SL IB Chemistry

Your notes

Functional Groups: Classification of Organic Compounds

Contents

Representing Formulas of Organic Compounds

Your notes

Representing Formulas of Organic Compounds

- Organic compounds can be represented using a variety of different formulae:
  - **Empirical**
  - **Molecular**
  - **Structural**
  - **Condensed Structural**
  - **Skeletal**
  - **Stereochemical**

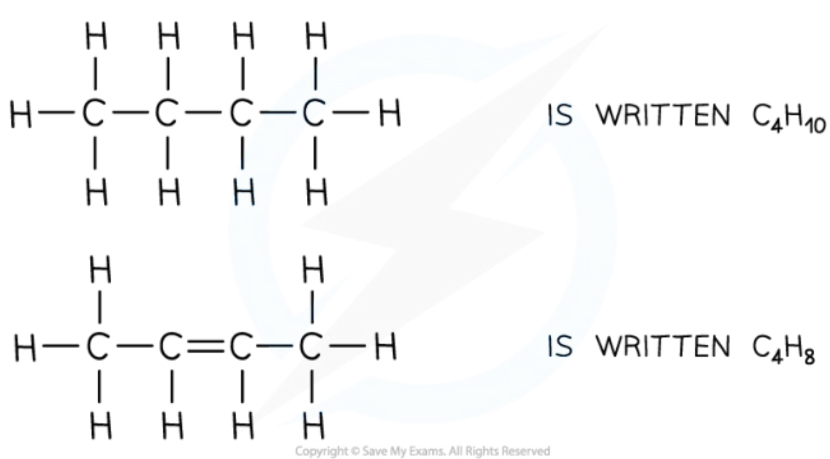
Empirical formula

- What is **empirical formula**?
  - The empirical formula shows the **simplest whole-number ratio of the atoms in a molecule**
- For example, if you were asked "What is the empirical formula of hydrogen peroxide?"
  - Hydrogen peroxide is H_2O_2
  - This shows that there are two hydrogen atoms and two oxygen atoms, but this is not the simplest whole-number ratio
  - Since there is a factor of 2, the empirical formula is HO

Molecular formula

- What is **molecular formula**?
  - The molecular formula shows the **actual number of atoms in a molecule**
- For example:

The molecular formulae of butane and butene



The molecular formula of butane is C_4H_{10} because it contains four carbon and ten hydrogen atoms, while butene is C_4H_8 because it contains four carbon and eight hydrogen atoms

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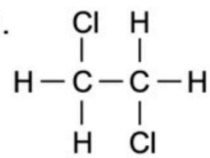
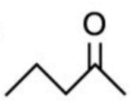
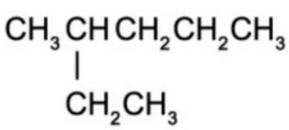
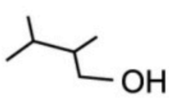
Worked example

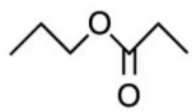
Deduce the molecular and empirical formula of the following compounds:

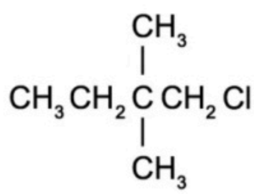
1. 

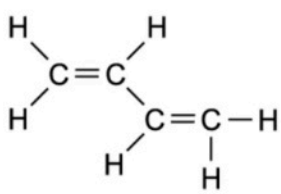
2. 

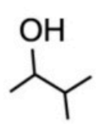
3. 

4. 

5. 

6. 

7. 

8. 

Answers:

Answer 1:

- Molecular formula = $C_2H_4Cl_2$
- Empirical formula = CH_2Cl

Answer 2:

- Molecular formula = $C_5H_{10}O$
- Empirical formula = $C_5H_{10}O$

Answer 3:

- Molecular formula = C_7H_{16}

Answer 5:

- Molecular formula = $C_6H_{12}O_2$
- Empirical formula = C_3H_6O

Answer 6:

- Molecular formula = $C_6H_{13}Cl$
- Empirical formula = $C_6H_{13}Cl$

Answer 7:

- Molecular formula = C_4H_6

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- Empirical formula = C_7H_{16}

- Empirical formula = C_2H_3

Answer 4:

- Molecular formula = $C_6H_{14}O$
- Empirical formula = $C_6H_{14}O$

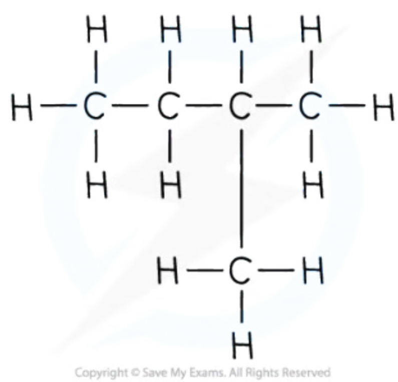
Answer 8:

- Molecular formula = $C_5H_{12}O$
- Empirical formula = $C_5H_{12}O$

Structural formula

- 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:

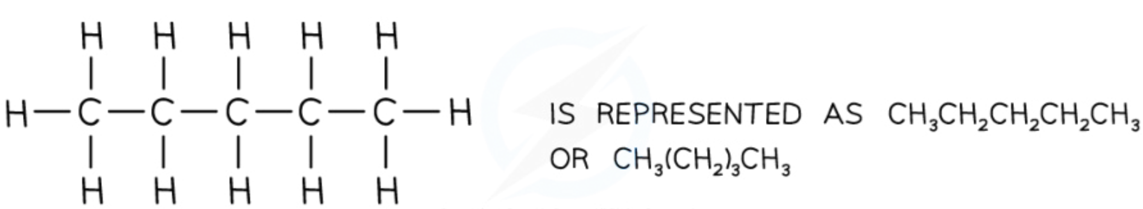
The structural formula of 2-methylbutane



The structural formula shows all of the bonds between all atoms

- In a **condensed structural formula**, 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:

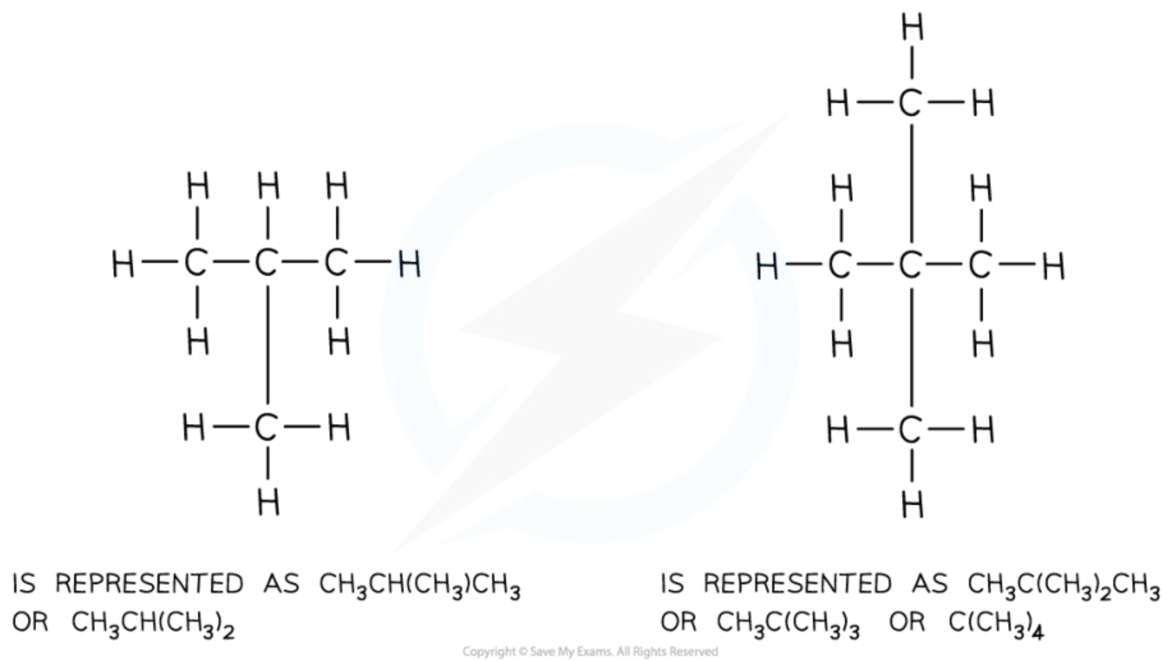
Representing the condensed structural formula of straight-chain alkanes



The full structural formula shows all bonds, while the condensed structural formula indicates the structure of the compound

- Side groups are shown using brackets:

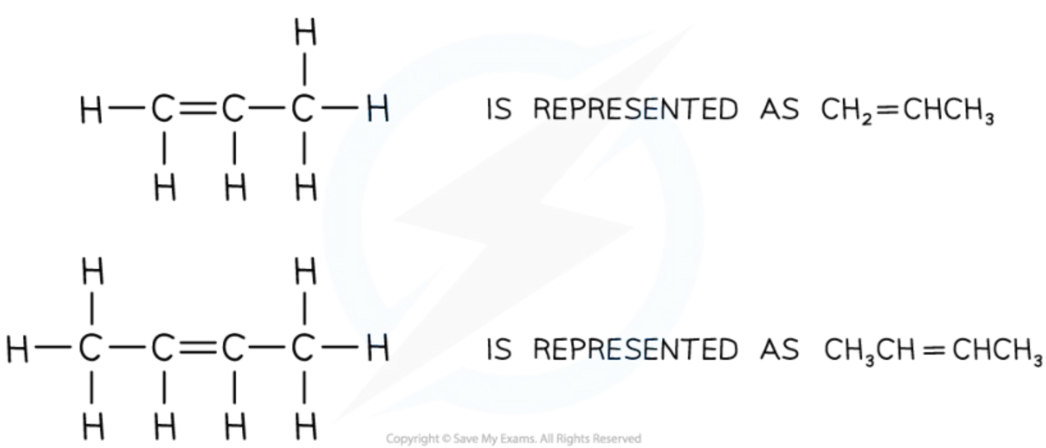
Representing the condensed structural formula of branched chain alkanes



The full structural formula shows all bonds, while the condensed structural formula includes functional groups in brackets to indicate the structure of the compound

- Specific bonds such as double (or triple) bonds are not always shown
  - It can be expected for you to deduce if there is a double (or triple) bond within the structure from the number of hydrogens attached to the carbon atoms

Representing the condensed structural formula of alkenes



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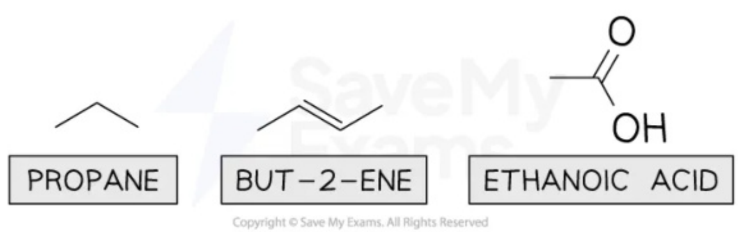
The condensed structural formula of an alkene can be shown with or without the carbon-carbon double bond

Your notes

Skeletal formula

- A **skeletal formula** is a simplified displayed formula with:
  - All of the carbon-carbon bonds are represented by lines
    - The end of each line and the point where two lines meet is a carbon atom
  - Most of the hydrogen atoms are removed except hydrogen atoms that are part of a functional group, e.g. OH
  - For more information about the different functional groups, see our revision not on Functional Groups
- For example:

The skeletal formula of propane, but-2-ene and ethanoic acid



Skeletal formulae do not show carbon atoms and only show hydrogen atoms that are contained within a functional group

- What is the skeletal formula of methane?
  - There is no skeletal formula for methane
  - This is because carbon-carbon bonds are replaced with lines, which means that two carbon atoms are required
  - Some answers suggest the skeletal formula of methane is a dot, but this is unlikely as it could easily be mistaken or confused with the symbol for a free radical
  - Other answers incorrectly suggest that the skeletal formula of methane is a carbon atom showing all four carbon-hydrogen bonds, but this is a structural formula

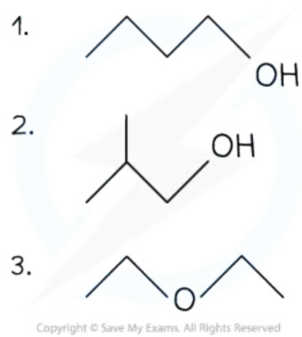
Your notes

Worked example

Draw the skeletal formula of the following molecules:

1. $CH_3(CH_2)_3OH$
2. $(CH_3)_2CHCH_2OH$
3. $CH_3CH_2OCH_2CH_3$

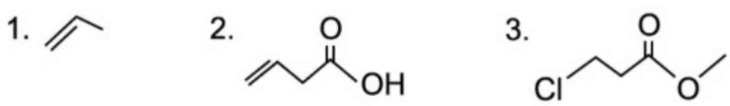
Answers:



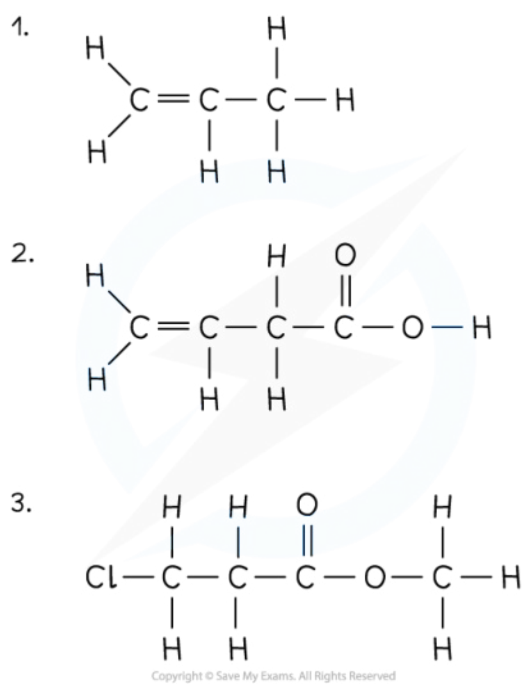
Your notes

Worked example

Draw the full structural formula of the following molecules:



Answers:

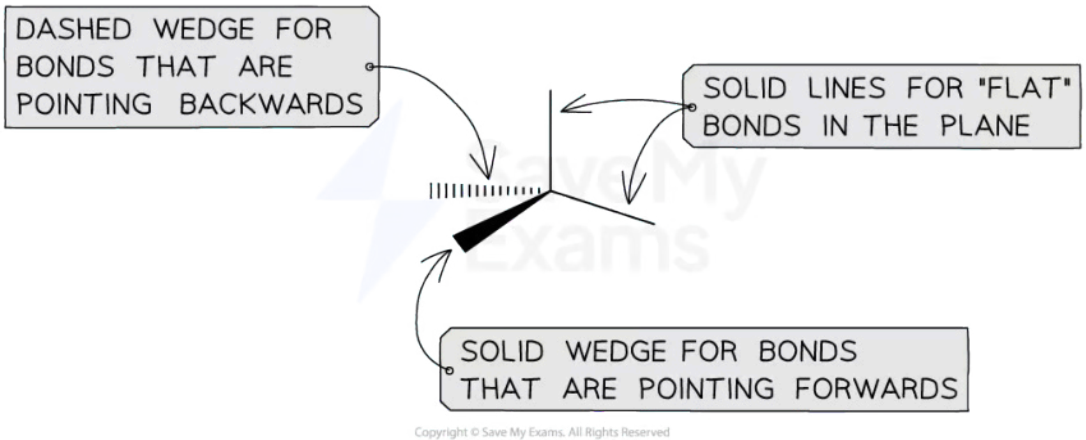


Stereochemical formula

- A **stereochemical formula** is a formula that attempts to show the relative positions and three-dimensional geometry of atoms and groups of atoms around a **chiral carbon**
  - For more information about chiral carbons, see our revision note on Enantiomers
- Stereochemical formulae follow a standard convention:
  - Bonds in the plane of the paper are drawn as solid lines
  - Bonds coming forward out of the plane (towards you) are drawn as a solid wedge
  - Bonds going backward out of the plane (away from you) are drawn as a dashed wedge

Diagram of the different bonds in a stereochemical formula

Your notes



Stereochemical formulae use solid lines, solid wedges and dashed wedges to illustrate if the bonds are in the plane of the paper, forwards from the paper or backwards from the paper

- Since the central, chiral carbon has four bonds / electron domains to different atoms or groups of atoms, the shape is tetrahedral with bond angles of 109.5^{o}
  - For more information about the shapes and bond angles of molecules, see our revision note on Shapes of Molecules

Functional Groups

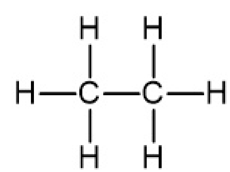
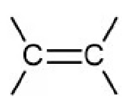
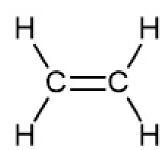
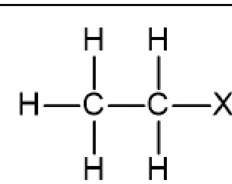
Your notes

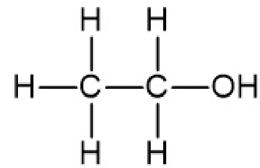
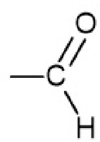
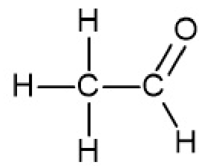
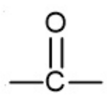
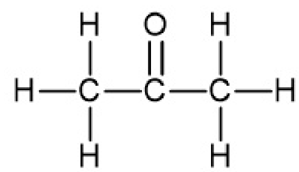
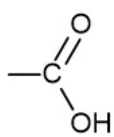
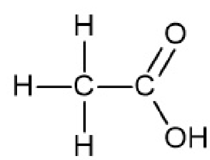
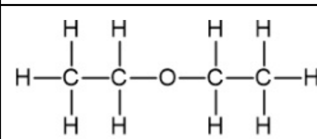
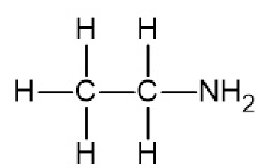
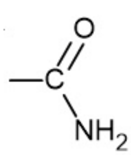
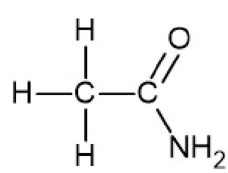
Functional Groups

What are functional groups in organic chemistry?

- Functional groups are atoms or groups of atoms that are found in organic compounds
- They give organic compounds their characteristic physical and chemical properties
- Organic compounds that contain the same functional group belong to the same **class**
  - **Careful:** This should not be confused with belonging to the same homologous series
- For example:
  - The class of organic compounds called the alkenes all contain the carbon-carbon double bond – **C=C**– functional group
  - The class of organic compounds called the aldehydes all contain the –**CHO** functional group

Classes of organic compounds table

Class	Functional group name	Functional group formula	IUAC prefix– or –suffix	Example
alkane	alkyl	–	–ane	 ethane
alkene	alkenyl		–ene	 ethene
alkyne	alkynyl		–yne	 ethyne
halogenoalkane	halogeno	F– Cl– Br– I–	fluoro– chloro– bromo– iodo–	

				if X = F, fluoroethane
alcohol	hydroxyl	—OH	hydroxy- -ol	 ethanol
aldehyde	carbonyl (aldehyde)		-al	 ethanal
ketone	carbonyl (ketone)		-one	 propanone
carboxylic acid	carboxyl (acid)		-oic acid	 ethanoic acid
ether	alkoxy	—O—	-	 ethoxyethane
amine	amino	$—NH_2$	-amine	 ethanamine
amide	amido		-amide	 ethanamide

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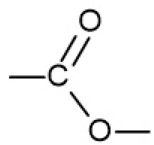
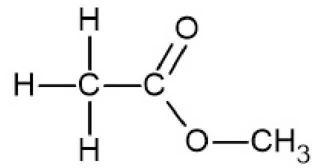
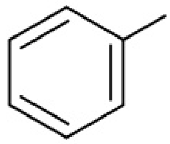
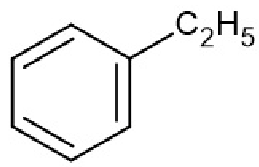
ester	ester (carboxyl)		-oate	 methyl ethanoate
aromatics*	phenyl		phenyl– -benzene	 phenylethene ethylbenzene

* The specification does not require specific knowledge of aromatics / arenes as a class of organic compound

Your notes

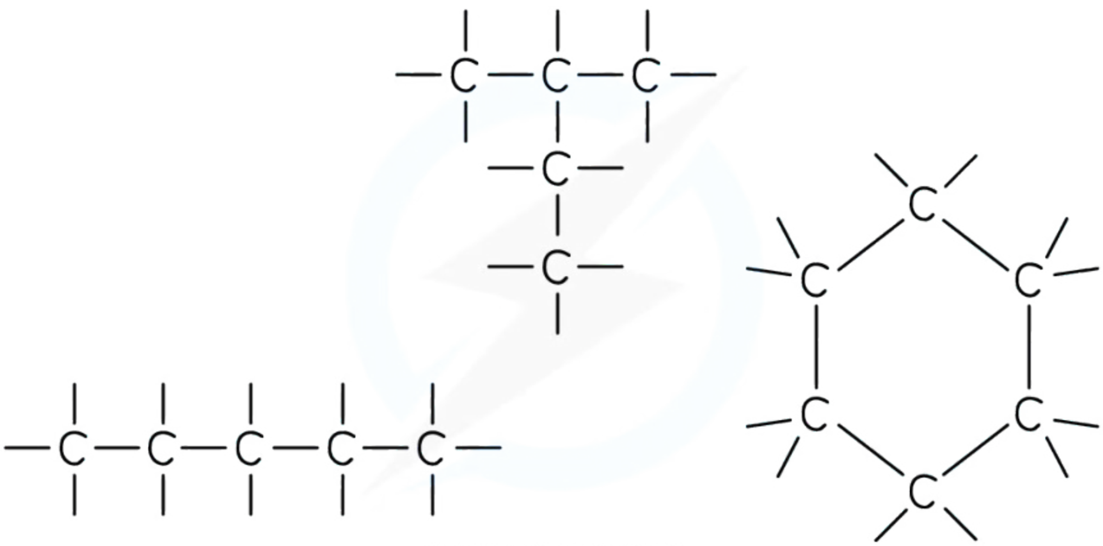
Homologous Series

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**

Examples of catenation using carbon



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

What is a homologous series?

- Organic compounds with the same functional group, but a different number of carbon atoms, are said to belong to the same **homologous series**
- One definition of a homologous series is:

A family of similar compounds, having the same functional group, and so similar chemical properties

- Every time a carbon atom is added to the chain, two hydrogen atoms are also added

Your notes

Homologous Series of Alkanes Table

Name of alkane	Number of carbons	Chemical formula	Melting point / °C	State at room temperature	Boiling point / °C
Methane	1	CH_4	–182	gas	–162
Ethane	2	C_2H_6	–183	gas	–89
Propane	3	C_3H_8	–188	gas	–42
Butane	4	C_4H_{10}	–138	gas	–1
Pentane	5	C_5H_{12}	–130	liquid	36

The characteristics of a homologous series

- The features of a homologous series are:
  - 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

General formulae of different homologous series

- Each homologous series can be described by a general formula

General formulae of homologous series table

Homologous series	General formula	Example
alkanes	C_nH_{2n+2}	Propane C_3H_8
alkenes**	C_nH_{2n}	Propene C_3H_6

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alkynes	C_nH_{2n-2}	Propyne C_3H_4
halogenoalkanes	$C_nH_{2n+1}X$	Chloropropane C_3H_7Cl
alcohols	$C_nH_{2n+1}OH$	Propanol C_3H_7OH
aldehydes	$C_nH_{2n}O$ (usually written as R–CHO)	Propanal C_3H_6O
ketones	$C_nH_{2n}O$ (usually written as R–(C=O)–R)	Propanal C_3H_6O
carboxylic acids	$C_nH_{2n+1}COOH$ (usually written as R–COOH)	Propanoic acid C_2H_5COOH
ethers	$C_nH_{2n+2}O$ (usually written as R–O–R)	Methoxymethane CH_3OCH_3
amines	$C_nH_{2n+1}NH_2$	Propylamine $C_3H_7NH_2$
amides	$C_nH_{2n+1}NO$ (usually written as R–CONH–R')	*N*-methylethanamide $CH_3CONHCH_3$
esters	$C_nH_{2n}O_2$ (usually written as R–COO–R')	Methyl methanoate $HCOOCH_3$

** Ethene is the smallest possible alkene as a minimum of two carbons are required to form the carbon-carbon double bond

Physical Trends in a Homologous Series

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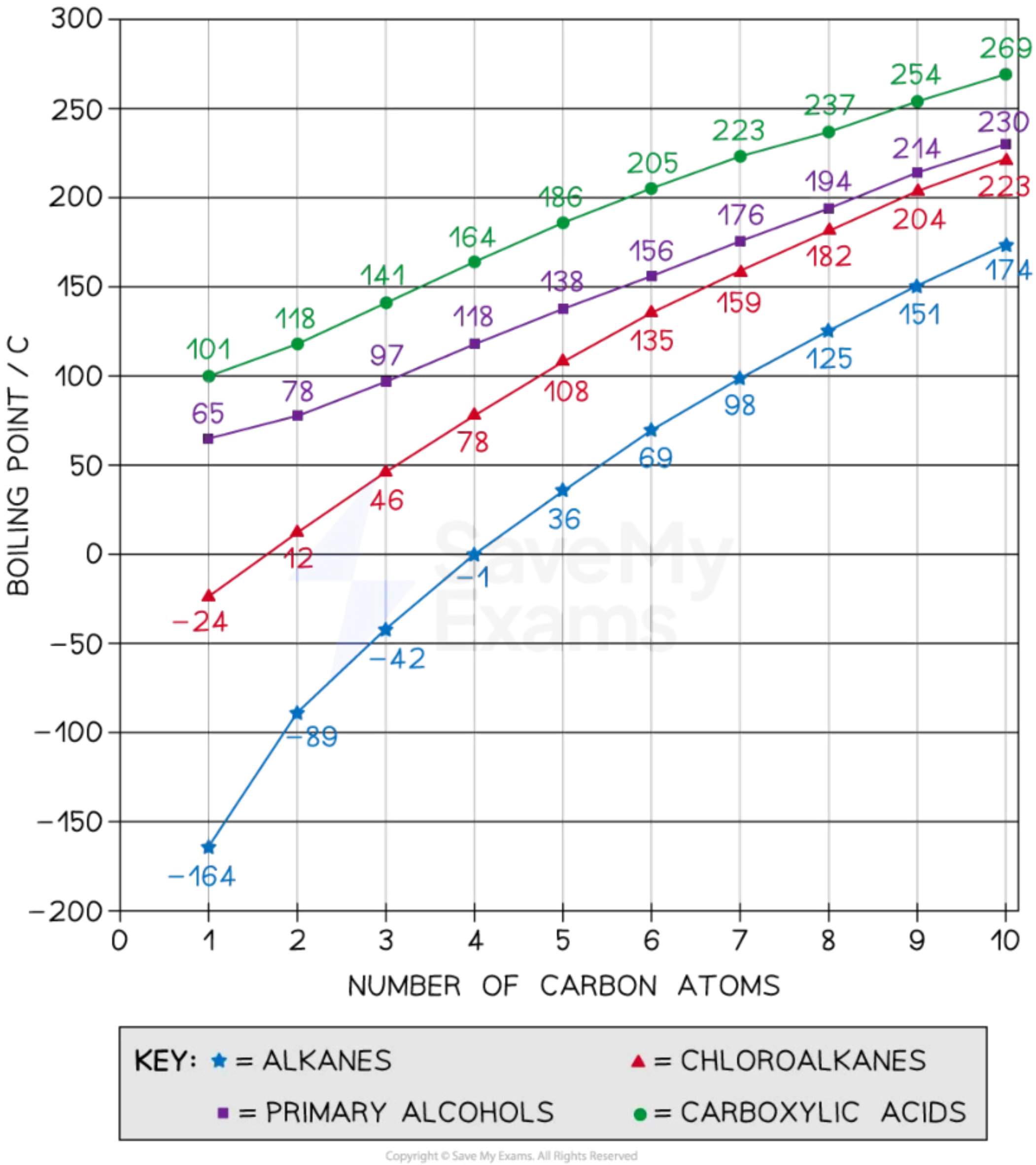
- Since successive members of a homologous series differ by a single $-CH_2-$ group, they show a trend in physical properties

Boiling point graph for four different homologous series



As the number of carbons in the straight-chain molecule increases, the boiling point increases

- 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**, which leads to a higher boiling point
- Similar trends are seen with other physical properties such as melting point, density and viscosity
- These trends are followed in other homologous series

Your notes

IUPAC Nomenclature

Your notes

IUPAC Nomenclature

- **IUPAC** or **systematic nomenclature** can be used to name organic compounds and therefore make it easier to refer to them

Naming hydrocarbons

- **Hydrocarbons** are compounds containing hydrogen and carbon only
- There are four families of hydrocarbons you should know:
  1. **Alkanes**
  2. **Alkenes**
  3. **Alkynes**
  4. **Arenes**

Naming alkanes

- **Alkanes** have the general molecular formula $\mathbf{C_nH_{2n+2}}$
  - 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 following table
- 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

IUPAC system of naming alkanes table

Number of carbon atoms	Molecular formula of straight-chain alkane	IUPAC 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-

Your notes

Examiner Tip

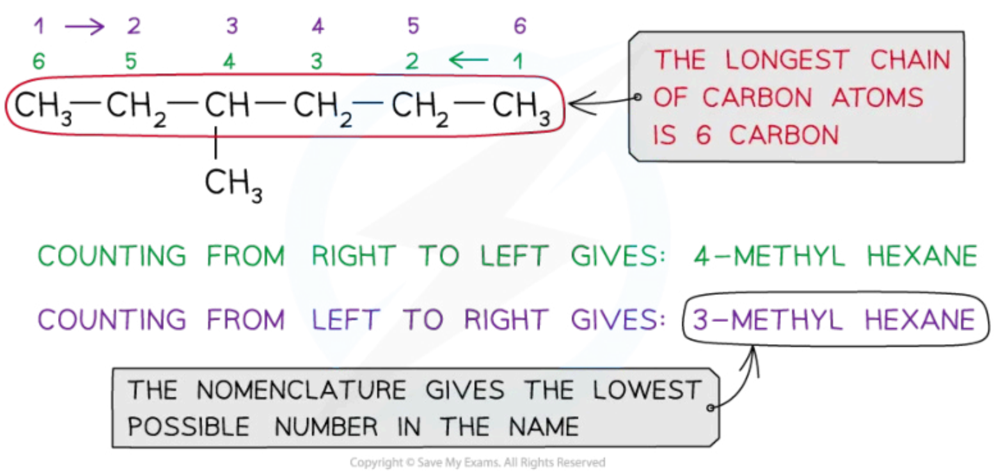
Although the table shows up to 10 carbons for reference, in your IB Chemistry exam you are only required to name molecules with up to 6 carbons

- If there are any side-chains or functional groups present, then the position of these groups is 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 organic compounds with one alkyl side chain



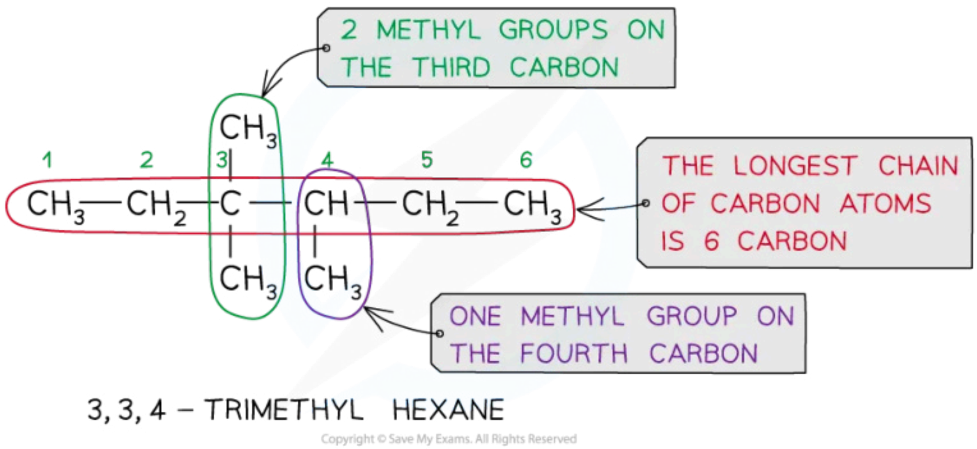
The longest chain provides the main name and the side chain is shown as a numbered alkyl prefix

- 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

Your notes

- The adjacent **numbers** have a comma between them
- **Numbers** are separated from **words** by a hyphen

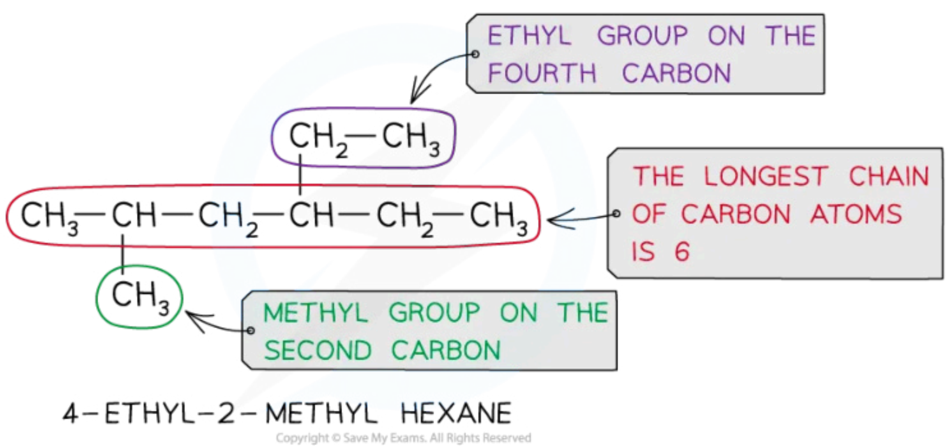
Naming organic compounds with multiple, identical side chains



The longest chain still provides the main name and the side chains are shown as numbered alkyl prefixes

- If there is more than one type of alkyl side chain, the same numbering system applies but the different side chains are listed in alphabetic order

Naming organic compounds with multiple, different side chains



The longest chain still provides the main name and the side chains are still shown as numbered alkyl prefixes but in alphabetical order

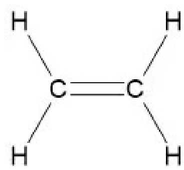
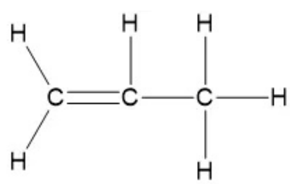
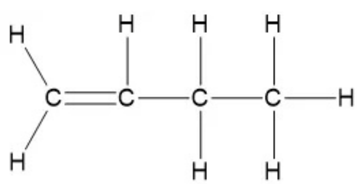
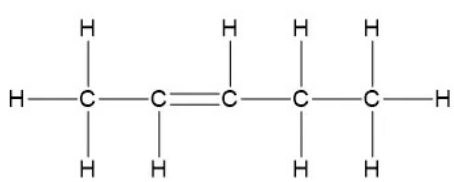
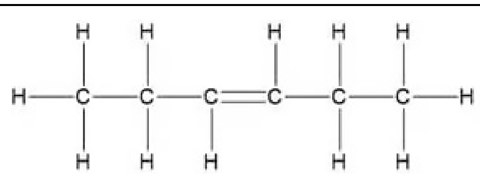
Naming alkenes

- **Alkenes** have the general molecular formula C_nH_{2n}
- They are said to be **unsaturated**
- Alkenes are named using the nomenclature rule **alk + ene**

Your notes

- 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:

IUPAC system of naming alkenes table

Number of carbon atoms	Displayed formula of straight-chain alkene	Molecular formula of alkene	IUPAC name of alkene
1	-	-	-
2		C_2H_4	ethene
3		C_3H_6	propene
4		C_4H_8	but-1-ene
5		C_5H_{10}	pent-2-ene
6		C_6H_{12}	hex-3-ene

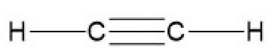
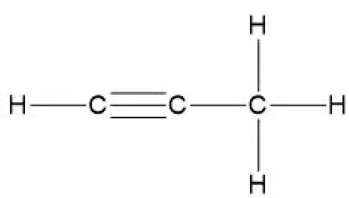
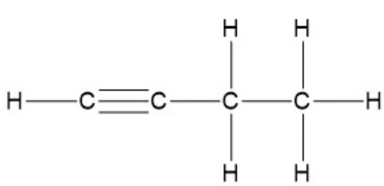
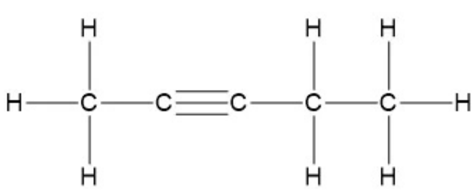
- There is a distinction to be made between the name of the **functional group** and the name of the **family**

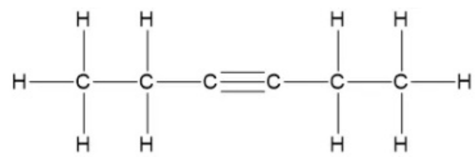
- The name of the family is **alkene**
- The name of the functional group is **alkenyl**

Naming alkynes

- **Alkynes** have the general molecular formula $\mathbf{C_nH_{2n-2}}$
- The triple bond makes them **unsaturated** molecules
- Alkenes are named using the nomenclature rule **alk + yne**
- In molecules with a straight chain of 4 or more carbon atoms, the position of the C=C 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:

IUPAC system of naming alkynes table

Number of carbon atoms	Displayed formula of straight-chain alkyne	Molecular formula of alkyne	IUPAC name of alkyne
1	-	-	-
2		C_2H_2	ethyne
3		C_3H_4	propyne
4		C_4H_6	but-1-yne
5		C_5H_8	pent-2-yne

6		C_6H_{10}	hex-3-yne

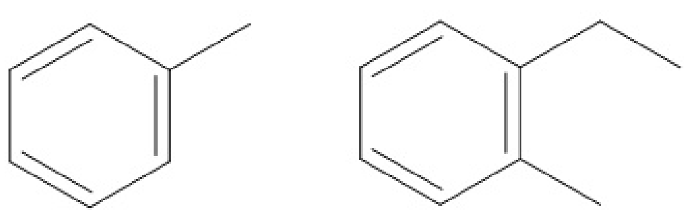
- There is a distinction to be made between the name of the **functional group** and the name of the **family**
  - The name of the family is **alkyne**
  - The name of the functional group is **alkynyl**

Naming arenes

- Arenes are **aromatic** compounds, i.e. compounds with one or more rings with **pi electrons** that are **delocalised** throughout the ring(s)

- **Benzene**, C_6H_6, is the only **aromatic hydrocarbon** that is covered in IB Chemistry and is covered in our Benzene revision note
- Naming aromatic compounds depends on whether the benzene ring is considered the main structure or a functional group
  - Benzene as the main structure:
    - Alkyl groups attached to benzene rings are named using the nomenclature rule **alkyl group + benzene**
    - If there is only one alkyl group attached, then no numbering system is applied to the benzene ring
    - If more than one alkyl group is attached, then a relative numbering system is applied
      - This is where the longest alkyl chain is considered as being attached to carbon-1 of the ring
      - The other alkyl groups are then numbered accordingly
      - The alkyl groups are still named in alphabetical order

Examples of alkyl substituted aromatic compounds

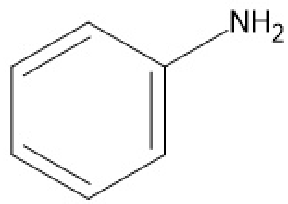


Methylbenzene is often called by the common name toluene. 1-ethyl-2-methylbenzene has the longest (ethyl) side chain set as carbon-1, so the methyl side chain is attached to carbon-2

  - Benzene as a functional group:
    - The functional group in **benzene** is known as a **phenyl group** when attached to other molecules

Benzene as the functional group

Your notes

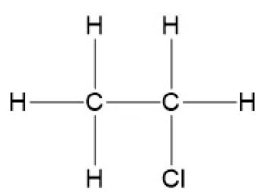
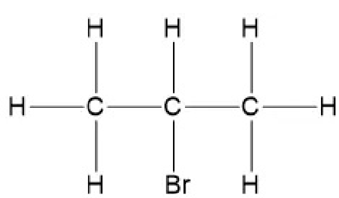
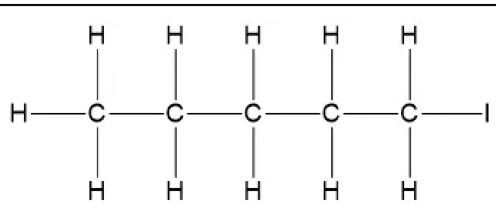


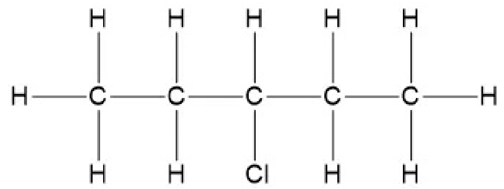
The benzene ring is considered a functional group in amine structures, which means that this aromatic compound is called phenylamine

Halogenoalkanes

- **Halogenoalkanes** have the general molecular formula, $\mathbf{C_nH_{2n+1}X}$, where X represents a halogen
- **Halogenoalkanes** 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:

Halogenoalkanes Examples Table

Displayed formula of halogenoalkane	Molecular formula of halogenoalkane	IUPAC name of halogenoalkane
	C_2H_5Cl	chloroethane
	C_3H_7Br	2-bromopropane
	$C_5H_{11}I$	1-iodopentane

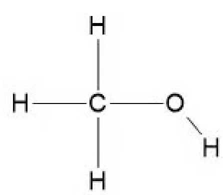
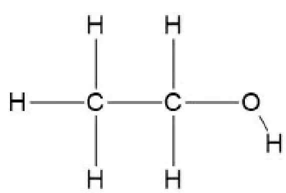
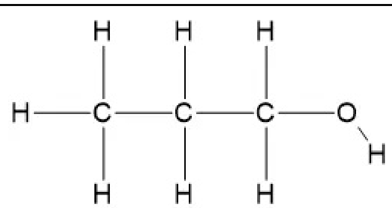
	$C_5H_{11}Cl$	3–chloropentane

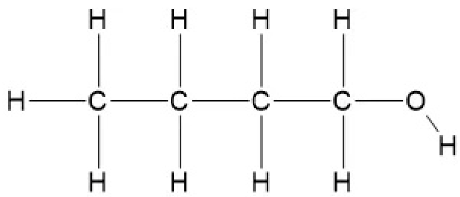
- For halogenoalkanes with multiple halogen functional groups, the position and type of functional group must be given
  - For example, an ethane chain with 2 chlorine functional groups on carbon-1 and one chlorine functional group on carbon 2 will be named 1,1,2–trichloroethane

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**

Primary alcohols examples table

Displayed formula of primary alcohol	Structural formula of primary alcohol	IUPAC name of primary alcohol
	CH_3OH	methanol
	CH_3CH_2OH	ethanol
	$CH_3CH_2CH_2OH$	propan-1-ol

	$CH_3CH_2CH_2CH_2OH$	butan-1-ol

Your notes

- Further information about the classification of alcohols as **primary, secondary** or **tertiary** can be found in our Structural Isomers revision note

Carbonyls

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

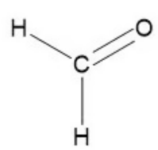
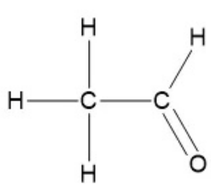
Aldehydes

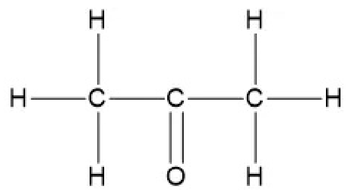
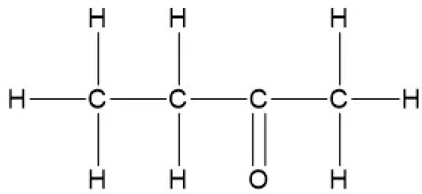
- If the carbonyl group is on the end of a chain then it is an **aldehyde** and has the functional group formula, **RCHO**
  - The H is written before the O so as not to confuse it with an alcohol
- The nomenclature of **carbonyls** follows the pattern **alkan + al**
- There is no need to use numbers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

Carbonyls examples table

Displayed formula of carbonyl	Structural formula of carbonyl	IUPAC name of carbonyl
	CH_2O	methanal (also known as formaldehyde)
	CH_3CHO	ethanal

	CH_3COCH_3	propanone (also known as acetone)
	$CH_3CH_2COCH_3$	butanone

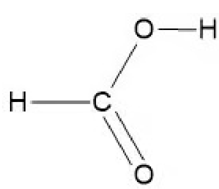
Your notes

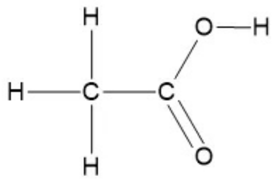
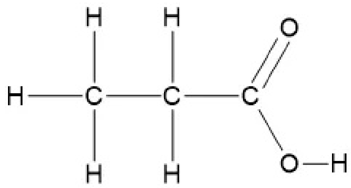
- As they have a very similar functional group arrangement, **aldehydes** and **ketones** show similar chemical reactions
- Differences in their chemistry are due to the reactions that involve the H on the **aldehyde** or the nature of the R group
- The difference in **electronegativity** between oxygen 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**

Carboxylic acids

- **Carboxylic acid** is the name given to compounds containing the functional group **carboxyl, -COOH**
- The general formula of a carboxylic acid is $\mathbf{C_nH_{2n+1}COOH}$ which can be shortened to just **RCOOH**
  - (In some countries the family is called alkanoic acid)
- The nomenclature of **carboxylic acids** 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

Displayed formula of carboxylic acid	Structural formula of carboxylic acid	IUPAC name of carboxylic acid
	HCO_2H	methanoic acid (also known as formic acid)

	CH_3CO_2H	ethanoic acid (also known as acetic acid)
	$CH_3CH_2CO_2H$	propanoic acid

Your notes

Your notes

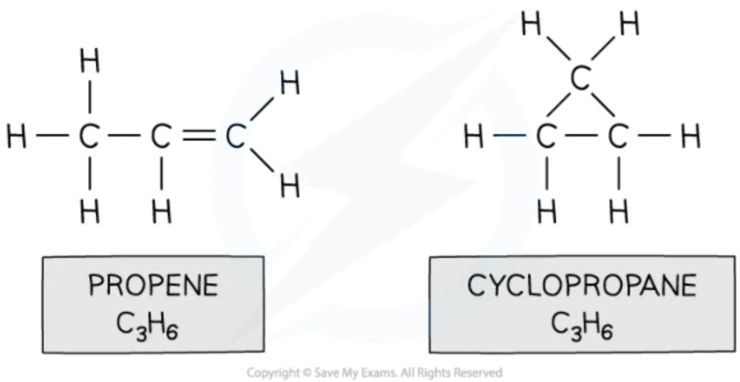
Structural Isomers

Structural Isomers

What are isomers?

- Isomers are compounds that have the same molecular formula but a different arrangement of atoms
- One group of isomers is the structural isomers
  - These are compounds that have the same molecular formula but different structural formulae

Isomers of C_3H_6



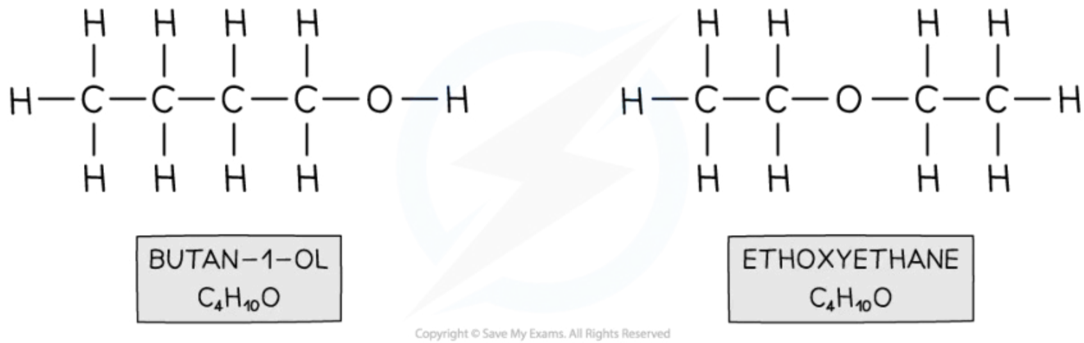
Propene and cyclopropane are both made of 3 carbon and 6 hydrogen atoms but the structure of the two molecules differs

- There are three different types of structural isomerism:
  1. **Functional group** isomerism
  2. **Positional** isomerism
  3. **Branched chain** isomerism

Functional group isomerism

- When different functional groups result in the same molecular formula, **functional group isomers** arise
- These isomers have very **different chemical properties** as they have different functional groups

Functional group isomers of $C_4H_{10}O$



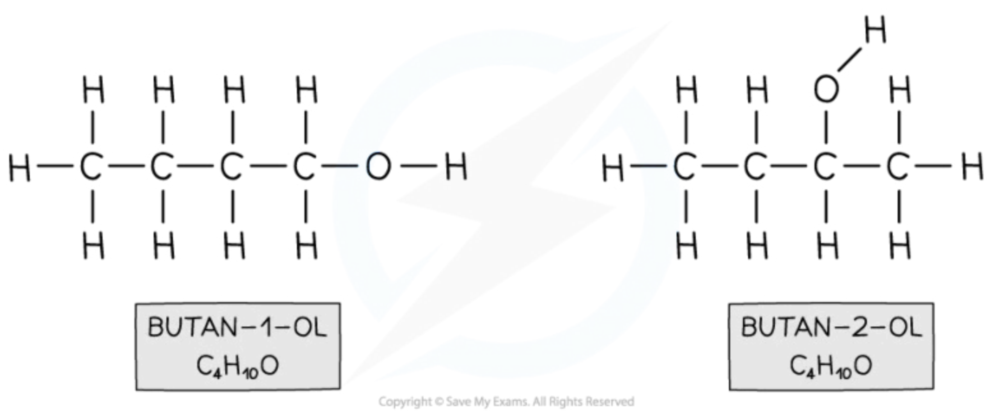
Both compounds have the same molecular formula however butan-1-ol contains an alcohol functional group and ethoxyethane an ether functional group

- It can help to be aware of which **homologous series** can be functional group isomers of each other:
  - Alkenes and cycloalkanes
  - Alcohols and ethers
  - Aldehydes and ketones

Positional isomerism

- Positional isomers arise from differences in the position of a functional group in each isomer
  - This literally means that the functional group is located on different carbon atoms

Position isomers of butanol, C_4H_9OH, diagram



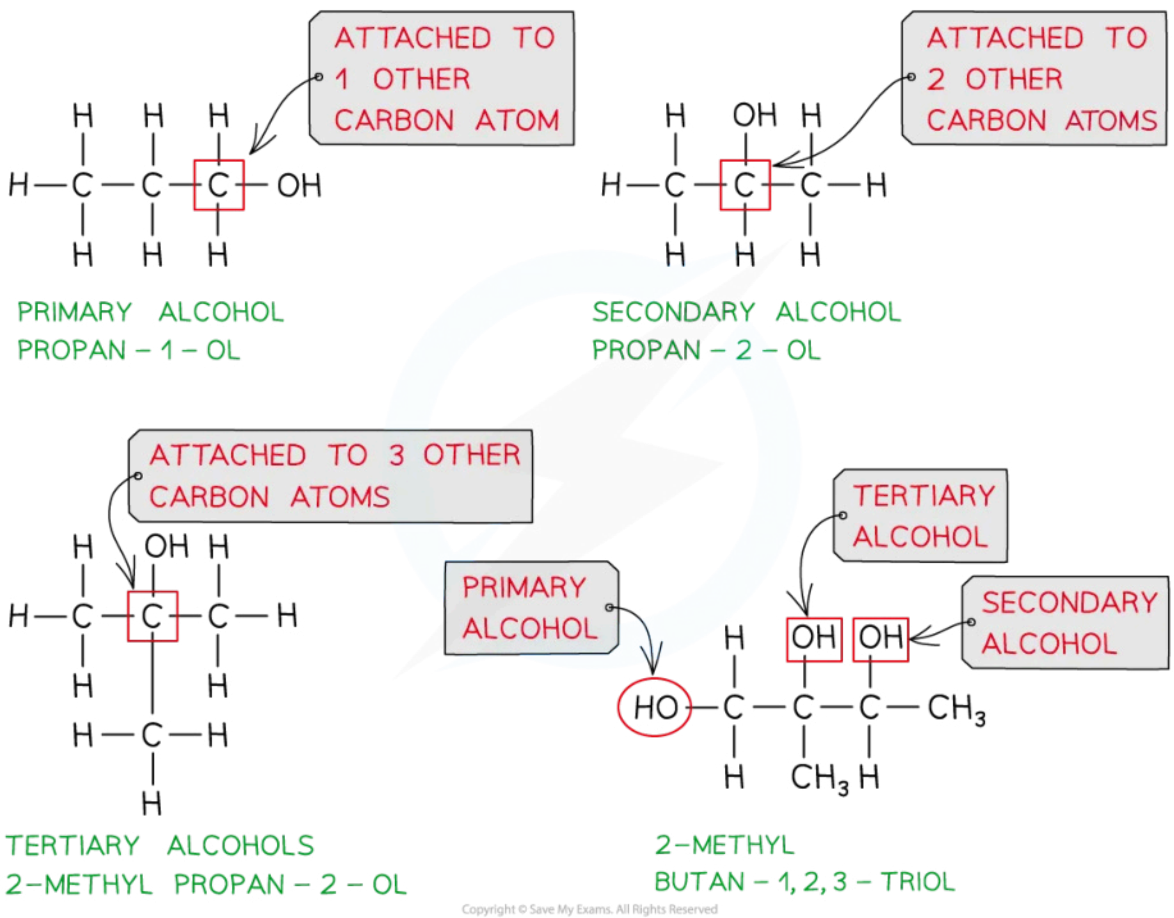
Both compounds are made up of 4 carbon, 10 hydrogen and one oxygen atom. However, the alcohol / OH group is located on different carbon atoms

- In the example above, the functional group is the alcohol / OH group
  - The OH group can be attached to carbon-1, which gives rise to butan-1-ol
  - The OH group can be attached to carbon-2, which gives rise to butan-2-ol
  - **Careful:** In the butan-1-ol diagram, it appears that the OH group is attached to carbon-4
    - If you imagine looking at the molecule from the other side, you would see that the OH group is attached to carbon-1

- The same is true of butan-2-ol, where the OH group appear to be attached to carbon-3

- Some organic compounds that can be described as having **primary**, **secondary** or **tertiary** structures will exhibit isomerism
  - The terms **primary**, **secondary** and **tertiary** relate to the number of carbon atoms that the functional group carbon is attached to

Demonstrating primary, secondary and tertiary structures in alcohols



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

- **Alcohols**, e.g. propanol
  - The primary alcohol propan-1-ol and the secondary alcohol propan-2-ol are position isomers of each other
  - **Careful:** The tertiary alcohol 2-methylpropan-2-ol is another isomer but it is branched chain **not** position isomerism
- **Halogenoalkanes**, e.g. $C_4H_{11}Br$
  - The primary halogenoalkane 1-bromobutane and the secondary halogenoalkane 2-bromobutane are position isomers of each other

Your notes

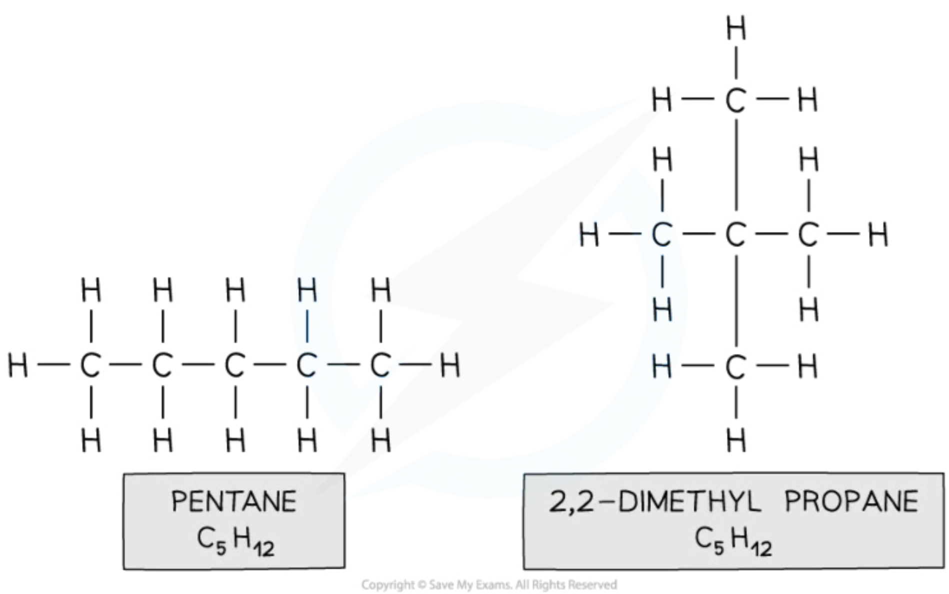
- **Careful:** The tertiary halogenoalkane 2–bromo–2–methylpropane is another isomer but, again, it is branched chain **not** position isomerism

Your notes

Branched 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, i.e. where the longest hydrocarbon is broken into smaller pieces and some of these smaller pieces are added as side-chains / branches

Isomers of C_5H_{12}



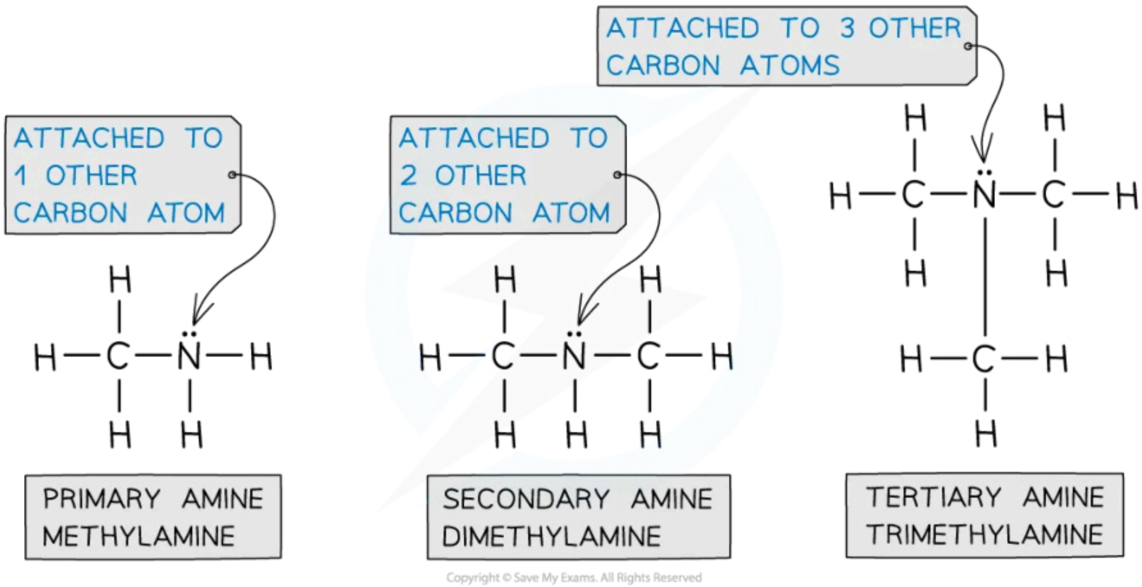
Both compounds contain 5 carbon and 12 hydrogen atoms. However, the longest carbon chain in pentane is 5 and in 2,2–dimethylpropane it is 3 (with two methyl branches)

Isomerism in amines

- **Amines** follow a slightly different classification system to alcohols and halogenoalkanes, 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)

Examples of primary, secondary and tertiary amines

Your notes



The number of carbons attached to the nitrogen atom indicate if an amine is primary (1 carbon), secondary (2 carbons) or tertiary (3 carbons)

- This means that amines do show isomerism
  - It is ambiguous whether isomerism in amines is position or branched chain

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

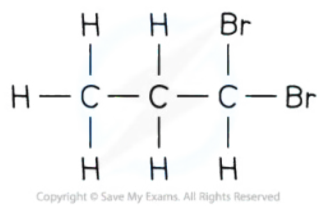
Your notes

Worked example

How many structural isomers are there of $C_3H_6Br_2$?

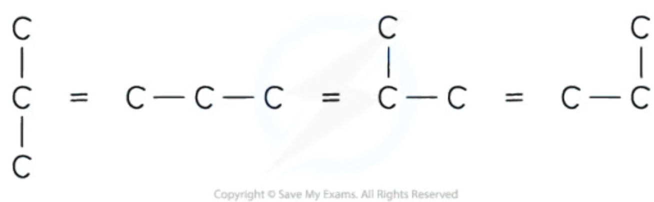
Answer:

Step 1: Draw a displayed formula of the compound



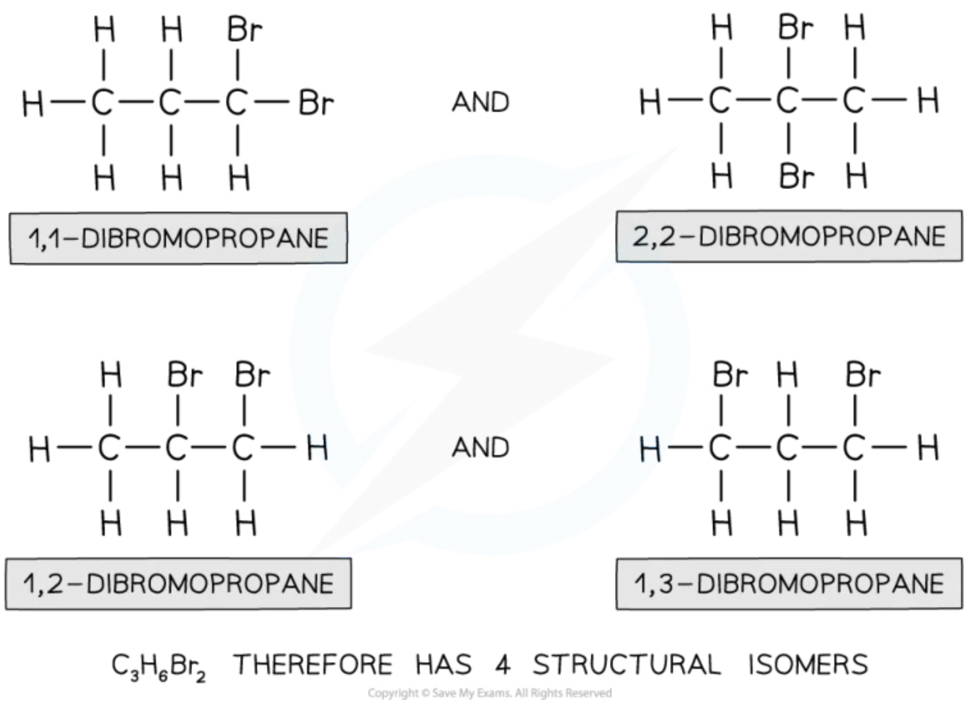
Step 2: Determine whether there is functional group, branched chain or positional isomerism

- Functional group?
  - No, Br is the only functional group present
- Branched chain?
  - No, the longest carbon chain is 3 carbons which cannot branch:



- Positional?
  - Yes, there are two bromine atoms that can be bonded to different carbon atoms

Your notes


1,1–DIBROMOPROPANE
AND
2,2–DIBROMOPROPANE
1,2–DIBROMOPROPANE
AND
1,3–DIBROMOPROPANE
$C_3H_6Br_2$ THEREFORE HAS 4 STRUCTURAL ISOMERS
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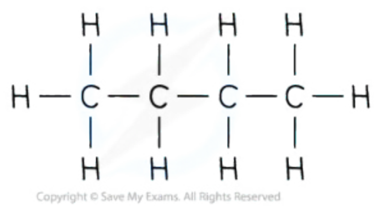
Your notes

Worked example

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

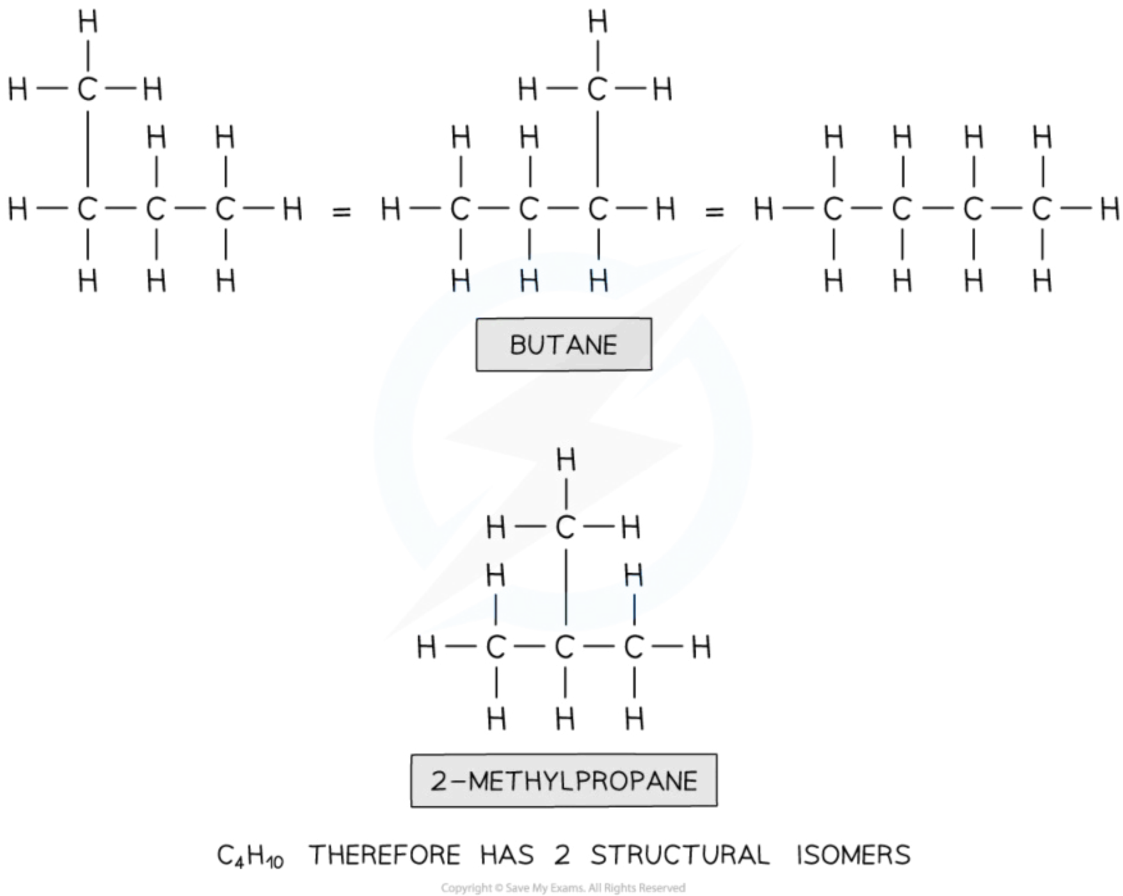
Answer:

Step 1: Draw one possible structural formula of the compound



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

- Functional group?
  - No, there are no functional groups
- Positional?
  - No, as there are no functional groups which can be positioned on different carbon atoms
- Branched chain
  - Yes, a carbon chain containing 4 carbons is the smallest chain that can exhibit branched chain isomerism



Your notes

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.