# Stereochemistry

CO5:- To evaluate and visualise the concept of configurations and conformations of various organic compounds.

Topic :- Isomerism, Types of isomerism i.e, Structural Isomerism & Stereoisomerism.

## 1. Isomerism :-

The organic compounds having same molecular formula but different physical and chemical properties. Such compounds are called isomers and the Phenomenon is known as isomerism.

→ There are two main types of isomerism.

a) Structural isomerism b) Stereoisomerism.

### a) Structural isomerism :-

It is due to different arrangements of atoms within the molecule.

It is further divided into :

(i) Chain isomerism (ii) Position isomerism

(iii) Functional isomerism (iv) Metamerism

(v) Tautomerism

### b) Stereoisomerism :-

It is due to difference in the arrangement of atoms around the carbon atom in space.

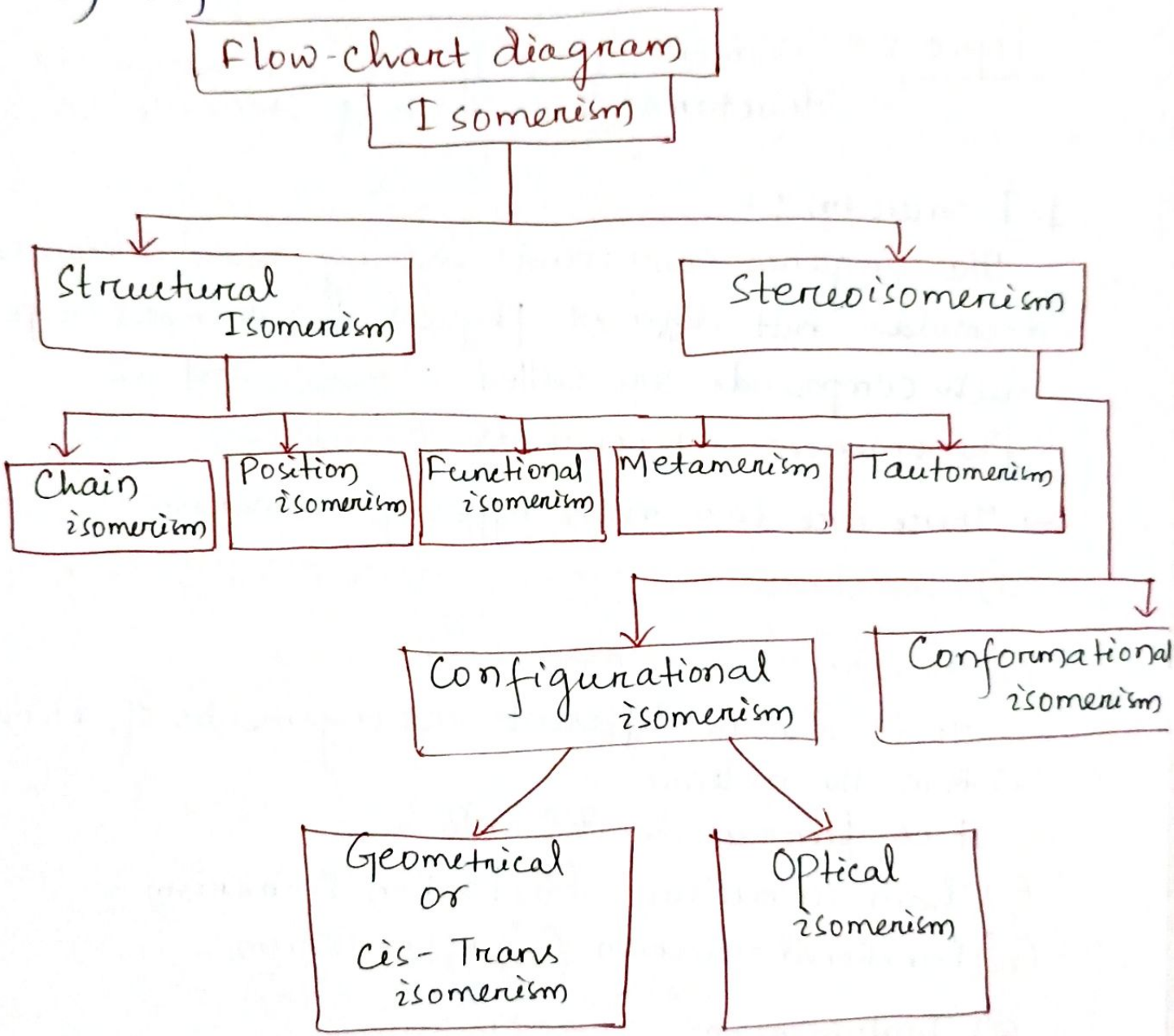
→ Stereoisomers have the same molecular as well as structural formulae but possess different spatial arrangements of atoms in space (3D geometry) i.e, configuration. It is also called space-isomerism.

- It is clasified as

a) Configurational isomerism. It is again divided into two types.
   (i) Geometrical or cis-trans isomerism
   (ii) Optical isomerism

b) conformational isomerism.

Flow-chart diagram




Examples :-

Isomerism :- Pentane ($C_5H_{12}$)

1. $CH_3-CH_2-CH_2-CH_2-CH_3$ [n-Pentane]

2. $CH_3-\underset{\underset{CH_3}{|}}{CH}-CH_2-CH_3$ [2-methyl butane]

3. $CH_3-\underset{\underset{CH_3}{|}}{\overset{\overset{CH_3}{|}}{C}}-CH_3$ [2,2-dimethyl Propane]

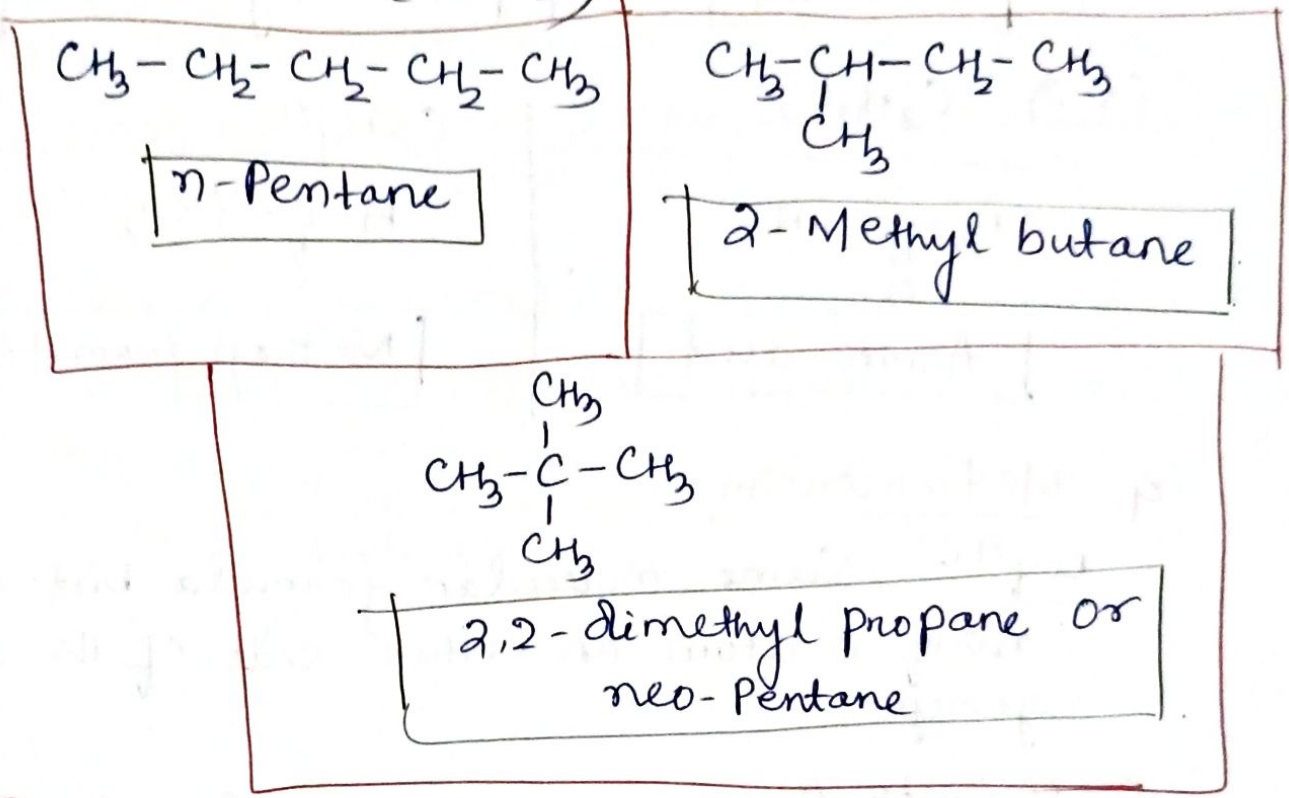
Topic :-

## Structural isomerism :- Types

### a) Chain isomerism :-

Defⁿ :- Same molecular formula but different arrangement of carbon chain.

Ex- Pentane ($C_5H_{12}$)




### b) Position Isomerism :-

Defⁿ :- Same structure of 'C' atom chain but different position.

Ex - But-1-ene | But-2-ene

$CH_3-CH_2-CH=CH_2$ | $CH_3-CH=CH-CH_3$

Ex-2 :- Propan-01-ol | Propan-2-ol

$CH_3-CH_2-CH_2-OH$ | $CH_3-CH(OH)-CH_3$

## 3. Functional isomerism :-

**Defⁿ :-** Same molecular formula but different functional group.

**Ex-1**

| $C_2H_6O$ | $C_2H_6O$ |
|---|---|
| $CH_3-CH_2-OH$ | $CH_3-O-CH_3$ |
| Ethanol | Methoxy methane |

**Ex-2**

| $C_2H_4O_2$ | $C_2H_4O_2$ |
|---|---|
| $CH_3-\overset{\overset{O}{\|\|}}{C}-OH$ | $H-\overset{\overset{O}{\|\|}}{C}-OCH_3$ |
| Acetic acid | Methyl formate |

## 4. Metamerism :-

**Defⁿ :-** Same molecular formula but different no. of 'C' atom on either side of the functional group.

**Ex-1** $C_5H_{10}O$

| $C_5H_{10}O$ | $C_5H_{10}O$ |
|---|---|
| $CH_3-CH_2-CO-CH_2-CH_3$ | $CH_3-CO-CH_2-CH_2-CH_3$ |
| Pentan-3-one | Pentan-2-one |

**Ex-2**

| $C_2H_5-CO-C_2H_5$ | $CH_3-CO-C_3H_7$ |
|---|---|
| Diethyl Ketone | Methyl propyl Ketone |
| $C_5H_{11}N$ | $C_4H_{11}N$ |
| $C_2H_5-N(C_2H_5)-H$ | $CH_3CH_2CH_2-N(CH_3)-H$ |
| Diethylamine | Methyl Propylamine |

Topic:-

5. Tautomerism :- (5)

Defⁿ :- Two different compounds having different functional group which exist in dynamic equilibrium with each other.

Ex (1) ~~Acetg~~ Acetaldehyde & vinyl alcohol are tautomers of each other.

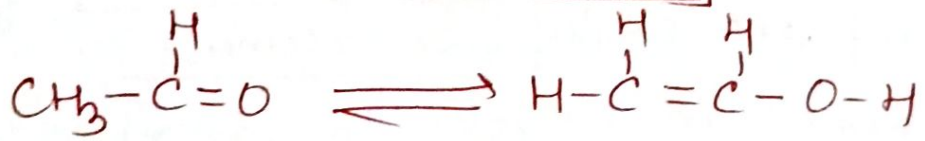
Where, Acetaldehyde being more stable isomer is in large amount as compared to vinyl alcohol.

→ Acetaldehyde contains a keto group ($-\overset{O}{\overset{\|}{C}}-O$)

→ Vinyl alcohol contains an enolic group ($=\overset{O}{\overset{|}{C}}-OH$)

→ This type of tautomerism is called as

**Keto-enol tautomerism**



(2) Stereoisomerism :- Types :-

(1) Configurational :-

Defⁿ :- When same molecular formula represent two or more compounds having different spatial arrangement.

(2) Geometrical Isomerism :- / cis-Trans isomerism

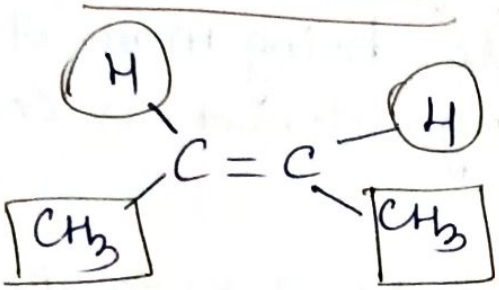
This isomerism is mostly shown by such compounds that contain at least one carbon-carbon double bond and in which each of the doubly bonded carbon atom has same or different.

- sets of two unlike atoms or groups.

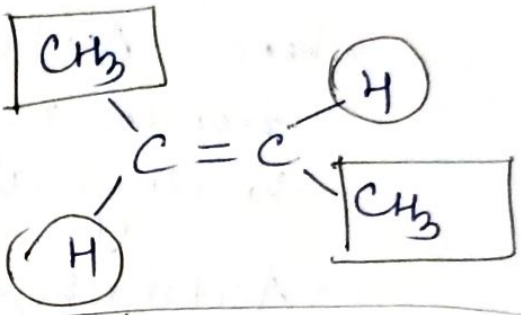
Thus compounds of the type

$abC=Cab$ or $abC=Cxy$ show geometrical isomerism

Ex- 2-butene :-




cis-2-Butene



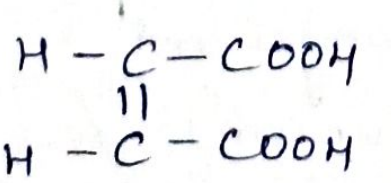

trans-2-Butene

→ Isomers in which similar atoms or groups lie on the same side of double bond are called cis-isomers.

→ Isomers in which the similar atoms or groups lie on the opposite side of double bond are called trans-isomers.

Ex-2 :- Maleic acid

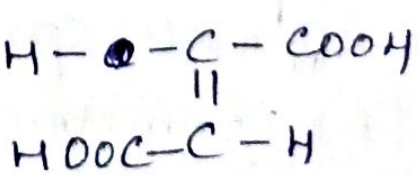
M.P = 130°C




cis-form

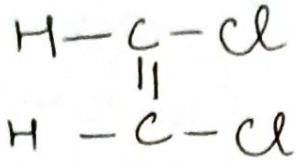
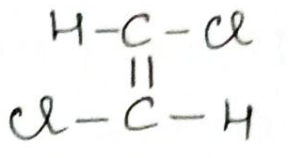
Fumaric acid

M.P = 302°C

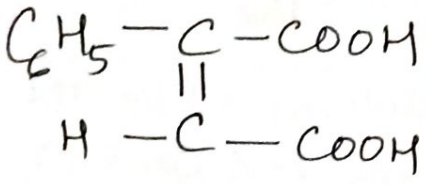



trans-form

## Ex-3 :- Geometrical Isomerism :-

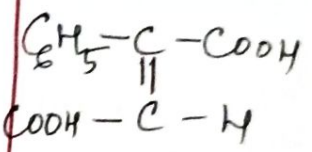
| Dichloroethene (B.P = 60°C) | Dichloroethene (B.P = 48°C |
|---|---|
|  |  |
| Cis-isomer | Trans-isomer |

## Ex-4 :- Allocinnamic acid (b.P = 68°C)



Cis-isomer

Cinnamic acid (b.P-13



Trans-isomer

## E & Z Notation :-

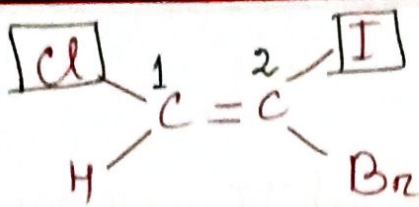
E - stands for - German word **Entgegen** means **against**

Z - stands for - German word **Zusammen** means **together**

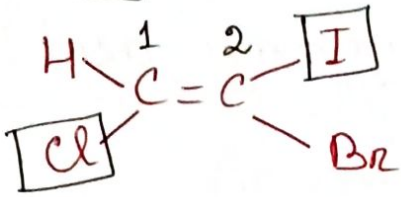
**E-notation :-** If the two groups of higher priority are on opposite sides of double bond, the isomer is **E-configuration**.

**Z-notation :-** If the two groups of higher priority are on same sides of the double bond, the isomer is **Z-configuration**.

Example:-

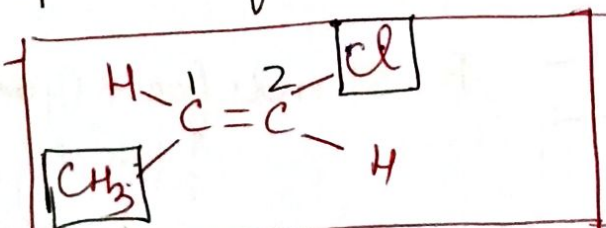



Here, Two groups on carbon 1 are Cl & H, out of which Cl has higher priority. Similarly, out of the on carbon '2' are I & Br, out of which I has Priority over Br. The group of higher priority on each carbon are (Cl & I) on the same side of the double bond. therefore the structure get Z-configuration.

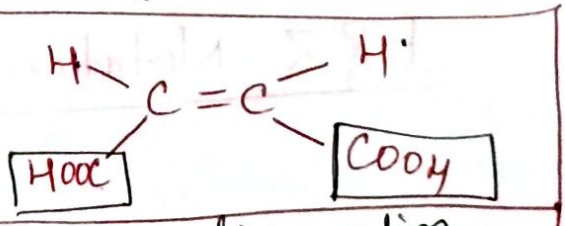



Similarly, above structure, for 1st carbon higher Priority is Cl and for 2nd carbon higher priority is I which is present opposite side of the double bond. therefore the structure get E-configuration

Ex-2:-

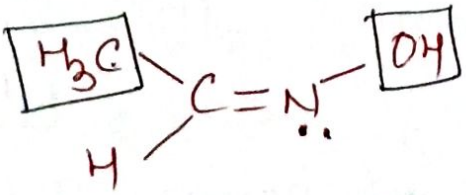



E-configuration



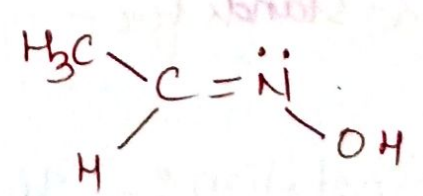

Z-configuration

Ex-3:-




Z-configuration

Acetaldoxime




E-configuration

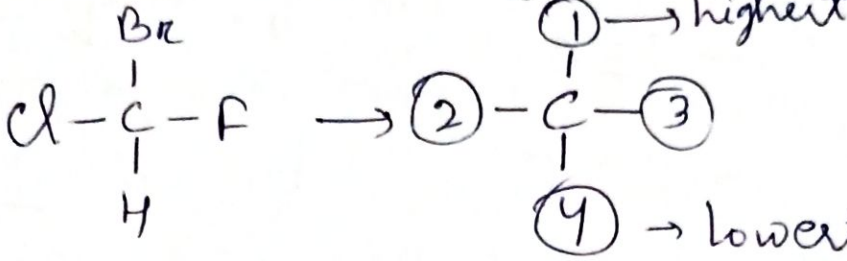
Acetaldoxime

## CIP Rule:-

### Rule-1:-

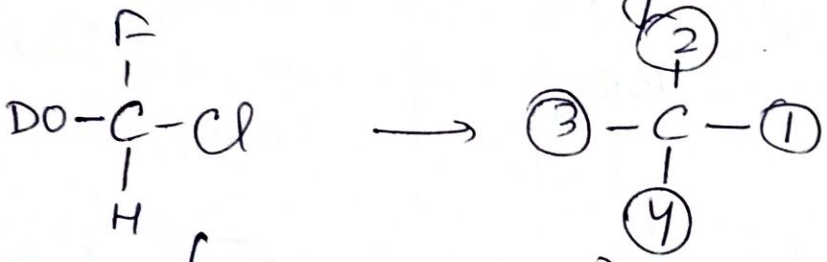
The atom linked to C-atom having higher atomic number gets more priority.

Ex-




### Rule-2:-

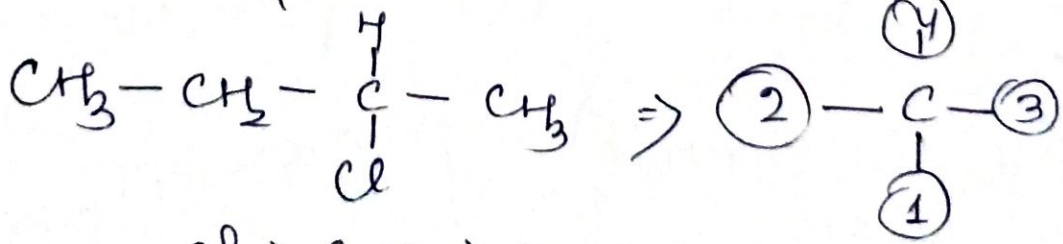
If two isotopes are present, then isotope of higher atomic mass gets higher priority.




(Cl > F > D > H)

### Rule-3:-

When two groups have identical first atom the priority is determined by considering the atomic no. of second atom & if the 2nd atom is also same, the third atom is considered & so on.




Cl > $C_2H_5$ > $CH_3$ > H

### Rule-4:-

When there is a (=) or (≡) bonded atom is present in a group, it is considered as

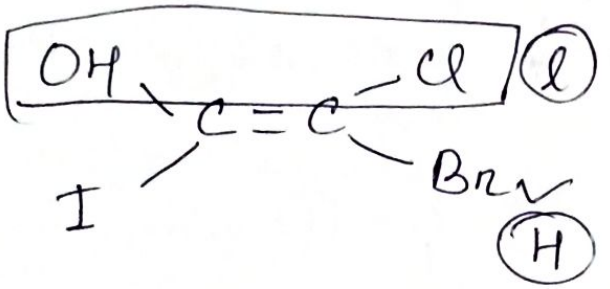
equivalent to two or three single bonded atom respectively

i.e., $-C=C-$ equivalent to $-C\overset{C}{\underset{C}{<}}$

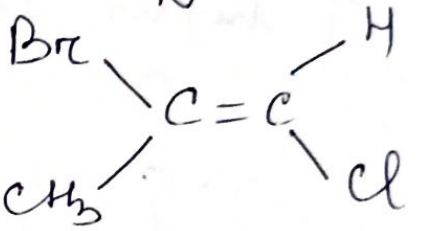
$-C\equiv C-$ " to $-C\overset{C}{\underset{C}{\overset{C}{<}}}$

$-C=O$ " " $-C\overset{O}{\underset{O}{<}}$

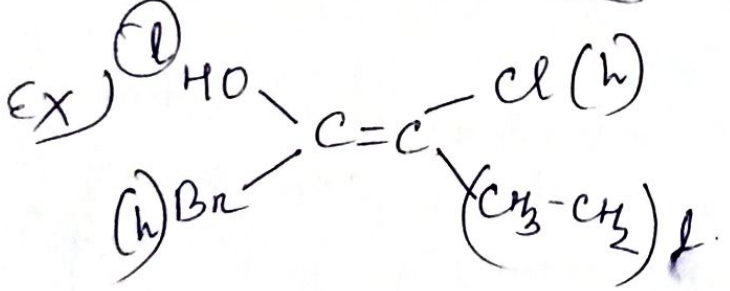
$-C\equiv N$ " " $-C\overset{N}{\underset{N}{\overset{N}{<}}}$

Ex) 

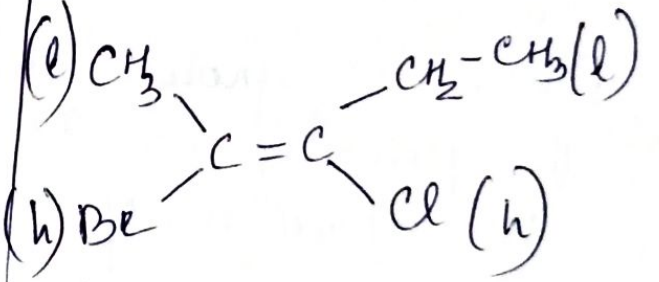

Z-form



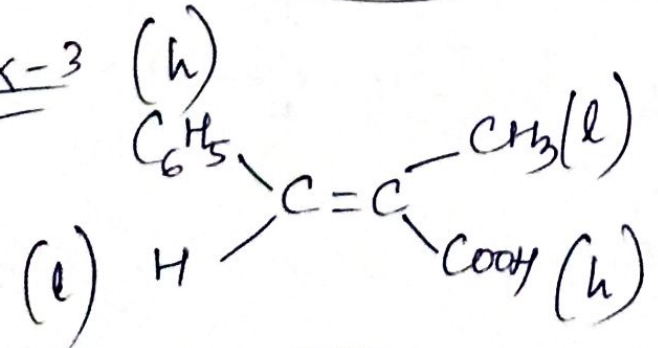

E-form

Ex) 

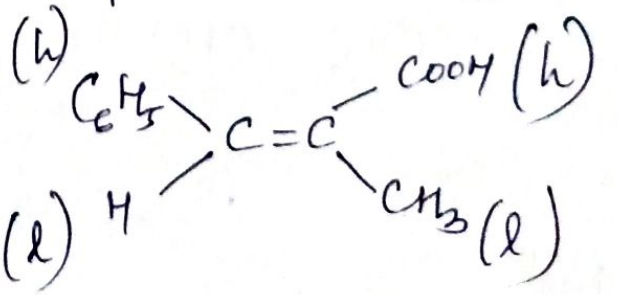

E-form




Z-form

Ex-3 


E-form




Z-form)

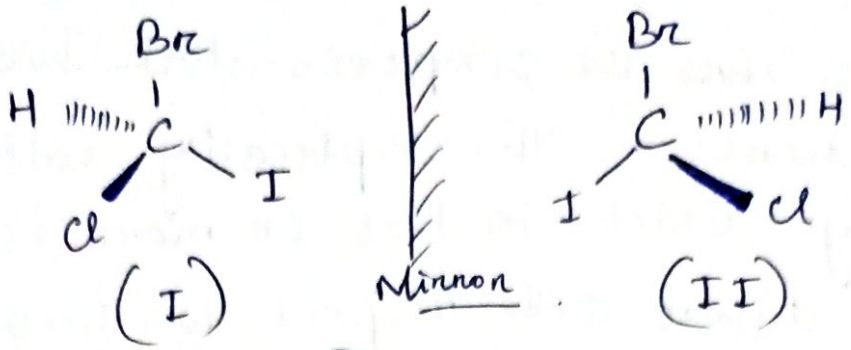
# Topic → Optical Isomerism :-

These are the complexes which have chiral - structures. The optically active compounds always exist in two or more isomeric form, and differ with respect to their optical activity.

There are two main types of optical isomerism

| a) Enantiomerism | (ii) Diastereomerism |
|---|---|
| → These stereoisomers have a mirror image relationship. | → These stereoisomers do not have a mirror image relationship. |
| → These have similar physical properties, such as melting Point, boiling Point, solubility in a given solvent, density. | → These have different Physical Properties such as melting Point, boiling Point, solubility in a given solvent, density etc. |
| → These cannot be separa- -ted by such methods. | → These can be separated by fractional distillation, fractional crystallization and adsorption Chromatography. |
| → They have optical rotation in opposite direction but to the same extent. | → They may have optical rotation in the same or opposite directions but to a different extent. |

Enantiomer :- Bromo-chloro iodomethane

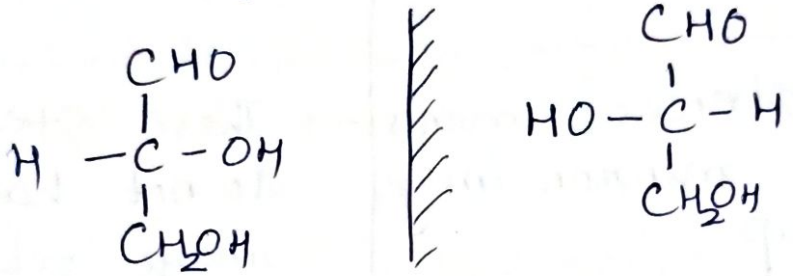



(I) (II)

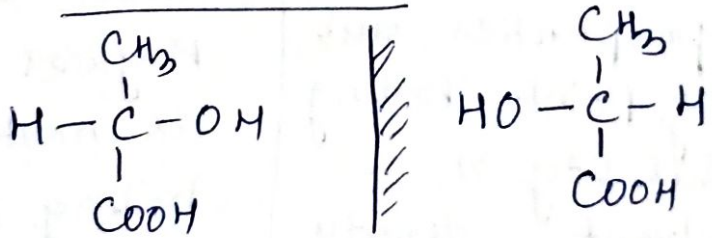
(D-isomer) [Rotate the plane clockwise dextro-]

L-isomer [Anti-clockwise (leavo)]

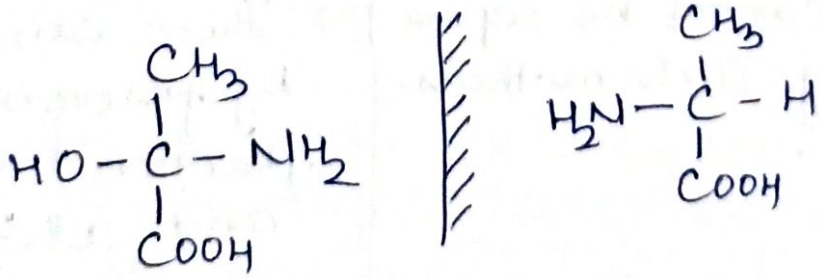
Ex-2 glyceraldehyde



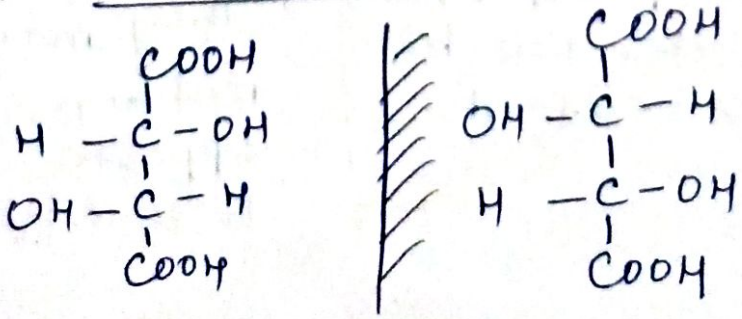

Ex-3 Lactic acid :-




Ex-4 Alanine :-

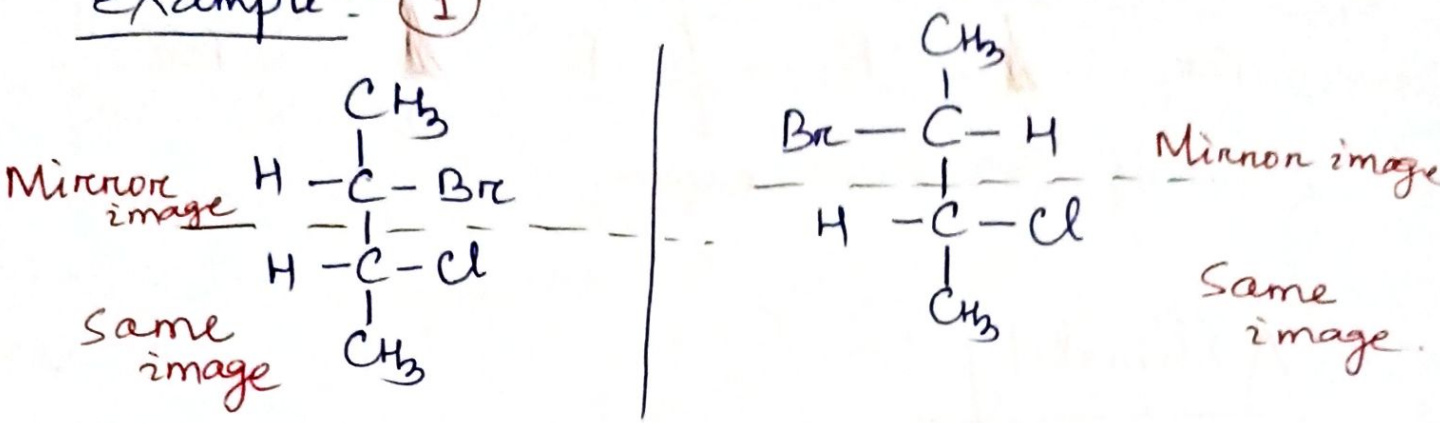



Ex-5 :- Tartaric acid :-



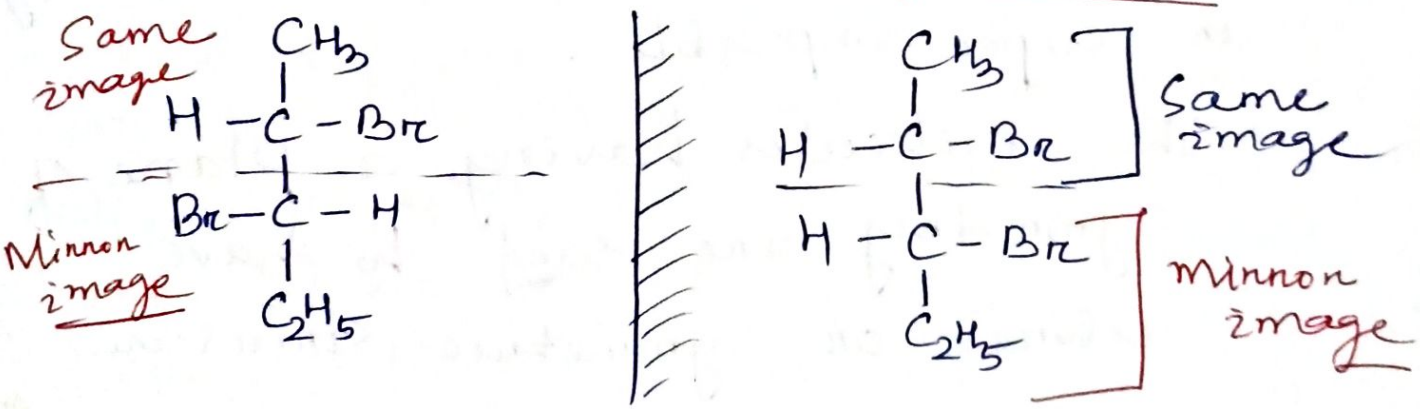
## Diastereomers :-

### Example :- (1)




* One half of the molecules are identical while the other half are mirror image

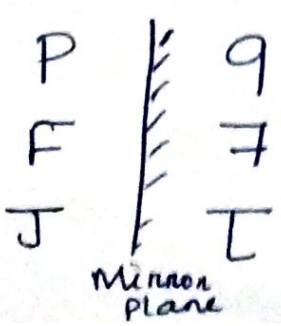
### Example - 2 :- 2 - 3 dibromopentane




## Chirality :-

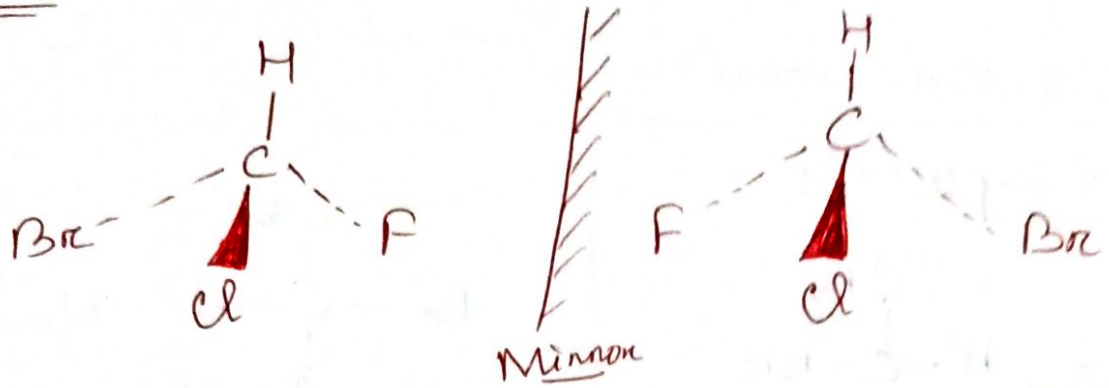
Def$^n$ :- An object that has no plane of symmetry and is not superimposable on its mirror image is said to be chiral or asymmetric structure.

Example :-




Chiral structure due to non-superimposable image

Ex- Bromochloro fluoro methane.




## Achirality :-

Def$^{n}$:- It is a real or an imaginary plane, which when passed through a substance, divides it into two symmetrical halves and the object and it is mirror image are super imposable.

→ The molecules having a plane of symmetry are said to have achiral or symmetric structure.

Example :-

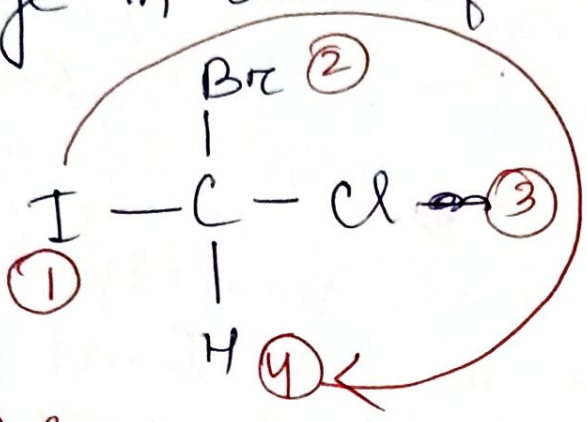
O | O → Achiral due to superimposable image
M | M → Achiral
A | A → Achiral

Mirror Plane

## R-S-Configuration Rule:-

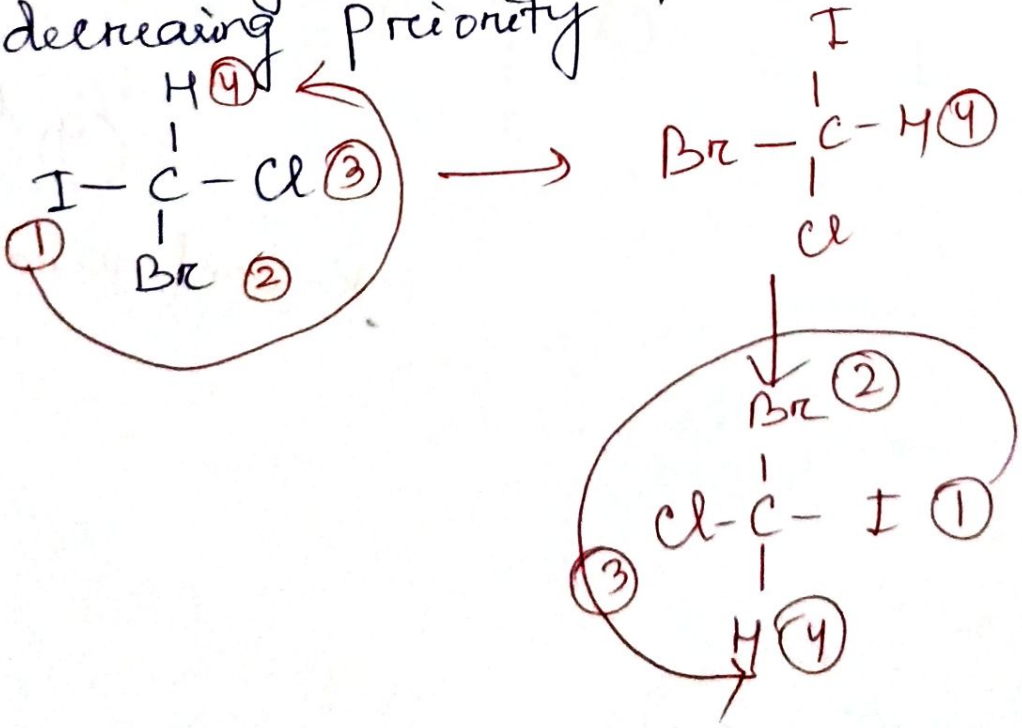
**Rule-1 :-** When the atom or group of least Priority is at the bottom, then simply rotate the eye in order of decreasing Priority.

Ex→



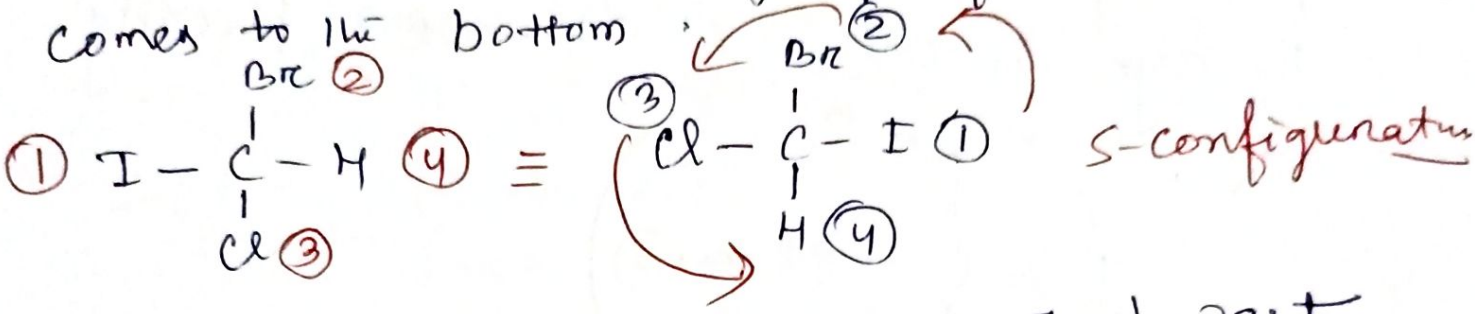

**Rule-2 :-**

When the group of lowest priority is at the top position, then rotate the molecule by 180°. so as to bring the atom or group of lowest Priority to the bottom Now, by rotating the eye in order of decreasing Priority.

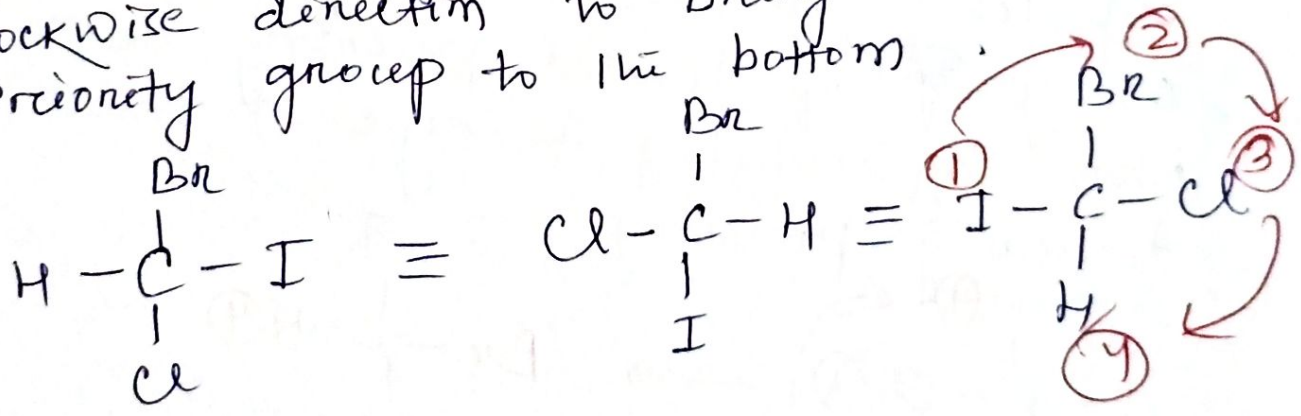



S - Configuration.

**Rule-3 :-** When the atom or group of lowest priority is at the right hand side of horizontal line. In such a case, keep the top position fixed and change the position of other atoms or groups in clockwise direction so that the atom or group of a lowest priority comes to the bottom.




**Rule-4 :-** When the group of lowest priority is at the left hand side of horizontal line. In such a case, keep the top position fixed & change the position of the remaining atom or groups in the clockwise direction to bring the lowest priority group to the bottom.



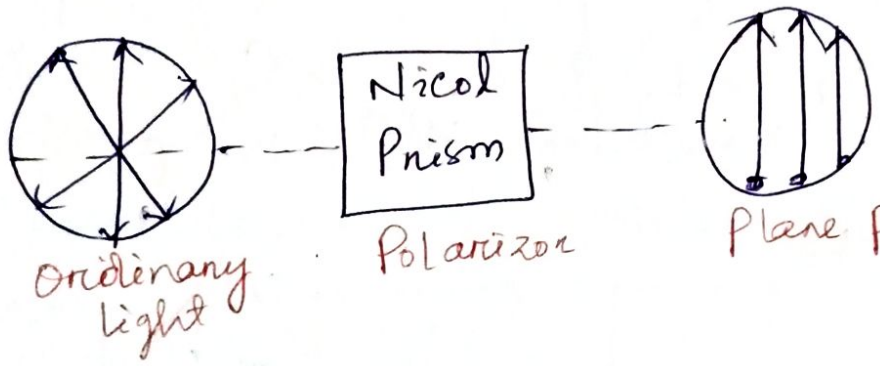
## Optical isomerism :-

### Monochromatic light :-

A beam of light with waves of same wave length is known as monochromatic light.

### → Plane-Polarized Light :-

Light wave vibrations takes place only in one plane is known as plane polarized light.




### R-S- Configuration :-

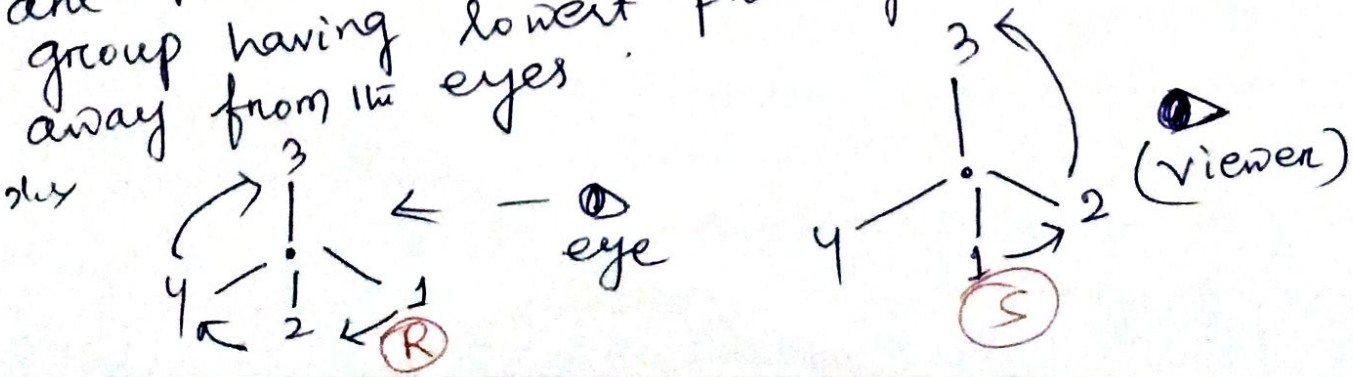
R → Rectus which means right or clockwise

S → Sinisten which means Left or anticlockwise.

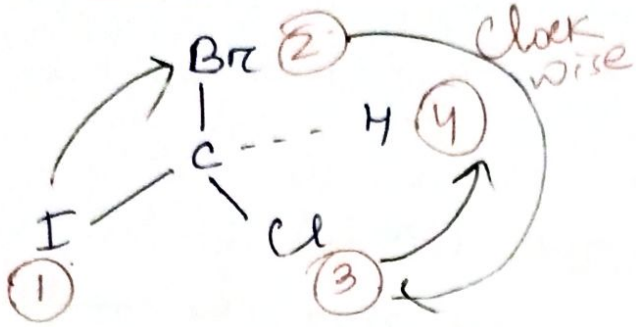
### Procedure :-

step-1 :- Priority is given to all four c' atoms according to CIP rule.

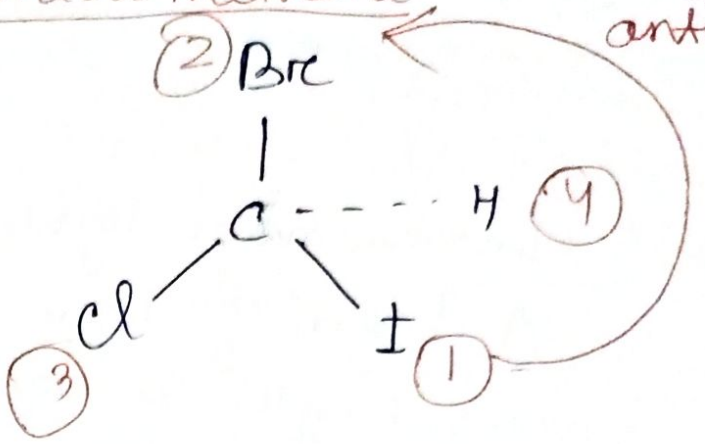
step-2 :- After giving Priority, the molecule are visualised in such a way that the group having lowest priority is directed away from the eyes.



Ex-1 :- Bromochloridomethane

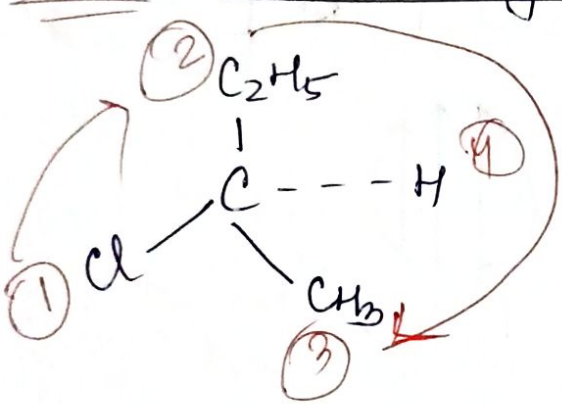



R-configuration

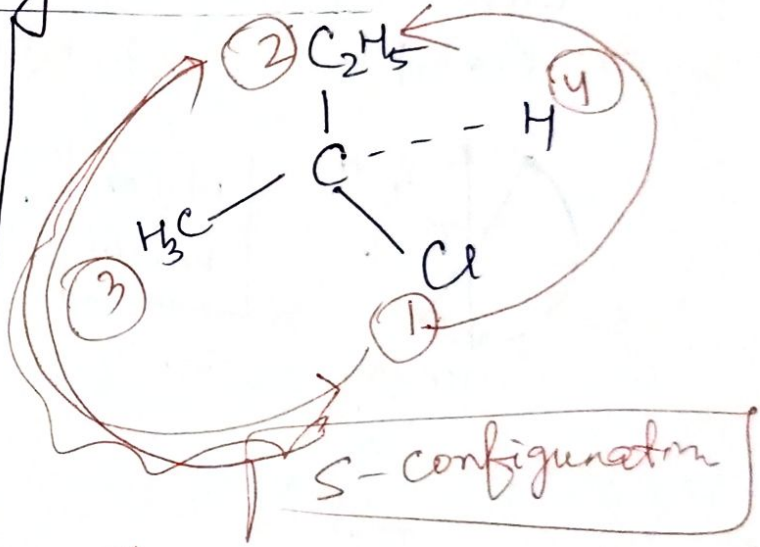



S-Configuration

Ex-2: Secondary Butyl chloride :-

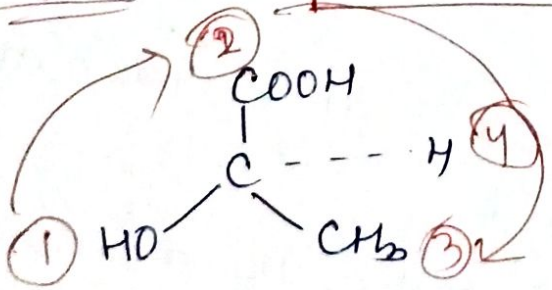



R-configuration

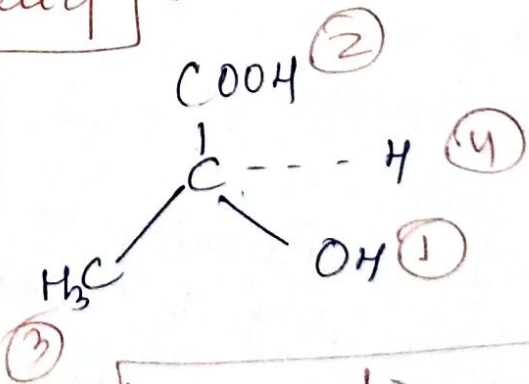



S-configuration

Ex-3 :- Lactic acid




R-configuration




S-configuration