

CHM 101: GENERAL CHEMISTRY I

INTRODUCTION TO ORGANIC CHEMISTRY AND IUPAC NOMENCLATURE

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LECTURE : C19 - 1

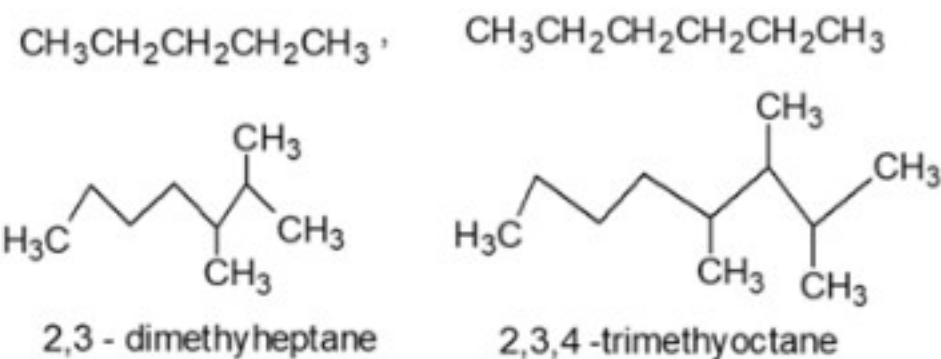
CHM 101

CHM 101 INTRODUCTION TO ORGANIC CHEMISTRY.

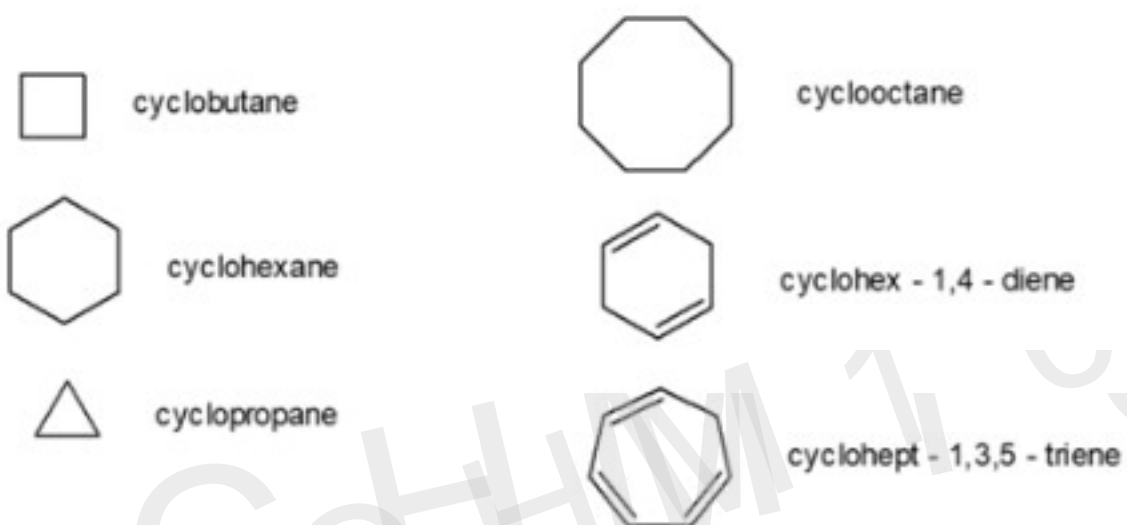
- Organic chemistry is the study of the structure, properties, composition, reactions, and preparation of carbon-containing compounds, which include not only hydrocarbons but also compounds with any number of other elements, including hydrogen (most compounds contain at least one carbon–hydrogen bond), nitrogen, oxygen. General Organic chemistry: Is a chemistry of carbon containing compounds
- Carbon has four valent electrons and it uses these four valent electrons to form covalent bonding with any incoming atom which is either hydrogen, oxygen, nitrogen even carbon itself, sulphur, chlorine fluorine etc.
- The simplest organic compound is CH_4 (methane gas) > It is colourless, found with crude oil or sometimes called Marsh gas during exploration of petroleum.
- CLASSIFICATION OF ORGANIC COMPOUNDS
- Organic compounds are classified into groups and subgroups according to the nature of the covalent bonds and the kind of atom present. I.e Saturated and unsaturated compounds. (single bond, double or triple bond).

CLASSES OF ORGANIC COMPOUNDS

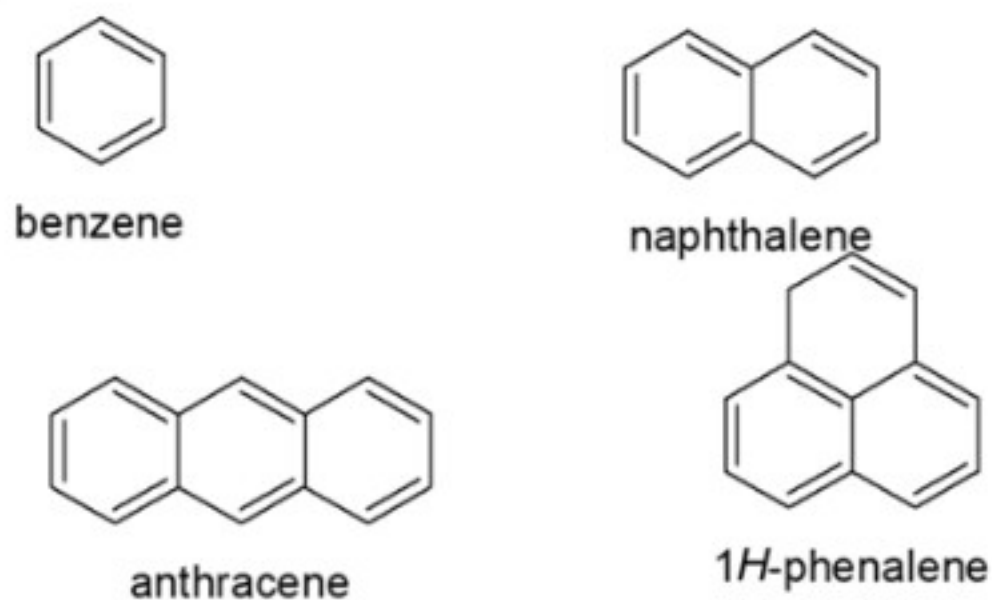
- Aliphatic compounds: Open chain (branched or unbranched) e.g. pentane, hexane, 2,3-dimethylheptane, 2,3,4-trimethyloctane



- Alicyclic Compounds: Compounds with closed ring of carbon atom. This ring may contain single or multiple bonds. Examples are:



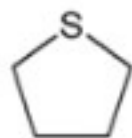
- Aromatic Compounds: Compounds containing at least one benzene ring . The pi electron in the p-orbitals are delocalized (alternating single and double ring) examples are



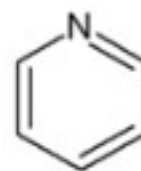
- Heterocyclic compounds: Compounds based on a closed ring made up carbon atom and one or more other elements. Example Furan



Furan



Thiophene



Pyridine

HOMOLOGOUS SERIES

This is a family of organic compound which follows a regular structural pattern in which each successive member differ in composition by CH_2 or molar mass – 14.

Examples are: Alkane - $\text{C}_n\text{H}_{2n+2}$ Alkene - C_nH_{2n} Alkyne - $\text{C}_n\text{H}_{2n-2}$
 Alkanol - $\text{C}_n\text{H}_{2n+1}\text{OH}$ etc.

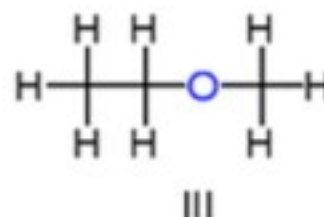
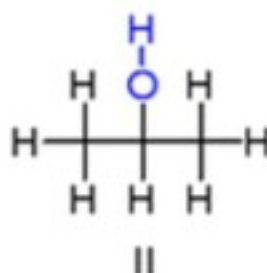
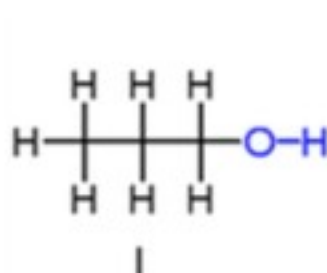
CHARACTERISTICS OF HOMOLOGOUS SERIES

- They differ in composition by CH_2 or 14 g/mol
- They are represented by a general formular
- They have similar method of preparation
- There are gradual changes in their physical properties as their carbon atom increases.
- They have identical methods of preparation.

ISOMERISM **Structural isomers** differ in terms of the connectivity of some or all constituent atoms.

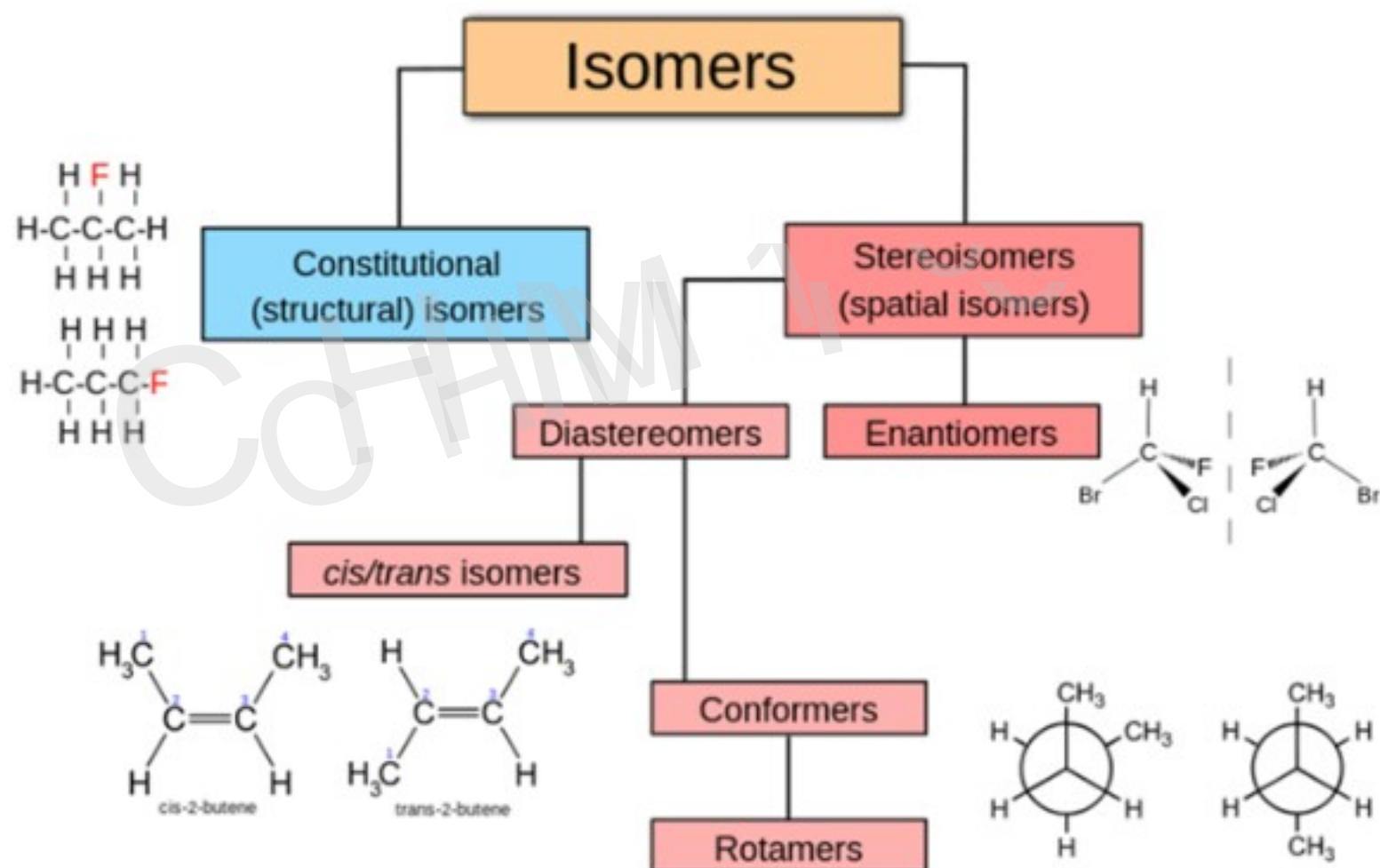
Example: propanols and methoxyethane

A simple example of isomerism is given by propanol: It has the formula $\text{C}_3\text{H}_8\text{O}$ (or $\text{C}_3\text{H}_7\text{OH}$) and occurs as two isomers: propan-1-ol (n-propyl alcohol; I) and propan-2-ol (isopropyl alcohol; II)

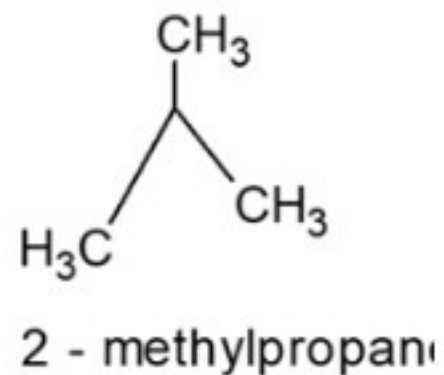
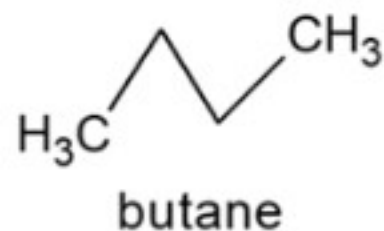


These two molecules are position isomers of each other, because the position of the hydroxyl group differs between the two: It is attached to an end carbon in the first isomer, and to the center carbon in the second.

Another isomer of C_3H_8O methoxyethane (ethyl-methyl-ether; **III**). Unlike the isomers of propanol, methoxyethane has an oxygen connected to two carbons rather than to one carbon and one hydrogen. Methoxyethane is an ether, not an alcohol, because it lacks a hydroxyl group, and it has chemical properties more similar to other ethers than to either of the above alcohol isomers.

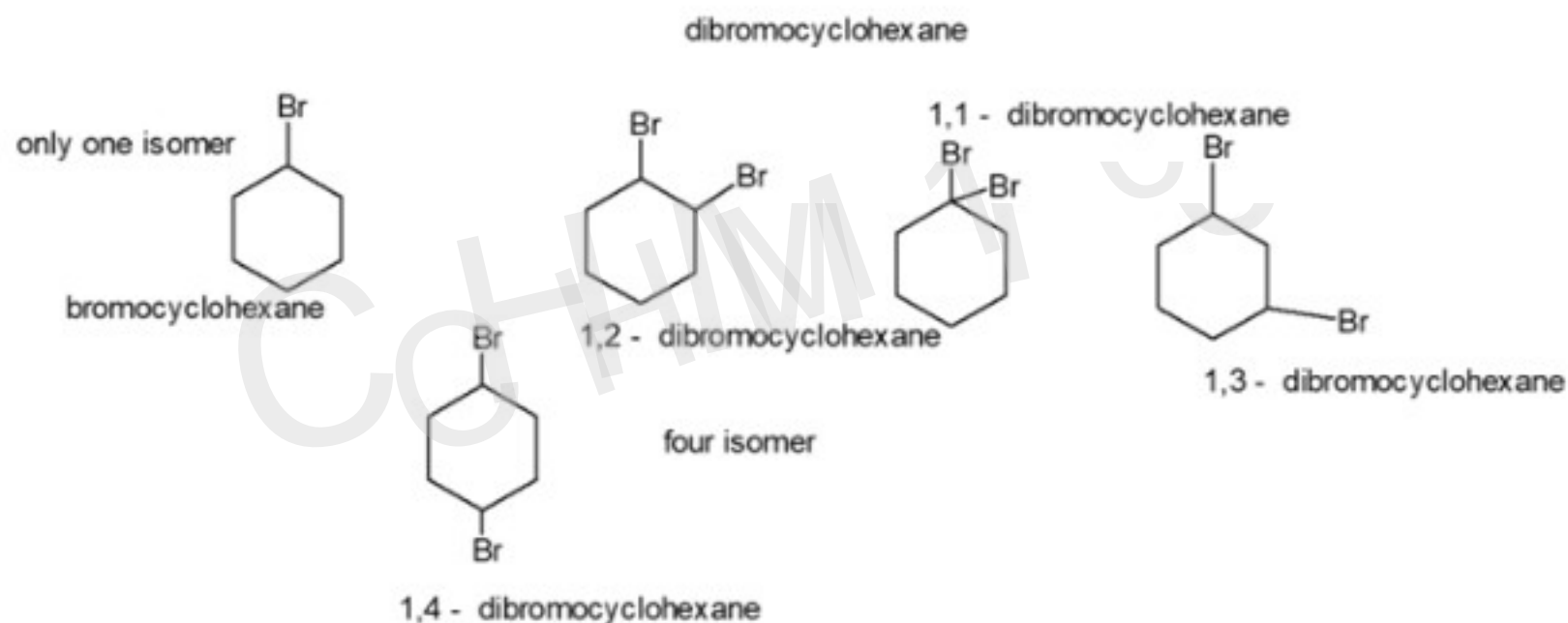


What are the possible isomer of C_4H_{10}



Exercise Try the possible isomer of C_5H_{12}

CYCLIC COMPOUNDS



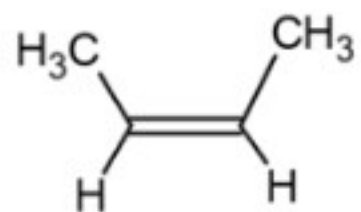
ISOMERISM: Can be divided into 2 groups which are (i) Structural isomerism (ii) Stereo Isomerism

However, the structural isomerism can be subdivided into

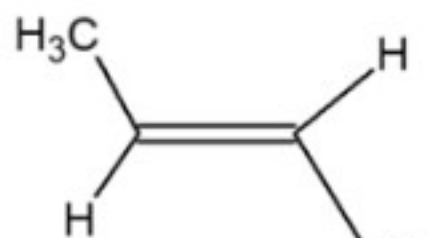
a). Positional Isomerism b). Functional group isomerism c) Chain-cycle isomerism d) Tautomerism

Stereoisomerism : (i) Geometric isomerism i.e. Cis and Trans configuration

(ii) optical isomerism.



Cis but - 2 - ene



Trans but - 2 - ene

Optical Isomerism : this has a set of isomers which are called ENANTIOMERS and DIASTEREOMERS

When a carbon in a compound has four different groups attached to it, such a compound is said to be ASSYMETRICAL.

ENANTIOMERS Are nonsuperposable mirror images. I.e when all the four sides of the objects or group attached to centre carbon atom can not coincide with its mirror image.

DIASTEREOMERS: Are superposable mirror images. i.e. when all the four sides of the objects or group of atoms attached to the centre carbon atom coincide with its mirror image.

Substances having a asymmetric carbon atom are said to be CHIRAL COMPOUND and are Non-superposable mirror image. That is one of the isomer will rotate the plane polarized light to right == DEXTROROTATORY (+). If it rotates the plane polarized light to the left, it is called LAEVOROTATORY (-).

FACTORS AFFECTING ORGANIC REACTIONS

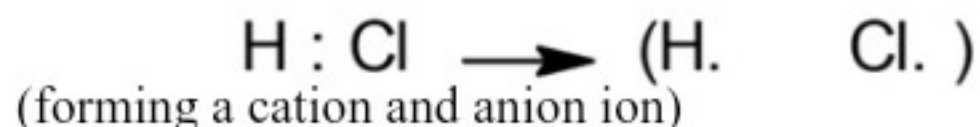
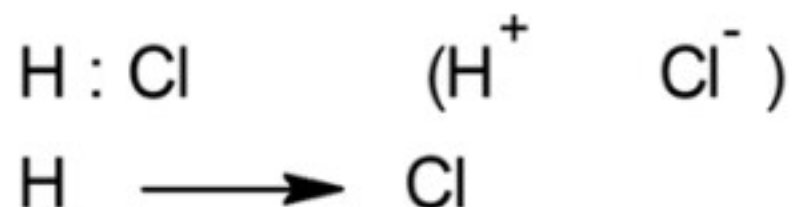
• Bonds and Polarisation (ii) Inductive effect (iii) Electromeric effect (iv) Mesomeric and Resonance effect (v) Steric effect (vi) Bond – breaking during reactions (vii) Types of bonds in organic chemistry.

BOND DISSOCIATION

In an organic molecule, there is bond formation and bond breaking (cleavage). When bonds are formed, there is release of energy (Exothermic) while energy is absorbed when bonds are broken (Endothermic).

Two ways to cleavage of bonds

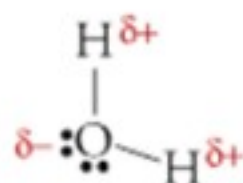
- Heterolytic cleavage: The electronegative atom carries all the electrons with it.



- Homolytic Cleavage: The two electrons that form the bond are shared by each atom to form a radical

BOND POLARITY

When a bond is formed between two atoms of different electronegative atom, the bond is said to be polar. That is the two electrons that make up the bond are not shared equally between the two atoms. The electron spend most of its time in the vicinity of the most electronegative atom. The electronegative atom is assigned relatively negative, other end = relatively positive



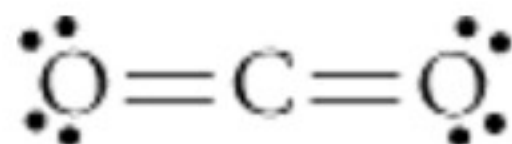
EXAMPLE – Predicting Molecular Polarity:

Decide whether the molecules represented by the following formulas are polar or nonpolar. (You may need to draw Lewis structures and geometric sketches to do so.)

a. CO_2 b. OF_2 c. CCl_4 d. CH_2Cl_2 e. HCN

Solution:

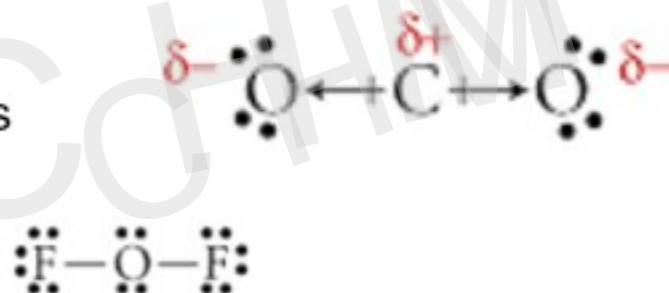
a. The Lewis structure for CO_2 is



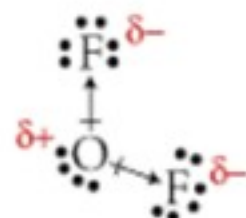
The electronegativities of carbon and oxygen are 2.55 and 3.44. The 0.89 difference in electronegativity indicates that the C-O bonds are polar, but the symmetrical arrangement of these bonds makes the molecule nonpolar.

If we put arrows into the geometric sketch for CO_2 , we see that they exactly balance each other, in both direction and magnitude. This shows the symmetry of the bonds.

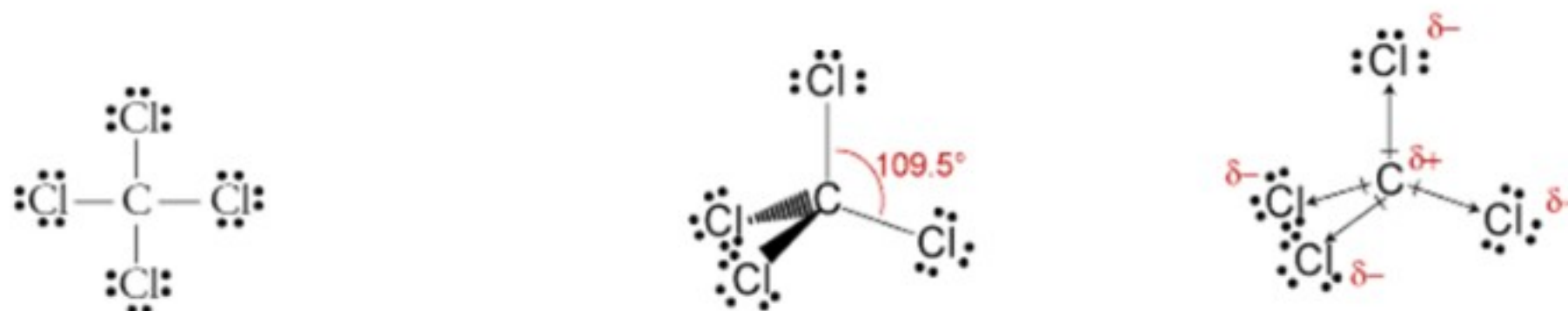
b. The Lewis structure for OF_2 is



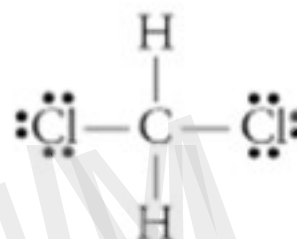
The electronegativities of oxygen and fluorine, 3.44 and 3.98, respectively, produce a 0.54 difference that leads us to predict that the O-F bonds are polar. The molecular geometry of OF_2 is bent. Such an asymmetrical distribution of polar bonds would produce a polar molecule.



c. The molecular geometry of CCl_4 is tetrahedral. Even though the C-Cl bonds are polar, their symmetrical arrangement makes the molecule nonpolar.



d. The Lewis structure for CH_2Cl_2 is



The electronegativities of hydrogen, carbon, and chlorine are 2.20, 2.55, and 3.16. The 0.35 difference in electronegativity for the H-C bonds tells us that they are essentially nonpolar. The 0.61 difference in electronegativity for the C-Cl bonds shows that they are polar. The following geometric sketches show that the polar bonds are asymmetrically arranged, so the molecule is polar. (Notice that the Lewis structure above incorrectly suggests that the bonds are symmetrically arranged. Keep in mind that Lewis structures often give a false impression of the geometry of the molecules they represent.)



e. The Lewis structure and geometric sketch for HCN are the same:



The electronegativities of hydrogen, carbon, and nitrogen are 2.20, 2.55, and 3.04. The 0.35 difference in electronegativity for the H-C bond shows that it is essentially nonpolar. The 0.49 difference in electronegativity for the C-N bond tells us that it is polar. Molecules with one polar bond are always polar.

How to name organic compounds using the IUPAC rules

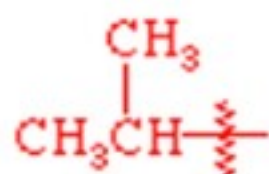
In order to name organic compounds you must first memorize a few basic names. These names are listed within the discussion of naming alkanes. In general, the base part of the name reflects the **number** of carbons in what you have assigned to be the **parent chain**. The **suffix** of the name reflects the type(s) of functional group(s) present on (or within) the parent chain. Other groups which are attached to the parent chain are called **substituents**.

Alkanes - saturated hydrocarbons

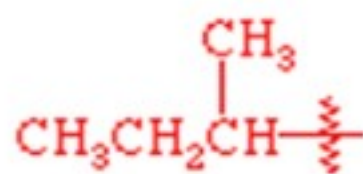
The names of the straight chain saturated hydrocarbons for up to a 12 carbon chain are shown below. The names of the substituents formed by the removal of one hydrogen from the end of the chain is obtained by changing the suffix **-ane** to **-yl**.

Number of Carbons	Name
1	methane
2	ethane
3	propane
4	butane
5	pentane
6	hexane
7	heptane
8	octane
9	nonane
10	decane
11	undecane
12	dodecane

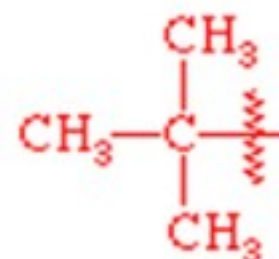
There are a few common branched substituents which you should memorize. These are shown below.



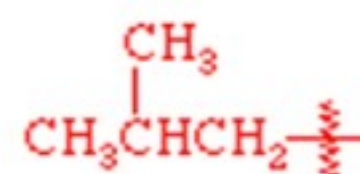
isopropyl



sec-butyl



tert-butyl



isobutyl



Here is a simple list of rules to follow.

1. Identify the longest carbon chain. This chain is called the parent chain.
2. Identify all of the substituents (groups appending from the parent chain).
3. Number the carbons of the parent chain from the end that gives the substituents the lowest numbers. When comparing a series of numbers, the series that is the "lowest" is the one which contains the lowest number at the occasion of the first difference. If two or more side chains are in equivalent positions, assign the lowest number to the one which will come first in the name.
4. If the same substituent occurs more than once, the location of each point on which the substituent occurs is given. In addition, the number of times the substituent group occurs is indicated by a prefix (di, tri, tetra, etc.).

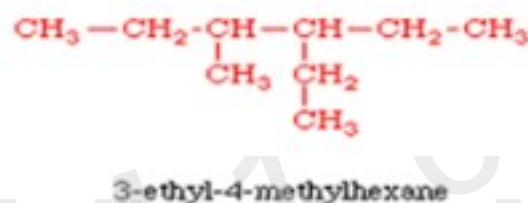
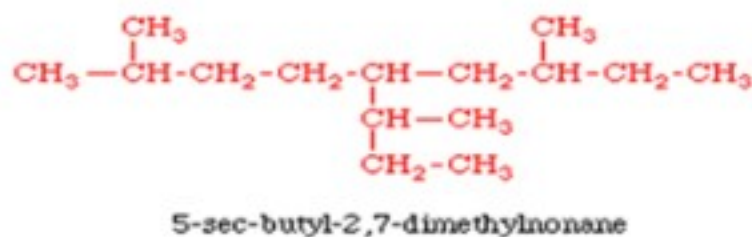
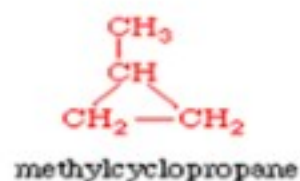
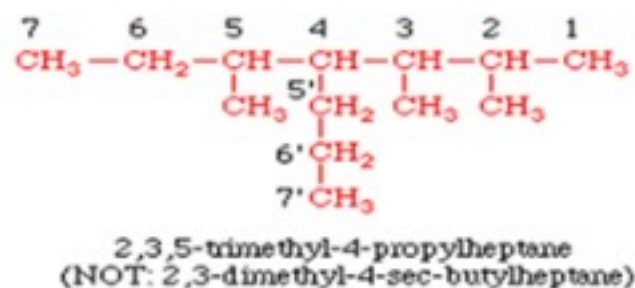
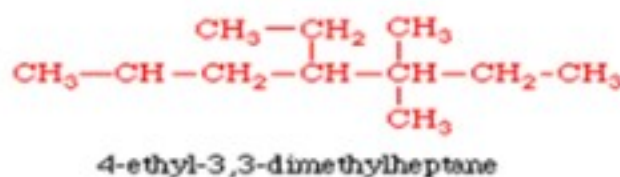
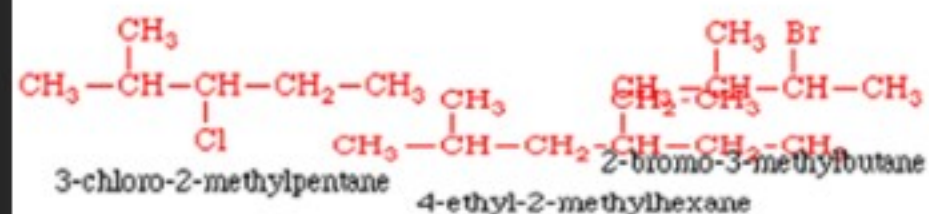
5. If there are two or more different substituents they are listed in alphabetical order using the base name (ignore the prefixes). The only prefix which **is** used when putting the substituents in alphabetical order is **iso** as in isopropyl or isobutyl. The prefixes sec- and tert- are not used in determining alphabetical order except when compared with each other.

6. If chains of equal length are competing for selection as the parent chain, then the choice goes in series to: a) the chain which has the greatest number of side chains. b) the chain whose substituents have the lowest- numbers. c) the chain having the greatest number of carbon atoms in the smaller side chain. d) the chain having the least branched side chains.

A cyclic (ring) hydrocarbon is designated by the prefix **cyclo-** which appears directly in front of the base name.

In summary, the name of the compound is written out with the substituents in alphabetical order followed by the base name (derived from the number of carbons in the parent chain). Commas are used between numbers and dashes are used between letters and numbers. There are **no** spaces in the name.

Here are some examples:



Alkyl halides

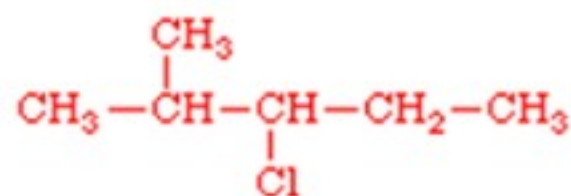
The halogen is treated as a substituent on an alkane chain. The halo- substituent is considered of equal rank with an alkyl substituent in the numbering of the parent chain. The halogens are represented as follows: F- fluoro, Cl - Chloro, Br – Bromo, I - iodo

Here are some examples:

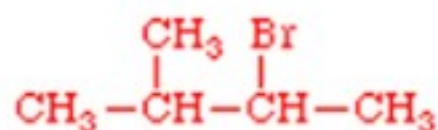
Alkyl halides

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Here are some examples:



3-chloro-2-methylpentane



2-bromo-3-methylbutane

- Alkenes and Alkynes - unsaturated hydrocarbons

Double bonds in hydrocarbons are indicated by replacing the suffix **-ane** with **-ene**. If there is more than one double bond, the suffix is expanded to include a prefix that indicates the number of double bonds present (**-adiene**, **-atriene**, etc.). Triple bonds are named in a similar way using the suffix **-yne**. The position of the multiple bond(s) within the parent chain is(are) indicated by placing the number(s) of the first carbon of the multiple bond(s) directly in front of the base name.

Here is an important list of rules to follow:

1. The parent chain is numbered so that the multiple bonds have the lowest numbers (double and triple bonds have priority over alkyl and halo substituents).
2. When both double and triple bonds are present, numbers as low as possible are given to double and triple bonds even though this may at times give "-yne" a lower number than "-ene". When there is a choice in numbering, the double bonds are given the lowest numbers.

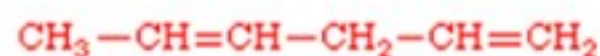
When both double and triple bonds are present, the -en suffix follows the parent chain directly and the -yne suffix follows the -en suffix (notice that the e is left off, -en instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the triple bond(s) is(are) indicated between the -en and -yne suffixes. See below for examples.

For a branched unsaturated acyclic hydrocarbon, the parent chain is the longest carbon chain that contains the **maximum number of double and triple bonds**. If there are two or more chains competing for selection as the parent chain (chain with the most multiple bonds), the choice goes to

(1) the chain with the greatest number of carbon atoms, (2) the # of carbon atoms being equal, the chain containing the maximum number of double bonds.

If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

Here are some examples:



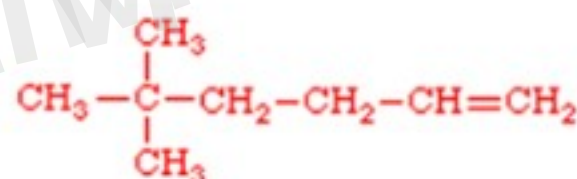
1,4-hexadiene



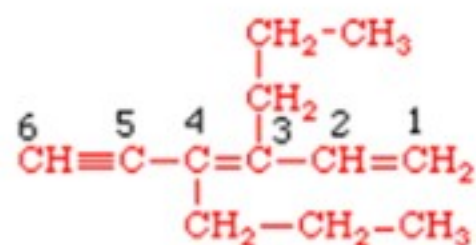
1,3-hexadien-5-yne



3-penten-1-yne



5,5-dimethyl-1-hexene



3,4-dipropyl-1,3-hexadien-5-yne



1,4,4-trimethylcyclobutene
(NOT: 2,3,3-trimethylcyclobutene)

Alcohols

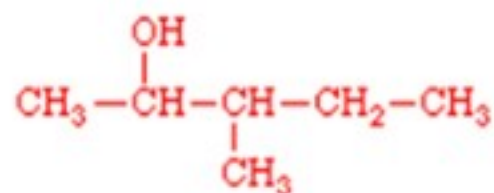
Alcohols are named by replacing the suffix **-ane** with **-anol**. If there is more than one hydroxyl group (-OH), the suffix is expanded to include a prefix that indicates the number of hydroxyl groups present (**-anediol**, **-anetriol**, etc.). The position of the hydroxyl group(s) on the parent chain is(are) indicated by placing the number(s) corresponding to the location(s) on the parent chain directly in front of the base name (same as alkenes).

Here is an important list of rules to follow:

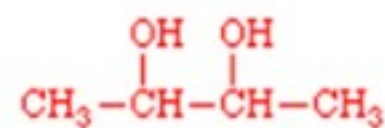
a. The hydroxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.

b. When both double bonds and hydroxyl groups are present, the **-en** suffix follows the parent chain directly and the **-ol** suffix follows the **-en** suffix (notice that the **e** is left off, **-en** instead of **-ene**). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the hydroxyl group(s) is(are) indicated between the **-en** and **-ol** suffixes. See below for examples. Again, the hydroxyl gets priority in the numbering of the parent chain.

c. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**. Here are some examples:



3-methyl-2-pentanol



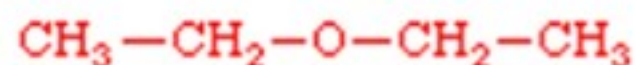
2,3-butanediol



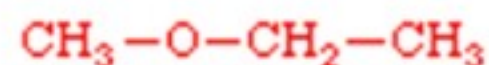
2-cyclopenten-1-ol

Ethers

You are only expected to know how to name ethers by their common names. The two alkyl groups attached to the oxygen are put in alphabetical order with spaces between the names and they are followed by the word ether. The prefix di- is used if both alkyl groups are the same. Here are some examples:



diethyl ether



ethyl methyl ether

Aldehydes

Aldehydes are named by replacing the suffix **-ane** with **-anal**. If there is more than one -CHO group, the suffix is expanded to include a prefix that indicates the number of -CHO groups present (**-anedial** - there should not be more than 2 of these groups on the parent chain as they must occur at the ends). It is not necessary to indicate the position of the -CHO group because this group will be at the end of the parent chain and its carbon is automatically assigned as C-1. Here is an important list of rules to follow:

- The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.
- When both double bonds and carbonyl groups are present, the -en suffix follows the parent chain directly and the -al suffix follows the -en suffix (notice that the e is left off, **-en** instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the -al suffix follows the -en suffix directly. Remember it is not necessary to specify the location of the carbonyl group because it will automatically be carbon #1. See below for examples. Again, the carbonyl gets priority in the numbering of the parent chain.

c. There are a couple of common names which are acceptable as IUPAC names. They are shown in the examples at the end of this list but at this point these names will not be accepted by the computer. Eventually they will be accepted.

d. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

Here are some examples:



propanal



3-methylbutanal



3-methyl-3-butenal



methanal

(common name: formaldehyde)



ethanal

(common name: acetaldehyde)



Benzaldehyde

Ketones

Ketones are named by replacing the suffix **-ane** with **-anone**. If there is more than one carbonyl group (C=O), the suffix is expanded to include a prefix that indicates the number of carbonyl groups present (**-anedione**, **-anetrione**, etc.). The position of the carbonyl group(s) on the parent chain is(are) indicated by placing the number(s) corresponding to the location(s) on the parent chain directly in front of the base name (same as alkenes).

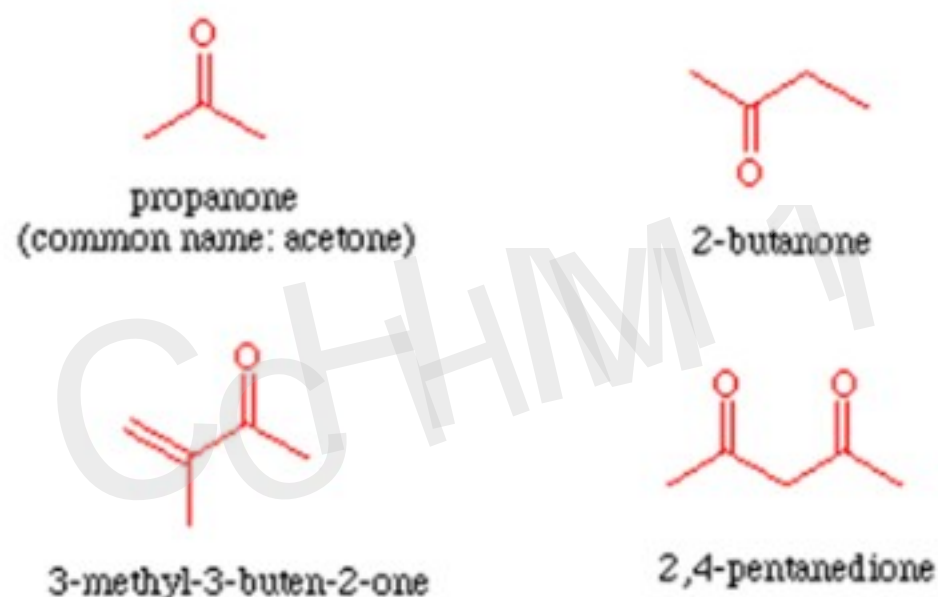
Here is an important list of rules to follow:

a. The carbonyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.

b. When both double bonds and carbonyl groups are present, the -en suffix follows the parent chain directly and the -one suffix follows the -en suffix (notice that the e is left off, **-en** instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the location of the carbonyl group(s) is(are) indicated between the -en and -one suffixes. See below for examples. Again, the carbonyl gets priority in the numbering of the parent chain.

- If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

Here are some examples:



Carboxylic Acids

Carboxylic acids are named by counting the number of carbons in the longest continuous chain including the carboxyl group and by replacing the suffix **-ane** of the corresponding alkane with **-anoic acid**. If there are two -COOH groups, the suffix is expanded to include a prefix that indicates the number of -COOH groups present (**-anedioic acid** - there should not be more than 2 of these groups on the parent chain as they must occur at the ends). It is not necessary to indicate the position of the -COOH group because this group will be at the end of the parent chain and its carbon is automatically assigned as C-1.

Here is an important list of rules to follow:

a. The carboxyl group takes precedence over alkyl groups and halogen substituents, as well as double bonds, in the numbering of the parent chain.

b. If the carboxyl group is attached to a ring the parent ring is named and the suffix -carboxylic acid is added.

c. When both double bonds and carboxyl groups are present, the -en suffix follows the parent chain directly and the -oic acid suffix follows the -en suffix (notice that the e is left off, **-en** instead of -ene). The location of the double bond(s) is(are) indicated before the parent name as before, and the -oic acid suffix follows the -en suffix directly. Remember it is not necessary to specify the location of the carboxyl group because it will automatically be carbon #1. See below for examples. Again, the carboxyl gets priority in the numbering of the parent chain.

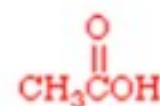
d. There are several common names which are acceptable as IUPAC names. They are shown in the examples at the end of this list **but** at this point these names will **not** be accepted by the computer. Eventually they will be accepted.

d. If there is a choice in numbering not previously covered, the parent chain is numbered to give the substituents the **lowest** number at the **first point of difference**.

Here are some examples:



methanoic acid
(common name: formic acid)



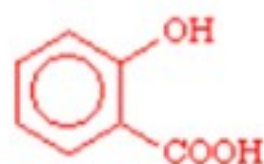
ethanoic acid
(common name: acetic acid)



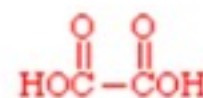
3-methylpentanoic acid



benzoic acid



salicylic acid
(common name)



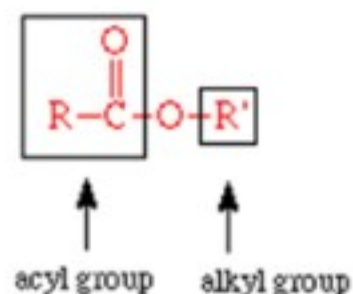
ethanedioic acid
(common name: oxalic acid)



3-butenic acid

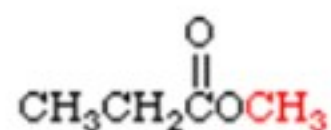
Esters

Systematic names of esters are based on the name of the corresponding carboxylic acid. Remember esters look like this:

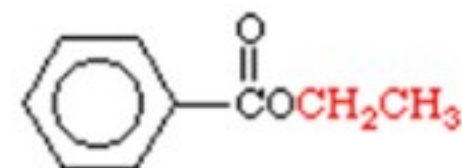


The alkyl group is named like a substituent using the **-yl** ending. This is followed by a space. The acyl portion of the name (what is left over) is named by replacing the **-ic acid** suffix of the corresponding carboxylic acid with **-ate**.

Here are some examples:



methyl propanoate



ethyl benzoate



tert-butyl acetate

Amines

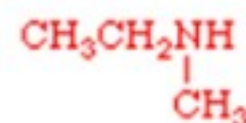
They are named like ethers, the alkyl (R) groups attached to the nitrogen are put in alphabetical order with no spaces between the names and these are followed by the word amine. The prefixes di- and tri- are used if two or three of the alkyl groups are the same.

NOTE: Some books put spaces between the parts of the name, but we will not. Follow the examples.

Here are some examples:



dimethylamine



ethylmethanamine

Summary of functional groups

FORMULA	FUNCTIONAL GROUP	PREFIX	SUFFIX
C_nH_{2n+2}	Alkane	None	ane
C_nH_{2n}	Alkene	None	ene
C_nH_{2n-2}	Alkyne	None	yne
$C_nH_{2n+1}OH$ (ROH)	ROH Primary alcohol	Hydroxyl	-ol
RCHO	Aldehyde	None	-al
RCOR'	Ketone	None	-one
$C_nH_{2n+1}COOH$ (RCOOH)	Carboxylic acids	None	-oic acid
RNH_2	Primary amine	Amino	amine
R_2NH	Secondary amine	None	none
$R_3N:$	Tertiary amine	None	none
ROR'	Ethers	Alkoxy-	-ether
RCOOR'	Ester	None	-ate
CONH ₂	Amide	None	-amide
RCOXY, X = F, Cl, Br, I	Acid halide	None	-acid

TYPES OF ORGANIC REACTIONS

It involves breakage of bond and formation of new ones. The main types of reactions include:

Substitution reactions (ii) Addition reactions (iii) Elimination reactions

SUBSTITUTION REACTION: In this kind, atoms or groups of atom are being replaced by another atom or group of atoms in the reactant molecule.



ADDITION REACTION: This involves combination of two molecules to yield a single molecule. This reaction is for unsaturated compounds ($C=C$) or ($C\equiv C$).



ELIMINATION REACTION: This is a reverse of addition reaction.
Atoms or groups of atoms are removed from a molecule to produce multiple bonds.

