Q.1 Explain the IUPAC system of nomenclature of organic compound with suitable examples. (15)

Ans:

The **IUPAC** (International Union of Pure and Applied Chemistry) system of nomenclature is a standardized method used to name chemical compounds systematically based on their molecular structure. This system ensures clarity and consistency in communication among chemists worldwide.

Steps for IUPAC system

1. **Identify the Main Functional Groups**
   The first step is to identify the main functional groups present in the molecule. Functional groups are specific arrangements of atoms that confer particular chemical properties to the compound.
2. **Choose the Longest Carbon Chain**
   In organic compounds, the backbone usually consists of a chain of carbon atoms. Select the longest continuous chain of carbon atoms (the parent chain). This chain may be straight or branched.
3. **Number the Carbon Atoms**
   Number the carbon atoms in the parent chain sequentially, starting from the end closest to the first substituent (functional group or side chain). This ensures that substituents are assigned the lowest possible numbers.
4. **Name Substituents**
   Substituents are groups of atoms attached to the main carbon chain. They are named as prefixes and their positions are indicated by the number of the carbon atom to which they are attached. Common substituents include methyl (CH_3-), ethyl (C_2H_5-), hydroxyl (-OH), and chloro (-Cl).
5. **Identify and Name Multiple Bonds**
   If there are multiple bonds present in the molecule, indicate their presence and location using appropriate prefixes such as "di-" (two bonds), "tri-" (three bonds), etc. The position of the multiple bonds is indicated by the lowest possible number.
6. **Order of Priority**
   If there are multiple functional groups present, prioritize them based on a predefined hierarchy established by IUPAC rules. The functional group with the highest priority determines the suffix of the compound name.
7. **Combine Prefixes and Suffixes**
   Combine the prefixes (indicating substituents) and the suffix (indicating the main functional group) to form the complete name of the compound. Ensure that the prefixes are listed in alphabetical order, ignoring any numerical prefixes like "di-" or "tri-".

Nomenclature of Organic Compound

"IUPAC"

(International Union of Pure and Applied Chemistry)

→ The purpose of IUPAC system of Nomenclature is to establish an international standard of naming the compounds to facilitate communication.

IUPAC

- **Prefix**
  - → Substituents (2°)
  - → Cyclo/bicyclo (1°)
- **Word Root**
  - → No. of 'C' atom in main chain
- **Suffix**
  - → Type of bond (1°)
  - → functional (2°) group

Naming: 2° Prefix + 1° prefix + Word Root + 1° suffix + 2° suffix

Note: 1° ⇒ Primary
2° → Secondary

Substituents

1) $-CH_3$ — Methyle
2) $-C_2H_5$ — ethyle
3) $-C_3H_7$ → Propyl
4) $-Br$ → Bromo
5) $-Cl$ → chloro
6) $-F$ → fluoro
7) $-NO_2$ → Nitro
8) $-I$ → Iodo

Bonds

(—) → -ane
(=) → ene
(≡) → yne

Word root

- 1 Carbon : Meth
- 2 Carbon : eth
- 3 - C : prop
- 4 - C : but
- 5 - C : Pent
- 6 - C : hex
- 7 - C : hept
- 8 - C : oct
- 9 - C : Non
- 10 - C : dec

Functional Group

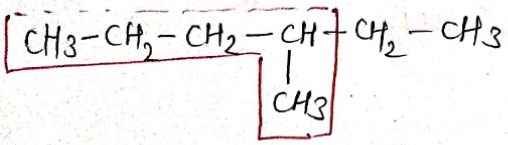
- $-OH$ → Alcohol (ol)
- $-CHO$ → Aldehyde (al)
- $-COOH$ → Carboxylic acid (oic acid)
- $-R-\overset{\overset{O}{\|}}{C}-R$ → Ketone (-one)
- $R-\overset{\overset{O}{\|}}{C}-OR$ → Ester (Alkyle alkanoate)
- $R-O-R$ → Ether (Alkoxy Alkane)
- $-\overset{\overset{H}{|}}{N}-H$ → Amin (Amino)
- $CO-NH_2$ → Amide
- $-X$ → halide (X = F, Cl, Br, I)

Rules for IUPAC Nomenclature

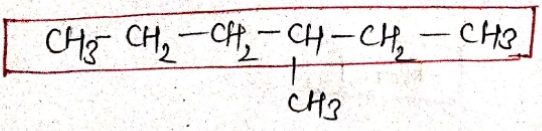
Alkane

① Longest chain rule

* Select the longest C-C chain (may be straight/not)

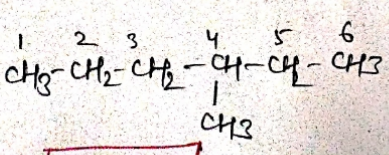


✗ wrong

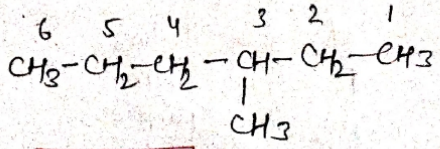


✓ Right

* Numbering from the end from branch get closer.

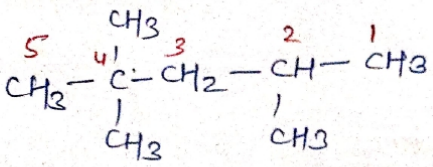


Wrong



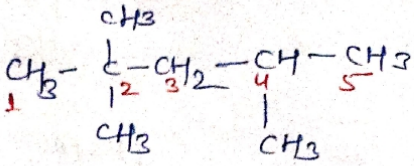
correct

* When branching is more then follow first point of difference.



(corong) ×

(2, 4, 4)

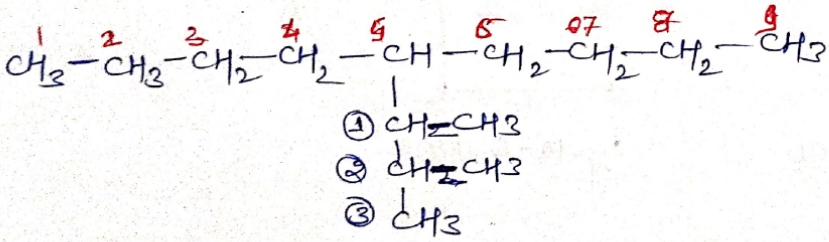


Right (✓)

(2, 2, 4)

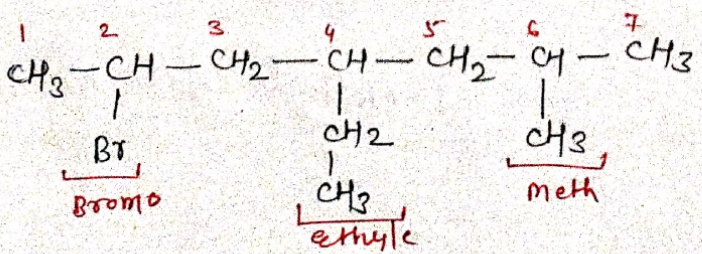
(2) Complex Substituents chain

- Give 1st number to the 'C' directly attached to chain (main)
- Then follow IUPAC system.



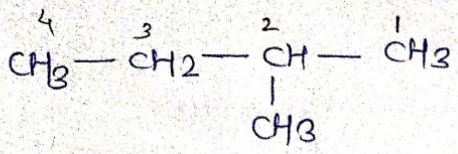
5 (1,2 dimethyl propyl) octane Nonan

- Naming done alphabatically always



(2-bromo, 4 ethyle - 6 methyle heptane)

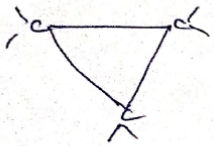
COMMON STRUCTURE FOR NAMING



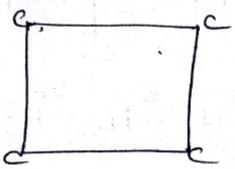
2- → Position of alkyl group + Methyl → Attached Alkyl group + butane → Longest chain

2. NOMENCLATURE FOR CYCLO ALKANE

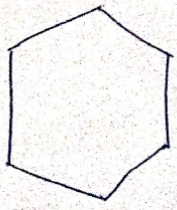
Structure: "cyclo + name of alkane"



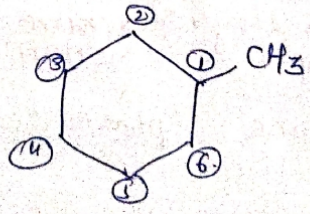
cyclo-Propane



cyclo-butane



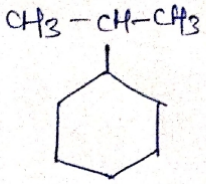
cyclo-hexane



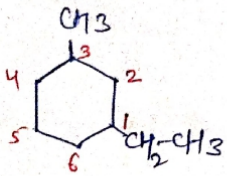
1-Methyle cyclo hexane

* Substituted cycloalkane are named as "alkyl cycloalkane"

* Substituent (according to alphabet) given lowest number in ring.



⇒ iso-propyl cycloalkane



1-ethyle 3 methyle cyclo hexane

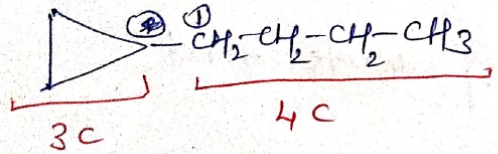
Prefix for alkane

n- for straight chain alkane
e.g. $CH_3-CH_2-CH_2-CH_3$ (n-butane)

iso → if methyle group attached to second last 'c'.
e.g. $CH_3-\underset{\underset{CH_3}{|}}{\overset{\overset{H}{|}}{C}}-CH_3$ (isobutane)

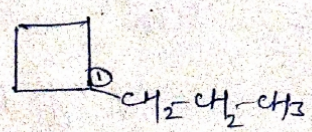
neo: if 2-methyl attached to second last carbon.
eg. $CH_2-\underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{C}}-CH_3$ (neo-pentane)

* Ring is designated as "substituent" if no. of carbon is less than 'c' chain.

(1) 

⇒ so △ = Substituent

✓(1-cyclo propyl butane) but not as Butyl cyclo propane ✗ (wrong)
(right)

(2) 

(1-propyl cyclo butane)

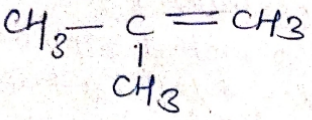
3. Nomenclature of Alkenes and Alkyne

⇒ C=C

⇒ Their name obtained by changing the ending -ane to -ylene.

$CH_2=CH_2$ - Ethylene.

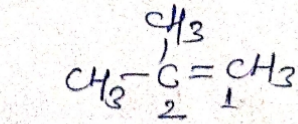
$CH_3-CH=CH_2$ Propylene



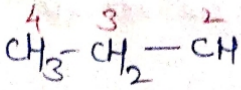
Isobutylene

Rules

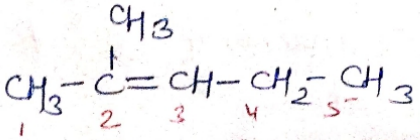
1) Select longest chain containing double bond.
2) Name the longest chain
3) Number the chain from the end closer to = bond.
4) Indicate the position of double bond. form = bond.
5) alkyl group/other substituents are numbered named, and placed as prefix in alphabatic order.

Ex. $CH_2=CH_2$ $CH_2-CH=CH_2$ 

Ethene Propene 2-methyl propene

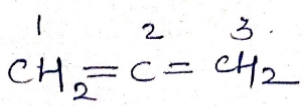


1- butene

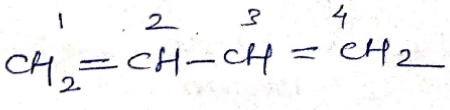


2- methyl pentene

* If two double bond present in alkene, so termed as "Alkadienes"

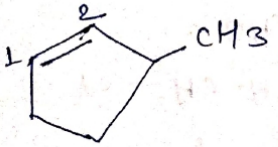


(1, 2 propdienes)

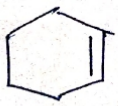


(1, 3 butadiene)

* In cyclo-alkene => Position of bond is not indicated.

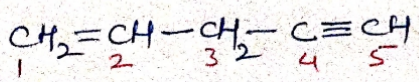


→ 3, Methyl cyclopentene



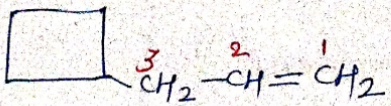
→ cyclohexene

* In case of =/≡ Bond
⇒ then => ≡



(Pent 1-ene 4 yne)

* If both ring and chain present, then select max =/≡ bonds (besides no. of Carbon)



3. cyclobutyl Prop-1-ene.

* Alkyne containing two triple bond are named as Alkadiynes

Naming of Alkyl halide (X = Cl, Br, I.)

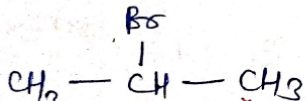
1) Select longest chain with which halide is attached

2) Prefix → chloro
Bromo
iodo etc.

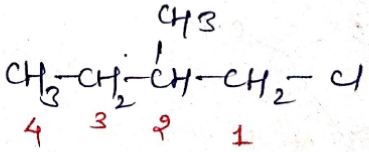
3) Number the chain.

4) Substituents are numbered, named & prefix as alphabetic order.

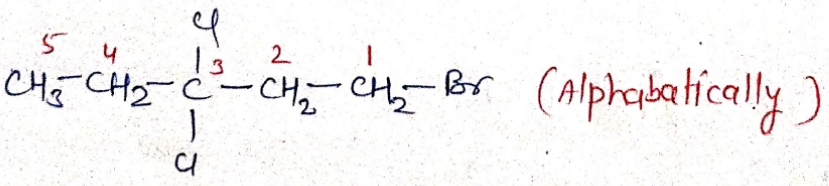
Ex.



2-bromo-propane



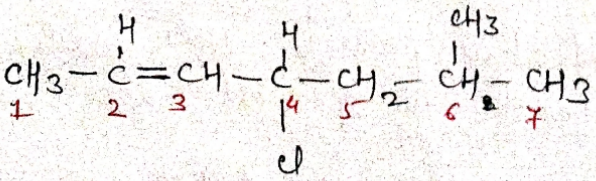
1-chloro-2-methyl butane



(Alphabatically)

1. bromo 3-3. dichloro pentane

⇒

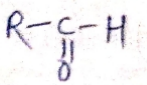
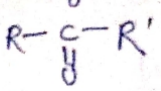
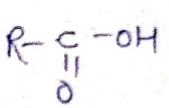
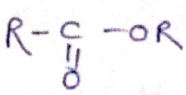


(4-chloro, 6 methyle hept 2-ene)

Priority
(=> ≡> halide)

Nomenclature of functional Group

→ Functional group are responsible for all property of compound.

	functional group	structure	suffix
1)	Alcohol	R–OH	-ol
2)	Aldehyde		-al
3)	Ketone		-one
4)	Carboxylic acid		-oic
5)	Ether	R–O–R'	alkoxy alkane
6)	Ester		alkyl alkanoate
7)	Amine	$R-NH_2$	-amine

Rules

1) Select longest chain having functional group.
2) Numbering from where functional group remain close.
3) Order for naming.

> functional group > = > ≡
> ∈ carbon chain

① Alcohols

→ Alcohol are compound in ⊆ hydroxyl group (-OH) is attached to a saturated carbon.

→ classified as Primary, Secondary, tertiary } depends on ⊆ carbon it is attached.

Alkane + ol → Alkanol

1) CH_3OH → Methanol

2) C_2H_5OH → Ethenol

3) $CH_3^{3}-CH^{2}(OH)-CH_3^{1}$ ⇒ 2-propanol

4) $CH_3^{4}-CH^{3}(CH_3)-CH_2^{2}-CH_2^{1}OH$

⇒ 3-methyl 1 butanol

* 2 or 3 alcohol group present

2 (-OH) = alkandiol

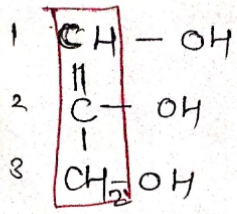
3 (-OH) = alkantriol

e.g.

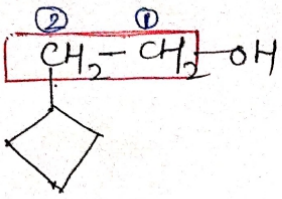
$CH_2(OH)-CH_2-CH_2(OH)$ 1, 3 propane-di-ol.

1 CH_2-OH
2 $CH-OH$
3 CH_2-OH

1, 2, 3 Propane triol



Prop 1-ene, 1,2,3 triol

* 

2- cyclobutyl ethane-1-ol
or
(2-cyclobutyl ethanol)

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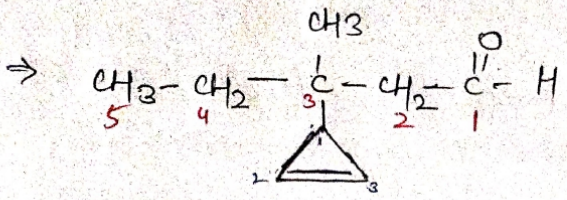
(2) Aldehyde (R-CHO), suffix -al

formula	common Name	IUPAC Name
$H-\overset{O}{\overset{\|\|}{C}}-H$	formaldehyde	Methanal
$CH_3-\overset{O}{\overset{\|\|}{C}}-H$	Acetaldehyde	Ethanal
$C_2H_5-\overset{O}{\overset{\|\|}{C}}-H$	Propanaldehyde	Propanal
$C_3H_7-\overset{O}{\overset{\|\|}{C}}-H$	Butaraldehyde	Butanal

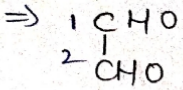
Structure.

$CH_3-CH_2-\overset{O}{\overset{\|\|}{C}}-H$ (3, 2, 1) — Propane-1-al

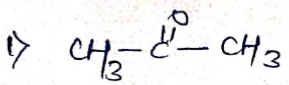
$CH_3-CH_2-\underset{\underset{CH_3}{|}}{CH}-\overset{O}{\overset{\|\|}{C}}-H$ (4, 3, 2, 1) ⇒ 2-methyl butane-1-al

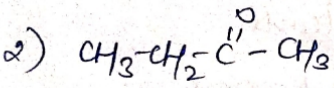
⇒ 

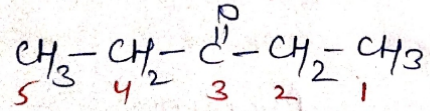
3 cyclo prop 2 enyl, 3 meth - Pent 1 - al

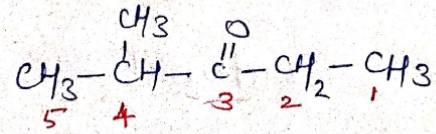
⇒  ⇒ Ethan 1, 2 di-al.

(8.) Ketones (-one)

1)  (acetone) Propanone

2)  ethyl methyl ketone } Butanone

3)  3-Pentanone

4)  4-Methyl-3 pentanone