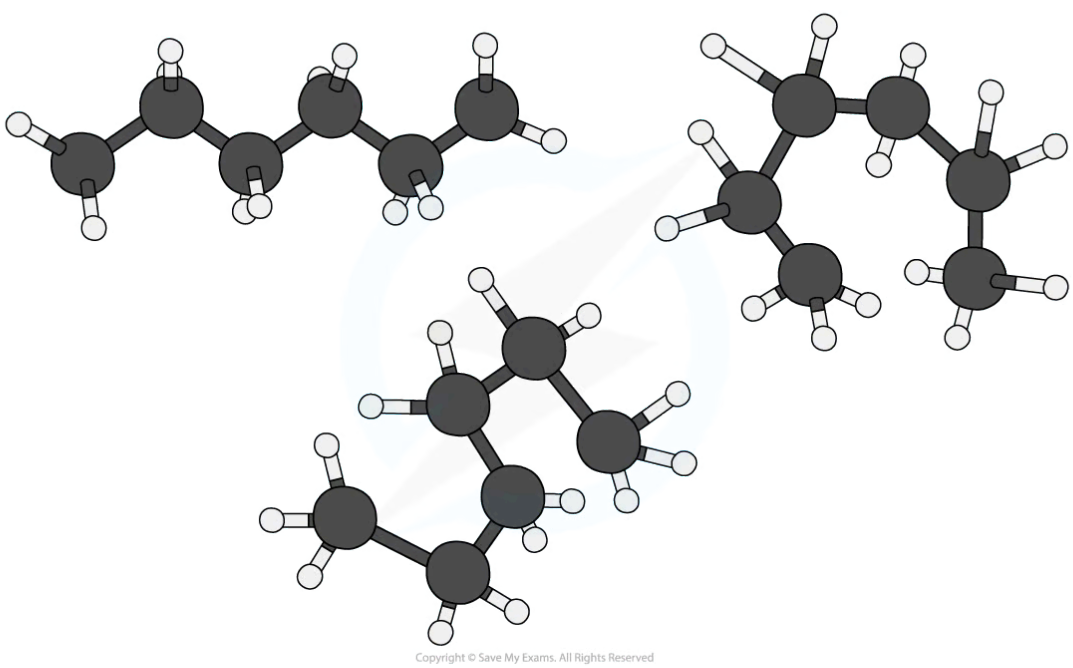
3-D Modelling

- 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:

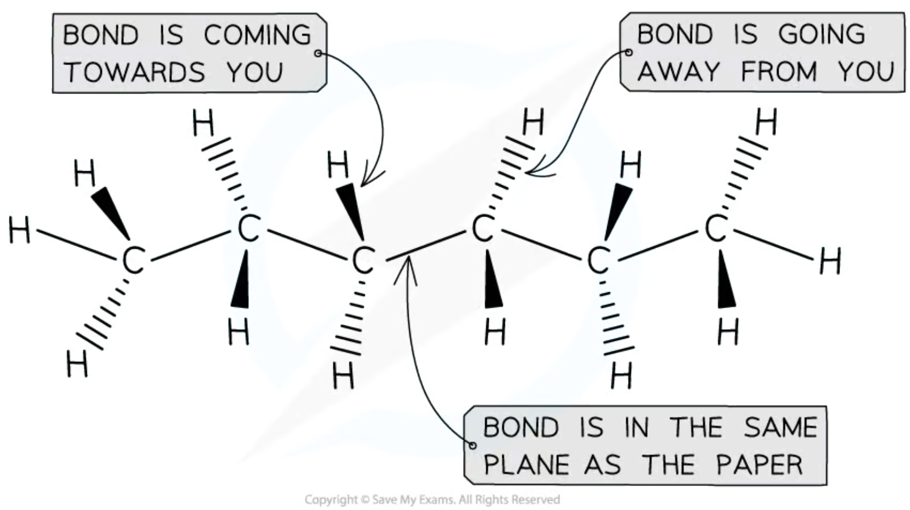


Different 3-D structures for hexane

- 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

Your notes

Exam 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

Your notes

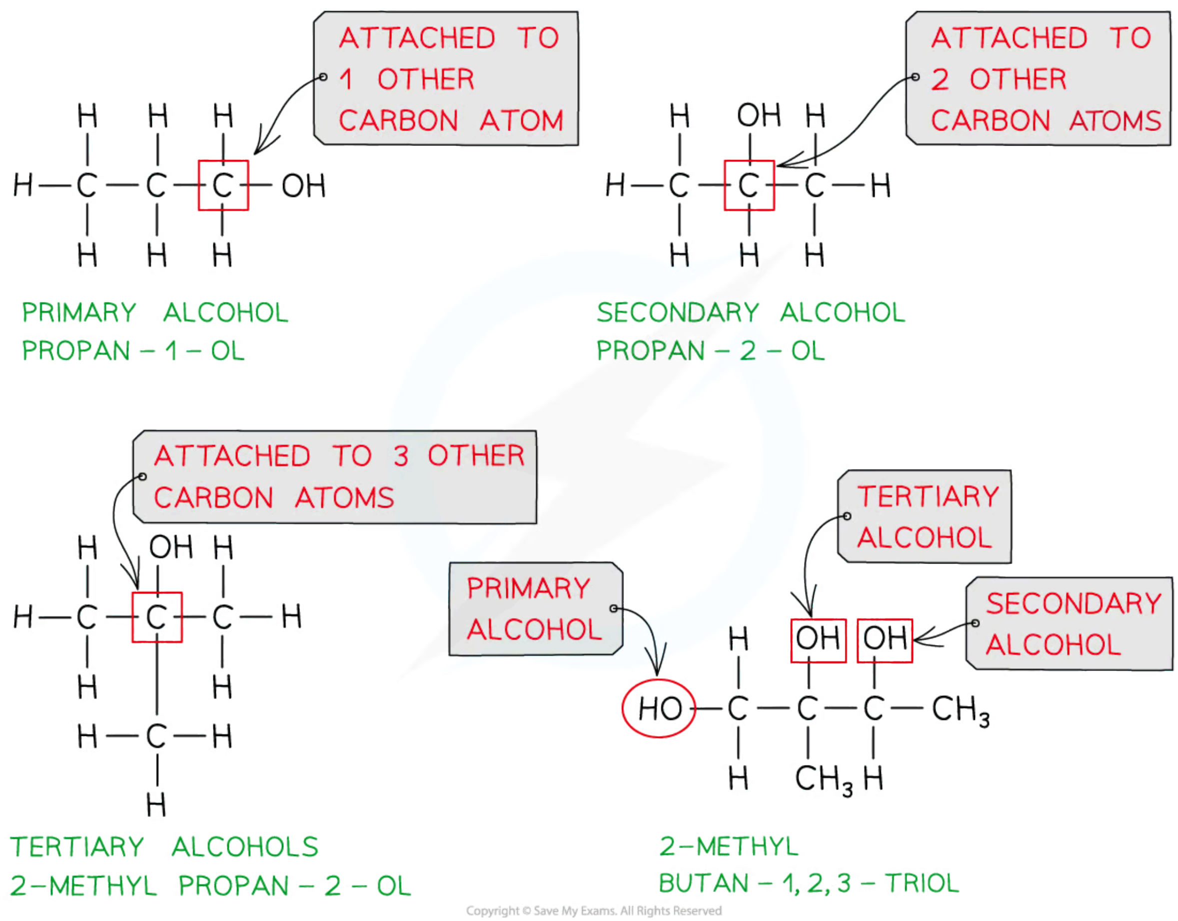
Your notes

10.1.11 Primary, Secondary & Tertiary atoms

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)

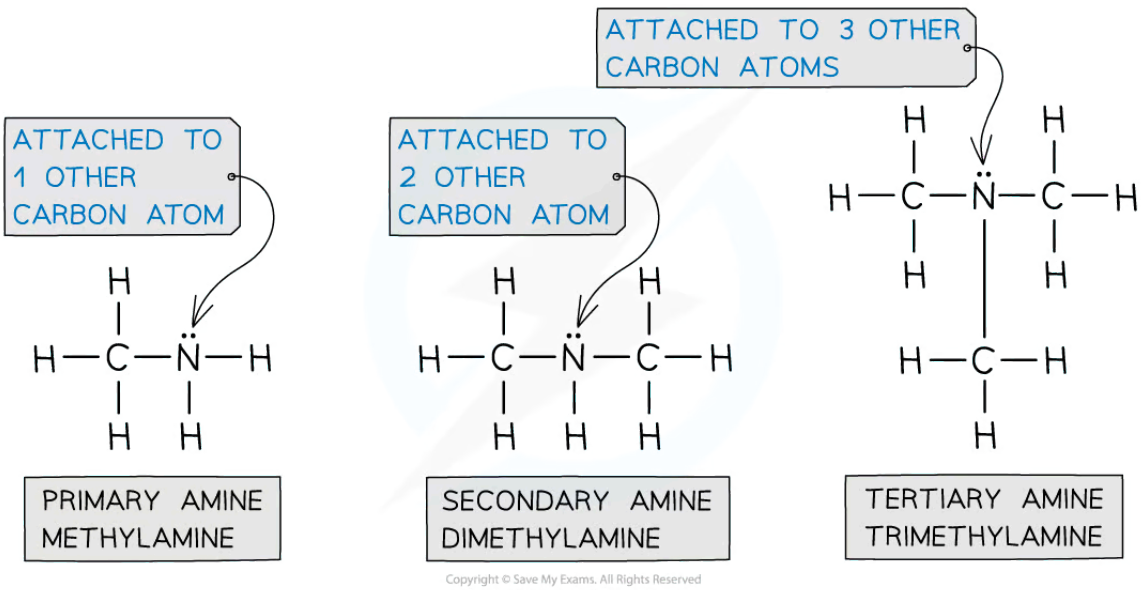


Classifying primary, secondary and tertiary alcohols and alcohols with more than one alcohol group

Your notes

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

Your notes

10.1.12 Benzene

Benzene

Kekulé structure for benzene

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

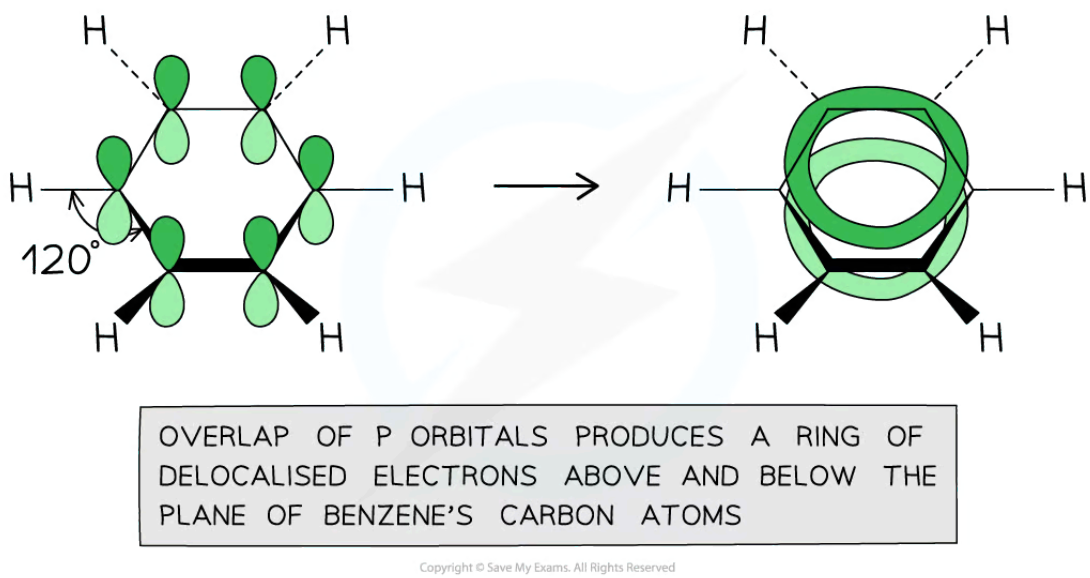
Problems with Kekulé's structure for benzene

- 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 sp^2 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**



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