

CHAPTER 14: An Introduction to Organic Chemistry

14.1 Organic Compounds

14.2 Organic Reactions

14.3 Isomerism

Learning outcomes:

(a) *interpret, and use the general, structural, displayed and skeletal formulae of the following classes of compound:*

- (i) *alkanes and alkenes.*
- (ii) *halogenoalkanes.*
- (iii) *alcohols (including primary, secondary and tertiary).*
- (iv) *aldehydes and ketones.*
- (v) *carboxylic acids and esters.*

[Candidates will be expected to recognise the shape of the benzene ring when it is present in organic compounds. Knowledge of benzene or its compounds is not required for AS.]

(b) *interpret, and use the following terminology associated with organic reactions:*

- (i) *functional group.*
- (ii) *homolytic and heterolytic fission.*
- (iii) *free radical, initiation, propagation, termination.*
- (iv) *nucleophile, electrophile.*
- (v) *addition, substitution, elimination, hydrolysis.*
- (vi) *oxidation and reduction.*

[in equations for organic redox reactions, the symbols [O] and [H] are acceptable]

(c) (i) *describe the shapes of the ethane and ethene molecules.*

(ii) *predict the shapes of other related molecules.*

(d) *explain the shapes of the ethane and ethene molecules in terms of σ and π carbon-carbon bonds.*

(e) *describe structural isomerism, and its division into chain, positional and functional group isomerism.*

(f) *describe stereoisomerism, and its division into geometrical (cis-trans) and optical isomerism.*

- (g) describe cis-trans isomerism in alkenes, and explain its origin in terms of restricted rotation due to the presence of π bonds.*
- (h) explain what is meant by a chiral centre and that such a centre gives rise to optical isomerism*
- (i) identify chiral centres and/or cis-trans isomerism in a molecule of given structural formula.*
- (j) deduce the possible isomers for an organic molecule of known molecular formula.*
- (k) deduce the molecular formula of a compound, given its structural, displayed or skeletal formula.*

14.1 Organic Compounds

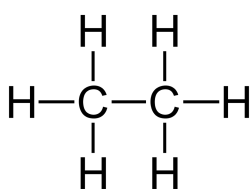
What is organic chemistry?

- 1) Organic chemistry is the study of carbon compounds (excluding simple compounds like CO , CO_2 , CO_3^{2-} , HCO_3^-).

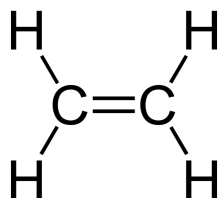
Formulae of organic compounds

- 1) There are five ways in which organic compounds/molecules can be presented:
- Empirical formula
 - Molecular formula
 - Structural formula
 - Displayed formula
 - Skeletal formula
- 2) i. **Empirical formula** gives the **simplest ratio** of the number of atoms of each element present in the compound.
- ii. **Molecular formula** gives the **actual number** of atoms of each element present in the compound.
- iii. These two formulae are least useful and rarely used in organic chemistry because they do not reveal much information about the compounds.
- 3) **Structural formula** shows the **order** of the atoms joined together in an organic compound. These formulae are usually written in one line.
- Examples: Ethane - CH_3CH_3
Ethene - $\text{CH}_2=\text{CH}_2$ (only double and triple bonds are shown)
Ethanoic acid - CH_3COOH
2-methylpentane - $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$
- 4) **Displayed formula** shows the **order** of the atoms joined together, as well as the **orientation** of the atoms and bond angles.

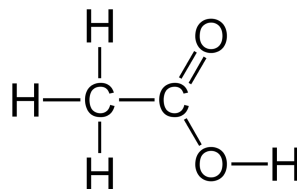
Examples:



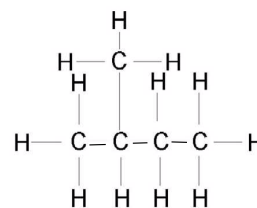
Ethane



Ethene

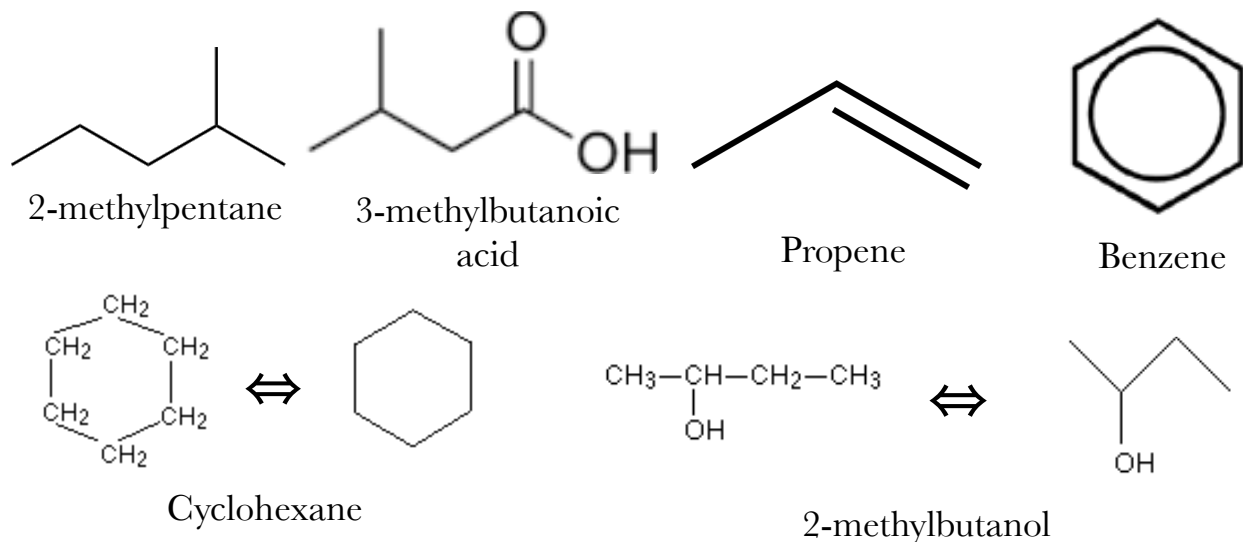


Ethanoic acid



2-methylbutane

- 5) **Skeletal formula** shows only the functional groups. The carbon and hydrogen atoms are simplified and hidden. In a skeletal formula:
- there is a carbon atom **at each junction** and **at the end of the bond**, there is no carbon atom at a place occupied by another functional group.
 - there is **enough hydrogen atoms** bonded to each carbon so that each carbon has four bonds only.



- 6) It is essential to learn to convert between different formulae of the same compound.

Names of organic compounds

- Organic compounds are named systematically according to the IUPAC (International **U**nion of **P**ure and **A**ppplied **C**hemistry) nomenclature.
- For details, **refer to the attached document** at the end of the notes.

- 3) Some examples to fill the page:

Compound	IUPAC Name	Remarks
$\begin{array}{c} \text{CH}_3\text{CHCH}_2\text{CH}_2\text{CH}_3 \\ \\ \text{CH}_3 \end{array}$	2-methylpentane	(<i>not</i> 4-methylpentane)
$\begin{array}{c} \text{CH}_3\text{CH}-\text{CHCH}_2\text{CH}_3 \\ \quad \\ \text{CH}_3 \text{CH}_3 \end{array}$	2,3-dimethylpentane	(<i>not</i> 3,4-dimethylpentane)
$\begin{array}{c} \text{CH}_3\text{CH}-\text{CHCH}_2\text{CH}_2\text{CH}_3 \\ \quad \\ \text{Cl} \quad \text{Br} \end{array}$	3-bromo-2-chlorohexane	substituent groups in alphabetical order.
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3-\text{C}-\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CH}_3 \\ \quad \\ \text{CH}_3 \text{CH}_2\text{CH}_3 \end{array}$	4-ethyl-2,2-dimethylheptane	substituent groups in alphabetical order. (ignore di- and tri- etc.)
$\text{CH}_2=\text{CHCH}_2\text{OH}$	prop-2-ene-1-ol	principal group on the smallest number.
	1,4-dibromobenzene	—

Functional groups

- 1) A *functional group* is a group of atoms in an organic compound that determines the chemistry of that particular compound.
- 2) A *homologous series* is a series of compounds with the same functional group, and the adjacent members differ in the number of carbon atoms.

Some common functional groups and their associated types of compounds:

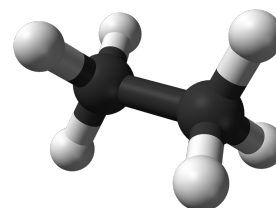
<i>Homologous series</i>	<i>Functional group</i>	<i>prefix or suffix</i>	<i>Example</i>
Alkene	$\begin{array}{c} \diagup \text{C} - \text{C} \diagdown \\ \diagdown \quad \diagup \end{array}$	-ene	$\text{H}_2\text{C}-\text{CH}_2$ ethene
Alkyne	$-\text{C}\equiv\text{C}-$	-yne	$\text{H}-\text{C}\equiv\text{C}-\text{H}$ ethyne
Halogen compound	$\begin{array}{c} -\text{X} \\ \\ \text{---C---} \\ \\ (\text{X} = \text{F}, \text{Cl}, \text{Br}, \text{I}) \end{array}$	halo-	$\text{CH}_3\text{CH}_2-\text{Cl}$ chloroethane
Alcohol	$-\text{OH}$	-ol	$\text{CH}_3\text{CH}_2-\text{OH}$ ethanol
Ether	$-\text{O}-$	alkoxy-	$\text{CH}_3\text{OCH}_2\text{CH}_3$ methoxyethane
Aldehyde	$\begin{array}{c} \text{O} \\ \\ \text{---C} \\ \\ \text{H} \end{array}$	-al	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{C} \\ \\ \text{H} \end{array}$ ethanal
Ketone	$\begin{array}{c} \text{O} \\ \\ \text{---C} \\ \\ \diagdown \end{array}$	-one	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{C} \\ \\ \text{CH}_3 \end{array}$ propanone
Carboxylic acid	$\begin{array}{c} \text{O} \\ \\ \text{---C} \\ \\ \text{OH} \end{array}$	-oic acid	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{C} \\ \\ \text{OH} \end{array}$ ethanoic acid
Ester	$\begin{array}{c} \text{O} \\ \\ \text{---C} \\ \\ \text{O---} \end{array}$	-oate	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{C} \\ \\ \text{O-CH}_3 \end{array}$ methyl ethanoate
Acid chloride	$\begin{array}{c} \text{O} \\ \\ \text{---C} \\ \\ \text{Cl} \end{array}$	-oyl chloride	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{C} \\ \\ \text{Cl} \end{array}$ ethanoyl chloride
Amide	$\begin{array}{c} \text{O} \\ \\ \text{---C} \\ \\ \text{NH}_2 \end{array}$	-amide	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{C} \\ \\ \text{NH}_2 \end{array}$ ethanamide
Amine	$-\text{NH}_2$	-amine	$\text{CH}_3\text{CH}_2-\text{NH}_2$ ethylamine
Nitrile	$-\text{C}\equiv\text{N}$	-nitrile	$\text{CH}_3\text{CH}_2-\text{CN}$ propanenitrile

[Note: You do not need to memorise the table above at this moment.]

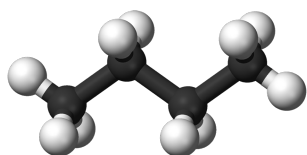
Bonding in organic molecules

- 1) Carbon atoms which are sp^3 hybridised (typically forming 4 bonds) have the atoms bonded to it arranged in **tetrahedral shape** with a bond angle of 109.5° .

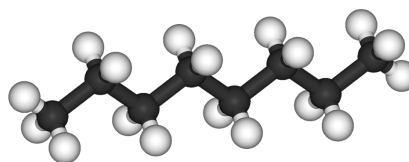
- 2) One such example is ethane. In an ethane molecule, the two carbon atoms undergo sp^3 hybridisation. All other atoms are bonded to the carbon atoms via σ bonds. All bond angles are 109.5° .



- 3) If the carbon chain is longer, all the bond angles are still 109.5° , the molecule has a zig-zag shape.

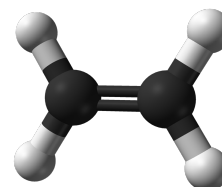


Butane



Octane

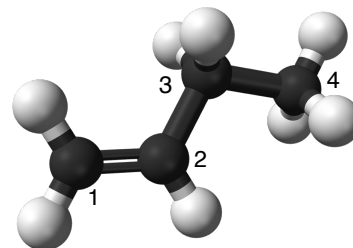
- 4) Carbon atoms which are sp^2 hybridised (typically forming 3 bonds) have the atoms bonded to it arranged in a **trigonal planar shape** with bond angle 120° .



- 5) One such example is ethene. In an ethene molecule, the two carbon atoms undergo sp^2 hybridisation. The two carbon atoms are connected via σ and π bonds, a double bond is formed between the two carbon atoms. The bond angle is 120° .

- 6) If the carbon chain is longer, depending on the number of double bonds, a mixture of trigonal planar and tetrahedral shape is possible. However, each carbon atom can only have either one.

- 7) Observe the but-1,2-ene molecule beside. Carbon 1 and 2 are sp^2 hybridised, so the atoms around it have a trigonal planar arrangement. Carbon 3 and 4 are sp^3 hybridised, so the atoms around it have a tetrahedral arrangement.



[Note : For greater detail on hybridisation and bonding, refer Chapter 4]

14.2 Organic Reactions

Reactions that organic compounds undergo

1) Organic reactions are classified using two ways:

i. By the type of reagent used:

- Nucleophilic
- Electrophilic

ii. By what happens during the reaction:

- Addition
- Substitution
- Elimination

2) Some common reactions:

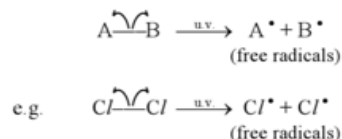
- Free-radical substitution
- Electrophilic addition
- Electrophilic substitution
- Nucleophilic addition
- Nucleophilic substitution
- Redox (oxidation and reduction)
- Hydrolysis

[Note : You do not need to be familiar with these names at this moment.]

Homolytic and heterolytic bond fission

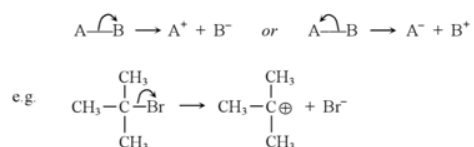
1) Organic reactions involve the breaking of covalent bonds. There are two ways in which a covalent bond can be broken, by homolytic or heterolytic fission.

2) *Homolytic fission* is the breaking of a covalent bond in such a way that one electron goes to each atom, forming free-radicals.



3) A *free-radical* is an atom or a group of atoms with an unpaired electrons formed from the homolytic fission of a covalent bond and is very reactive.

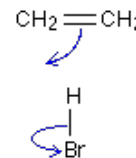
4) *Heterolytic fission* is the breaking of a covalent bond in such a way that both electrons go to the same atom, forming cation and anion.



Curly arrows

1) Curly arrows are used in organic chemistry to represent the **movement of electron(s)**. It is often used in the presentation of an organic mechanism.

2) The tail of the arrow shows where the electron(s) originates from while the head shows the place where electron(s) is/are moved to. The electrons can either originate **from a lone pair or from a bond**.



3) Half arrows show the movement of **one** electron while a full arrow shows the movement of **two** electrons. In the diagram above, the first is a half arrow while the second is a full arrow.

4) Curly arrows can only be used to represent the movement of electron(s), they may not be used for other purposes to avoid ambiguity.

Nucleophiles and electrophiles

1) A *nucleophile* is a species which contains a lone pair of electrons and is attracted to regions of positive charge or electron-deficient sites. They are often negatively-charged or carry a partial negative charge.

2) Some examples of nucleophiles are NH_3 , CN^- , OH^- , Cl^- , Br^- and H_2O .

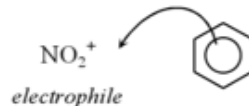
3) An *electrophile* is an electron-deficient species which can accept electrons and is attracted to regions of negative charge or electron-rich sites. They are often positively-charged or carry a partial positive charge.

4) Some examples of electrophiles are H^+ , Br^+ , Cl^+ and NO_2^+ .

Nucleophiles will attack *electron deficient* regions, e.g.



Electrophiles will attack *electron rich* regions, e.g.

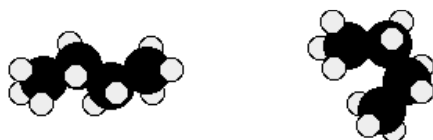


[Note : A benzene ring is an electron-rich region]

14.3 Isomerism

What are isomers?

- 1) *Isomers* are two or more compounds with the same molecular formula but a different arrangement of atoms in space. Organic molecules which exhibit this property show isomerism.
- 2) **This excludes any different arrangements which are simply due to the molecule rotating** as a whole, or rotating about particular bonds. For example, both of the following are the same molecule. They are not isomers, both are butane.

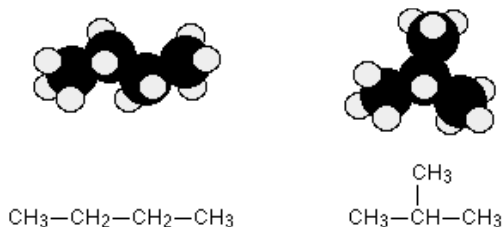


- 3) Isomers **must have different names**. A good way to identify isomers is by naming the molecules, molecules with the same name are not isomers.
- 4) There are two types of isomerism
- Structural isomerism
 - Stereoisomerism

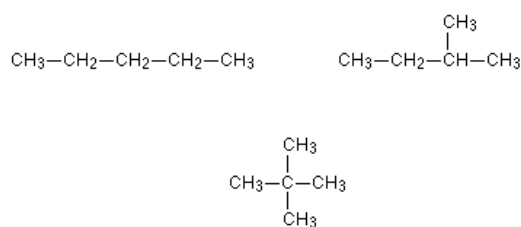
<i>isomerism</i>	
<i>structural isomerism</i> - chain isomerism - positional isomerism - functional group isomerism	<i>stereoisomerism</i> - geometrical (<i>cis-trans</i>) isomerism - optical isomerism
<i>Structural Isomerism</i>	<i>Stereoisomerism</i>
<ul style="list-style-type: none">➤ Structural isomers have the same molecular formula but different structural formula.➤ Arises from the different ways in which atoms can join together to form molecules.➤ The atoms are linked in different sequences and in different ways.	<ul style="list-style-type: none">➤ Stereoisomers have same molecular and structural formulae but <i>different arrangement of their atoms in space</i>.➤ Arises from the different ways in which the various groups in the molecule can arrange in space.➤ The atoms are linked in the same sequence and in the same way but differ in their <i>arrangement in space</i>.

Structural isomerism

- 1) **Chain isomerism** arises due to the **different arrangement of carbon atoms in a chain**. The carbon atoms may be arranged in a straight chain or branched chain.

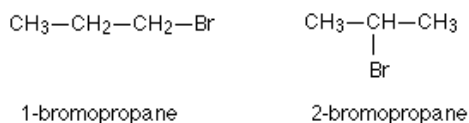


Isomers of butane, C_4H_{10}

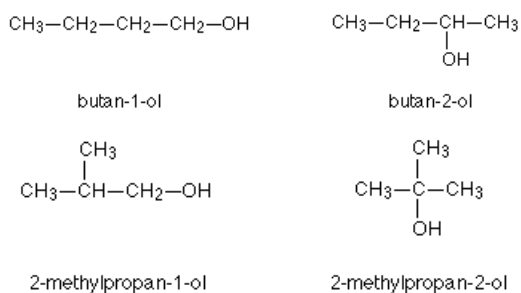


Isomers of pentane, C_5H_{12}

- 2) **Positional isomerism** arises due to **different positions of functional group** in the carbon chain.



Isomers of $\text{C}_3\text{H}_7\text{Br}$



Isomers of butanol, $\text{C}_4\text{H}_9\text{OH}$

- 3) **Functional isomerism** arises due to **different functional groups**.



Some isomers of $\text{C}_3\text{H}_6\text{O}$

[Note : Propanal is an aldehyde while propanone is a ketone, they belong to different homologous series]

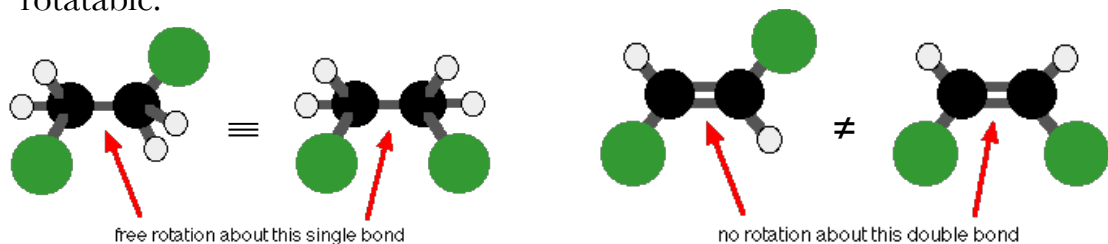
4) More examples:

Molecular formula	Structural isomers		
C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$ pentane	$CH_3CHCH_2CH_3$ CH_3 2-methylbutane	CH_3 CH_3-C-CH_3 CH_3 2,2-dimethylpropane
$C_4H_{10}O$	$CH_3CH_2CH_2CH_2OH$ butan-1-ol CH_3CHCH_2OH CH_3 2-methylpropan-1-ol	$CH_3CHCH_2CH_3$ OH butan-2-ol $CH_3CH_2-O-CH_2CH_3$ ethoxyethane $CH_3-O-CH_2CH_2CH_3$ 1-methoxypropane	CH_3 CH_3-C-CH_3 OH 2-methylpropan-2-ol $CH_3-O-CHCH_3$ CH_3 2-methoxypropane
$C_3H_6Br_2$	$CH_3CH_2CHBr_2$ 1,1-dibromopropane	$CH_3CHBrCH_2Br$ 1,2-dibromopropane $CH_2BrCH_2CH_2Br$ 1,3-dibromopropane	Br CH_3-C-CH_3 Br 2,2-dibromopropane
$C_3H_6O_2$	$CH_3CH_2C(=O)OH$ propanoic acid	$CH_3C(=O)OCH_3$ methyl ethanoate	$H-C(=O)OCH_2CH_3$ ethyl methanoate

Stereoisomerism - Geometrical (*cis-trans* or E-Z) isomerism

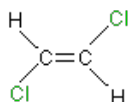
1) Geometrical isomerism arises due to the **rotation about a bond is restricted**. It is common in compounds containing **carbon-carbon double bond (C=C bond)** and certain **ring systems**.

2) i. A C=C bond cannot be rotated due to the **presence of π bond**. A π bond will break if a rotation occurs. Conversely, a carbon-carbon single bond is rotatable.

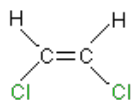


ii. In ring systems, rotation about a bond is restricted due to the **linkage of the ring** because the C-C bond is now part of the ring system.

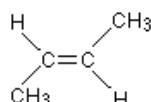
- 3) Geometrical isomers occur in pairs, differing from each other in the **positioning of the two groups across the double bond**.
- A *cis*-isomer has the two groups on the **same side** of the double bond.
 - A *trans*-isomer has the two groups on the **opposite sides** of the double bond.



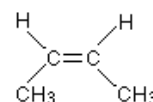
trans-1,2-dichloroethene



cis-1,2-dichloroethene

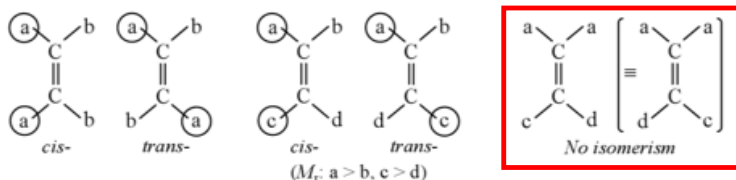


trans-but-2-ene



cis-but-2-ene

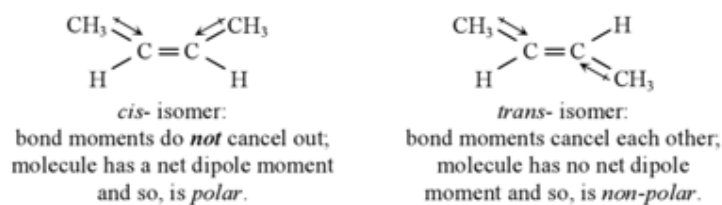
- 4) To identify geometrical(*cis-trans*) isomers, it is essential to draw the groups around the double bond showing the correct bond angles(120°).
- 5) Geometrical(*cis-trans*) isomerism **cannot exist if either carbon carries identical groups**. In short, to have geometrical isomers, it is essential to have two different groups on the left and two different groups on the right.



- 6) More examples:

Compound	Geometrical (<i>cis-trans</i>) isomers	Remarks
BrCH=CHBr	 <i>cis</i> -isomer <i>trans</i> -isomer	—
CH ₃ CH=CCl/Br	 <i>cis</i> -isomer <i>trans</i> -isomer	In the <i>cis</i> -isomer, the group of higher priority (higher M _r) on each C are on the same side of C=C bond.
 1,2-dichloro cyclopropane	 <i>cis</i> -isomer <i>trans</i> -isomer	—

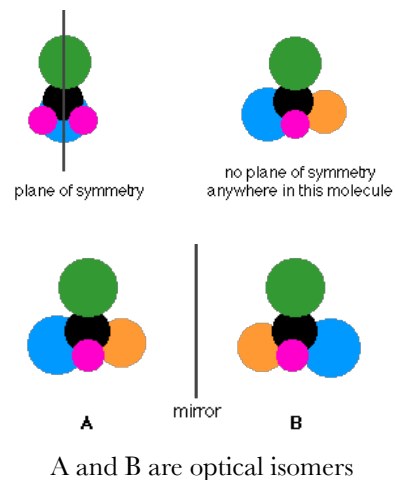
- 7) Geometrical isomers have similar(not identical) chemical properties but different physical properties.
- 8) *cis*-isomer generally has a **higher boiling point** than *trans*-isomer. This is because dipoles in a *cis*-isomer do not cancel out each other, causing the entire molecule to have a **net dipole moment** and it is **polar**. Permanent dipole-dipole forces exist and more energy is required to overcome it.



- 9) *trans*-isomer generally has a **higher melting point** than *cis*-isomer. This is because in the solid state, trans-isomers pack more efficiently in the crystalline lattice due to its shape.

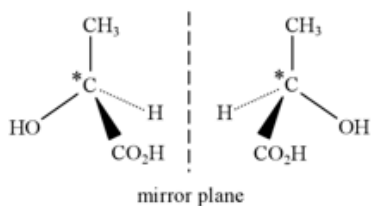
Stereoisomerism - Optical isomerism

- 1) Optical isomerism arises due to the **ability of compounds to rotate the plane of polarisation of a plane-polarised light**.
- 2) A compound is said to be **optically-active**(optical isomerism exists) if it rotates the plane of polarised light. If it does not, it is said to be optically-inactive.
- 3) For a compound to be optically active:
 - i. It needs to have an **asymmetrical carbon** with **four different groups** attached to it so that there is no plane of symmetry. The carbon atom with four different groups attached to it is called the **chiral carbon** or **chiral centre**.
 - ii. The isomers must be mirror-images of each other and are non-superimposable. That is, no matter how the molecules are rotated, they never fully resemble each other.



4) An example:

e.g. 2-hydroxypropanoic acid has a chiral carbon (marked *) and so, shows optical activity. It has no plane of symmetry and its mirror images are non-superimposable.

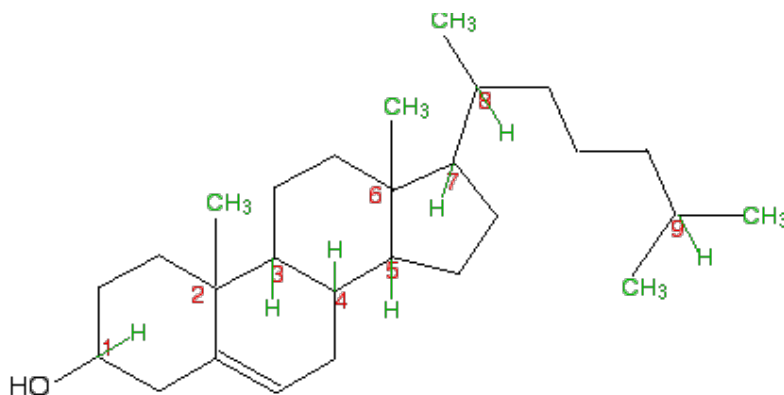


NB. When drawing a pair of optical isomers, the three-dimensional structures should be indicated according to the convention used in this example.

Note: — represents a bond lying *on the plane* of the paper,
--- represents a bond sticking out *behind the plane* of the paper, and
▴ represents a bond sticking out *in front of the plane* of the paper.

5) To identify optical isomers:

- In chain systems, check which carbon has four different groups attached to it.
- In ring systems, check also which carbon has four different groups attached to it. A different group here can be identified by **tracking around that ring** from a particular carbon atom in either clockwise or anti-clockwise direction. If the pattern along the way is the same, that carbon atom is not chiral, and the converse is also true.
- An example:



Only carbon 9 is not a chiral carbon in this cholesterol molecule

Attachment

NOMENCLATURE OF ORGANIC COMPOUNDS

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Organic chemistry is the chemistry of carbon compounds. Carbon has the ability to bond with itself to form long chains and, as a result, millions of compounds from simple hydrocarbons to large biomolecules such as proteins, lipids, carbohydrates, and nucleic acids. Originally it was believed that these compounds had to come from a living organism, now they are synthesized in the laboratory.

The simplest organic compounds are composed of carbon and hydrogen and are known as hydrocarbons. There are four types, or classes, of hydrocarbons:

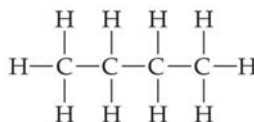
Alkanes: contain all C-C single bonds. These are known as **saturated hydrocarbons**.

Alkenes: contain at least one C=C double bond.

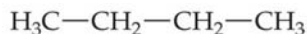
Alkynes: contain at least one C≡C triple bond. Both alkenes and alkynes are known as **unsaturated hydrocarbons**

Aromatic hydrocarbons: contain a benzene structure

Lewis structures of alkanes look like this:



These are also called structural formulas. Since these take up a lot of space, condensed structural formulas are used.



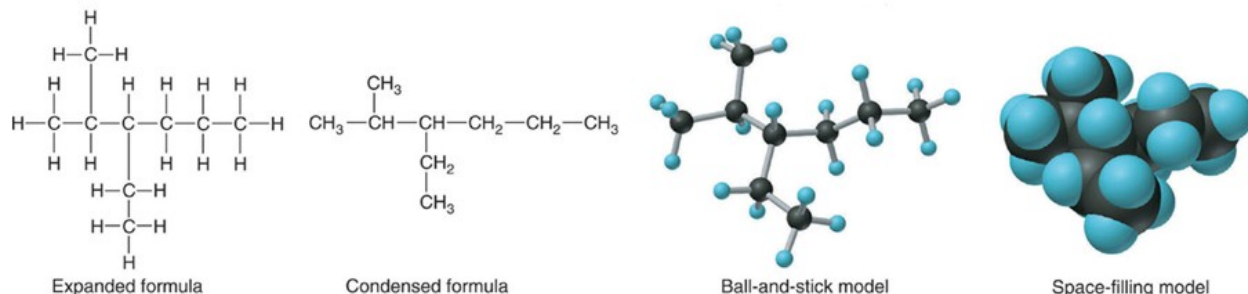
or



Even simpler than condensed structures are skeletal or line structures:

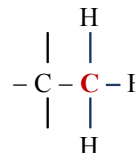


There are a range of structures used to represent organic compounds:

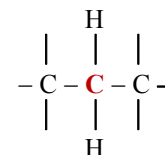


Before we start naming organic compounds, it is important to understand how carbon atoms are bonded. Every carbon atom will try to form 4 bonds.

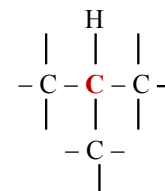
A carbon atom on the end of a chain of single bonded carbon atoms will be bonded to one carbon atom and three hydrogen atoms:



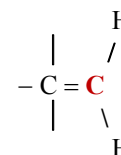
A carbon atom in the middle of a chain of single bonded carbon atoms will be bonded to two carbon atoms and two hydrogen atoms.



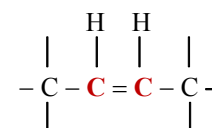
A carbon atom bonded to 3 other single bonded carbon atoms will be bonded to one hydrogen.



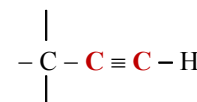
A carbon atom on the end of a chain that is double bonded to another carbon atom be bonded to two hydrogen atoms.



A carbon atom in the middle of a chain of that is double bonded to another carbon atom will be bonded to one carbon atom and one hydrogen atom.



A carbon atom on the end of a chain that is triple bonded to another carbon atom will be bonded to one hydrogen atom. The second carbon atom in that chain is only bonded to another carbon atom, but no hydrogen atoms.

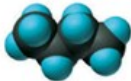
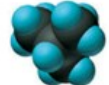
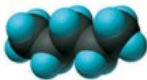
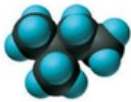
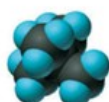


I. Naming Saturated Hydrocarbons - The Alkanes

The names of the alkanes are derived from the Greek prefix for the particular number of carbon atoms in the compound with an -ane ending. The names of the first ten alkanes are given in the following table.

Molecular Formula	Condensed Structural Formula	Name	Boiling Point (°C)
CH ₄	CH ₄	Methane	-161
C ₂ H ₆	CH ₃ CH ₃	Ethane	-89
C ₃ H ₈	CH ₃ CH ₂ CH ₃	Propane	-44
C ₄ H ₁₀	CH ₃ CH ₂ CH ₂ CH ₃	Butane	-0.5
C ₅ H ₁₂	CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	Pentane	36
C ₆ H ₁₄	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	Hexane	68
C ₇ H ₁₆	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	Heptane	98
C ₈ H ₁₈	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	Octane	125
C ₉ H ₂₀	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	Nonane	151
C ₁₀ H ₂₂	CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	Decane	174

Not all the alkanes are straight chained compounds, as shown in the previous table, they can have side chains or branches. These variations of compounds which have the same number of carbon and hydrogen atoms, but a different arrangement are known as **isomers**. Some isomers are shown in the diagram below.

Systematic Name (Common Name)	Condensed Formula	Expanded Formula	Space-filling Model	Density (g/mL)	Boiling Point (°C)
Butane (<i>n</i> -butane)	$\text{CH}_3\text{—CH}_2\text{—CH}_2\text{—CH}_3$	$ \begin{array}{cccc} \text{H} & \text{H} & \text{H} & \text{H} \\ & & & \\ \text{H—C—C—C—C—H} \\ & & & \\ \text{H} & \text{H} & \text{H} & \text{H} \end{array} $		0.579	−0.5
2-Methylpropane (isobutane)	$ \begin{array}{c} \text{CH}_3\text{—CH—CH}_3 \\ \\ \text{CH}_3 \end{array} $	$ \begin{array}{ccc} \text{H} & \text{H} & \text{H} \\ & & \\ \text{H—C—C—C—H} \\ & & \\ \text{H—C—H} \\ \\ \text{H} \end{array} $		0.549	−11.6
Pentane (<i>n</i> -pentane)	$\text{CH}_3\text{—CH}_2\text{—CH}_2\text{—CH}_2\text{—CH}_3$	$ \begin{array}{ccccc} \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \\ & & & & \\ \text{H—C—C—C—C—C—H} \\ & & & & \\ \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \end{array} $		0.626	36.1
2-Methylbutane (isopentane)	$ \begin{array}{c} \text{CH}_3\text{—CH—CH}_2\text{—CH}_3 \\ \\ \text{CH}_3 \end{array} $	$ \begin{array}{ccc} \text{H} & \text{H} & \text{H} & \text{H} \\ & & & \\ \text{H—C—C—C—C—H} \\ & & & \\ \text{H—C—H} & & \text{H} & \text{H} \\ & & & \\ \text{H} & & & \end{array} $		0.620	27.8
2,2-Dimethylpropane (neopentane)	$ \begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3\text{—C—CH}_3 \\ \\ \text{CH}_3 \end{array} $	$ \begin{array}{c} \text{H} \\ \\ \text{H—C—H} \\ \\ \text{H—C—C—C—H} \\ & & \\ \text{H—C—H} & \text{H—C—H} & \text{H—C—H} \\ & & \\ \text{H} & \text{H} & \text{H} \end{array} $		0.614	9.5

Rules for Naming of Branched Hydrocarbons.

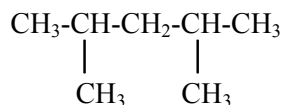
There are four parts to the name of a branched hydrocarbon

1. The **parent chain**: Tells how many carbons are in the longest continuous chain.
meth = 1 eth = 2 prop = 3 but = 4 pent = 5
2. The **suffix**: Tells what type of compound it is.
ane = an alkane ene = an alkene yne = an alkyne
3. The **prefix**: Tells what groups, or branches are attached to the parent chain.
methyl = —CH_3 ethyl = $\text{—CH}_2\text{—CH}_3$ propyl = $\text{—CH}_2\text{—CH}_2\text{—CH}_3$
4. The **location**: Tells where groups, or branches, are attached to the parent chain.

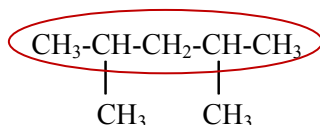
2 = 2nd carbon atom 3 = 3rd carbon atom 4 = 4th carbon atom

Note: alkyl groups, or branches cannot be located on the 1st or last carbon

Example 1:

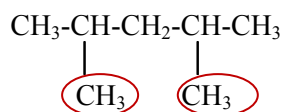


1. Select as the **parent chain** the LONGEST CONTINUOUS CHAIN of carbon atoms. The compound is considered to have been derived from the parent structure by the replacement of hydrogens by various alkyl groups.



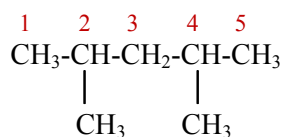
The longest continuous chain of carbon atoms in this example contains five carbon atoms. Since the carbon atoms in this compound all contain The alkane that contains five carbon atoms is **pentane**.

2. Identify the branches, or side chains, attached to the parent chain.



Both branches consist of single carbon atoms, there are called **methyl** groups

3. Starting from either end of the longest carbon chain, number the carbon atoms in the parent chain consecutively so that the alkyl groups (or branches) are attached to the carbon atoms with the lowest possible numbers.



For this compound, it makes no difference which end you start the numbering. In both cases the alkyl groups, or branches are attached to the second and fourth carbon atoms in the parent chain.

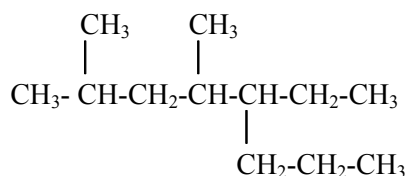
4. Name the compound in order of: number of carbon atom-alkyl group attached(number of carbon atom-alkyl group attached- etc...) name of parent compound. If there are several different alkyl groups attached to the parent chain, name them in order of increasing size or in alphabetical order.

The name for this compound looks like it would be called would be called 2-methyl-4-methylpentane, however, all branches with the same name are grouped together. The number of these branches have a prefix:

di = 2 tri = 3 tetra = 4 penta = 5

But, each branch needs a specified location, so, the correct name is **2,4-dimethylpentane**

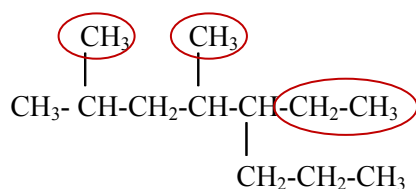
Example 2



In this compound, the longest continuous chain is **8 carbon atoms long**. Note that the longest continuous chain does not have to be straight. This longest chain is **oct-** (for 8 carbons)

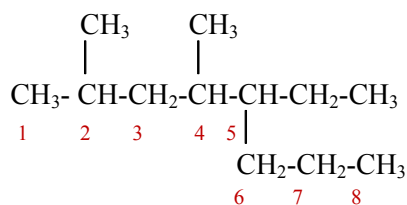
All the bonds are single bonds, so this is an alkane. The suffix is **-ane**

This parent chain is **octane**



There are three branches attached to the parent chain. Two of these are **methyl** groups and one is an **ethyl** group.

Number the carbon atoms, so that the groups are attached to the carbon atoms with the lowest possible numbers.



The two methyl groups in this compound are attached on the 2nd and 4th carbon atoms and the ethyl group is attached to the 5th carbon atom.

This compound is named **5-ethyl-2,4-dimethyloctane**. Note that the branches are named in alphabetical order.

II. Naming Unsaturated Hydrocarbons – Alkenes and Alkynes

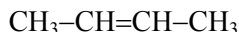
Rules for Naming Alkenes and Alkynes

Alkenes contain at least one carbon to carbon double bond. The suffix used is **-ene**.

Alkynes contain at least one carbon to carbon triple bond. The suffix used is **-yne**.

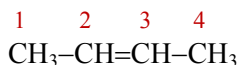
Naming is the same as used for alkanes, except that the parent structure is the longest continuous chain of carbon atoms that contains the carbon-carbon double bond or triple bond. The name is derived by changing the suffix of the corresponding alkane name to **-ene** for an alkene and **-yne** for an alkyne and a number is added to denote the location of the multiple bond.

Example:



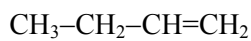
The longest continuous chain in this compound contains four carbon atoms. The parent structure would be named **but + ene** (to denote the double bond)

Number the carbon atoms in the longest chain in such a way that the carbon atoms containing the double bond have the lowest possible numbers.



For this compound, the numbering should start on the left side so the double bond will be located between carbon atom no. 2 and carbon atom no. 3. Although the double bond involves two carbon atoms, its position is designated by the number of the first doubly-bonded carbon atom when numbering from the end of the parent chain nearest the double bond. So, this compound would be named **2-butene**.

Example:

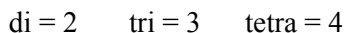


In this compound the double bond is located between the 1st and 2nd carbon atoms. The compound is named **1-butene**.

Example:

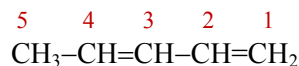


The longest continuous chain in this compound contains five carbon atoms. The parent structure would be named **pent-** however, the compound contains **two** carbon-carbon double bonds. The number of double bonds, if greater than 1, is denoted by a prefix added to the suffix.



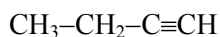
The parent chain is named **pentadiene**. Note that an "a" is added to the name to make it easier to pronounce.

Number the carbon atoms in the longest chain in such a way that the carbon atoms containing the double bond have the lowest possible numbers.



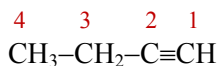
For this compound, the numbering should start on the right side so the double bonds will be located between carbon atom no. 1 and carbon atom no. 2 and carbon atom no. 3 and carbon atom no. 4. The name of the compound is **1,3-pentadiene**.

Example



The longest continuous chain in this compound contains four carbon atoms. The parent structure would be named **but + yne** (to denote the triple bond)

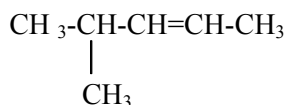
Number the carbon atoms in the longest chain in such a way that the carbon atoms containing the triple bond have the lowest possible numbers.



For this compound, the numbering should start on the right side so the triple bond will be located between carbon atom no. 1 and carbon atom no. 2. This compound would be named **1-butyne**.

If the compound is branched, the name is determined similar to that used for the alkanes.

Example.

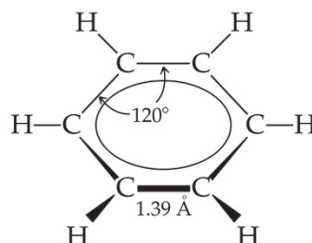
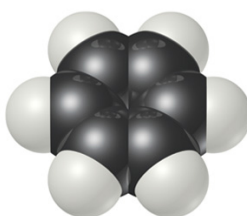


This compound is named **4-methyl-2-pentene**. Note that the double bond takes precedence in naming.

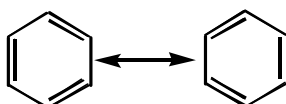
III. Naming Aromatic Compounds

Aromatic Compounds are cyclic hydrocarbons containing a benzene structure.

AROMATIC
Benzene C_6H_6



Benzene can be represented by the resonance structures:



The actual structure of benzene, however, is a resonance hybrid of these two structures usually written as:



Benzene rings can be fused together. These compounds have common names.



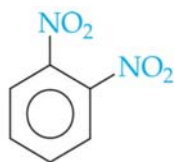
Naphthalene



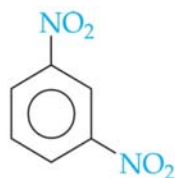
Anthracene

An aromatic compound which is formed by having an alkyl group attached to a benzene ring is named by prefixing the alkyl group name to the word benzene. An example of this is named **methylbenzene** or **toluene**

If there are only two groups attached to the benzene ring, their relative positions can be designated by numbers or by the terms ortho, meta, or para, abbreviated o-, m-, or p-.



1,2-dinitrobenzene
ortho-dinitrobenzene



1,3-dinitrobenzene
meta-dinitrobenzene



1,4-dinitrobenzene
para-dinitrobenzene

Ortho = the 1 and 2 positions on the ring (adjacent carbon atoms)

Meta = the 1 and 3 positions on the ring (alternate carbon atoms)

Para = the 1 and 4 positions on the ring (opposite carbon atoms)

IV. Naming Functional Group Compounds

Derivatives are formed by replacing one or more of the hydrogens in a hydrocarbon by a FUNCTIONAL GROUP. The functional group is responsible for giving what is ordinarily an inactive compound the characteristic chemical and physical properties of another class of compounds.

A. Halogen Derivatives of Hydrocarbons

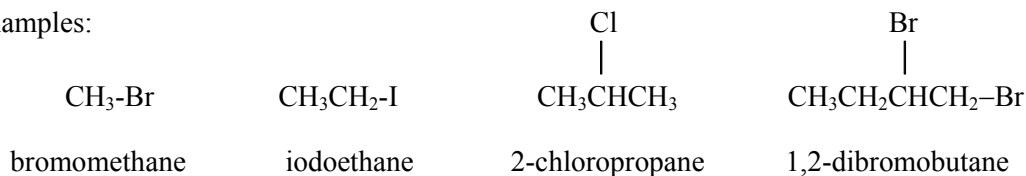
Functional Group: - X (F, Cl, Br, I)

General Formula: R-X

Naming of Halides

Halogens attached to a hydrocarbon chain are named by replacing the -ine ending of the halogen name with **-o**. When naming a compound, halogens are named in the same manner as alkyl group branches.

Examples:



B. Oxygen Derivatives of the Hydrocarbons

These functional group compounds contain at least one oxygen atom in its structure.

1. Alcohols

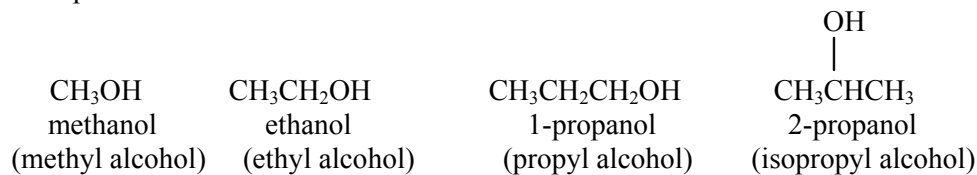
Functional Group: -OH

General Formula: R-OH

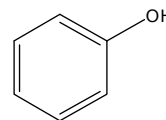
Naming of alcohols:

Number the longest carbon chain so that the -OH group is attached to the carbon atom with the lowest possible number. Name the parent compound by using the alkane name and replacing the -e ending with an **-ol** ending. Indicate the position of the hydroxyl group with a number in any alcohol containing three or more carbon atoms.

Examples:



Aromatic alcohols are called phenols and contain the structure:



2. Ethers

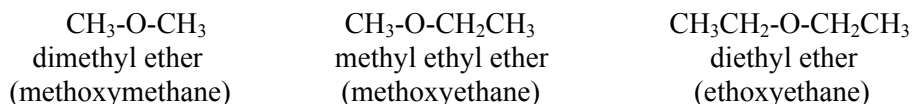
Functional Group: -O-

General formula: R-O-R

Naming of ethers

Ethers are commonly named by naming each group attached to the oxygen followed by the word **ether**. If one group has no simple name, the ether can be named as an alkoxy derivative of the larger group.

Examples:

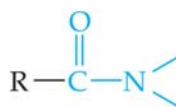


3. Carbonyl Compounds

Carbonyl compounds all contain a $\text{C}=\text{O}$

This includes several types of compounds:

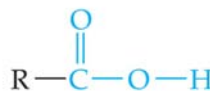
- Aldehydes
- Ketones
- Carboxylic acids
- Esters
- Amides



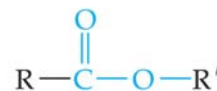
Amide



Aldehyde



Carboxylic
acid

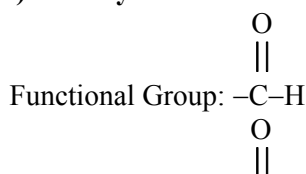


Ester



Ketone

a) Aldehydes

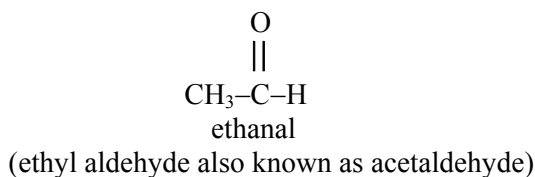
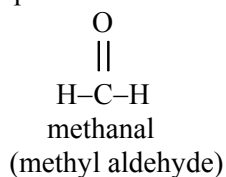


General formula: $\text{R}-\text{C}-\text{H}$ or shorthand as $-\text{CHO}$ (The oxygen is bonded to a terminal carbon atom)

Naming of aldehydes:

Number the longest carbon chain starting with the $-\text{CHO}$ group. Name the parent compound by using the alkane name and replacing the $-e$ ending with an **-al** ending.

Examples:



b) Ketones

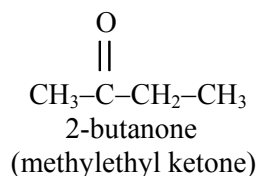
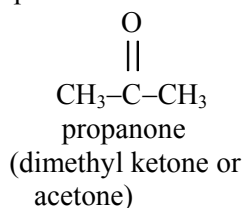


General formula: $\text{R}-\text{C}-\text{R}$ (The oxygen is bonded to a carbon atom in the middle of the chain)

Naming of Ketones:

Number the longest carbon chain starting so that the $-\text{C}=\text{O}$ group is attached to the carbon atom with the lowest number. Name the parent compound by using the alkane name and replacing the $-e$ ending with an **-one** ending.

Examples:



c) Carboxylic acids

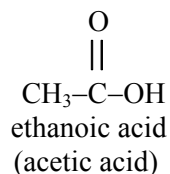
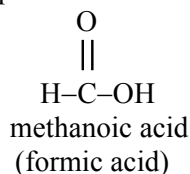


$$\begin{array}{c} \text{O} \\ || \\ \text{General formula: R--C--OH or shorthand as --COOH} \end{array}$$
 (The carboxyl group is bonded to a terminal carbon atom)

Naming of acids:

Number the longest carbon chain starting with the -COOH group. Name the parent compound by using the alkane name and replacing the -e ending with an **-oic acid** ending.

Examples:



d) Esters

An ester is formed from the combination of a carboxylic acid and an alcohol. They are often highly aromatic compounds and are used for flavors and fragrances.

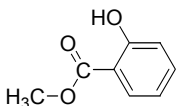


$$\begin{array}{c} \text{O} \\ || \\ \text{General formula: R--C--O--R'} \end{array}$$
 (The R' may be the same or different from R)

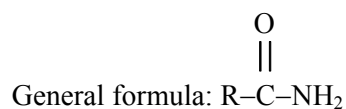
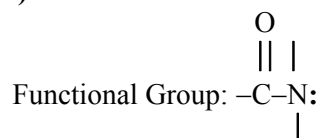
Naming of esters

Esters are usually named by naming the R' group [from an alcohol] as an alkyl group first followed by the acid name [the R-C group] with ending **-oate**. Esters are often called by their common names.

Examples of esters and their flavor/odor properties are given in the table below.

Formula	Common name	IUPAC name	Flavor/odor
$\begin{array}{c} \text{O} \\ \\ \text{HC-O-CH}_2\text{-CH}_3 \end{array}$	ethyl formate	ethyl methanoate	rum
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-C-O-CH}_2\text{-(CH}_2\text{)}_3\text{-CH}_3 \end{array}$	n-amyl acetate	pentyl ethanoate	pears, bananas
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-C-O-CH}_2\text{-CH}_2\text{-CH(CH}_3\text{)}_2 \end{array}$	isoamyl acetate	3-methylbutyl ethanoate	pears, bananas
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-C-O-CH}_2\text{-(CH}_2\text{)}_6\text{-CH}_3 \end{array}$	n-octyl acetate	octyl ethanoate	oranges
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-CH}_2\text{-C-O-CH}_2\text{-CH(CH}_3\text{)}_2 \end{array}$	isobutyl propionate	2-methylpropyl propanoate	rum
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-CH}_2\text{-CH}_2\text{-C-O-CH}_3 \end{array}$	methyl butyrate	methyl butanoate	apples
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-CH}_2\text{-CH}_2\text{-C-O-CH}_2\text{-CH}_3 \end{array}$	ethyl butyrate	ethyl butanoate	pineapples
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-CH}_2\text{-CH}_2\text{-C-O-CH}_2\text{-(CH}_2\text{)}_2\text{-CH}_3 \end{array}$	n-butyl butyrate	butyl butanoate	pineapples
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-CH}_2\text{-CH}_2\text{-C-O-CH}_2\text{-(CH}_2\text{)}_3\text{-CH}_3 \end{array}$	n-amyl butyrate	pentyl butanoate	apricots
$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C-(CH}_2\text{)}_3\text{-C-O-CH}_2\text{-CH}_2\text{-CH(CH}_3\text{)}_2 \end{array}$	isoamyl valerate	3-methylbutyl butanoate	apples
	methyl salicylate	methyl 2-hydroxybenzoate	oil of wintergreen

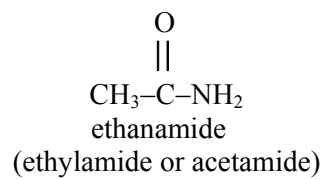
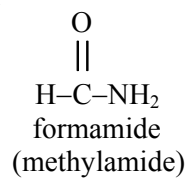
e) Amides





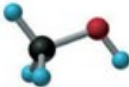
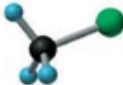
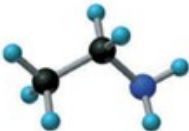
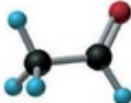
Naming of Amides

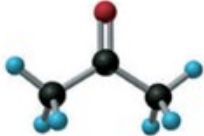
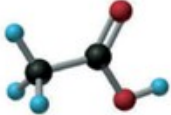
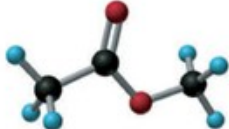
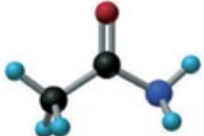

Amides are commonly named similar to a carboxylic acid, replacing the **–oic acid** suffix with **amide**.

Examples:



A summary of the functional group compounds, their structures and names is listed in tables on the next two pages.

Functional Group	Compound Type	Suffix or Prefix of Name	Example		Systematic Name (Common Name)
$\begin{array}{c} \diagup \\ \text{C}=\text{C} \\ \diagdown \end{array}$	alkene	-ene	$\begin{array}{c} \text{H} & & \text{H} \\ & \diagdown & / \\ & \text{C}=\text{C} \\ & / & \diagdown \\ \text{H} & & \text{H} \end{array}$		ethene (ethylene)
$\text{—C}\equiv\text{C—}$	alkyne	-yne	$\text{H—C}\equiv\text{C—H}$		ethyne (acetylene)
$\begin{array}{c} \\ \text{—C—}\ddot{\text{O}}\text{—H} \\ \end{array}$	alcohol	-ol	$\begin{array}{c} \text{H} \\ \\ \text{H—C—}\ddot{\text{O}}\text{—H} \\ \\ \text{H} \end{array}$		methanol (methyl alcohol)
$\begin{array}{c} \\ \text{—C—}\ddot{\text{X}}\text{:} \\ \\ (\text{X}=\text{halogen}) \end{array}$	haloalkane	halo-	$\begin{array}{c} \text{H} \\ \\ \text{H—C—}\ddot{\text{Cl}}\text{:} \\ \\ \text{H} \end{array}$		chloromethane (methyl chloride)
$\begin{array}{c} \\ \text{—C—}\ddot{\text{N}}\text{—} \\ \end{array}$	amine	-amine	$\begin{array}{c} \text{H} & \text{H} \\ & \\ \text{H—C} & \text{—C—}\ddot{\text{N}}\text{—H} \\ & & \\ \text{H} & \text{H} & \text{H} \end{array}$		ethylamine
$\begin{array}{c} \text{:O:} \\ \\ \text{—C—H} \end{array}$	aldehyde	-al	$\begin{array}{c} \text{H} & \text{:O:} \\ & \\ \text{H—C} & \text{—C—H} \\ \\ \text{H} \end{array}$		ethanal (acetaldehyde)

Functional Group	Compound Type	Suffix or Prefix of Name	Example		Systematic Name (Common Name)
$\begin{array}{c} \text{:O:} \\ \parallel \\ -\text{C}-\text{C}-\text{C}- \\ \quad \quad \end{array}$	ketone	-one	$\begin{array}{c} \text{H} \quad \text{:O:} \quad \text{H} \\ \quad \parallel \quad \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$		2-propanone (acetone)
$\begin{array}{c} \text{:O:} \\ \parallel \\ -\text{C}-\ddot{\text{O}}-\text{H} \end{array}$	carboxylic acid	-oic acid	$\begin{array}{c} \text{H} \quad \text{:O:} \\ \quad \parallel \\ \text{H}-\text{C}-\text{C}-\ddot{\text{O}}-\text{H} \\ \\ \text{H} \end{array}$		ethanoic acid (acetic acid)
$\begin{array}{c} \text{:O:} \\ \parallel \\ -\text{C}-\ddot{\text{O}}-\text{C}- \\ \quad \end{array}$	ester	-oate	$\begin{array}{c} \text{H} \quad \text{:O:} \quad \text{H} \\ \quad \parallel \quad \\ \text{H}-\text{C}-\text{C}-\ddot{\text{O}}-\text{C}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$		methyl ethanoate (methyl acetate)
$\begin{array}{c} \text{:O:} \\ \parallel \\ -\text{C}-\ddot{\text{N}}- \\ \end{array}$	amide	-amide	$\begin{array}{c} \text{H} \quad \text{:O:} \\ \quad \parallel \\ \text{H}-\text{C}-\text{C}-\ddot{\text{N}}-\text{H} \\ \quad \\ \text{H} \quad \text{H} \end{array}$		ethanamide (acetamide)
$-\text{C}\equiv\text{N:}$	nitrile	-nitrile	$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{C}\equiv\text{N:} \\ \\ \text{H} \end{array}$		ethanenitrile (acetonitrile, methyl cyanide)