UNIT - I

CLASSIFICATION, NOMENCLATURE AND ISOMERISM

(1) CLASSIFICATION OF ORGANIC COMPOUND

Organic Chemistry

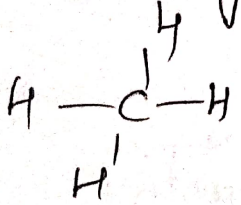
→ Contain Carbon

Total Eliment = 118.

1 — C

117 — inorganic

→ Also called Hydrocarbon.



H — C — H — methane

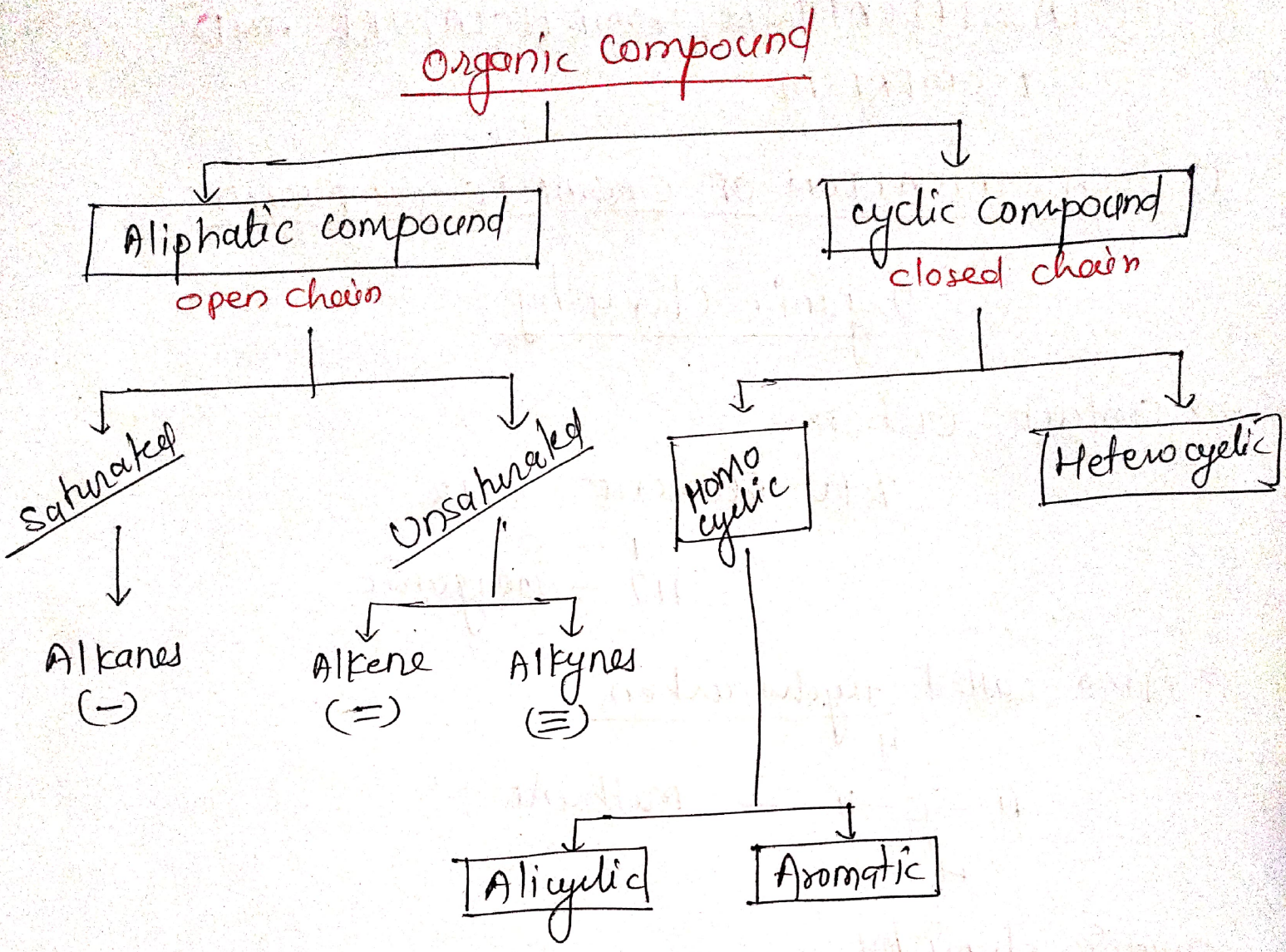
H

Organic chemistry

It is a branch of science that deals ~ molecules ≤ are made of 'C'.

Organic Compound:

The compounds that are made ~ carbon i.e. CH_4, C_6H_6, C_3H_7 etc.



(1) Aliphatic Compounds

→ Also k/n as open chain structure.

→ 'C' atoms are attached in the form of straight / branched chain, not in cyclic / closed structure

eg. CH_4 , $CH_3-CH_2-CH_3$ (Propane)

(a) Saturated compound

• 'C' attached ∈ C with single bond.

e.g. Alkanes

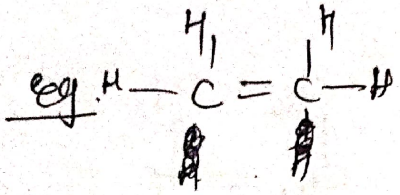
→ General formula → C_nH_{2n+2}

$C_1H_{2\times1+2} \rightarrow CH_4$ → Methane

$C_2H_{2\times2+2} \rightarrow C_2H_6$ – Ethane

(b) Unsaturated compounds

→ double bond is present among C & C or triple bond

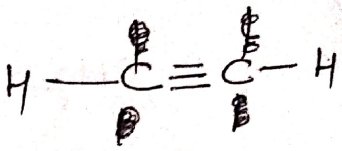
eg. 

C_2H_4 (Ethene)

Alkene

→ C_nH_{2n}

→ (=)



C_2H_2 (Ethyne)

Alkyne

C_nH_{2n-2}

(≡)

= } Co-valent bond

≡ }

σ

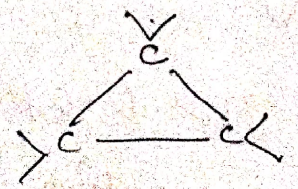
π

σ > π (stronger)

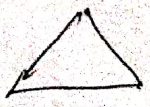
(2) cyclic Compound

* compounds c have closed ring structure.

Ex. cyclopropane,



or



(a) Homocyclic compound

→ Compounds having cyclic structure and ring forming

→ Also called Carbocyclic compound

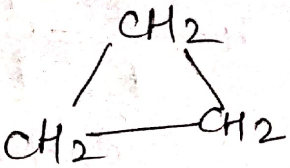
Types

(1) Alicyclic

→ Compounds in which carbon atom are attached in closed structure but do not have aromatic character.

→ It may be saturated or unsaturated.

ex. cyclopropane



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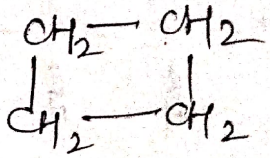


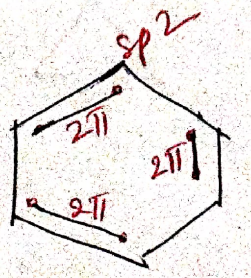
(cyclobutane)

(2) Aromatic Compound

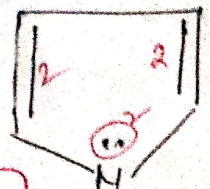
→ organic compound which follow hückles rule of aromaticity.

* for being aromatic, following rules must be followed.

(1) cyclic compound
(2) must be planner/(sp^2) Hybridization
(3) having π electron $(4n+2)\pi$
(4) must follow conjugation (— = — = — =)



✓ π = 6 electron
✓ conjugation
✓ cyclic
✓ sp^2

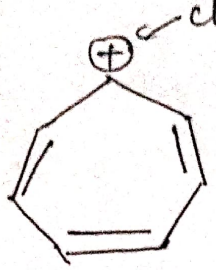


(Pyrole)

L.P → DLP
delocalised lone pair surround by single bond only

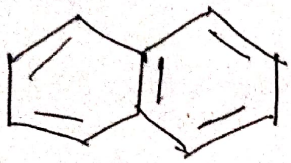
cyclic ✓
Conjugation ✓ (– = – = – ⊙)
π electron = 6

LLP
Localise lone pair.
L.P. is attached to single/double bond around it. in ring system.



cyclohepta-trienylium

cyclic = ✓
conj = – = – = – = ⊕
π electron = 6
n = 1 (single ring)
4n+2 = 6
(4×1)+2 = 6, hence. follow Huckle rule.



= 10 π electron.

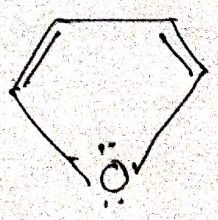
here = n = 2
∴ 4n+2 ⇒ 4×2+2 = (10) ✓

Heterocyclic Compound

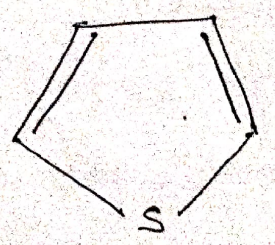
→ In ring structure single/multiple hetero atom attached ≥ carbon.

Hetero atom = H, S, O etc.

⇒ Ex.



(furan)



(Thiophene)

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

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

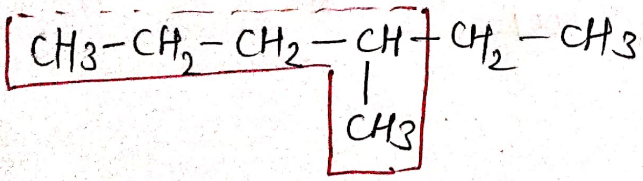
- $-OH$ → Alcohol (ol)
- $-CHO$ → Aldehyde (al)
- $-COOH$ → Carboxylic acid (oic acid)
- $-R-\overset{\overset{O}{\|}}{C}-R$ → Ketone (-one)
- $R-\overset{\overset{O}{\|}}{C}-OR$ → Ester (Alkyle alkanoate)
- $R-O-R$ → Ether (Alkoxy Alkane)
- $-\overset{\overset{H}{|}}{N}-H$ → Amin (Amino)
- $CO-NH_2$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

Rules for IUPAC Nomenclature

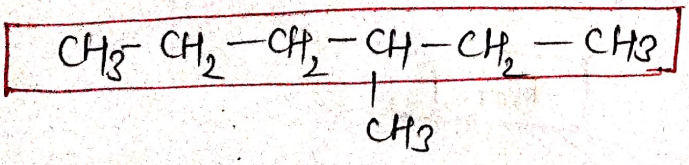
Alkane

① Longest chain rule

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

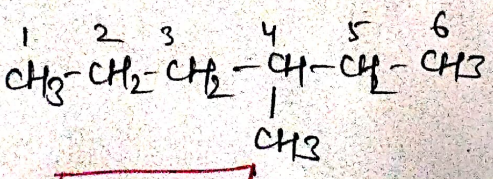


✗ wrong

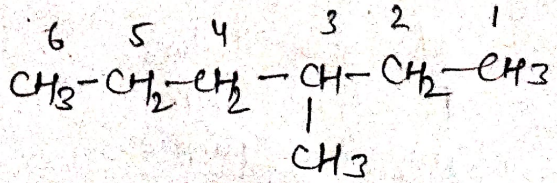


✓ Right

* Numbering from the end from branch get closer.

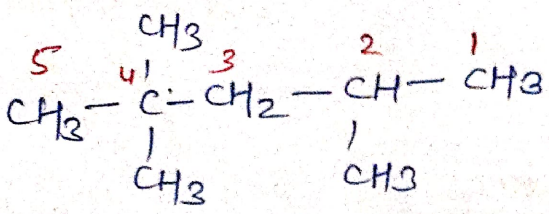


wrong



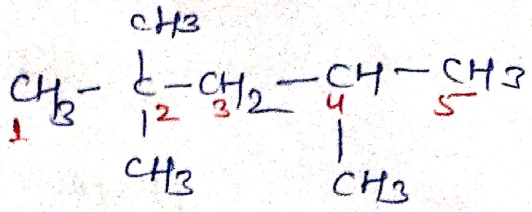
correct

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



(corong) ×

(2, 4, 4)

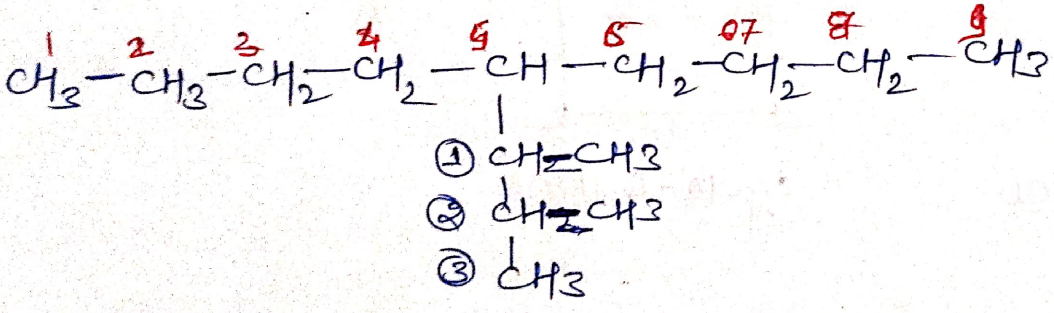


Right (✓)

(2, 2, 4)

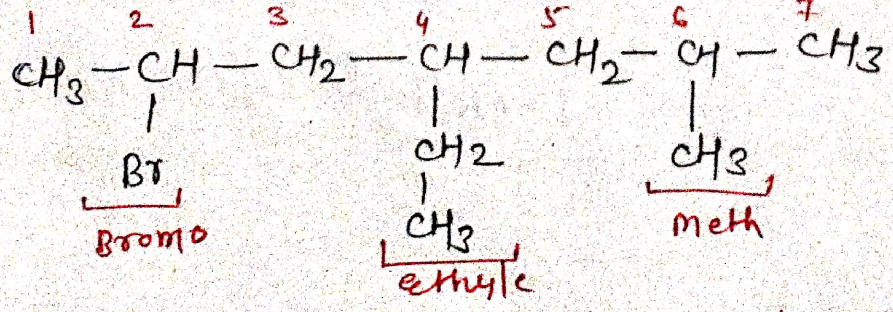
(2) Complex Substituents chain

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



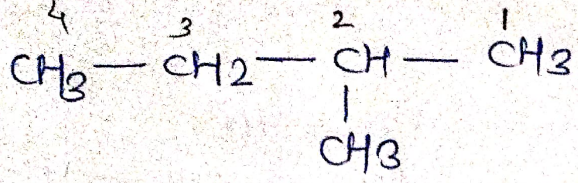
5 (1,2 dimethyl propyl) octane Nonan

- Naming done alphabatically always



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

COMMON STRUCTURE FOR NAMING

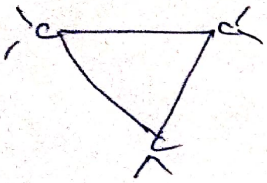


2- Methyl butane

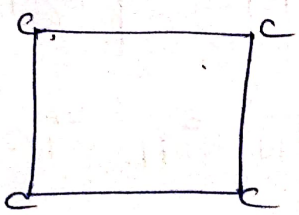
Position of alkyl group + Attached Alkyl group + Longest chain

2. NOMENCLATURE FOR CYCLO ALKANE

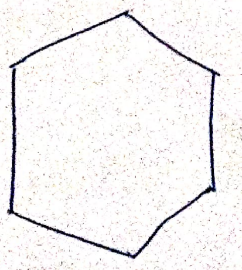
structure : "cyclo + name of alkane"



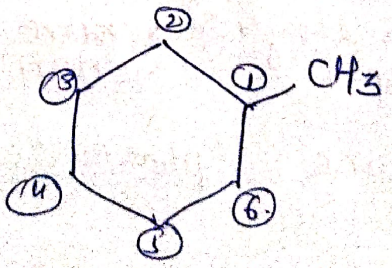
cyclo-Propane



cyclo-butane



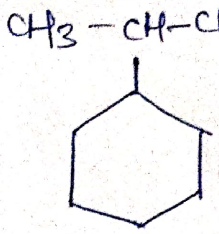
cyclo-hexane



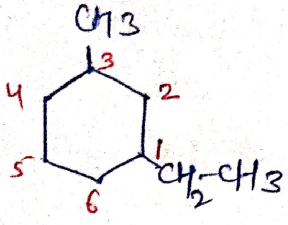
1-Methyle cyclo hexane

* Substituted cyclo alkane are named as "alkyl cyclo alkane"

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



⇒ iso-propyl cyclo alkane



1- ethyle 3 methyle cyclo hexane

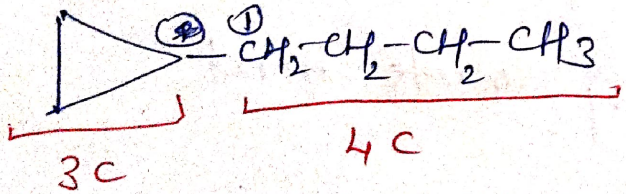
Prefix for alkane

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)

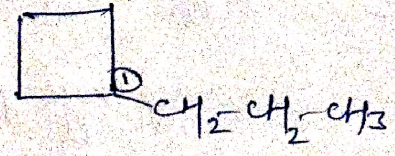
neo : if 2-methyl attached to second last carbon.
eg. $CH_2-\underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{C}}-CH_3$ (neo-pentane)

* 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)

(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

$CH_3-\underset{\underset{CH_3}{|}}{\overset{1}{C}}=CH_3$ Isobutylene

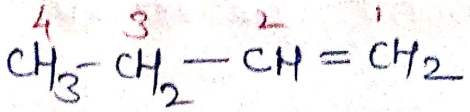
Rules

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.

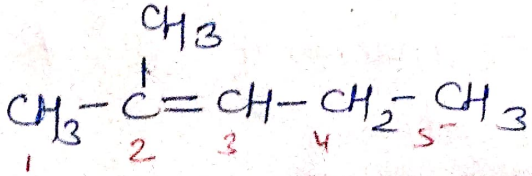
Ex. $CH_2=CH_2$ Ethene

$CH_2=CH-CH_3$ Propene

$CH_3-\overset{\overset{CH_3}{|}}{\underset{2}{C}}=\underset{1}{CH_2}$ 2-methyl propene

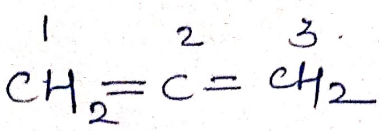


1- butene

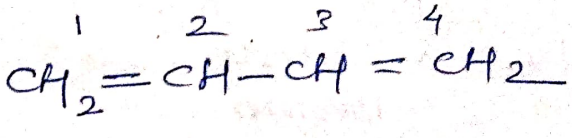


2- methyl pentene

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

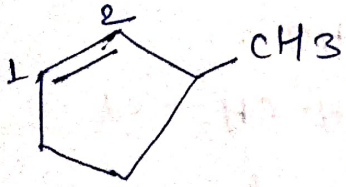


(1, 2 propdienes)

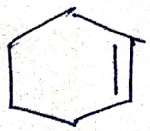


(1, 3 butadiene)

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

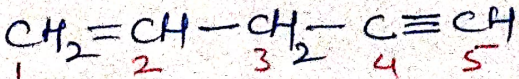


→ 3, Methyl cyclopentene



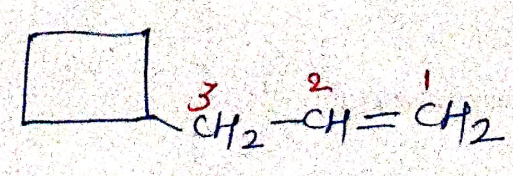
→ cyclohexene

* In case of =/≡ Bond
⇒ then => ≡



(Pent ~~ene~~ 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.)

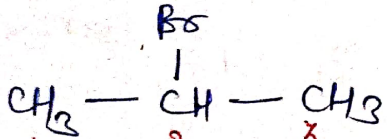
1) Select longest chain c/h ⊆ halide is attached

2) Prefix → chloro
Bromo
iodo etc.

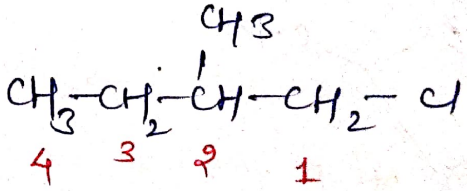
3) Number the chain.

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

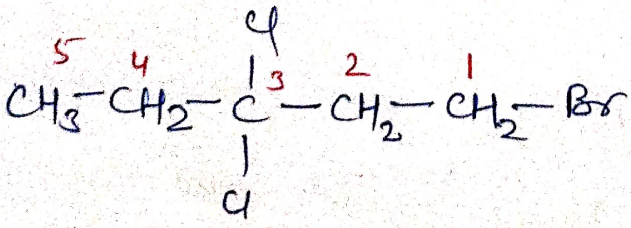
ex.



2-bromo-propane



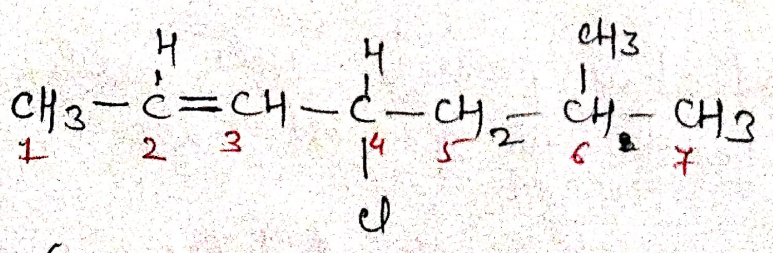
1-chloro-2-methyl butane



(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	R–C(=O)–H	-al
3) Ketone	R–C(=O)–R'	-one
4) Carboxylic acid	R–C(=O)–OH	-oic
5) Ether	R–O–R'	alkoxy alkane
6) Ester	R–C(=O)–OR	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 → Ethanol

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

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

⇒ 3-methyl 1 butanol

* 2 or 3 alcohol group present

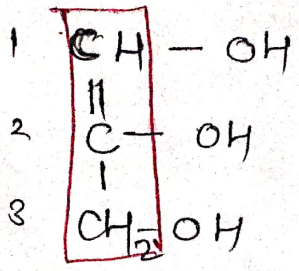
2 (-OH) = alkandiol

3 (-OH) = alkantriol

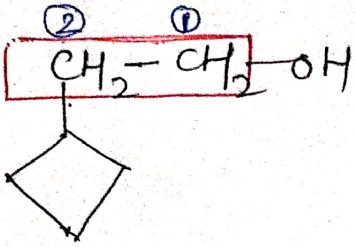
e.g.

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

$CH_2(OH)-CH(OH)-CH_2(OH)$ 1, 2, 3 Propane tri-ol



Prop 1-ene, 1,2,3 triol

* 

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

---

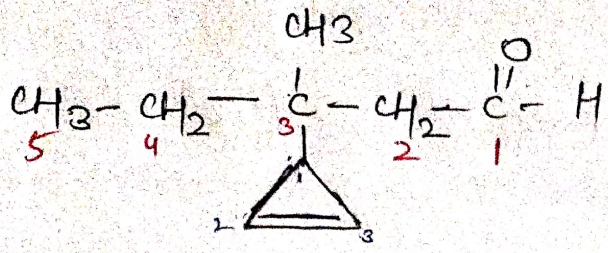
(2) Aldehyde (R-CHO), suffix -al

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

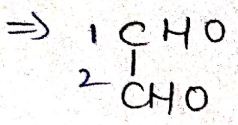
structure.

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

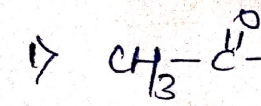
$CH_3-CH_2-\underset{\underset{CH_3}{|}}{CH}-\overset{\overset{O}{\|\|}}{C}-H$ (4, 3, 2, 1) ⇒ 2-methyl butane-1-al

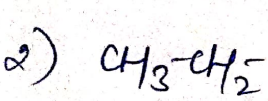
⇒ 

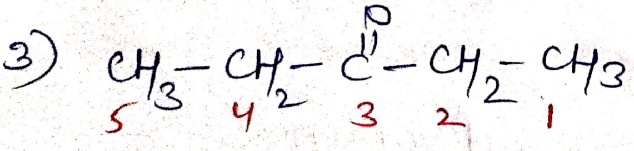
3 cyclo prop 2 enyl, 3 meth-Pent 1-al

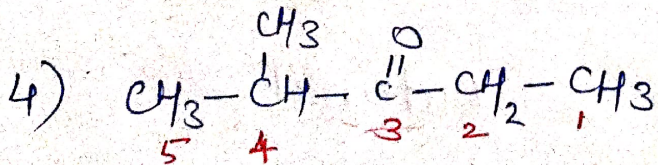
⇒  ⇒ Ethan 1, 2 di-al.

(8.) Ketones (-one)

1)  (acetone) Propanone

2)  ethyl methyl ketone } Butanone

3)  **3-Pentanone**

4)  4-Methyl-3 pentanone

(4) Carboxylic Acid (-COOH, -oic acid)

Formula	Comm. Name	IUPAC
$H-\overset{O}{\overset{\|\|}{C}}-OH$	formic acid	Methanoic acid
$CH_3-\overset{O}{\overset{\|\|}{C}}-OH$	Acetic acid	Ethanoic acid
$CH_3-CH_2-\overset{O}{\overset{\|\|}{C}}-OH$	Propanoic acid	Propanoic acid.

$CH_3-\overset{CH_3}{\overset{|}{CH}}-CH_2-\overset{O}{\overset{\|\|}{C}}-OH$ (4, 3, 2, 1) $\Rightarrow$ 3-methyl butanoic acid

$CH_3-CH_2-\overset{CH_3}{\overset{|}{CH}}-CH_2-\overset{O}{\overset{\|\|}{C}}-OH$ (5, 4, 3, 2, 1) $\Rightarrow$ 3-methyle pentonoic acid

(5) Carboxylic Acid Derivative

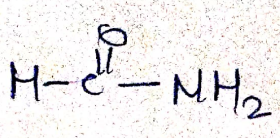
(1) Acid chloride

		IUPAC
$CH_3-\overset{O}{\overset{\|\|}{C}}-Cl$	Acetyl chloride	Ethanoyl chloride
$CH_3-CH_2-\overset{O}{\overset{\|\|}{C}}-Cl$	Propionyl chloride	Propanoyl chloride

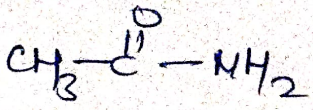
(2) Ester

$H-\overset{O}{\overset{\|\|}{C}}-OCH_3$	Methyl formate	Methyl methanoate
$CH_3-\overset{O}{\overset{\|\|}{C}}-OC_2H_5$	Ethyle Acetate	Ethyle ethanoate

Amide



→ formamide → Methanamide

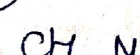


→ Acetamide → Ethanamide

⑥ Nitro compounds

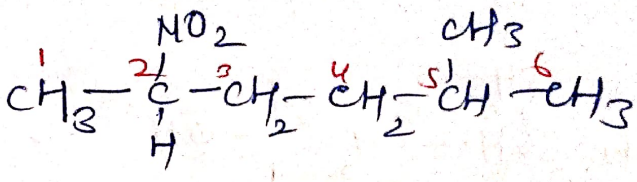
Prefix : - nitro.

①



(nitro methane)

②



5- methyle 2- nitro hexane

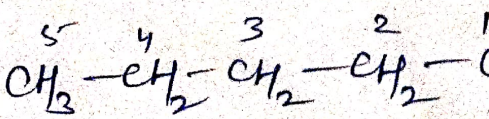
⑦ CYANIDES OR NITRILES

comm. Name = alkyl cynide } No. includes nitril
IUPAC = Alkanenitrile } 'C' atom

Ex.

IUPAC = Ethane nitril

(methyl cynide)



→ Pentane nitrile.

(n-butyl cynide)

(8) Amine

R (alkyl group)

$NH_3 \longrightarrow NH_2-(H) \longrightarrow R-NH_2$

Types

- $R-NH_2$ (Primary amin)
- R_2-NH (Secondary)
- R_3-N (tertiary)

eg- CH_3NH_2 → methylamine

$(CH_3)_2NH$ → Dimethylamine

$(CH_3)_3N$ → Trimethylamine

$CH_3-CH(CH_3)-NH_2$
Isopropylamine

$CH_3-NH-C_2H_5$
(Ethyl methylamine)

Common Names.

⇒ $CH_3CH_2NH_2$ → Ethanamine

$CH_3-CH(CH_3)-NH_2$ → 2-Propanamine
(Propanamine)

NOMENCLATORE OF POLY FUNCTIONAL GROUP

Priority order (most prior at first)

$-\overset{O}{\overset{\|}{C}}-OH > SO_3H > R-\overset{O}{\overset{\|}{C}}-O > -\overset{O}{\overset{\|}{C}}-X > R-\overset{O}{\overset{\|}{C}}-NH_2$

Ester — acid halide — Amide.

$> -CN > R-\overset{O}{\overset{\|}{C}}-H > R-\overset{O}{\overset{\|}{C}}-R' > -OH$

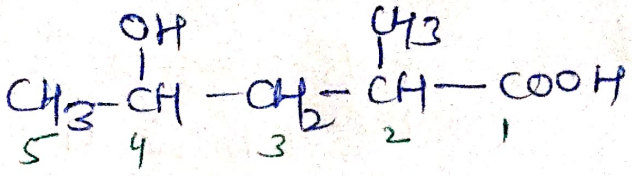
nitril — (aldehyde) — (ketone) — (alcohol)

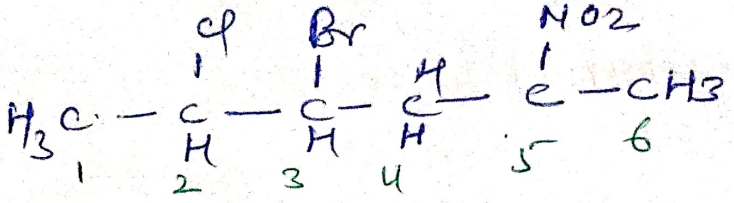
$> \text{amine} > \overset{C=C}{-ene} > \overset{C\equiv C}{-yne}$

Prefix used for functional group

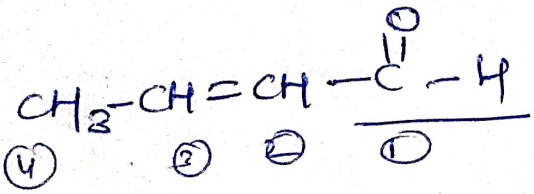
1. $R-\overset{O}{\overset{\|}{C}}-$ = oxo
2. $-NO_2$ = Nitro
3. $-NO$ = Nitroso
4. $-CN$ = cyno
5. $-OH$ = al / hydroxy.

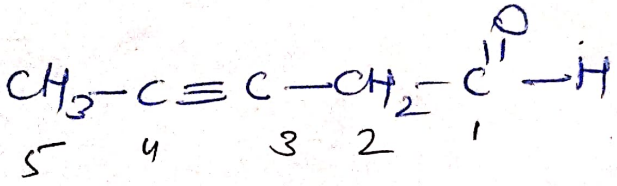
Ex.

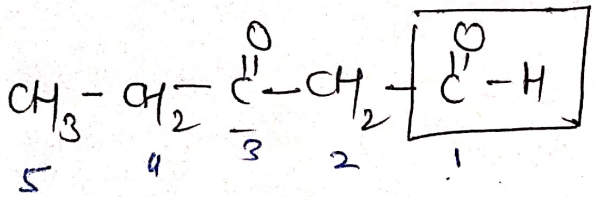
(1)  = 4-hydroxy 2 methyl pentanoic acid.

(2)  (None of them are principle functional group, so all are as substituents)

(2-bromo, 2-chloro 5 nitrohexane)

(3)  ⇒ 2 butenal

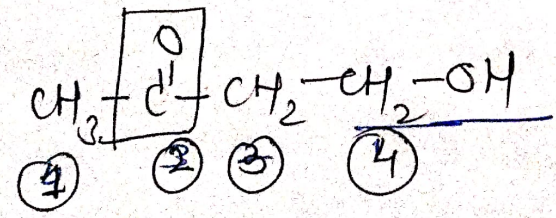
(5)  3 pentynal

(6) 

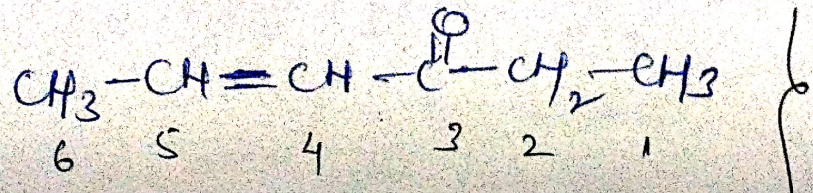
-CHO = Principle functional group.

C=O = Substituents.

(3-oxo pentanal)

(7) 

(4-hydroxy butanone)

(8)  4-hexene 3-one

ISOMERISM

ISOMERS: Compounds having same molecular formula but differ in their physical & chemical property.

⇒ This phenomenon is also **Isomerism.**

Types of Isomerism

- **Structural Isomerism**
  - chain Isomerism
  - Position Isomerism
  - functional Isomerism
  - Ring-chain isomerism
  - metamerism
  - Tautomerism
- **Stereo-isomerism**
  - (a) Configurational Isomerism
    - → Geometrical
    - → optical
  - (b) Conformational isomerism

⇒ STRUCTURAL ISOMERISM

→ when Isomerism is due to difference in arrangement of atoms in molecule or

we can say.

compounds having same molecular formula but different in structural formula.

(1) Chain Isomerism

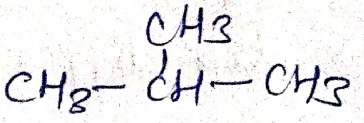
→ Same molecular formula but the order in ≤ Carbon atom are bonded to each other

example:

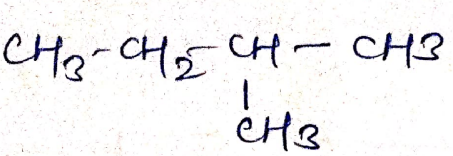
(i) n-Butane

$CH_3-CH_2-CH_2-CH_3$

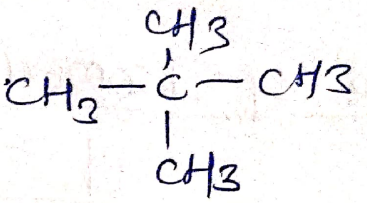
(ii) isobutane



(3) 2-methyl butane



2,2-Dimethyl propane

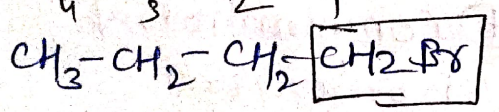


(2) Position Isomerism

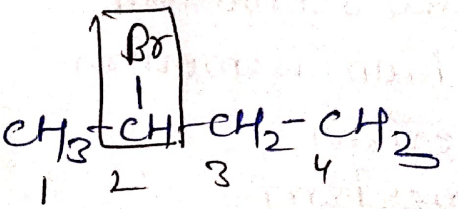
→ same molecular formula.

→ functional group position differs.

eg.



1-bromo butane



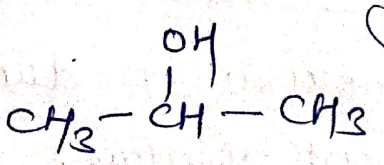
2-bromo butane

eg. (C_3H_8)

$CH_3-CH_2-CH_2-OH$

(n-propyl alcohol)

(C_3H_8)



(iso-propyl alcohol)

BONDS

(1) $CH_3-CH_2-CH=CH_2$

(1-butene)

(2) $CH_3-CH=CH-CH_3$

(2-butene)

(3) functional Isomerism

→ same molecular formula.

→ Differ in functional group.

eg.

CH_3-CH_2-OH

(ethanol)

C_2H_6O ⇐ mol. formula ⇒ C_2H_6O

CH_3-O-CH_3

(Dimethyl ether)

e.g.

$CH_3-\overset{O}{\overset{\|}{C}}-CH_3$

(Acetone)

C_3H_6O ⇜ molecular formula ⇝ C_3H_6O

$CH_3-CH_2-\overset{O}{\overset{\|}{C}}-H$

(Propionaldehyde)

(4) RING CHAIN ISOMERISM

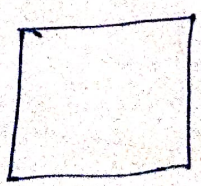
→ same molecular formula.

→ They have different mode of C-C linkage. like (ring/chain)

e.g.

$CH_3-CH_2-CH_2-CH_3$

(butane)



(cyclobutane)

(5) METAMERISM

→ Same molecular formula.
→ Same functional group.
→ But unequal distribution of 'C' on both side of functional group.

e.g.

$C_2H_5-O-C_2H_5$
(di-ethyl ether)

$CH_3-O-CH_2-CH_2-CH_3$
(Methyl propyl ether)

$C_2H_5-NH-C_2H_5$
(diethyl amine)

$CH_3-CH_2-CH_2-NH-CH_3$
(Methyl propyl amine)

(6) Tautomerism

→ same molecular formula
→ Exist in two different interconvertible structure (dynamic equillibrium).

e.g.

$$CH_3-\overset{\overset{O}{\|}}{C}-CH_3 \rightleftharpoons CH_2=\overset{\overset{OH}{|}}{C}-CH_3$$

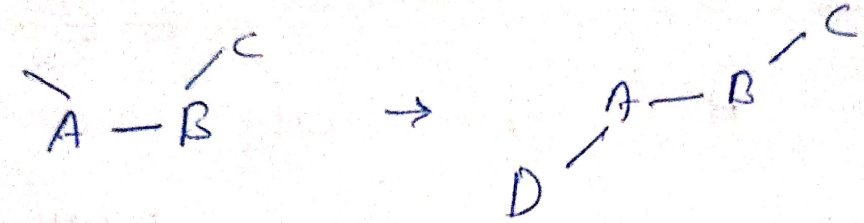
(Keto form) (enol form)

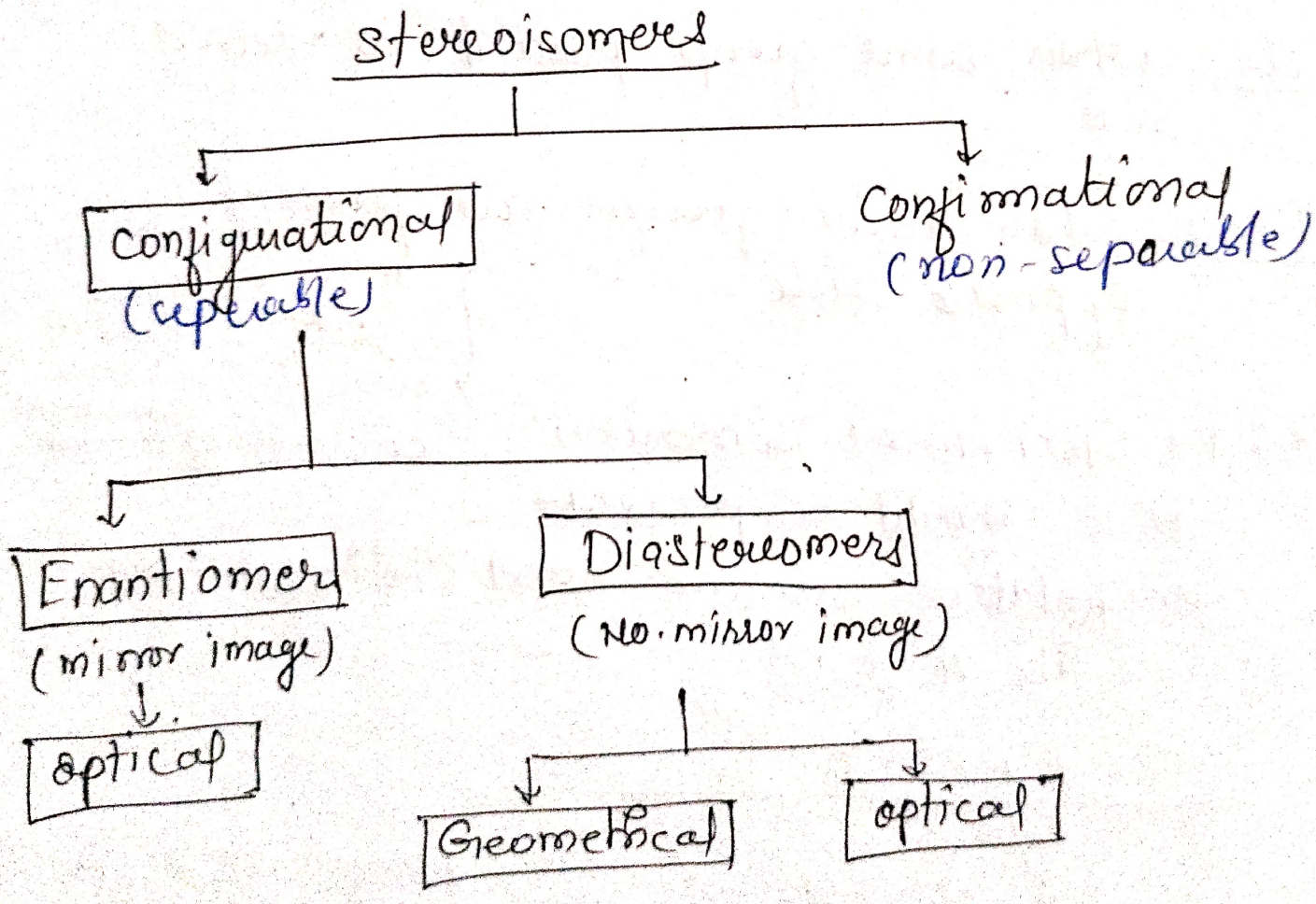
STEREO-ISOMERISM

→ Same molecular formula

→ Same structural formula

→ Different spatial arrangement of atom/grp

e.g. 

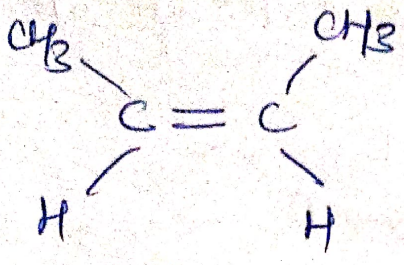


Note: optical isomers, it may be ~~enantiomer~~ mirror image or non mirror image.

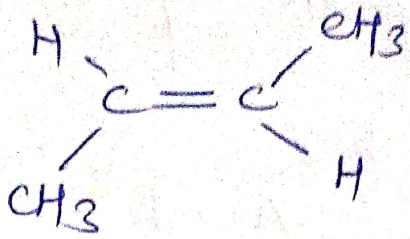
✡ Geometrical is always non-mirror image.

Geometrical Isomerism

e.g. lets understand example.



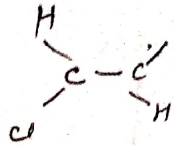
cis
(but-2-ene)



trans
(but-2-ene)

cis : when same group present at same side.

Trans : when same groups are present opposite side.



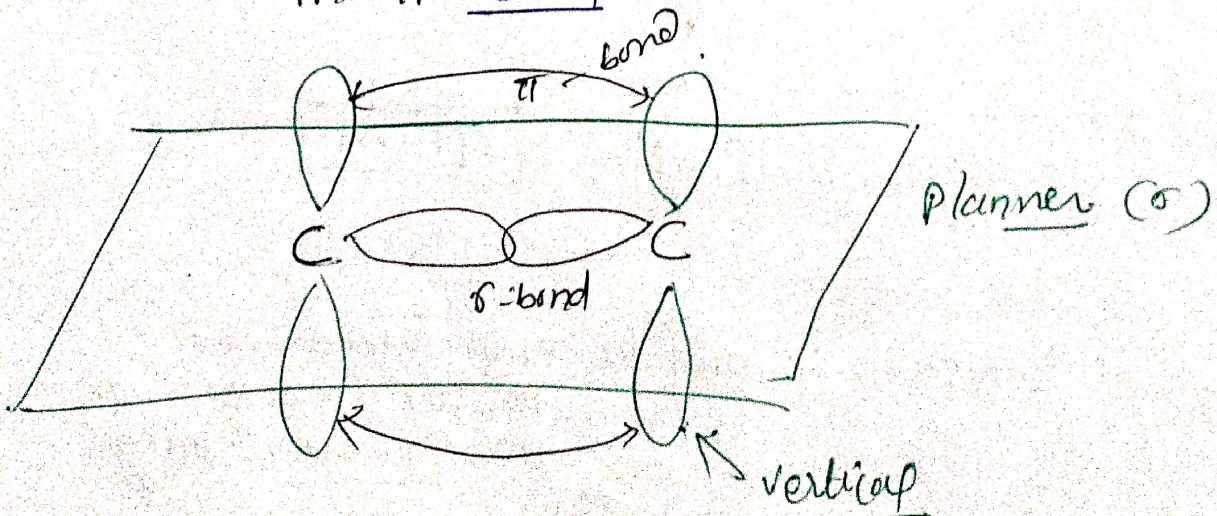
single bond do not have geometrical isomerism

(conformational)

Note : for Geometrical isomerism

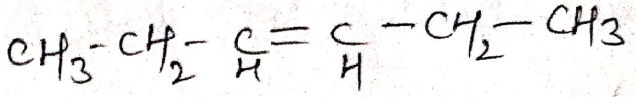
i) = should be present

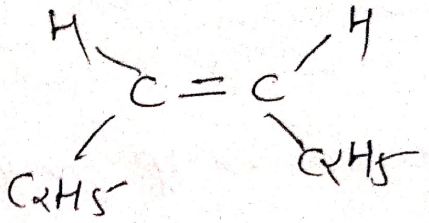
ii) Rotation around bond is restricted.
in π bond.



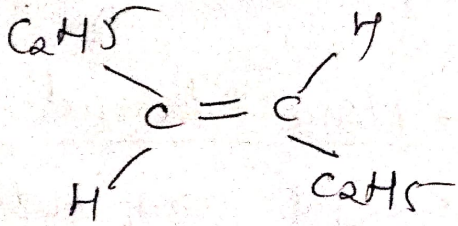
* cis & trans both have different property.

e.g. cis-trans of hex-3-ene



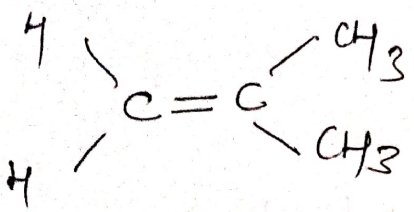


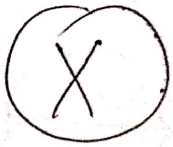
(cis)

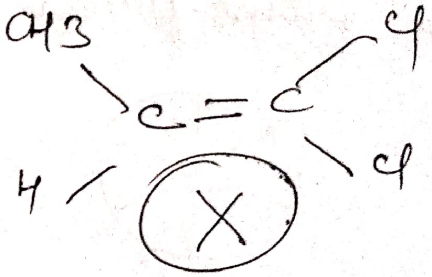


(Trans)

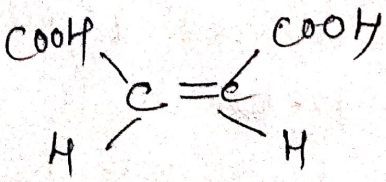
☆ If only 1-C have same group then G.I. is not possible





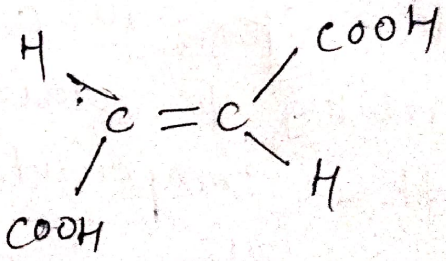


Ex. But-2-ene, 1,4-dioic acid



(cis)

Maleic acid



(Trans)

(fumeric acid)