

Unit III:-

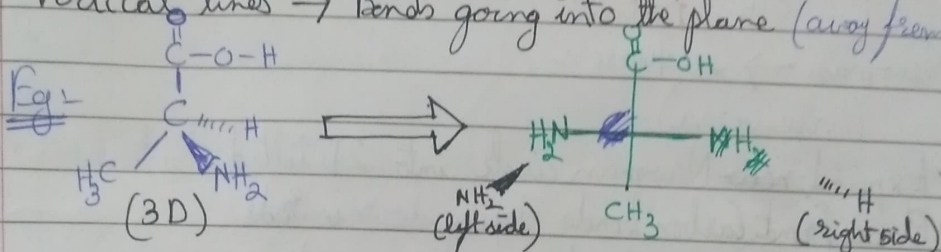
- 1) Study on the projections to represent the organic compounds and interconversions.

Sol:- Projection Types:-

1) Fischer Projection:-

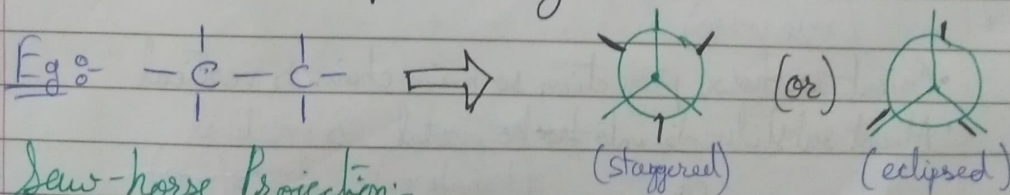
Organic compounds represented by:-

- Represent molecule in 2D plane
- Horizontal lines \rightarrow Bonds coming out of plane (towards observer)
- Vertical lines \rightarrow Bonds going into the plane (away from observer)



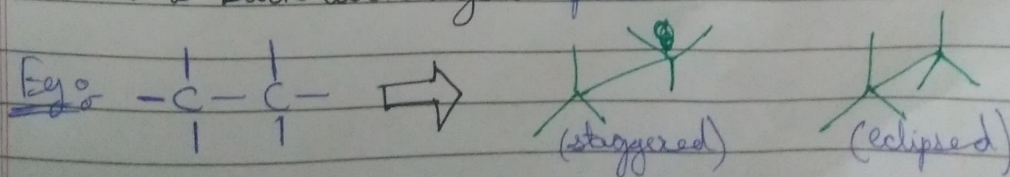
2) Newman Projection:-

- Visualize conformation by looking along C-C bond axis
- Front Carbon \rightarrow Represented by dot
- Back Carbon \rightarrow Represented by circle



3) Saw-horse Projection:-

- Tilted 2D view of molecule
- Bonds to Front Carbon goes downward
- Bonds to Back Carbon goes upward



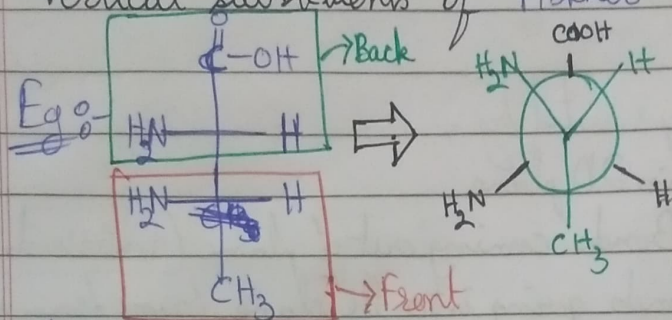
Interconversion :-

1) Fischer \rightarrow Newman :- (vice versa)

- Identify bond of interest (C-C bond)

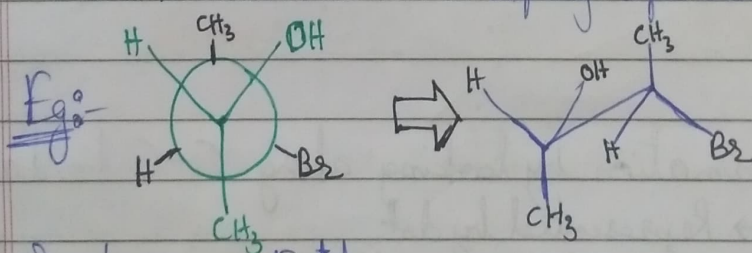
• Horizontal substituents of Fischer \Rightarrow Front carbon of Newman

• Vertical substituents of Fischer \Rightarrow Back carbon of Newman



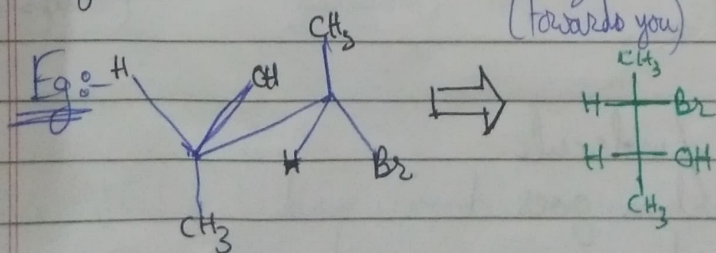
2) Newman \rightarrow Sawhorse :- (vice versa)

- Expand ~~new~~ Newman circle into 2D tilted structure
- Place Front Carbon bonds sloping downwards
- Place Back Carbon bonds sloping upwards



3) Sawhorse \rightarrow Fischer :- (vice versa)

- Orient sawhorse projection so main chain is vertical
- Adjust substituents into ~~the~~ horizontal & vertical
(towards you) (away from you)



2) Explain the steps to determine R/S configuration using Cahn-Ingold-Prelog (CIP) rules

Sl:- To determine R/S configuration, CIP rules are as follows:-

1) Assign Priorities/Rank to Substituents

- Rank the 4 substituents attached to chiral center (Based on Atomic no.)
- Higher Atomic number (Z) \rightarrow Higher Priority/Rank
- If two atoms are same, compare the next set of atoms along the chain until a difference is found
- Alkyl group (CH_3) $<$ Alkene ($\text{CH}_2=\text{CH}_2$) $<$ Alkyne ($\text{CH}\equiv\text{CH}$)

2) Orient the Molecule:-

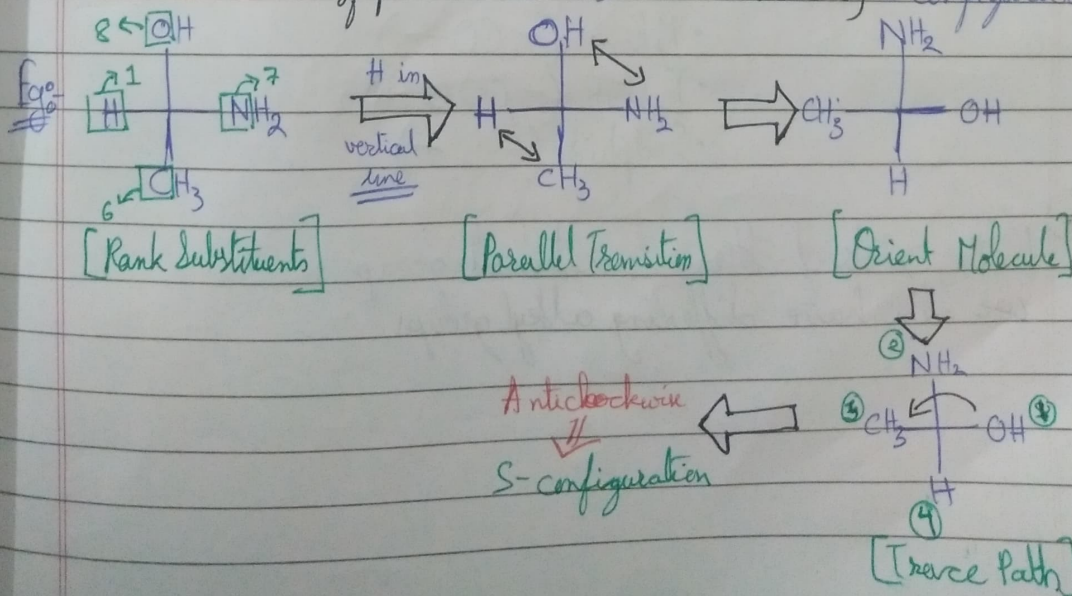
- Position molecule such that the substituent with lowest priority (4) is pointing away from observer (dashed line) / (vertical line)

3) Trace a Circle:-

- Trace a circular path from highest (1) to lower priority (2)
- Ignore lowest priority (4)

4) Determine Direction

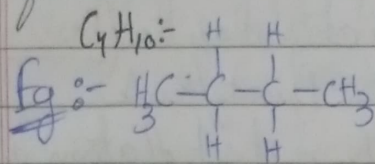
- Clockwise:- If path $1 \rightarrow 2 \rightarrow 3$ is clockwise, R configuration
- Anti-clockwise:- If path $1 \rightarrow 2 \rightarrow 3$ is anti-clockwise, S configuration



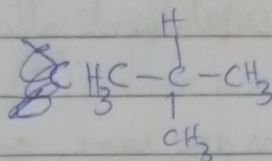
3) Mention the types of structural isomerism of organic compounds with examples.

Sol: Types of structural isomerism of organic compounds are:-

i) Chain Isomerism:- Same chemical formula but differ in structural formula.

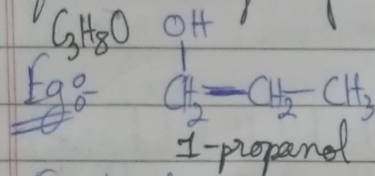


n-butane

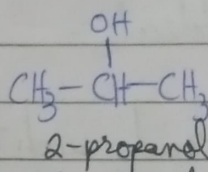


iso-butane

ii) Position Isomerism:- Same chemical formula but differ in position of functional group

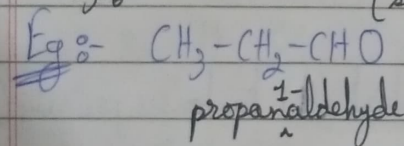


1-propanol

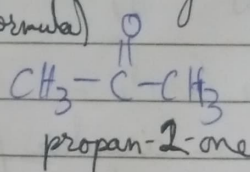


2-propanol

iii) Functional Isomerism:- Differing ~~chem~~ functional group present (same chemical formula)



propanaldehyde



propan-2-one

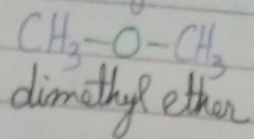
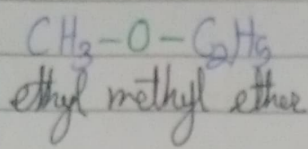
iv) Metamerism:- Differing alkyl group in same functional group

This is applicable for:-

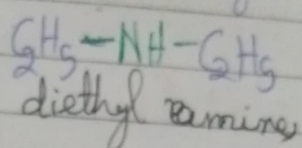
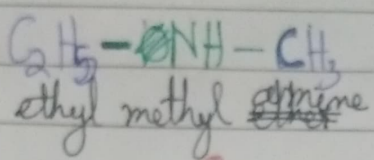
- Ether (-O-)
- Amine (-NH-)
- Ketone (-CO-)
- Ester (-COO-)
- Sulphide (-S-)

Either side of these functional groups, we can have differing alkyl groups

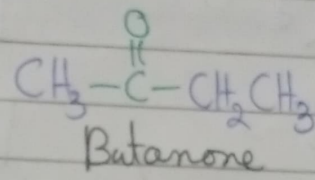
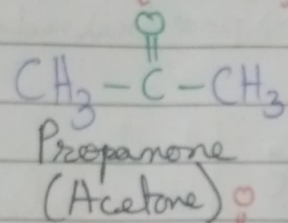
• For Ether ($-O-$): [Naming: Right alkyl + Left alkyl + ether]



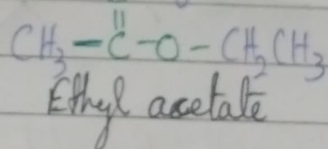
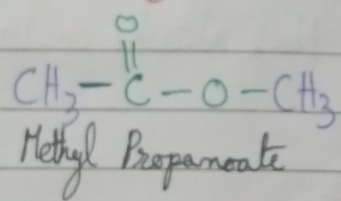
• For Amine ($-NH-$ or $-NR-$): [Naming: Left alkyl + Right alkyl + amine]



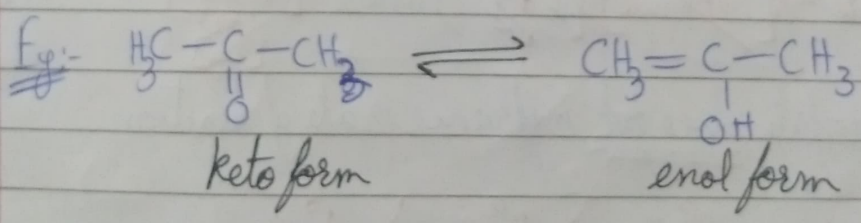
• For Ketone ($-C(=O)-$):



• For Ester ($-C(=O)-O-$): [Naming: Right alkyl + Left alkyl + oate]



✓ Tautomerism: 2 functional isomers exist together in \rightleftharpoons



Keto form is more stable than Enol form :-

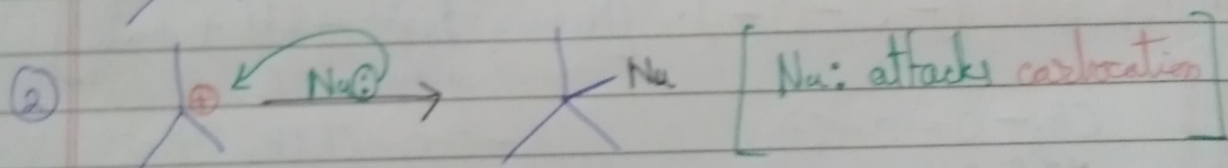
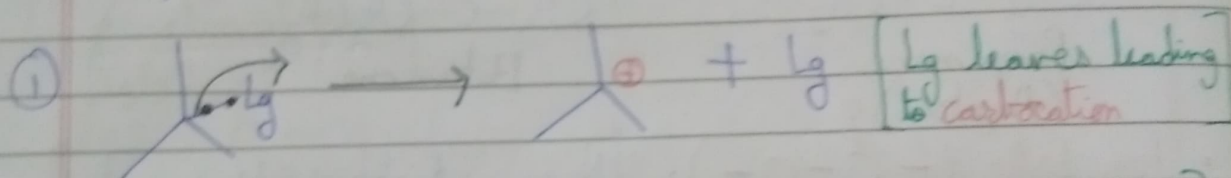
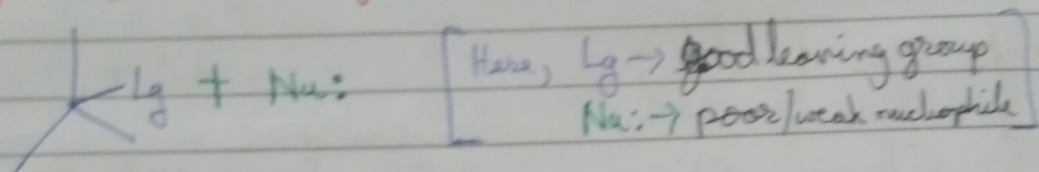
- 1) Resonance stability in keto form
- 2) Bond strength greater in $C=O$ (keto) $>$ $C=C$ (enol)
- 3) Hydrogen Bonding (in enol) $<$ Resonance stability (in keto)

4) Discuss in detail SN1 and SN2 mechanisms with examples and compare them.

Self SN1 :- Unimolecular Nucleophilic Substitution

Here, Nucleophile \rightarrow proton loving
Unimolecular \rightarrow reaction takes place 1 molecule at a time
(1st order reaction)

Steps :- (Mechanism)



The 1st step is the Rate determining step

$$\text{Rate} = k [\text{Substrate}]^1 [\text{Lg}]^0, \text{ where } [\text{Substrate}] \rightarrow \text{conc. of Lg}$$

Here, nucleophile does not influence rate of reaction

For stability :- $3^\circ > 2^\circ > 1^\circ$
fastest SN1 slowest SN1

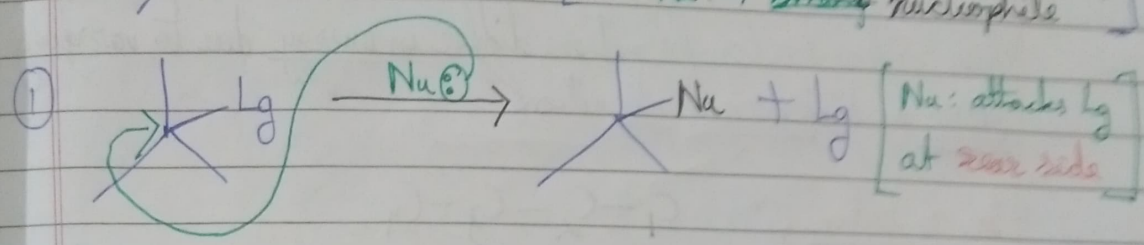
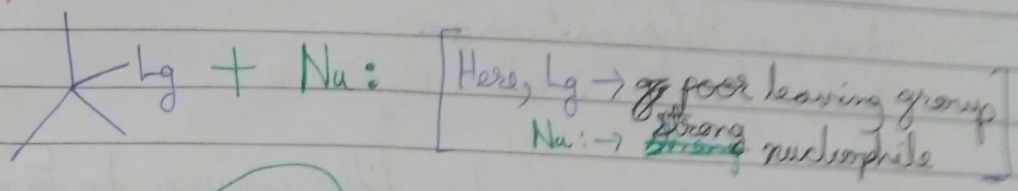
• $\text{Lg} \rightarrow$ good leaving group = Faster SN1
bad leaving group = slower SN1

• Polar Protic (Eg: H_2O , ROH) \rightarrow favours SN1

SN2:- Bimolecular Nucleophilic Substitution

Here, Nucleophile \rightarrow proton loving
Bimolecular \rightarrow reaction takes place 2 molecules at a time
(2nd order reaction)

Steps :- (Mechanism)



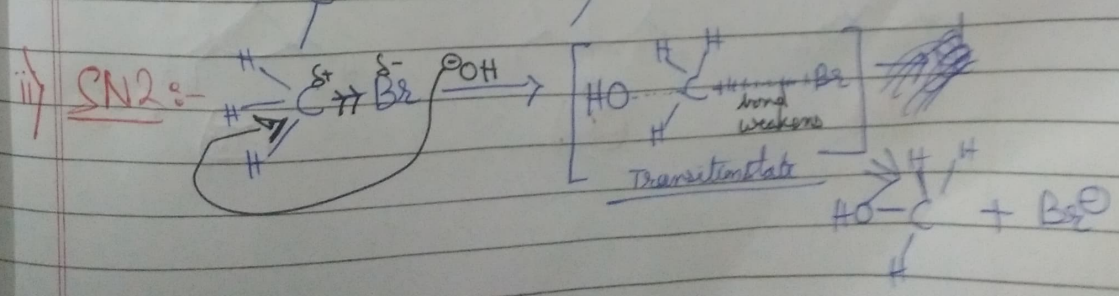
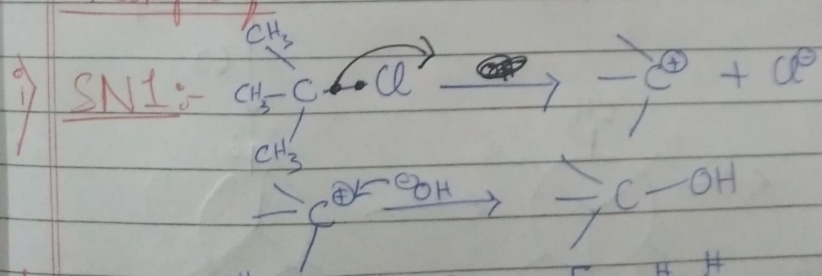
SN² is single-step reaction which is the rate determining step

Rate = $k [Nu:] [R-X]$, where $[Nu:] \rightarrow$ conc. of nucleophile
 $[R-X] \rightarrow$ conc. of substrate

Here, nucleophile influences rate of reaction

- For stability :-
- $Kg \rightarrow Nu:$ strength \rightarrow strong nucleophile = Faster SN2
weak nucleophile = Slower SN2
 - Polar Aprotic (Acetone, DMF) \rightarrow favours SN2

Example of :-



Q) Explain with a neat diagram about the conformational analysis of n-butane

Sol: Conformational Analysis:-

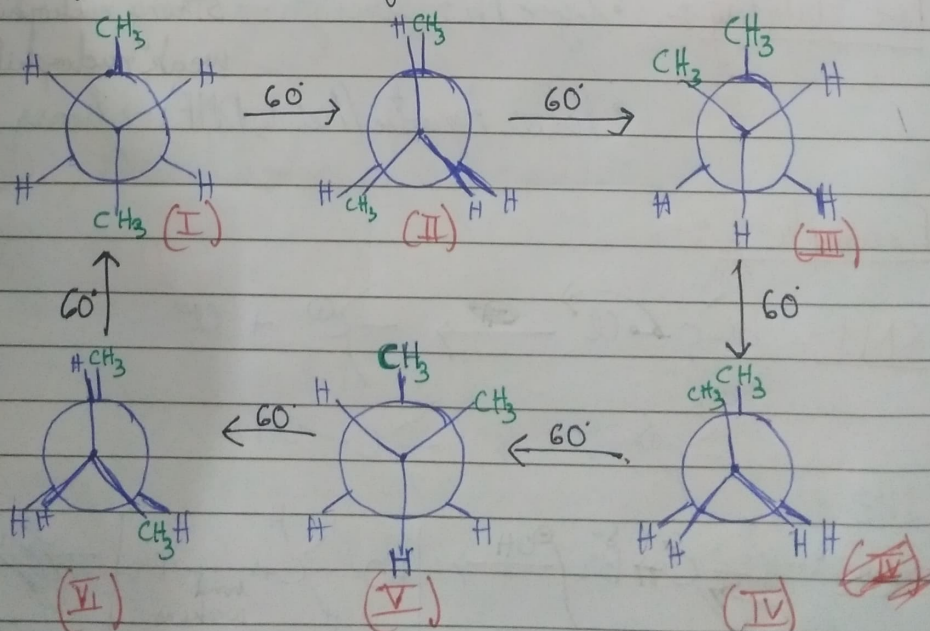
It is the study of the different spatial arrangements of atoms in molecule known as conformations.

Each conformation is called conformer.

These conformers/conformations differ in energy due to varying steric and torsional interactions.

In n-butane, $C_1 - C_2 - C_3 - C_4$

- The C-C bond connecting the 2 middle carbons ($C_2 - C_3$) is symmetrical about nuclear axis.
- This symmetry allows free rotation of $C_2 - C_3$ without breaking the C-C bond.
- This free rotation ~~allows~~ leads to various arrangements of methyl groups and hydrogen attached to $C_2 - C_3$.



Types of Conformations :-

- 1) Anti-Conformation :-
When two methyl groups (CH_3) are 180° apart
Energy \rightarrow lowest
- 2) Gauche Conformation :-
When two methyl groups (CH_3) are 60° apart
Energy \rightarrow moderate
- 3) Eclipsed Conformation :-
When two methyl groups (CH_3) are 0° or 120° apart
Energy \rightarrow highest

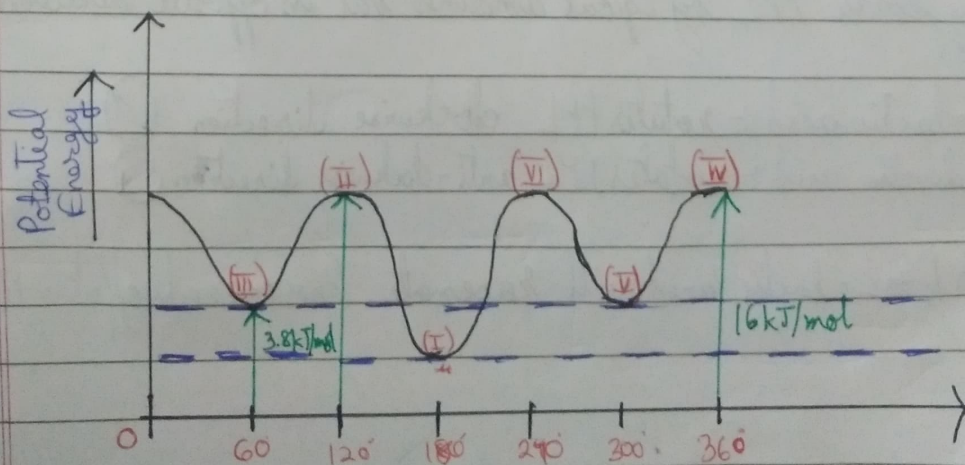
Based on these types :-

- (I) \Rightarrow Anti-conformation, staggered (stable)
- (II), (IV), (VI) \Rightarrow Eclipsed conformation, eclipsed (unstable)
- (III), (V) \Rightarrow Gauche conformation (relatively stable)

In Eclipsed conformation, repulsion betⁿ the 2 methyl groups is high. Hence, highly unstable

In Gauche conformation, repulsion betⁿ the 2 methyl groups is moderate. Hence, relatively stable

In Anti-conformation/staggered, repulsion betⁿ the 2 methyl groups is low as they are on opposite sides. Hence, highly stable



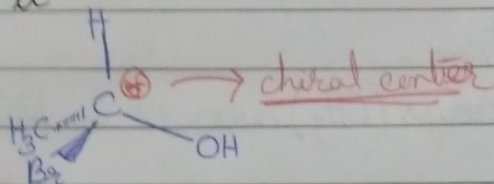
Q) Provide a brief account of Enantiomers and Diastereomers

Solⁿ Stereoisomers have same molecular formula and connectivity but differ in spatial arrangement of atoms

Optical isomers are stereoisomers that can rotate plane-polarized light which arises due to presence of chiral centers

Here, Chiral center is an atom that has 4 different groups attached to it

Eg:-



There are 2 types of Optical Isomers:-

Enantiomers

Diastereomers

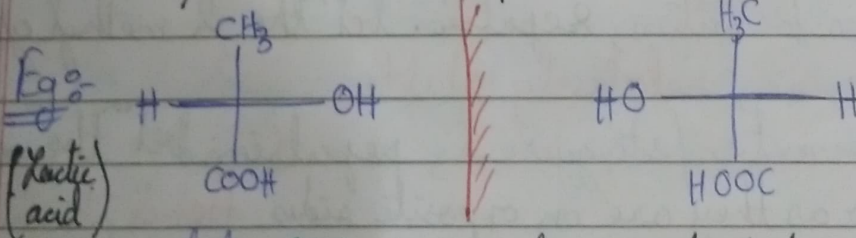
1) Enantiomers:-

Optical

• Isomers which are non-super imposable mirror images of each other.

• They are distinguished by:-

i) +/- ii) ~~D/L~~ D/L (dextro/levo)



They rotate PPL by equal amounts but in opposite directions

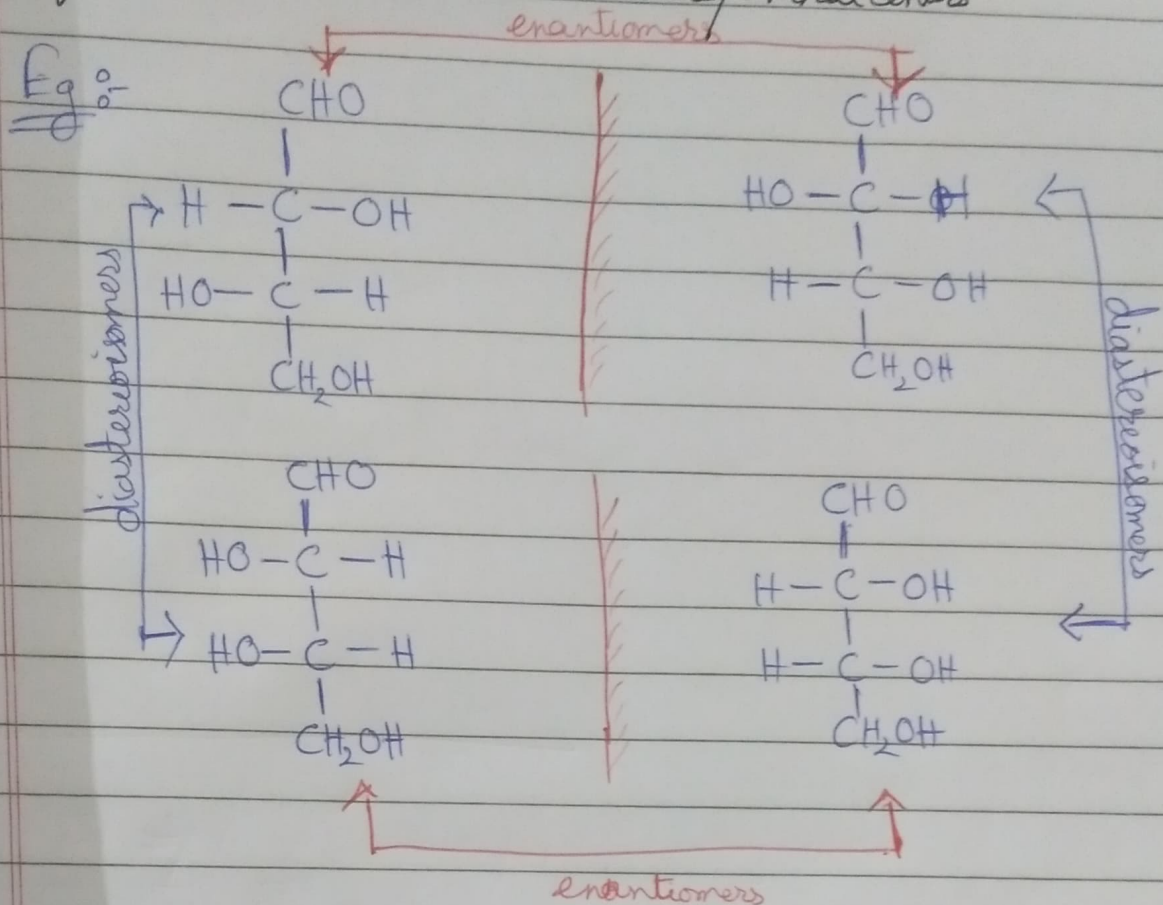
D-lactic acid :- rotates PPL clockwise direction ↻

L-lactic acid :- rotates PPL anti-clockwise direction ↺

Both D & L-lactic acid will racemate (no overall effect on PPL)

2) Diastereomers:-

- Optical Isomers which are non-super imposable non-mirror image
- They have 2 or more stereocenters/chiral centers



Racemic Mixture:-

A Racemic Mixture contains equal amounts of two enantiomers in the ratio (1:1)

It means it contains D & L Enantiomers

∴ No optical activity no change in PPL

Hence Racemic Mixtures are optically inactive