BP 202T - PHARMACEUTICAL ORGANIC CHEMISTRY - I

UNIT: 1 CLASSIFICATION, NOMENCLATURE & ISOMERISM

CLASS: 2

TOPIC: IUPAC NOMENLATURE OF ALKANES, ALKENES, ALKYNES & ALKYL HALIDES

International Union of Pure and Applied Chemistry: To establish an international name and to correlate each name with a unique name.

Structure:

Secondary prefix	+	Primary prefix	+	Root word	+	Primary suffix	+	Secondary suffix

Secondary prefix represents substituent's or branches (Cl, Br, F, I, CH_3 etc)

Primary prefix represents cyclic compounds

Root word represents the number of carbon atoms present in the carbon chain

Primary suffix represents saturation or unsaturation in carbon chain (alkane, alkene or alkyne)

Secondary suffix represents the functional group present in the organic molecule.(-COOH,- OH, -CHO etc)

Functional Groups: A functional group is an atom or group of atoms in a molecule that gives that molecule its characteristic properties. It is the reactive part of an organic molecule

CH_3-CH_2-CH_2-CH_2-CH_2-OH

Hydrocarbon portion Functional group

Each functional group undergoes characteristic reactions. By recognizing a functional group in a molecule, it is possible to predict the reactions which that molecule will undergo.

A functional group is a chemical reactivity in a molecule. Molecules can contain more than one functional group then it is said to be a poly functional group.

Common names or Trivial names: An ordinary name given to a compound without reference to its structure is called common name or trivial name. The common names are like nicknames.

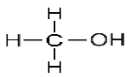
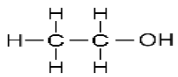
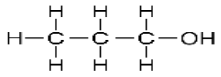
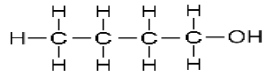
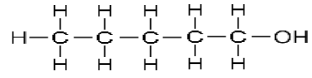
In early days of organic chemistry, each new compound was given an individual name based on

the source, some property or so some other trivial reason.

Example: Formic acid (HCOOH) is obtained from the distillation of red ants. In latin; Formica means ants.

Class of compounds	Functional group structure	IUPAC group prefix	IUPAC group suffix	Example
Alkanes	-	-	-ane	Butane, $CH_3(CH_2)_2CH_3$
Alkenes	>C=C<	-	-ene	But-1-ene, $CH_2=CHCH_2CH_3$
Alkynes	-C≡C-	-	-yne	But-1-yne, $CH{\equiv}CCH_2CH_3$
Arenes	-	-	-	Benzene, 
Halides	-X (X=F,Cl,Br,I)	halo-	-	1-Bromobutane, $CH_3(CH_2)_2CH_2Br$
Alcohols	-OH	hydroxy-	-ol	Butan-2-ol, $CH_3CH_2CHOHCH_3$
Aldehydes	-CHO	formyl, or oxo	-al	Butanal, $CH_3(CH_2)_2CHO$
Ketones	>C=O	oxo-	-one	Butan-2-one, $CH_3CH_2COCH_3$
Nitriles	-C≡N	cyano	nitrile	Pentanenitrile, $CH_3CH_2CH_2CH_2CN$
Ethers	-R-O-R-	alkoxy-	-	Ethoxyethane, $CH_3CH_2OCH_2CH_3$
Carboxylic acids	-COOH	carboxy	-oic acid	Butanoic acid, $CH_3(CH_2)_2CO_2H$
Carboxylate ions	$-COO^-$	-	-oate	Sodium butanoate, $CH_3(CH_2)_2CO_2^-\ Na^+$
Esters	-COOR	alkoxycarbonyl	-oate	Methyl propanoate, $CH_3CH_2COOCH_3$
Acyl halides	-COX (X=F,Cl,Br,I)	halocarbonyl	-oyl halide	Butanoyl chloride, $CH_3(CH_2)_2COCl$
Amines	$-NH_2$, >NH,>N-	amino-	-amine	Butan -2-amine , $CH_3CHNH_2CH_2CH_3$
Amides	$-CONH_2$, -CONHR, $-CONR_2$	-carbamoyl	-amide	Butanamide, $CH_3(CH_2)_2CONH_2$
Nitro compounds	$-NO_2$	nitro	-	1-Nitrobutane, $CH_3(CH_2)_3NO_2$
Sulphonic acids	$-SO_3H$	sulpho	sulphonic acid	Methylsulphonic acid CH_3SO_3H

Homologous Series: A homologous series is a series of compounds in which the adjacent members differ by CH_2 unit or 14amu (atomic mass unit).The individual members are called Homologs.

ALCOHOL	CARBON NUMBER	FORMULA	STRUCTURE
METHANOL	1	CH_3OH	
ETHANOL	2	CH_3CH_2OH	
PROPANOL	3	$CH_3CH_2CH_2OH$	
BUTANOL	4	$CH_3CH_2CH_2CH_2OH$	
PENTANOL	5	$CH_3CH_2CH_2CH_2CH_2OH$	

- All the compounds in the series contain the same elements and the functional groups
- All compounds in the series are represented by a general formula
- The molecular formula of each monolog differs by a single CH_2unit.
- All compounds in the series can be prepared by similar method.
- All compounds in the series have similar chemical properties.
- There is a gradual variation of physical properties with increasing molecular weight.

ALKANES:

Alkanes are the hydrocarbons that contain only carbon carbon single bond. Hydrocarbons are the compounds that contain only carbon and hydrogen.

Homologous series	General formula	Functional group
Alkanes	C_nH_{2n+2}	
Alkenes	C_nH_{2n}	C=C
Alkynes	C_nH_{2n-2}	C≡C
Alkanols	$C_nH_{2n+1}OH$	R – OH
Alkanoic acids	$C_nH_{2n+1}COOH$	R – COOH
Alkanals	$C_nH_{2n+1}CHO$	R – CHO

Table *Names, molecular formulae and condensed structural formulae of the first ten members of the alkane family*

Member	Name	Molecular formula	Condensed structural formula
1	Methane	CH_4	CH_4
2	Ethane	C_2H_6	CH_3CH_3
3	Propane	C_3H_8	$CH_3CH_2CH_3$
4	Butane	C_4H_{10}	$CH_3CH_2CH_2CH_3$
5	Pentane	C_5H_{12}	$CH_3CH_2CH_2CH_2CH_3$
6	Hexane	C_6H_{14}	$CH_3CH_2CH_2CH_2CH_2CH_3$
7	Heptane	C_7H_{16}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
8	Octane	C_8H_{18}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
9	Nonane	C_9H_{20}	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
10	Decane	$C_{10}H_{22}$	$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

Prefix: All isomeric alkanes have the same parent name. The names of various isomers are distinguished by prefixes. The prefix indicates the type of branching present in the molecule.

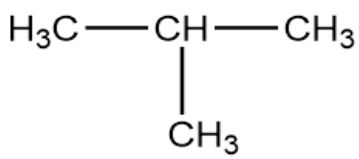
1. **Prefix"n":** Prefix 'n' is used for alkanes in which all carbons are in one continuous chain. The prefix 'n' stands for straight chain compounds.

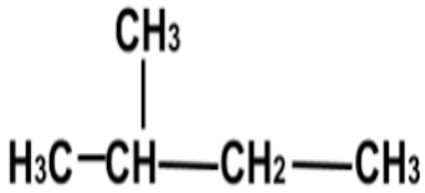
   Example: CH_3-CH_2-CH_2-CH_3 CH_3-CH_2-CH_2-CH_2-CH_3

   n-Butane **n-Pentane**

2. **Prefix "Iso":** It is used for those alkanes which have a methyl group (CH_3-) attached to the second last carbon of the continuous chain.

   Example:

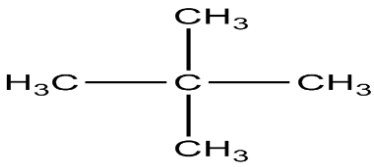




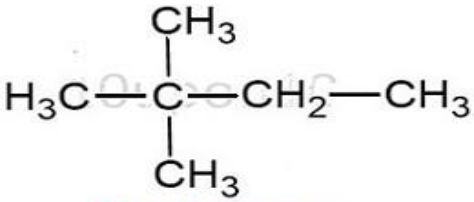
   Isobutane **Isopentane**

3. **Prefix "Neo":** It is used for those alkanes which have two methyl groups (CH_3-) attached to the second last carbon of the continuous chain

   Example:



Neopentane

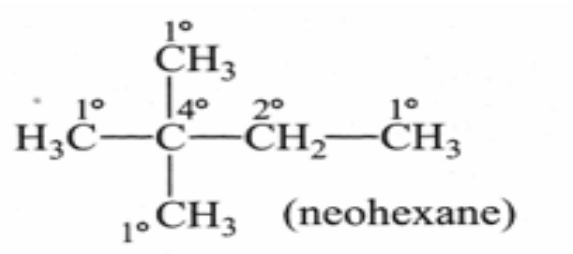


Neohexane

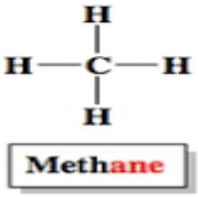
Classification of Carbon Atoms: The structural formula of alkanes contain four types of carbon

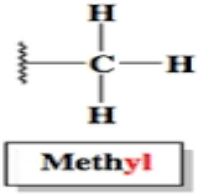
1. Primary carbon atom: A carbon atom attached to one other or no other carbon (1°Carbon)
2. Secondary carbon atom: A carbon atom attached to two other carbon atoms (2°Carbon)
3. Teritary carbon atom: A carbon atom attached to three other carbon atoms (3°Carbon)
4. Quaternary carbon: A carbon atom attached to four other carbon atoms (4°Carbon)

Example:



Alkyl Groups: Alkyl groups are formed by removing one hydrogen atom from an alkane.





No. of C atoms	Name of alkane	Molecular formula	Name of alkyl group	Formula
1	Methane	CH_4	Methyl	$-CH_3$
2	Ethane	C_2H_6	Ethyl	$-C_2H_5$
3	Propane	C_3H_8	Propyl	$-C_3H_7$
4	Butane	C_4H_{10}	Butyl	$-C_4H_9$
5	Pentane	C_5H_{12}	Pentyl	$-C_5H_{11}$
6	Hexane	C_6H_{14}	Hexyl	$-C_6H_{13}$
7	Heptane	C_7H_{16}	Heptyl	$-C_7H_{15}$
8	Octane	C_8H_{18}	Octyl	$-C_8H_{17}$
9	Nonane	C_9H_{20}	Nonyl	$-C_9H_{19}$
10	Decane	$C_{10}H_{22}$	Decyl	$-C_{10}H_{21}$

Non-alkyl Groups: A number of non-alkyl groups are used in naming an organic compound.

Group	Name
—F	fluoro
—Cl	chloro
—Br	bromo
—I	iodo
—NO_2	nitro
—NH_2	amino

IUPAC Nomenclature Rules:

Rule1: Select the longest continuous carbon chain

Rule2: Name the longest carbon chain. These are called the Parent names.

Rule 3: Give numbering to the longest continuous carbon chain. The numbering is started from the end which will give numbers having the lowest value to the carbon carrying substituent

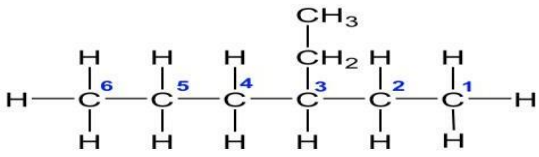
Rule 4: Identify the substituent. Name the substituent. Indicate its position by the number of the carbon atom to which it is attached.

Rule 5: Prefix the position number and name of the substituent onto the parent name. The whole name is written as one word. The name and number of the substituent are separated by a "Hyphen".

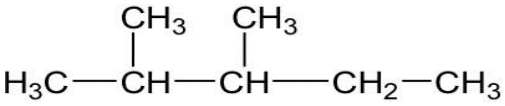
Rule 6: Identify the substituents by their names and position numbers. When the same substituent is present two or three times in the molecule then the prefix di, tri, tetra, penta. etc., are used. Position of each substituent is indicated bya separate number. These position numbers are separated by comma's and are placed just before the name of the substituent. The hyphen before and after the number are necessary.

Rule 7: When two or more different substituent's are present, their names are arranged in alphabetical order and added to the name of the parent alkane.

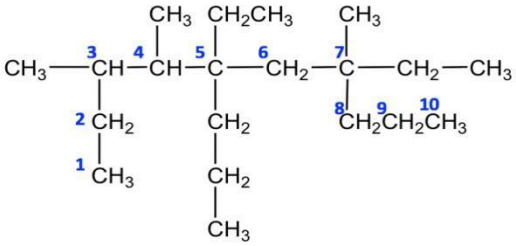
Examples:



3-ethylhexane



2,3-dimethylpentane

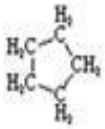
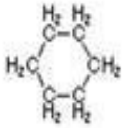
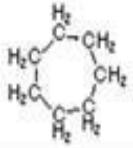
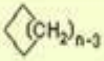


Find the parent chain correctly is the key step for naming this structure.

5,7-diethyl-3,4,7-trimethyl-5-propyldecane

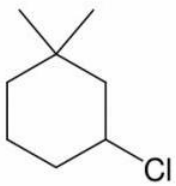
CYCLOALKANES:

Cyclo alkanes are the alkanes in which the carbon atoms are arranged in a ring. Theyare named by placing the prefix –*Cyclo* to the name of the alkane having the same number of carbons similar to ring.

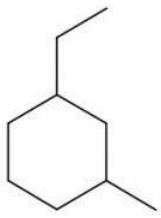
Name	Cyclopropane	Cyclobutane	Cyclopentane	Cyclohexane	Cycloheptane	Cycloalkane
Molecular Formula	C_3H_6	C_4H_8	C_5H_{10}	C_6H_{12}	C_7H_{14}	C_nH_{2n}
Structural Formula						$(CH_2)_n$
Line Formula						

- Substituted cyclo alkanes are named as **Alkyl cyclo alkanes.**
- The substituent's on the ring are named and their positions are indicated by numbers.
- The ring is numbered so that the substituent's are given the lowest possible numbers.
- The ring is designated as substituent if the alkane chain contains a greater number of carbon atoms than the ring structure.

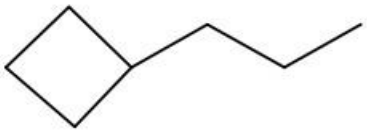
Examples:



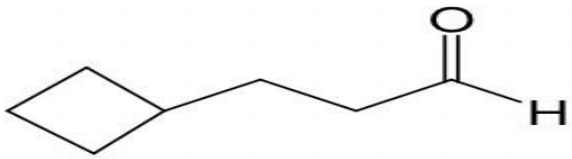
1,1-dimethyl-3-chlorocyclohexane



1-ethyl-3-methylcyclohexane



propylcyclobutane

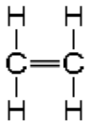
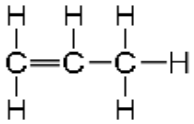
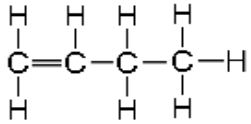
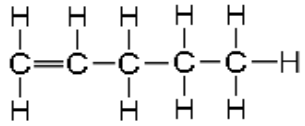
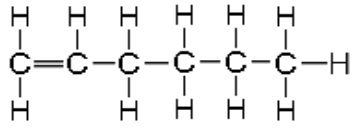


3-cyclobutylpropanal

ALKENES:

Alkenes are the hydrocarbons that contain a carbon-carbon double bond (C=C)

The names are written by changing the ending–*ane* of the corresponding alkane to-*ylene* (Alkane–ane+ylene) is Alkylene Or (Alkane–ane+ene)is Alkene

ALKENE	CARBON NUMBER	FORMULA	STRUCTURE
ETHENE	2	C_2H_4	
PROPENE	3	C_3H_6	
BUTENE	4	C_4H_8	
PENTENE	5	C_5H_{10}	
HEXENE	6	C_6H_{12}	

N. SIVA NAGA TEJASWINI, M. Pharm
Assistant Professor

IUPAC RULES FOR ALKENES:

Rule1: Select the longest carbon chain containing the double bond. This is the parent chain.

Rule2: Name the longest chain. (Alkane–ane+ene) is Alkene

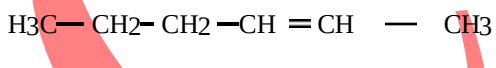
Rule3: Give numbering to the chain from the end closer to the double bond.

Rule 4: Indicate the position of the double bond by the number of the first (Lower number) carbon atom involved in the double bond.

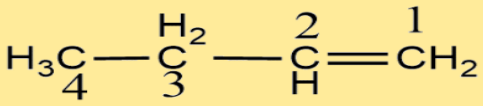
Rule 5: Alkyl groups and other substituent's are numbered, named and placed as prefixes in the alphabetical order

Rule6: Alkenes containing two double bonds are named as **Alkadienes**

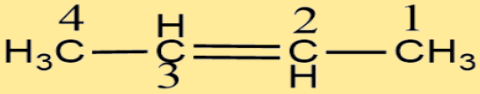
Rule 7: In naming Cycloalkenes, number the rings to give the double bonded carbons the lowest numbers i.e., the numbers 1 and 2. Choose the direction of numbering so the substituent's get the lowest numbers.



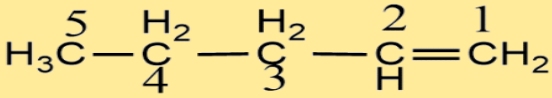
2-hexene



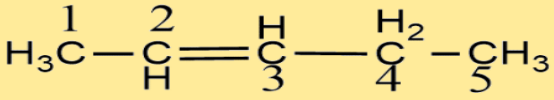
but-1-ene



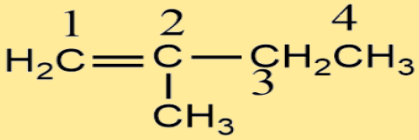
but-2-ene



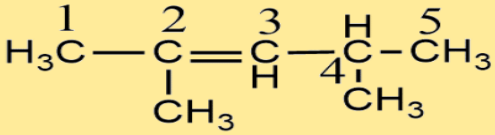
pent-1-ene



pent-2-ene



2-methyl but-1-ene



2,4-dimethyl pent-2-ene

buta-1,3-diene

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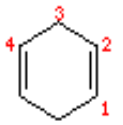
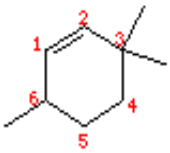
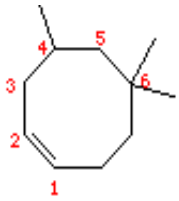

1,4-cyclohexadiene


3,3,6-trimethylcyclohexene


4,6,6-trimethylcyclooctene

ALKYNES:

Alkynes are the hydrocarbons that contain carbon-carbon triple bond. The simplest alkyne is commonly known as Acetylene. (Alkane – ane + yne) = Alkyne.

IUPAC RULES FOR ALKYNES:

Rule1: Select the longest carbon chain containing the triple bond. This is the parent chain.

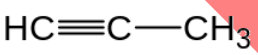
Rule2: Name the longest chain.(Alkane–ane+yne) is Alkyne

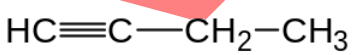
Rule3: Give numbering to the chain from the end closer to the triple bond.

Rule 4: Indicate the position of the triple bond by the number of the first (Lower number) carbon atom involved in the triple bond.

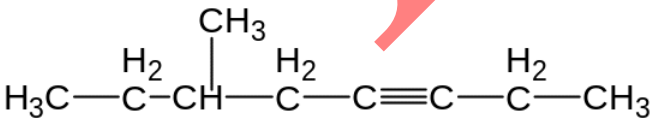
Rule 5: Alkyl groups and other substituent's are numbered, named and placed as prefixes in the alphabetical order

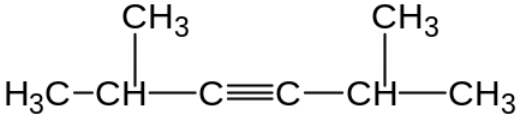
Rule6: Alkynes containing two triple bonds are named as **Alkadiynes**


Propyne


But-1-yne


But-2-yne


6-Methyl-3-octyne


2,5-Dimethylhex-3-yne

ALKYL HALIDES: Alkyl halides are the compounds which contain carbon – halogen bonds. The names of alkyl halides are obtained by naming the alkyl group attached to the halogen and adding the name of the halide as a separate word.

IUPACRULESFORALKYLHALIDES:

Rule 1: Select the longest carbon chain to which halogen is attached and give its corresponding alkane name.

Rule2: Prefix the name of the alkane by chloro, bromo, iodo or fluoro.

Rule 3: Give numbering to the chain as the carbon containing halogen atom the lowest possible number.

Rule 4: Alkyl groups and other substituent's are numbered, named and placed as prefixes in the alphabetical order. If two or more identical halogen substituents are present in the molecule then the prefix di, tri, tetra, penta. etc., are used.

Formula	Common name	IUPAC name
$CH_3 - Cl$	Methyl chloride	chloromethane
$CH_3 - CH_2 - Br$	Ethyl bromide	bromoethane
$CH_3 - CH_2 - CH_2 - I$	n-propyl iodide	1-iodopropane
$CH_3 - \underset{\displaystyle Cl}{\underset{\vert}{CH}} - CH_3$	Isopropyl chloride	2-chloropropane
$CH_3 - CH_2 - CH_2 - CH_2 - Br$	n-butyl bromide	1-bromobutane
$CH_3 - CH_2 - \underset{\displaystyle Br}{\underset{\vert}{CH}} - CH_3$	sec-butyl bromide	2-bromobutane
$CH_3 - \underset{\displaystyle CH_3}{\underset{\vert}{C}} - Br$ $\vert$ CH_3	tert-butyl bromide	2-bromo-2-methylpropane
$CH_3 - \underset{\displaystyle CH_3}{\underset{\vert}{CH}} - CH_2 - Br$	Isobutyl bromide	1-bromo-2-methylpropane
$CH_3 - \underset{\displaystyle CH_3}{\underset{\vert}{C}} - CH_2 - Br$ $\vert$ CH_3	Neopentyl bromide	1-bromo-2,2-dimethylpropane

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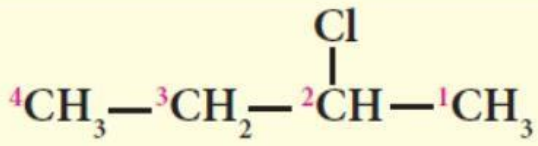
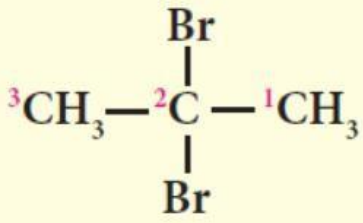
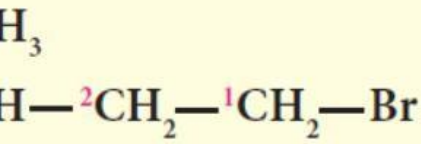
Compound	Systemic name of compound
	2-chlorobutane
	2,2- dibromopropane
	2-bromo-3-chlorobutane
	1-bromo-3-methylbutane

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