# BP202T. PHARMACEUTICAL ORGANIC CHEMISTRY –I (Theory)

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# UNIT-I

## UNIT-I 07 Hours

## Classification, Nomenclature and Isomerism

- Classification of Organic Compounds
- Common and IUPAC systems of nomenclature of organic compounds (up to 10 Carbons open chain and carbocyclic compounds)

# PART 1

## Organic Compounds:

Organic chemistry is defined as the study of carbon compounds and its classified as;

## Classification of Organic Compounds:

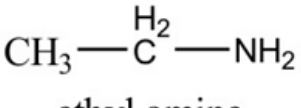
1. Aliphatic compounds:
   - ✓ ethane
   - ✓ ethy alcohol,
   - ✓ n-butyl amine
2. Saturated and unsaturated compound :
   - ✓ Ethane – saturated
   - ✓ Ethylene – Unsaturated
   - ✓ Acetylene- Unsaturated
3. Aromatic compounds:
   - ✓ Benzene
   - ✓ Aniline
   - ✓ Napthalene
4. Alicycliccompounds:
   - ✓ Cyclobutane
   - ✓ cyclopropane
5. Heterocyclic compound:
   - ✓ Pyrrole,
   - ✓ Pyridine
   - ✓ Quinoline

### 1. Aliphatic compounds:

The compound which contains open chain of carbon atoms are called aliphatic compounds.

ethane

ethyl alcohol



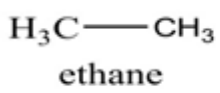
ethyl amine

### 2. Saturated compound :

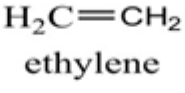
The compound which contains carbon carbon single bond are known are Saturated compound.

**3Unsaturated compound :**

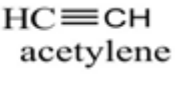
The compound which contains carbon carbon double or triple bond are known are unsaturated compound.



ethane



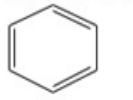
ethylene

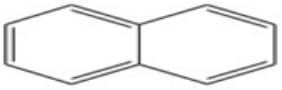


acetylene

**4.Aromatic compounds**:

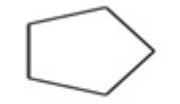
The compound which that have structures and chemical properties resembling with benzene are called as aromatic compound.

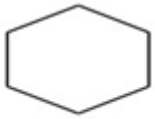

benzene


naphthalene

6. **Alicyclic compounds:**

   Cyclic compound conatins only carbon carbon atom are called as alicyclic compounds

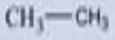
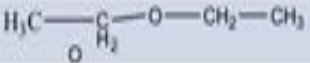
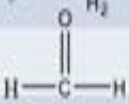
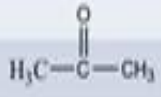

cyclopentane


cyclohexane

7. **Heterocyclic compound :**

   Cyclic compound which contain carbon and hetero atom known as Heterocyclic compound.

**Functional groups:** Functional group is the reactive part of an organic molecule

| Sr. No | Class of compounds | example | structure |
|---|---|---|---|
| 1. | Alkane | Ethane |  |
| 2. | Alkene | Ethylene |  |
| 3. | Alkyne | Acetylene |  |
| 4 | Alcohol | Ethyl alcohol |  |
| 5 | Ether | Diethyl ether |  |
| 6 | Aldehyde | formaldehyde |  |
| 7 | Ketone | acetone |  |
| 9 | Carboxylic acid | Acetic acid | $CH_3COOH$ |
| 10 | Ester | Mthyl acetate | $CH_3COOCH_3$ |
| 11 | Amine | Ethyl amine | $CH_3CH_2NH_2$ |
| 12 | Nitro compounds | Nitro methane | $CH_3NO_2$ |
| 13 | Alkyl Halide | Methyl chloride | $CH_3Cl$ |
| 14 | Amide | Formamide | HCONH2 |
| 15 | Thiol | Ethanethiol | $CH_3CH_2SH$ |

## Common and IUPAC systems of nomenclature of organic compounds (up to 10 Carbons open chain and carbocyclic compounds)

### Alkanes

Alkanes are aliphatic hydrocarbons having C—C and C— H σ bonds. They can be categorized as acyclic or cyclic.

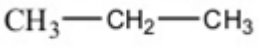
Acyclic alkanes have the molecular formula CnH2n+2 (where n = an integer) and contain only linear and branched chains of carbon atoms. They are also

called saturated hydrocarbons because they have the maximum number of hydrogen atoms per carbon.

Cycloalkanes contain carbons joined in one or more rings. Because their general formula is CnH2n, they have two fewer H atoms than an acyclic alkane with the same number of carbons.

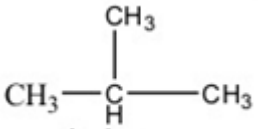
**Nomenclature of alkanes:**

- ✓ The first four member of the series are called by their names i.e, methane, ethane, propane , butane and higher alkanes are derived from the greek prefixes that indicates the carbon atom in the molecule .
- ✓ Eg: pentane has 5 carbon atom
- ✓ The prefix n- is used for those alkanes in which all carbons are in one continuous chain



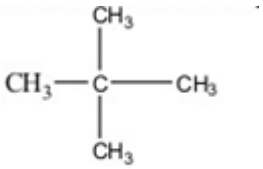
n-propane

- ✓ Prefix iso is used for those alkanes which have a methyl group attached to second last carbon atom of continuous chain.



isobutane

- ✓ Prefix neo is used for those alkanes which have two methyl groups attached to the second last carbon atom



neo pentane

- ✓ Alkyl group is formed by removing one hydrogen from an alkane. The suffix of this group is –yl
- ✓ Non alkyl groups: F-Fluro, Cl- Chloro, Br- Bromo, I- Iodo, NO2- Nitro, NH2- Amino, OH- Hydroxy.

**Parent alkanes**

| Sr.No | Name | structure |
|---|---|---|
| 1 | Methane | $CH_4$ |
| 2 | Ethane | $CH_3$-$CH_3$ |
| 3 | Propane | $CH_3$-$CH_2$-$CH_3$ |
| 4 | Butane | $CH_3$-$CH_2$-$CH_2$-$CH_3$ |
| 5 | Pentane | $CH_3$-$CH_2$-$CH_2$-$CH_2$-$CH_3$ |
| 6 | Hexane | $CH_3$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_3$ |
| 7 | Heptane | $CH_3$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_3$ |
| 8 | Octane | $CH_3$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_3$ |
| 9 | Nonane | $CH_3$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_3$ |
| 10 | Decane | $CH_3$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_2$-$CH_3$ |

## IUPAC Nomenclature

| Sr. No | Functional group | Prefix | Suffix |
|---|---|---|---|
| 1 | Alkane | alkyl | -ane |
| 2 | Alkene | - | -ene |
| 3 | Alkyne | - | -yne |
| 4 | Carboxylic acid | carboxyl | -Oic acid |
| 5 | Acid Halide | -yl halide | -oyl halide |
| 6 | Acid Amide | -amide | -amide |
| 7 | Acid Anhydride | -ic anhydride | Oic anhydride |
| 8 | Ester | - | -ate |
| 9 | Aldehyde | -oxo | -al |
| 10 | Ketone | -oxo | -one |
| 11 | Alcohol | -hydroxy | -ol |
| 12 | Amine | -amino | -amine |
| 13 | -Cl, F, Br, I | Fluoro, Chloro, Bromo, iodo | - |
| 14 | NO2 | -Nitro | - |

**Rules for IUPAC nomenclature**

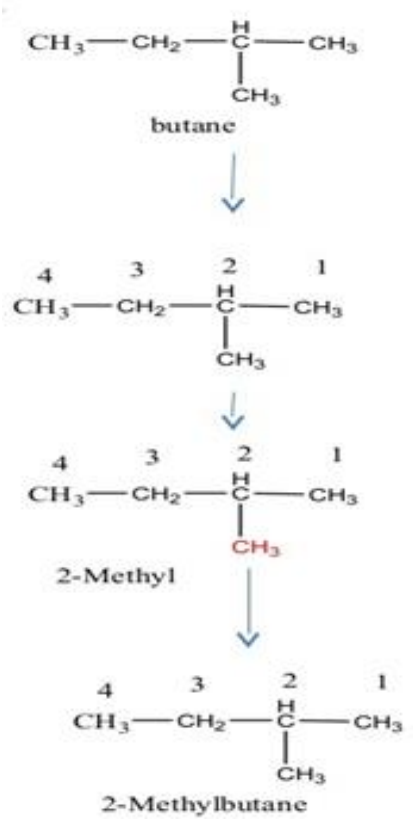
- ✓ Find the longest continuous carbon chain.
- ✓ Determine the root name for this parent chain.
- ✓ Number the chain in the direction such that the position number of the first substituent is the smaller number.
- ✓ If the first substituents from either end have the same number, then number so that the second substituent has the smaller number
- ✓ Determine the name and position number of each substituent.
- ✓ Indicate the number of identical groups by the prefixes di, tri, tetra, etc.
- ✓ Place the position numbers and names of the substituent groups, in alphabetical order, before the root name

**IUPAC Nomenclature of alkanes**

The steps for alkanes= Prefix------Parent--------Suffix.

***Rules for nomenclature of alkanes***

- ✓ Name the longest chain- the longest continuous carbon chain is chosen and given parent name.
- ✓ Number the longest chain- the carbon atoms in longest chain are numbered and numbering started from the end where substituent is attached
- ✓ Locate and name of substituent's- Each substituent is named and position of each substituent is indicated by number.
- ✓ Combine the longest chain and substituent's- The position and name of substituent are added to the name of the longest chain and written as one word.
- ✓ Indicate the number and position of substituent's- If the same substituent is present two or more time in the molecule at that time substituent is indicated by prefix di, tri, tetra, penta and location is indicated by separate numbers
- ✓ If two or more substituents are present, their names are alphabetized and added to the parent alkane

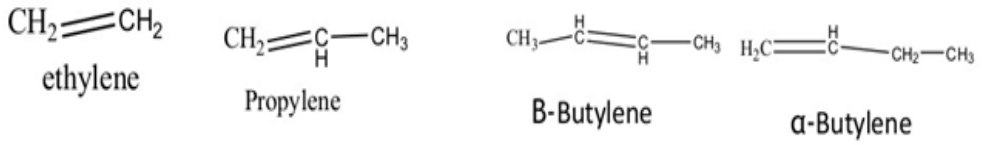



**Nomenclature of alkene**

**Common system-**

1. the common names of the first four members named by changing –ane to –ylene.

2. The Greek letters are used to distinguish isomers having double bond at the first and second carbon of the chain




**IUPAC Nomenclature alkene**

1. The IUPAC names of alkenes are derived from those of the corresponding alkanes by changing the ending –ane to –ene.

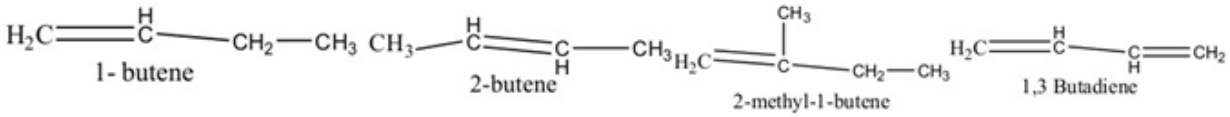
2. Select the longest continuous carbon chain that contains the double bond and use this as the parent compound.

3. Number this longest continuous chain so that the double bond has the lowest possible number.

4. To indicate the position of the carbon- carbon double bond, add the number of lower numbered carbon atom of carbon carbon double bond in front of the alkene name.

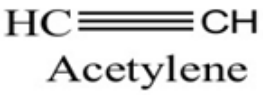
5. Side chain and substituents are named as usual and their position is indicated by number to show to which carbon atom they are attached.

6. When there are two or three double bonds in a molecule, the –ane is replaced by –adiene and –atriene.



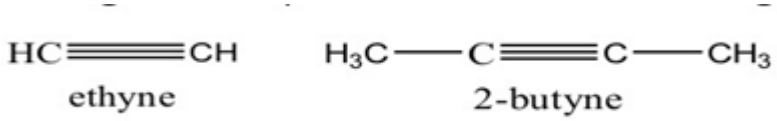

**Nomenclature of alkyne**

• **Common system:** acetylene is the common name of for the first member of the series.




• **Derived system:** Higher alkynes are regarded as alkyl derivatives of acetylene.

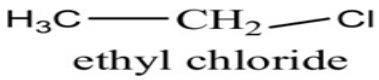

• **IUPAC Nomenclature:** The IUPAC names of alkynes are obtained by dropping the ending –ane of parent alkanes and adding the suffux –yne.



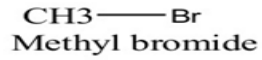

**Nomenclature for alkyl halide**

•Common system: in this system the alkyl group attached to the halogen atom is named first alkane and then chloride, fluoride and bromide will come.

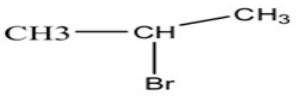
• Suffix for alkyl halides is –yl halide



ethyl chloride



Methyl bromide

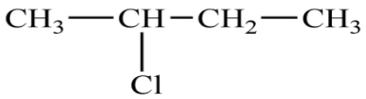


Isopropyl bromide

**Nomenclature for alkyl halide**

**IUPAC Nomenclature:**

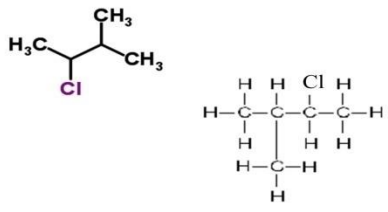
1. The longest continuous chain of carbon atoms is chosen as the parent. if parent chain has no branching alkyl group, the position of halogen atom is given by a number that corresponds to the carbon atom to which it is attached. The carbon chain is numbered so that the carbon atom bearing the halogen atom has the lowest number.



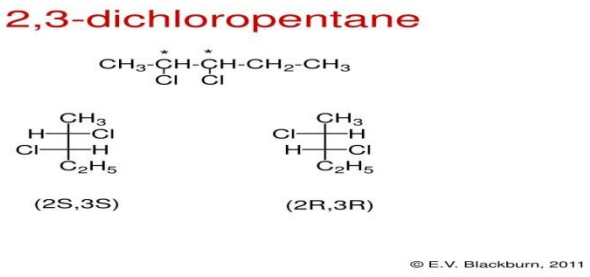
2-chlorobutane

2. If the parent chain has branching alkyl group, number the chain from the end near to first substituent. 3. If the compound contains two or more halogen atoms of the same type, they are indicated with prefixes di-, tri-, etc.

**2-chloro-3-methylbutane**




4. If the compound contains different substituent's, they are numbered according to their positions on the chain and listed in alphabetical order.




**Nomenclature of alcohol**

• **Common system:** In this system alcohols(R-OH) are named as alkyl alcohol.

**IUPAC Nomenclature :**

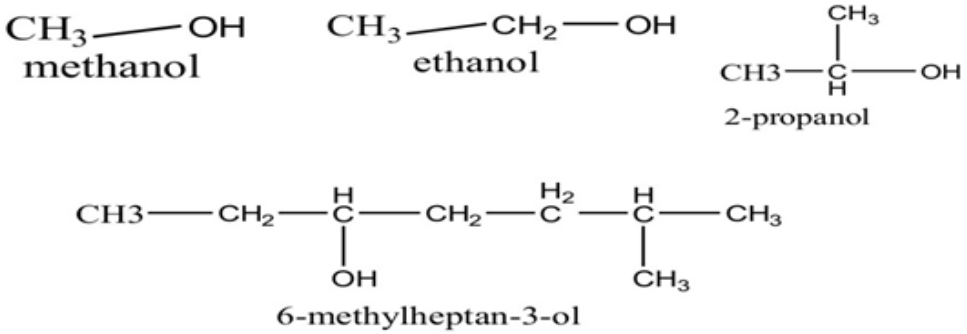
1. Select the longest continuous carbon chain containing the –OH group.

2. Change the name of the alkane corresponding to this chain by dropping the ending –e and adding suffix –ol.

3. Number the chain so as to give the carbon carrying the –OH group, the lowest possible number. The possition of -OH group is indicated by this number.

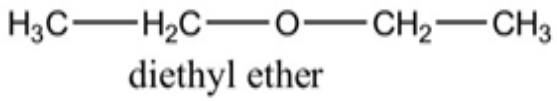
4. Indicate the positions of other substituents or multiple bonds by numbers.

5. When –OH is part of higher priority class of compound, it is named as hydroxy.




**Nomenclature of ethers**

- ✓ **Common system:** The two alkyl groups attached to oxygen are named in alphabetical order and word ether is added.
- ✓ If the two alkyl groups are same (R-O-R), the prefix di- is used.

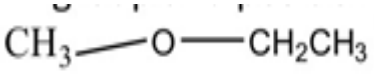



diethyl ether

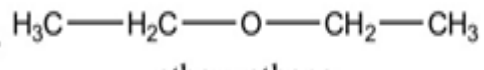

ethyl methyl ether

**IUPAC Nomenclature:**

- ✓ ethers are named as alkoxy alkanes.
- ✓ The larger alkyl group is considered to be alkanes or parent.
- ✓ The name of the alkane is prefixed by the name of alkoxy group and position number.




methoxyethane




ethoxyethane

**Nomenclature of oxiranes**

• **Common system:** usually they alkene epoxide because they are made from alkenes

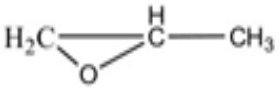

ethylene oxide
(epoxy ethane)


Propylene oxide
(epoxy propane)

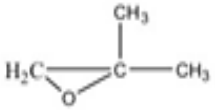
. • **IUPAC Nomenclature:**

In this system ethylene oxide is called as oxirane and epoxides are named as substituted oxiranes


oxirane




2-methyloxirane

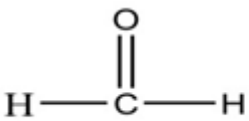


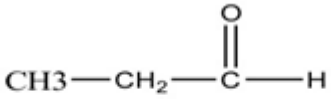

2,2-dimethyloxirane

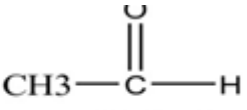
**Nomenclature of aldehyde**

- ✓ Common system: The name of simple aldehydes are derived from the common names of corresponding carboxylic acid.

- ✓ The characteristic –ic acid ending in the common name of carboxylic acid is dropped and replaced by- aldehyde.
- ✓ E.g. one carbon carboxylic acid is formic acid, so the name of the corresponding aldehyde is formaldehyde.


formaldehyde


propionaldehyde


acetaldehyde

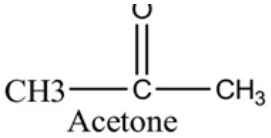
**IUPAC Nomenclature of aldehyde**

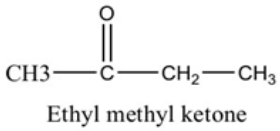
- ✓ The IUPAC system of naming aldehyde uses the parent alkane name corresponds to the longest continuous chain containing the aldehyde group.
- ✓ The final –e of alkane name is dropped and replaced by-al.
- ✓ The numbering of longest continuous chain starts with C-1 as the carbon bearing the aldehyde group. 4. The substituents are indicated by name and position number.

**Nomenclature of ketone**

**Common system:**

- ✓ ketones are named as dialkyl ketones.
- ✓ First member of the series CH3COCH3 is, however, popularly called acetone.
- ✓ The common names of unsymmetrical ketones are obtained by naming the alkyl groups as separate words in alphabetic order and adding the third word 'ketone'

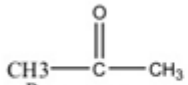

Acetone

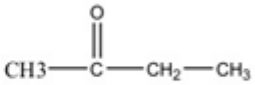

Ethyl methyl ketone

**Nomenclature of ketone**

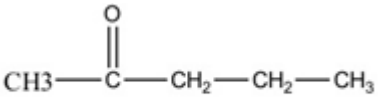
**IUPAC Nomenclature:**

- ✓ The IUPAC name of ketones is alkanones and the name of an individual member on the system is derived by dropping the final 'e' of the parent hydrocarbon and adding the suffix one‘.


Propanone


Butanone

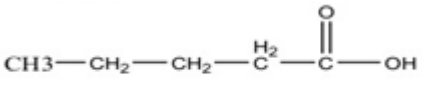
- ✓ While naming higher ketones on IUPAC system, it becomes necessary to assign positional number to the carbonyl group.

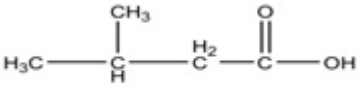

2-pentanone

**Nomenclature of carboxylic acid**

**• Common system:**

The longest carbon chain containing the carboxylic group is selected and the carboxylic acid is named by replacing the 'e' of the corresponding alkane by '-ic acid'.

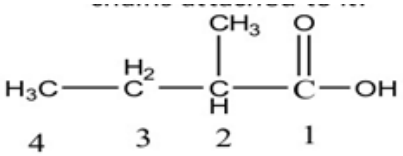

Valeric acid

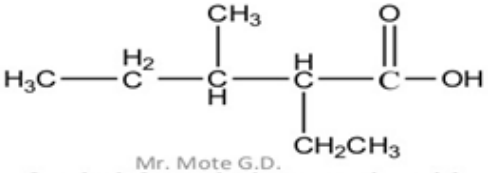

isovaleric acid

**IUPAC Nomenclature:**

The longest carbon chain containing the carboxylic group is selected and the carboxylic acid is named by replacing the 'e' of the corresponding alkane by '-oic acid'.

The selected carbon chain is numbered I, 2, 3, 4 etc to indicate the position of the side- chains attached to it.


2-methyl butanoic acid


2-ethyl-3-methylpentanoic acid

| Sr. No | Common Name | structure | IUPAC name |
|---|---|---|---|
| 1 | Formic acid | HCOOH | Methanoic acid |
| 2 | Acetic acid | $CH_3COOH$ | Ethanoic acid |
| 3 | Propionic acid | $CH_3CH_2COOH$ | Propanoic acid |
| 4 | Butyric acid | $CH_3CH_2CH_2COOH$ | Butanoic acid |
| 5 | Valeric acid | $CH_3CH_2CH_2CH_2COOH$ | Pentanoic acid |
| 6 | Caproic acid | $CH_3CH_2CH_2CH_2CH_2COOH$ | Hexanoic acid |

**Nomenclature of Acid halides, anhydrides, Acid amide and ester**

| Sr. No | Common Name | structure | IUPAC name |
|---|---|---|---|
| 1 | Formyl chloride | HCOCl | Methanoyl chloride |
| 2 | Acetyl chloride | $CH_3COCl$ | Ethanoyl chloride |
| 3 | Acetic anhydride | $CH_3CO\text{-}O\text{-}COCH_3$ | Ethanoic anhydride |
| 4 | Propionic anhydride | $CH_3CH_2CO\text{-}O\text{-}COCH_2CH_3$ | Propanoic anhydride |
| 5 | Formamide | $HCONH_2$ | Methanamide |
| 6 | Acetamide | $CH_3CONH_2$ | ethanamide |
| 7 | Ethyl acetate | $CH_3COOCH_2CH_3$ | Ethyl ethanoate |
| 8 | Ethyl propionate | $CH_3CH_2COOCH_2CH_3$ | Ethyl propanate |

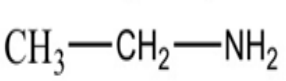
## Nomenclature of amine

**Common system:**

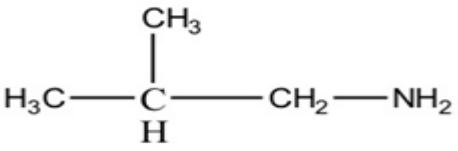
The longest carbon chain containing the amine group is selected and the amine is named by replacing the 'e' of the corresponding alkane by '-alkylamine'. .

**IUPAC Nomenclature:**

- ✓ The longest carbon chain containing the amine group is selected and the amine is named by replacing the 'e' of the corresponding alkane by '-amine
- ✓ The selected carbon chain is numbered I, 2, 3, 4 etc to indicate the position of the side-chains attached to it.



ethyl amine



iso butyl amine

**Rules for IUPAC nomenclature for polyfunctional group**

1. In naming molecules containing one or more of the functional groups in Group A, the group of highest priority is indicated by suffix; the others are indicated by prefix, with priority equivalent to any other substituents.

2. Priority of function group: Carboxylic acid> ester> acyl halide>amide>aldehyde>ketone>alcohol>amine>alkene>alkyne>alkane>ether> alkyl halide>nitro alkane

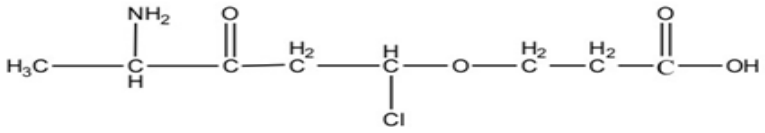
3. Find the highest priority functional group. Determine and name the longest continuous carbon chain that includes this group.

4. Number the chain so that the highest priority functional group is assigned the parent chain

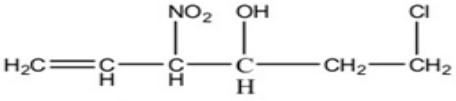
5. If the carbon chain includes multiple bonds (Group B), replace “ane” with “ene” for an alkene or “yne” for an alkyne. Designate the position of the multiple bond with the number of the first carbon of the multiple bond.

6. If the molecule includes Group A functional groups, replace the last “e” with the suffix of the highest priority functional group, and include its position number.

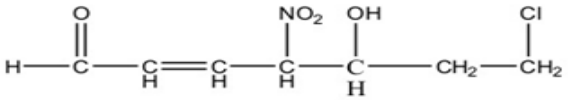
7. Indicate all Group C substituents, and Group A functional groups of lower priority, with a prefix. Place the prefixes, with appropriate position numbers, in alphabetical order before the root name.



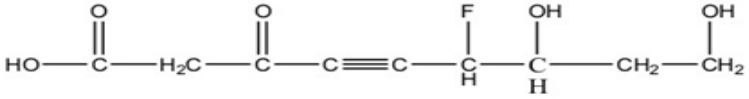
3-(4-amino-1-chloro-3-oxopentyloxy)propanoic acid



1-chloro-4-nitrohex-5-en-3-ol



7-chloro-5-hydroxy-4-nitrohept-2-enal



6-fluoro-7,9-dihydroxy-3-oxonon-4-ynoic acid

**References:**


- A textbook of organic chemistry,22nd edition, Arun bahl,B S Bahl,S.Chand publishing. Pg no;199-233,234-271,272-292,293-318-365,333-365.
- Organic chemistry;7thedition;RobertThortonMorrision,S.K.Bhattarcharje, Pearson,Pg no:120-291-326,411-423382-385,507-510,544-559.570-597,624-649