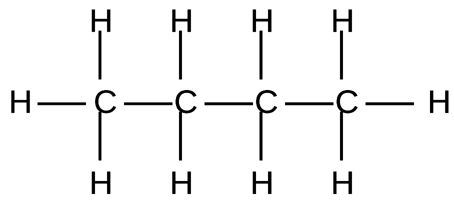
Module 1A – Basic concepts

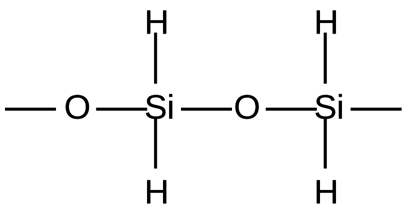
Introduction to organic chemistry

- **Organic Chemistry** is the study of carbon chemistry as carbon has an amazing ability to join together in chains, rings, balls etc.
- Pre – petrochemical industry almost all carbon compounds were extracted from living things. It was Lavoisier in 1784 who first suggested that all compounds extracted from living things contain **carbon and hydrogen** and are called **Hydrocarbons**.
- Carbon also joins with other elements easily such as oxygen, hydrogen, nitrogen, phosphorous and the halogens.
- Hydrocarbons make up over 90% of all known compounds.
- Carbon can join in many different ways and shapes.
- Organic compounds also contain other elements giving rise to functional groups (later).

Why carbon and not silicon?

Carbon compounds frequently contain long chains of carbon atoms





- Silicon does not, it forms a compound made of silicon and oxygen.

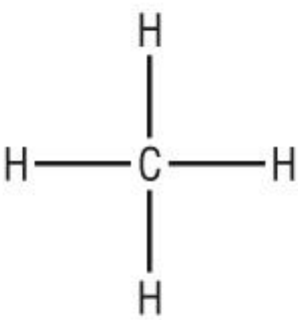
Bond energies give us the answers

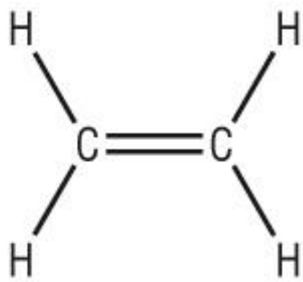
E(C – C) = 347 $KJMol^{-1}$
E(C – H) = 413 $KJMol^{-1}$
E(C – O) = 358 $KJMol^{-1}$

- All the bond energies are of similar magnitude (strong) which means there is little tendency of one of these bonds being replaced by another.
  E(Si – Si) = 226 $KJMol^{-1}$
  E(Si – H) = 318 $KJMol^{-1}$
  E(Si – O) = 466 $KJMol^{-1}$
- The Si – Si bond is the weakest of the bonds and has a tendency to be replaced by the stronger Si – O bond.

Bonding in organic compounds:

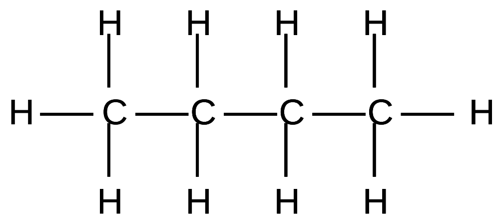
- As carbon is in Gp4 of the periodic table it has 4 single outer shell electrons meaning it forms **4 covalent bonds only**.
- Carbon can form more than one bond with itself:

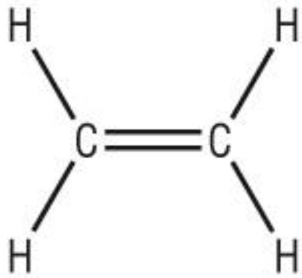




4 bonds only **A double bond and 2 single bonds to hydrogen = 4**

Saturated and unsaturated hydrocarbons:

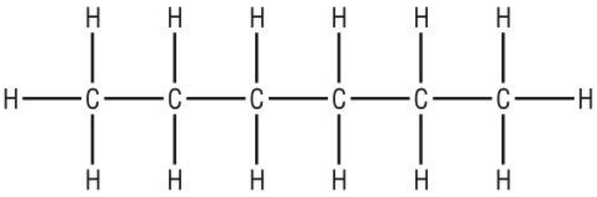




Saturated - is a hydrocarbon with single bonds only

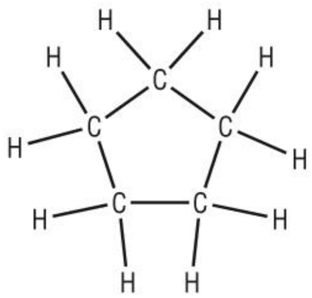
Unsaturated - is a hydrocarbon with carbon carbon multiple bonds

Aliphatic and alicyclic hydrocarbons:



Aliphatic

Aliphatic - is a hydrocarbon in which the carbon atoms are all joined in a straight lines (branched or unbranched)

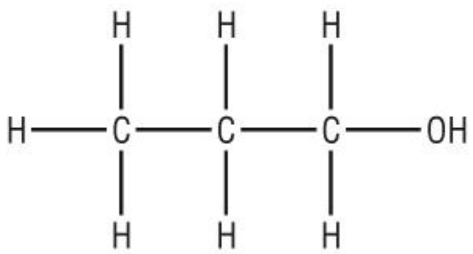


Alicyclic

Alicyclic - is a hydrocarbon in which the carbon atoms are joined together in a ring structure

Functional groups:

- This is the part of the molecule that is responsible for its chemical properties:



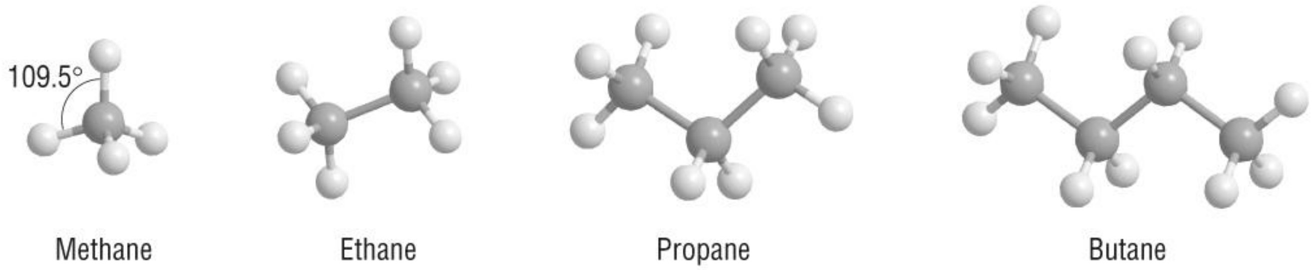
- The OH group in this molecule is the functional group.
- All molecules with the same functional group react in similar ways.

Homologous series:

- This is a family of molecules with the same functional group.
- This means they react in a similar way.
- The differences in the molecules are one carbon (and 2 hydrogens).

The Alkanes:

- This is a homologous series of saturated hydrocarbons:
- All the molecules end in **'ane'**



- The alkanes and their names are outlined in the table below:
- The number of carbons represent a name (later):

No of C's	Name	Formula
1	Methane	CH_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}
6	Hexane	C_6H_{14}
7	Heptane	C_7H_{16}
8	Octane	C_8H_{18}
9	Nonane	C_9H_{20}
10	Decane	$C_{10}H_{22}$

Naming hydrocarbons

Naming organic compounds:

- Because there are so many organic compounds we have to have a systematic way of naming them.
- This is called **Nomenclature**
- Organic molecules are usually made up from:

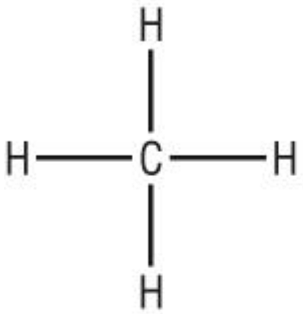
  Carbon chain
  Side chains (alkyl groups)
  Functional groups

Stems, prefix and suffix:

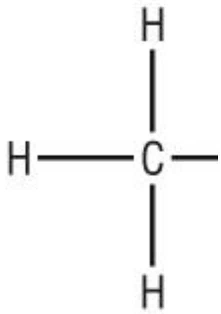
Stem The longest carbon chain - the main name (in the middle) (carbon chain)
Prefix Added before the main name - pre - main name (side chains)
Suffix Added after the main name - post - main name (functional groups)

Alkyl groups:

- If you remove a hydrogen from an alkane you have a group that has a bond that can join to the main carbon chain.
- Based on the alk**anes** the ending of these are changed to alk**yl**



Meth**ane**



Meth**yl**

- The first six alkyl side chains are in the table below:

No of C's	Name	Formula
1	Methyl	CH_3 -
2	Ethyl	C_2H_5 -
3	Propyl	C_3H_7 -
4	Butyl	C_4H_9 -
5	Pentyl	C_5H_{11} -
6	Hexyl	C_6H_{13} -

Naming alkanes:-

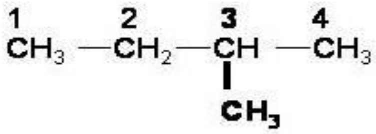
1) Look for the longest carbon chain alkane

2) Look for the functional groups

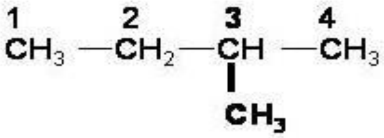
3) Look for the position of the functional group and assign a number. Use the lowest number possible counting from one end of the carbon chain.

4) The name goes in reverse order of the 3 points above.

Example:-



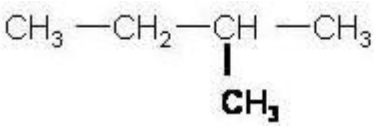
1) Look for the longest straight chain alkane



_____________Butane

The longest carbon chain is in bold. It is 4 carbons long which makes it **butane**

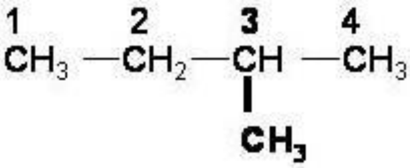
2) Look for the functional groups



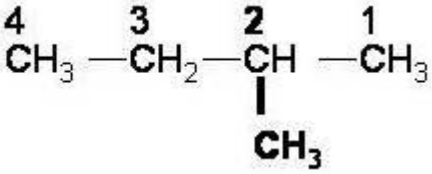
_______Methylbutane

A functional group is any side chain off the straight chain. CH_3 is a derivative of methane (CH_4) which we call **methyl**. See the table below

3) Look for the position of the functional group and assign a number. Use the lowest number possible counting from one end of the carbon chain.



Numbering from one end we get **3 – Methylbutane**. This is incorrect because if we number from the other end we get a lower number.



2 – Methylbutane

Numbering from the other end we get **2 – Methylbutane**. This is correct because if we get a lower number.

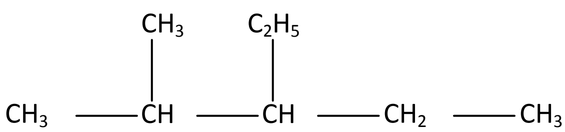
4) The name goes in reverse order of the 3 points above.

2 - Methyl butane

(3) (2) (1)

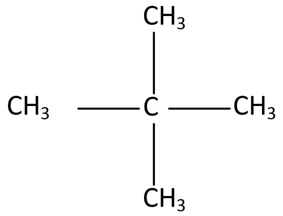
5) Additional side chains or stems

- If there is more than 1 side chain we write the names in alphabetical order:-



3-ethyl 2 methyl pentane

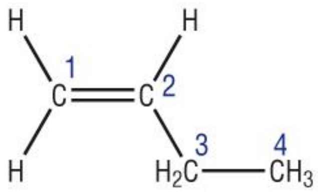
- If there is more than 1 chain on the same carbon we use di, tri, tetra etc:



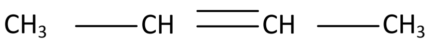
2,2-dimethyl propane

Naming alkenes

- These contain a C=C, the ending of the name changes to 'ene' and we have to put a number to where the double bond is in the carbon chain:-



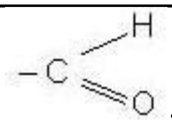
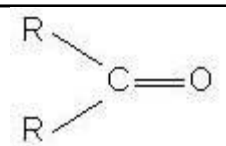
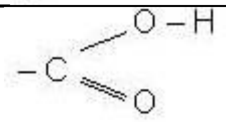
But – 1 – ene



But – 2 – ene

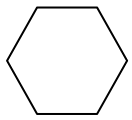
<u>Naming compounds with functional groups</u>

- Organic Chemistry is studied in a systematic way because each different group of atoms attached to a carbon atom has its own characteristic set of reactions.
- These are known as **Functional groups:-**

Functional group	**Formula**	**Prefix (side chains)**	**Suffix (functional group)**
Alkane	C - C		-ane
Alkene	C = C		-ene
Halogenoalkane	– F	Floro -	
	– Cl	Chloro -	
	– Br	Bromo -	
	– I	Iodo -	
Alcohols	– OH	Hydroxy - (if other functional groups are present)	- ol
Aldehydes	 - CHO		- al
Ketones			- one
Carboxylic acids			- oic acid

If a suffix starts with a vowel then the stem has 'an' added

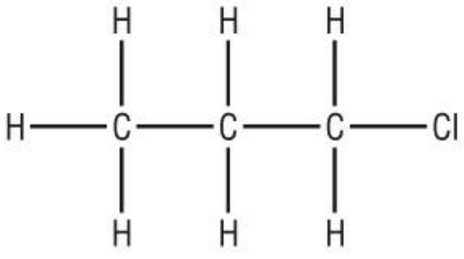
Names for alkanes containing a ring of carbon atoms



- If an alkane is cyclic we use the prefix '**Cyclo**'

cyclohexane

Names for Halogenoalkanes



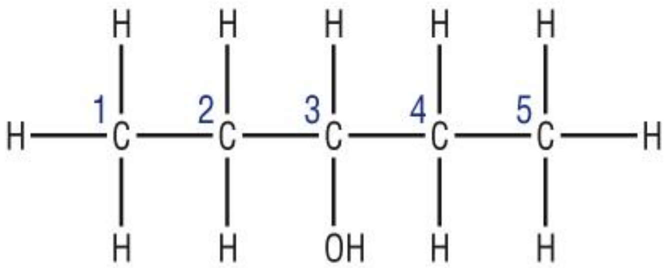
Longest chain = 3C = **prop**

Functional group = Cl (prefix) = **Chloro**prop

Chloro is on carbon 1 = **1** chloroprop

No suffix = ane = 1 chloroprop**ane**

Names for alcohols

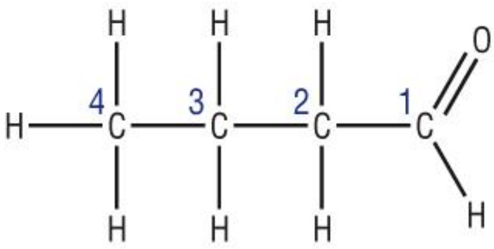


Longest chain = 5C = **pent**

Functional group =OH (suffix starts with a vowel) = pent**an ol**

OH is on carbon 3 = pentan **- 3 -** ol

Names for aldehydes

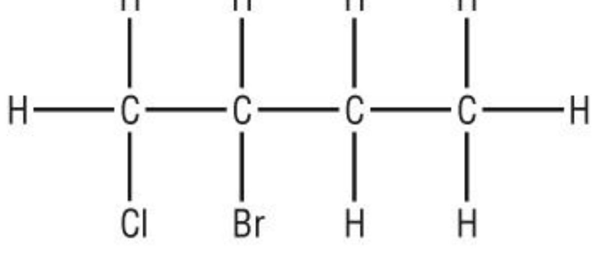


Longest chain = 4C = **but**

Functional group = CHO (suffix starts with a vowel) = but**anal**

The 'al' does not need a number as all aldehydes are at the end of the molecule.

More than one of the same type of functional group



Longest chain = 4C = **but**

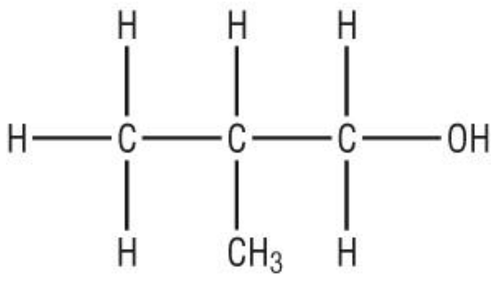
Functional group = Cl on carbon 1 (prefix) = **1 - chloro**

Functional group = Br on carbon 2 (prefix)n = **2 - bromo**

Functional groups are named alphabetically: **2 - bromo - 1 - chlorobut**

No suffix = ane = 2 - bromo - 1 - chlorobut**ane**

Names for 2 different functional groups:

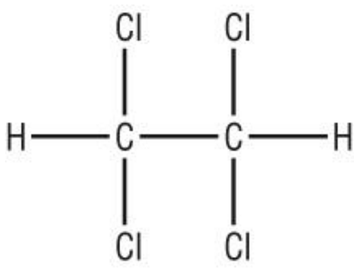


Longest chain = 3C = **prop**

Functional group = OH on carbon 1 (suffix, starts with a vowel so add 'an') = prop**an - 1 - ol**

Side chain = CH_3 on carbon 2 (prefix) = **2 - methyl**propan - 1 - ol

Names for many of the same functional groups:



Longest chain = 2C = **eth**

Functional group = Cl, (2 x on carbon 1) and 2 x on carbon 2 (prefix), numbers first then how many chlorines: **1,1,2,2 - tetrachloro**eth

No suffix = ane = 1,1,2,2 - tetrachloroeth**ane**

Note: di = 2, tri = 3, tetra = 4

<u>Formulae of organic compounds:</u>

Empirical formula:

Definition: Empirical Formula is the simplest ratio of atoms of elements in a compound.

Molecular formulae

Definition: Molecular formulae is the actual ratio of atoms of elements in a compound.

- This can be calculated using moles from percentage composition:-

Recap from Module 1:

Example 1
A sample of iron oxide was found to have 11.2g of iron and 4.8g of oxygen. Calculate the formula of this compound

Element	**Fe**		**O**
Masses	**11.2**		**4.8**
Divide by Ar	**11.2 / 55.8**		**4.8 / 16**
Moles	**0.2**	**:**	**0.3**
Divide by smallest	**0.2 / 0.2**	**:**	**0.3 / 0.2**
Ratio	**1**	**:**	**1.5**
Whole No Ratio	**2**	**:**	**3**
Empirical formula	**Fe_2O_3**		

Example 2

A sample of hydrocarbon was found to have 1.20g of carbon and 0.25g of hydrogen. Calculate the Empirical formula of this compound. Then find out the molecular formula if the Mr = 58

Element	**C**		**H**
Masses	**1.20**		**0.25**
Divide by Ar	**1.20 / 12**		**0.25 / 1**
Moles	**0.10**	**:**	**0.25**
Divide by smallest	**0.10 / 0.10**	**:**	**2.5 / 0.10**
Ratio	**1**	**:**	**2.5**
Whole No Ratio	**2**	**:**	**5**
Empirical formula		**C_2H_5**	**(29 x 2 = 58)**
Molecular formula		**C_4H_{10}**	

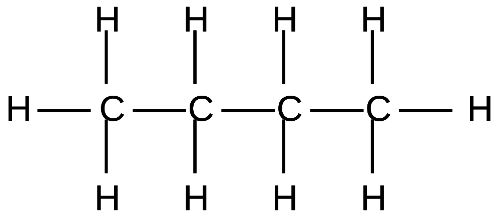
General Formula:

Definition: This is the simplest algebraic formula for a member of a homologous series (of the same functional group)

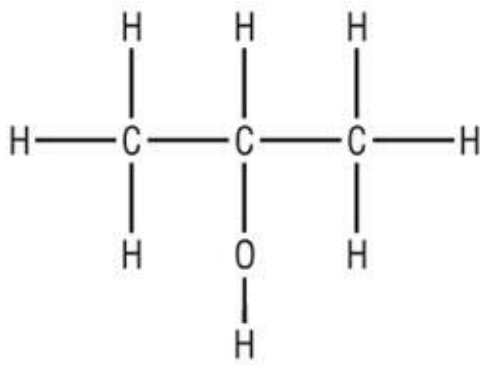
Alkanes	**C_nH_{2n+2}**	**Alkenes**	**C_nH_{2n}**	**Alcohols**	**$C_nH_{2n+1}OH$**
Methane	CH_4			Methanol	CH_3OH
Ethane	C_2H_6	Ethene	C_2H_4	Ethanol	C_2H_5OH
Propane	C_3H_8	Propene	C_3H_6	Propanol	C_3H_7OH

Displayed formula:

Definition: Shows the relative positioning of all the atoms in a molecule, and all the bonds between them



Butane: All the atoms and bonds are shown



Propan-2-ol: Even O - H bonds are shown

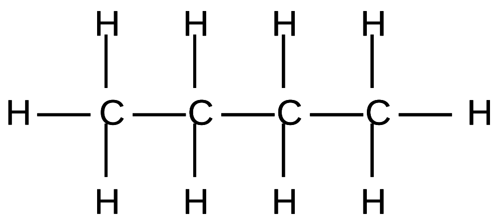
Questions 1-3 P109

Structural and skeletal formula:

Structural formula:

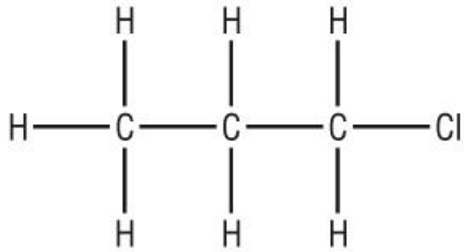
Definition: shows the minimum detail for the arrangement of atoms in a molecule

- Typically we show the ratio of all the atoms attached to each carbon atom in a molecule:



Butane:

$CH_3CH_2CH_2CH_3$

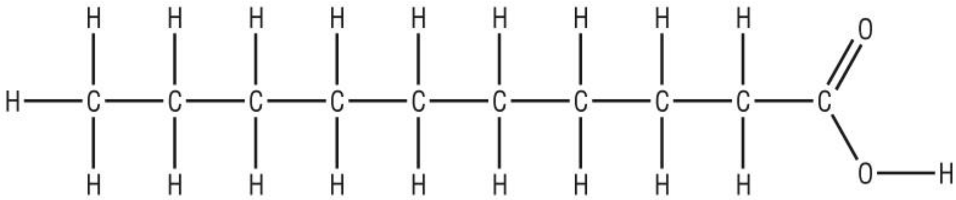


1 - Chloropropane:

$CH_3CH_2CH_2Cl$

- With many CH_2's we can put them in brackets:

Displayed formula:



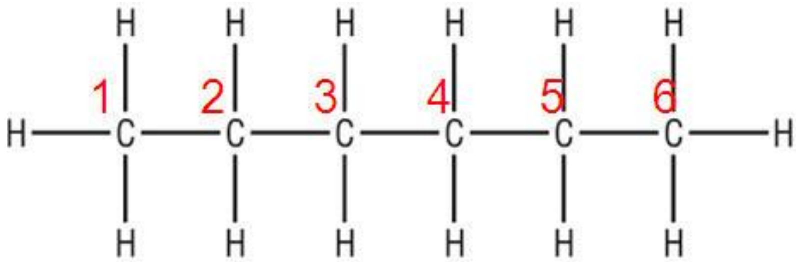
Structural formula: $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2COOH$

This can be simplified to: $CH_3(CH_2)_8COOH$

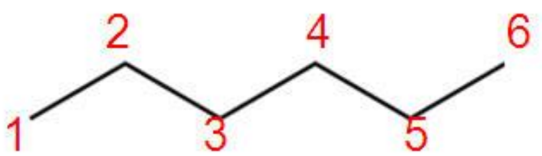
Skeletal formula:

Definition: The hydrogen's are removed leaving a carbon skeleton and associated functional groups

- A good way to approach this is to count and number the carbons. This can then be transposed to the carbon skeleton:

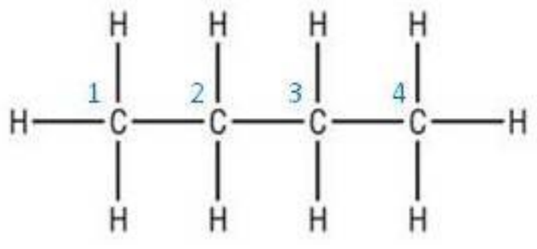


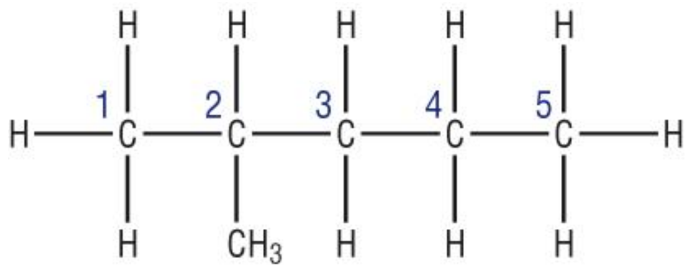
Displayed formula



Skeletal formula

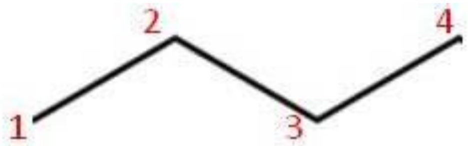
Other examples:

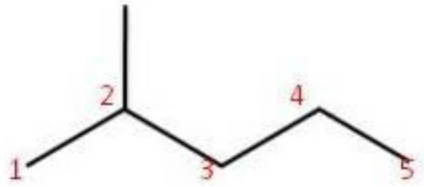




Structural formula: $CH_3CH_2CH_2CH_3$

Structural formula: $CH_3CH(CH_3)CH_2CH_2CH_3$

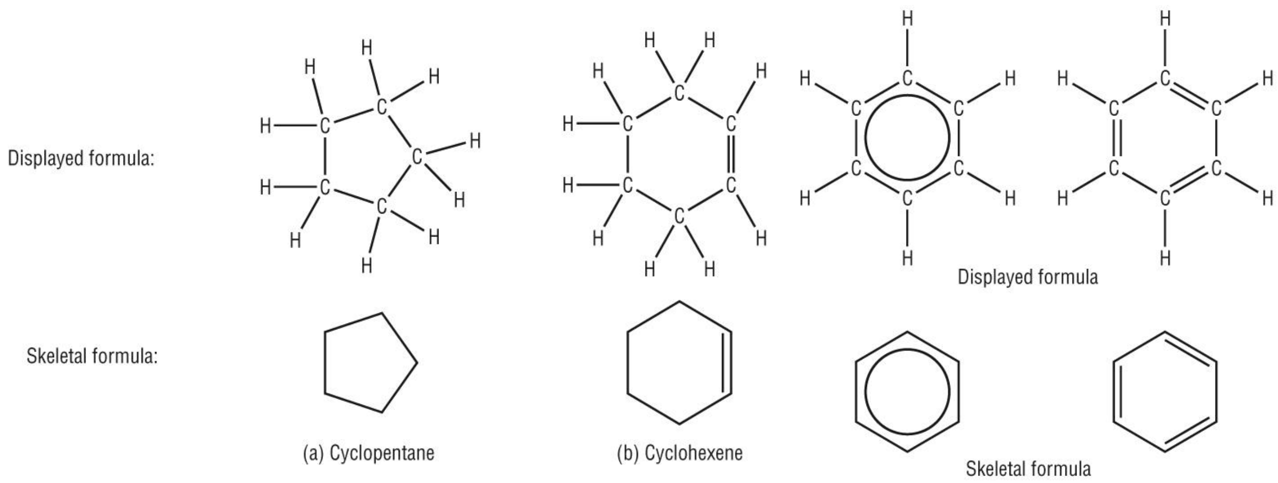




- No carbon or hydrogen atoms are shown
- A carbon atom exists at the ends
- A carbon atom exists at each point

Cyclic compounds:

- Cyclic compounds are usually drawn as skeletal:



Questions: 1-3 P111

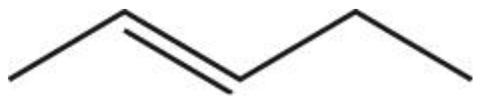
<u>Skeletal formulae and functional groups</u>

Unsaturated hydrocarbons:

- Add numbers to the carbons on the skeletal formulae. This is how many carbons in the molecule.
- Add a double bond between the corresponding carbons from the skeletal to the displayed:

Skeletal formulae:

Fill in the displayed formula:

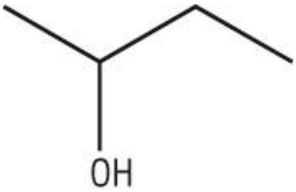


Pent-2-ene

Compounds with functional groups:
Butan-2-ol:

- Functional groups must be included in skeletal formulae
- The end of the side chain off carbon 2 is now an OH instead of a CH_3

Skeletal formulae: **Fill in the displayed formula:**

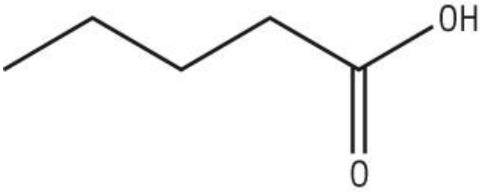


Butan-2-ol

Pentanoic acid:

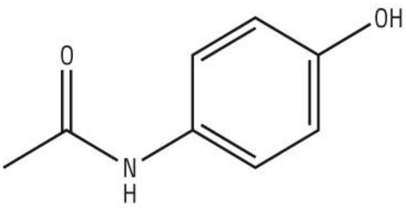
- **Coming off the final carbon is an =O and an -OH, these must be added to the end carbon:**

Skeletal formulae: **Fill in the displayed formula:**

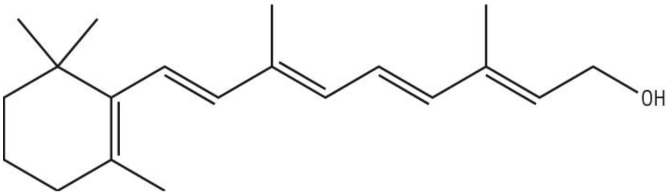


pentanoic acid

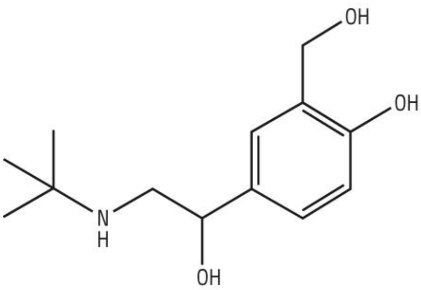
More complex AS / A2 structures:



Paracetamol



Retinol, vitamin A



Salbutamol

Salbutamol

Note:

- If a carbon in the skeletal structure is replaced with another element then we have to write the symbol of that element in its place

Questions: 1-4 P113

Isomerism

Structural isomers:

Activity 1:

- Use the molymods to make and draw as many molecules as possible using all of 5 carbons and 12 hydrogens, C_5H_{12}.
- There are 3 different shapes.
- All of the molecules above contain the same number of atoms but they are arranged differently. These are called structural isomers.
- This is one reason why we use a systematic method to name organic molecules.

Definition: These are compounds with the same molecular formula but with different structural arrangements of atoms

Activity 2:

- Using the molymods make and draw as many molecules as possible using 3 carbons, 8 hydrogens, and 1 oxygen, C_3H_8O.
- Some of these structures that you have made will be from different homologous groups / have different functional groups.
- This means that although they have the same empirical formula, they will have very different physical and chemical properties.

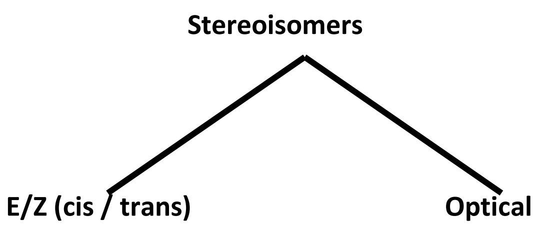
Steroeisomerism:

Activity 3:

- Build but-2-ene using the molymods.
- Look at your neighbours model, are they exactly the same?

Definition: The same atoms are joined to each other in different spatial arrangements

- There are 2 types of Stereoisomerism: E/Z and optical (optical is covered in A2):



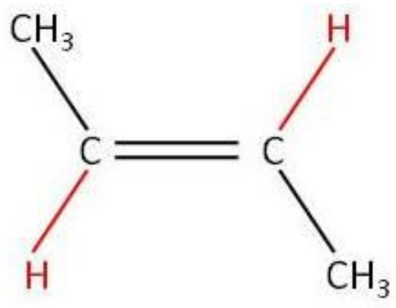
E/Z Isomerism: (of which cis / trans is one type)

- For this 2 things must be present in a molecule:

1) A carbon - carbon double bond, C=C
2) Each carbon must be attached to 2 different functional groups:

From GCSE: Cis / trans - But-2-ene:

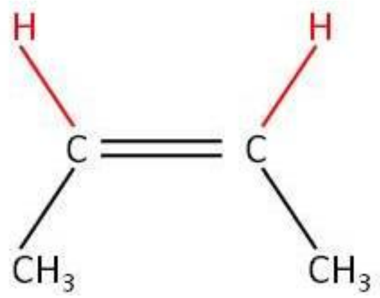
Cis trans is a specific type based upon having a hydrogen and a non hydrogen group on each of the carbons on the C=C:



Trans but-2-ene

(E-but-2-ene)

No free rotation around the C=C



Cis but-2-ene

(Z-but-2-ene)

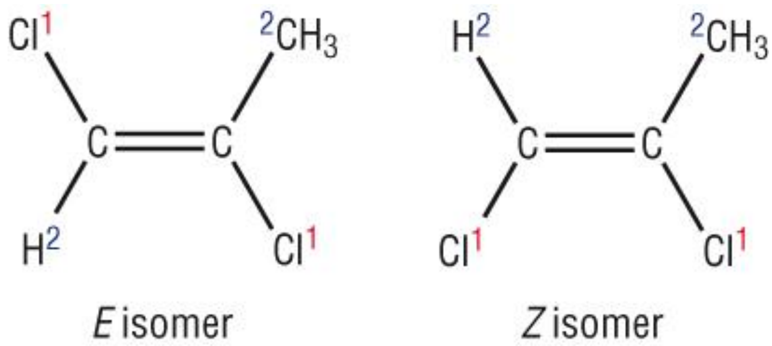
- The easiest way to spot which is which is to place a ruler along the C=C

If the hydrogen's are on different sides of the ruler = TRANS = ACROSS / Trans Atlantic (across Atlantic).

If the hydrogen's are on the same side of the ruler = CIS = SAME

Cahn - Ingold - Prelog nomenclature:

- Cis trans isomers are one specific type of stereoisomeism.
- Cis / trans isomers are when you have a hydrogen and another group on each of the carbon atoms.
- This is not always the case as some molecules may not fulfil this criteria:



- This molecule only has one hydrogen on one of the carbons so it does not fall into the Cis / trans category
- It can be solved by introducing a system where the priority is given based upon atomic number.
- Chlorine has the highest atomic number so it is given priority.
- Using you ruler apply the same principle as before:

If the chlorine's are on different sides of the ruler = E = 'ENTGEGEN' = OPPOSITE
If the chlorine's are on the same side of the ruler = Z = 'ZUSAMMEN' = TOGETHER

You will be expected to assign E/Z to molecules but not necessarily using CIP nomenclature
ET = across the molecule (ET flew 'across' the galaxy!!)

<u>Organic reagents and their reactions:</u>

Organic reactions

- **For a reaction to occur:**

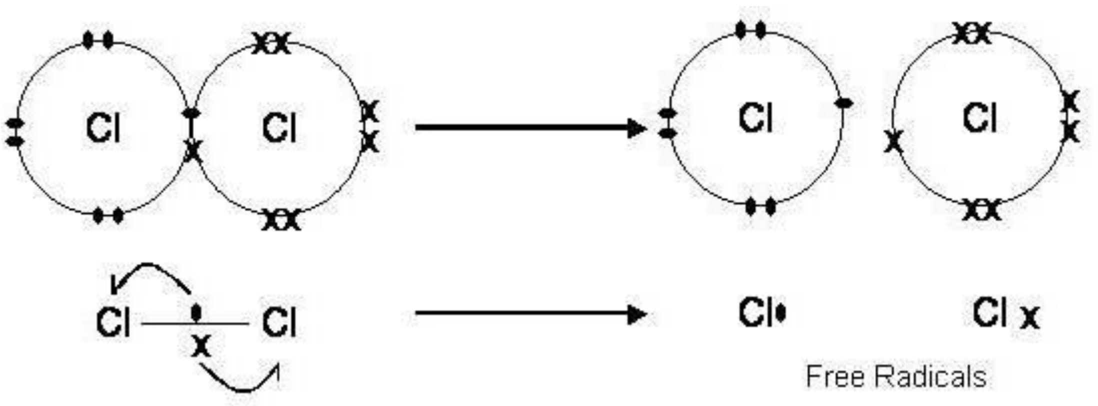
A) A bond must break.
B) The breaking of a bond will form a reagent.
C) The reaction must take place

A) Bond breaking:

- For an organic reaction to occur, a covalent bond must be broken.
- Bond breaking is called **fission** and it can be broken in one of 2 ways:

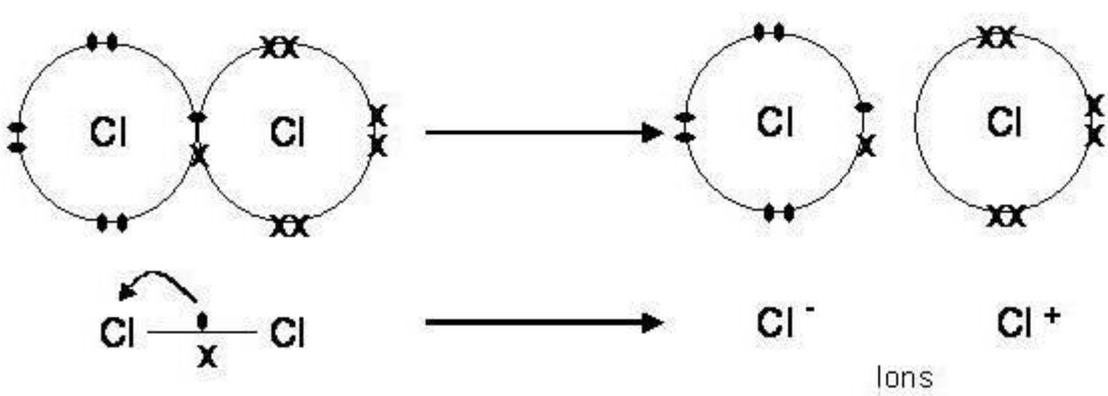
1) Homolytic fission
2) Heterolytic fission

1) Homolytic fission



- This is when the electrons in the bond go **'HOME'** to their parent atom. Each atom is the same. Homo….
- A half headed arrow represents the movement of 1 electron. This is because most reactions involve the movement of 2 electrons for which we use a normal headed arrow.
- **Free radicals** are atoms or groups of atoms with an unpaired electron, they are **extremely reactive** and are said to be **'short lived'**.

Heterolytic fission



- This is when the electrons in the bond go to one of the atoms.
- A double headed arrow represents the movement of 2 electrons, a pair of electrons.
- The 2 resulting ions have a different number of electrons.
- It gives a positive ion and a negative ion.
- These are different from each other = hetero...

B) Types of reactants:

- Reactants start a reaction going.
- There are 3 types of reactants:

1) Free radicals: these have an unpaired electron and are extremely reactive (as above)

2) Nucleophiles: these are attracted to electron deficient atom, δ+ and donate a pair of electrons to form a new covalent bond

- These are often negative ions but must have a lone pair of electrons as these are donated to form a new covalent bond.
- Br^-, OH^-, H_2O, NH_3

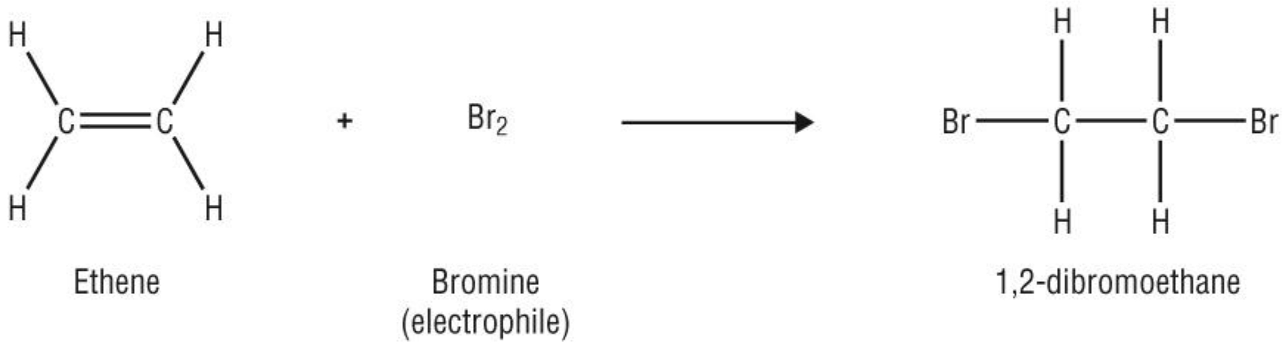
3) Electrophiles: these are attracted to electron rich atom, δ- and accept a pair of electrons to form a new covalent bond

- These are often positive ions.
- Br_2, HBr, NO_2^+

C) Types of reaction:

1) Addition reactions

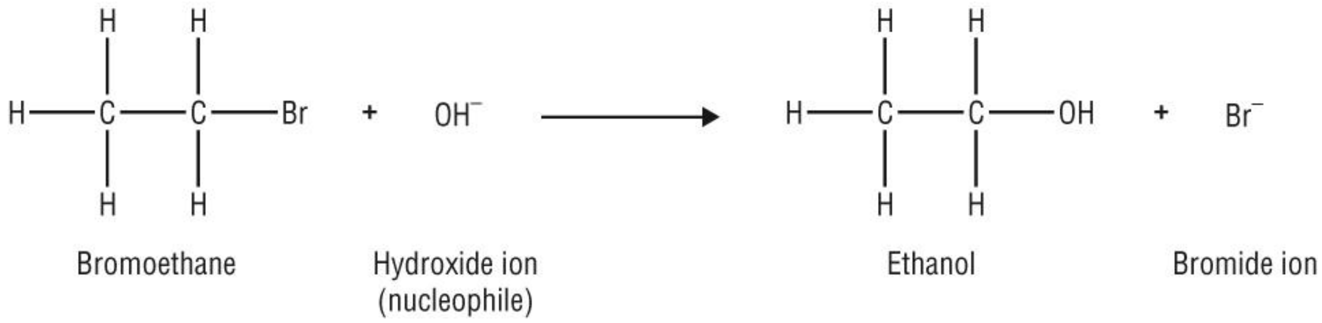
- Involves **2 molecules** joining to become **1 molecule**



- Bromine has been **added** to ethene.

2) Substitution reactions

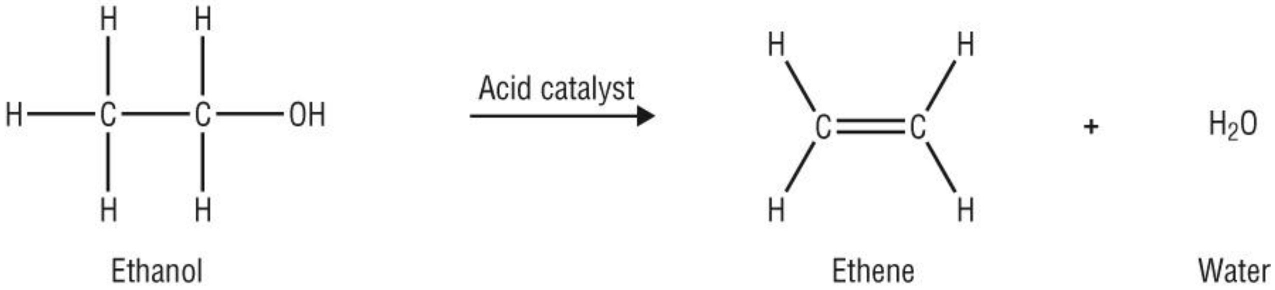
- Involves an atom (or group of atoms) being replaced by another atom (or group of atoms):
- **2 molecules** make **2 (new) molecules**



- You can see that the Br is being **substituted** by OH.

3) Elimination reactions

- Involves the removal of one molecule from another.
- **1 molecule** gives **2 molecules**:



- Water has been **eliminated** from ethanol