

MODULE IV

STEREOCHEMISTRY AND POLYMER CHEMISTRY

Kavitha S

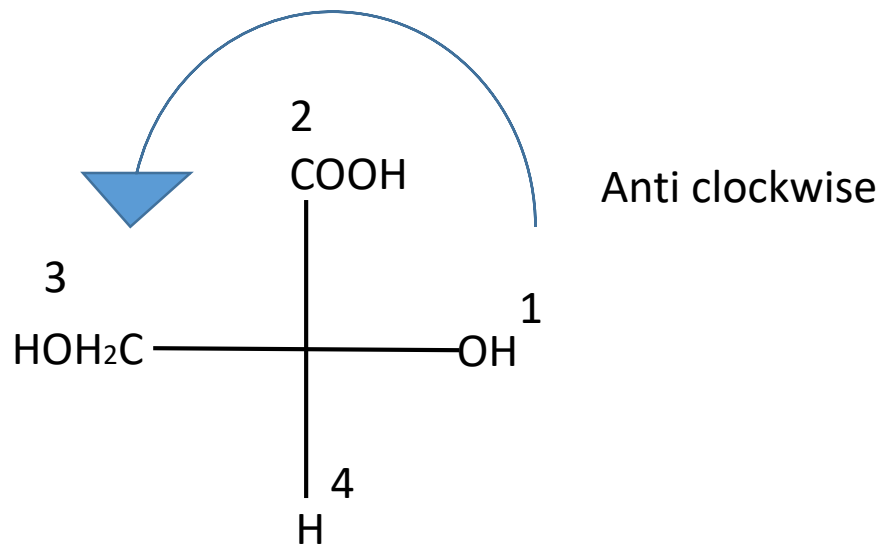
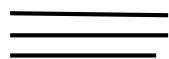
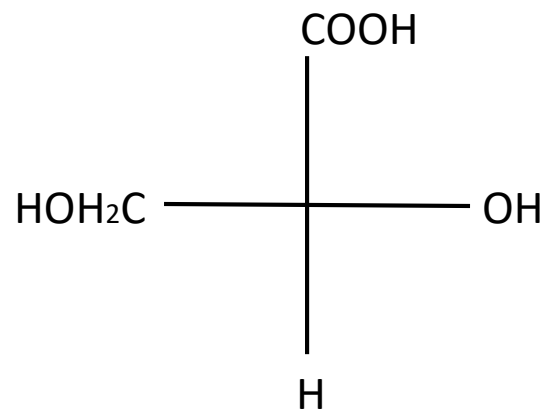
R and S Configuration for Optical Isomers

□ This nomenclature is applied to chiral molecules based on a priority sequence assigned to groups around an asymmetric carbon atom.

The rules are:

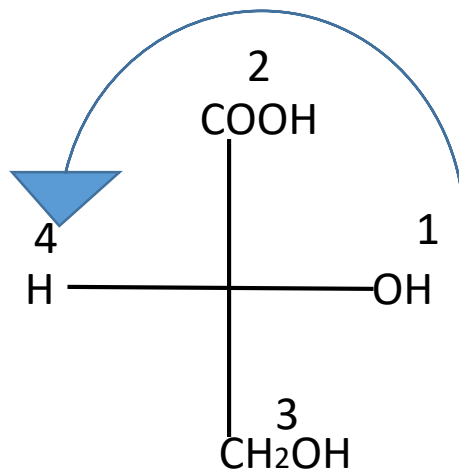
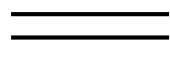
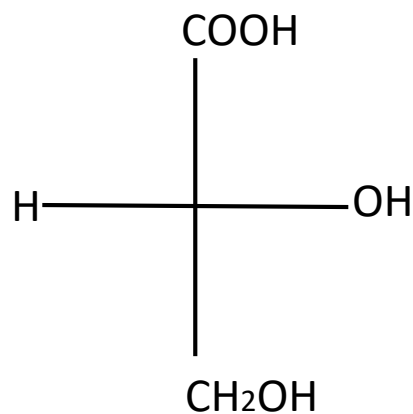
1. The directly attached atom having highest atomic number has highest priority.
2. When two directly attached atoms are same then look for the atomic number of the next linked atom.
3. For double bonds like -C=O , -C=C are treated as two oxygen attachment and two carbon attachment respectively to first atom.
4. The molecule is viewed such that the lowest priority group is away from us and look for priority order, if the sequence is clockwise the notation **R** is given, if it is anticlockwise notation **S** is given.
5. If lowest priority group given in a structure is towards us take opposite rotation of what obtained from front side.

1. Assign R, S notation to Fischer formula:



Anti clockwise

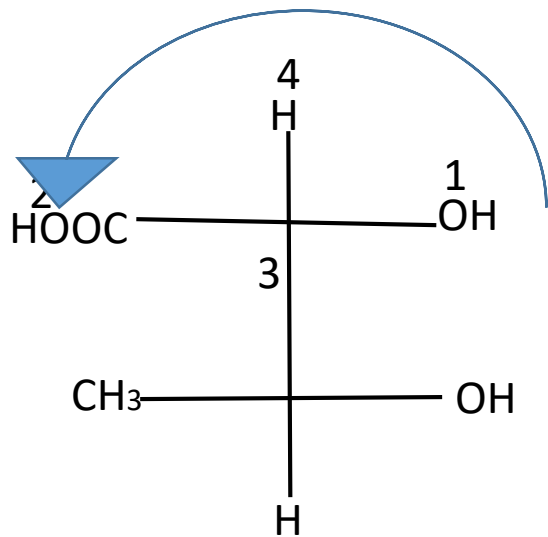
Lowest priority group back side
(S)-2,3 dihydroxypropanoic acid



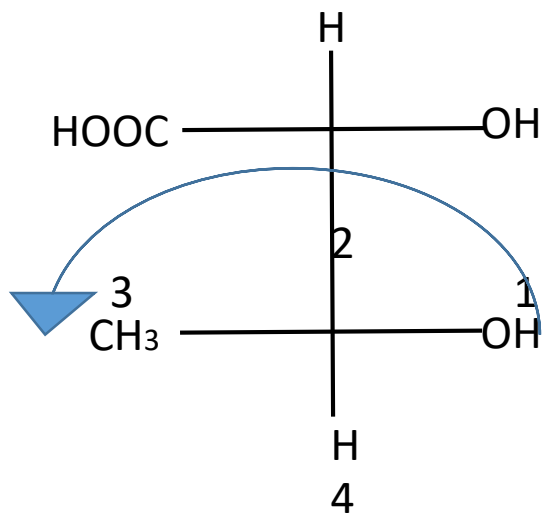
Lowest priority group front side
Anticlock from front so clockwise from back

(R)-2,3 dihydroxypropanoic acid

2. Assign R,S notation to Fischer projection formula for two chiral carbon molecules



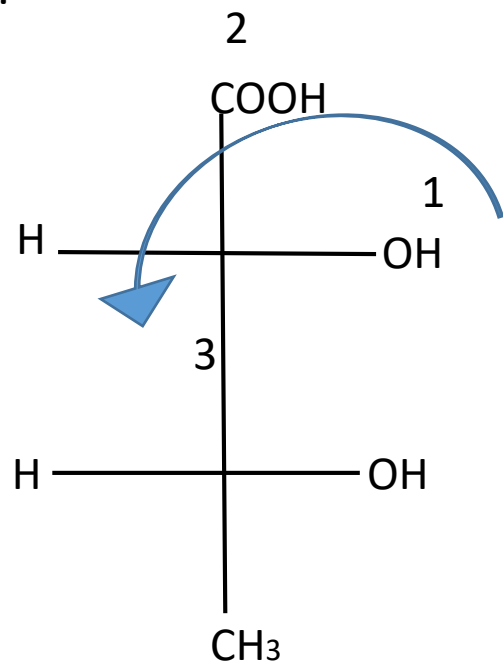
Carbon 2
H-atom is on vertical line
Anticlockwise
S notation



Carbon 3
H-atom is on vertical line
Anticlockwise
S notation

2(S) 3(S) – dihydroxybutanoic acid

3.

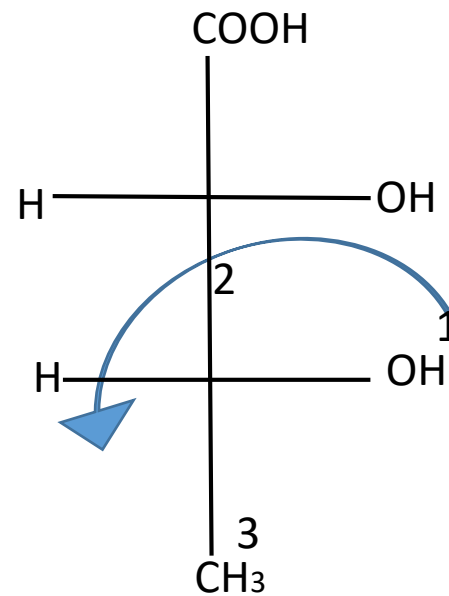


Carbon 2

H-atom is on horizontal line

Anticlockwise from front, so clockwise from back

Notation R



Carbon 3

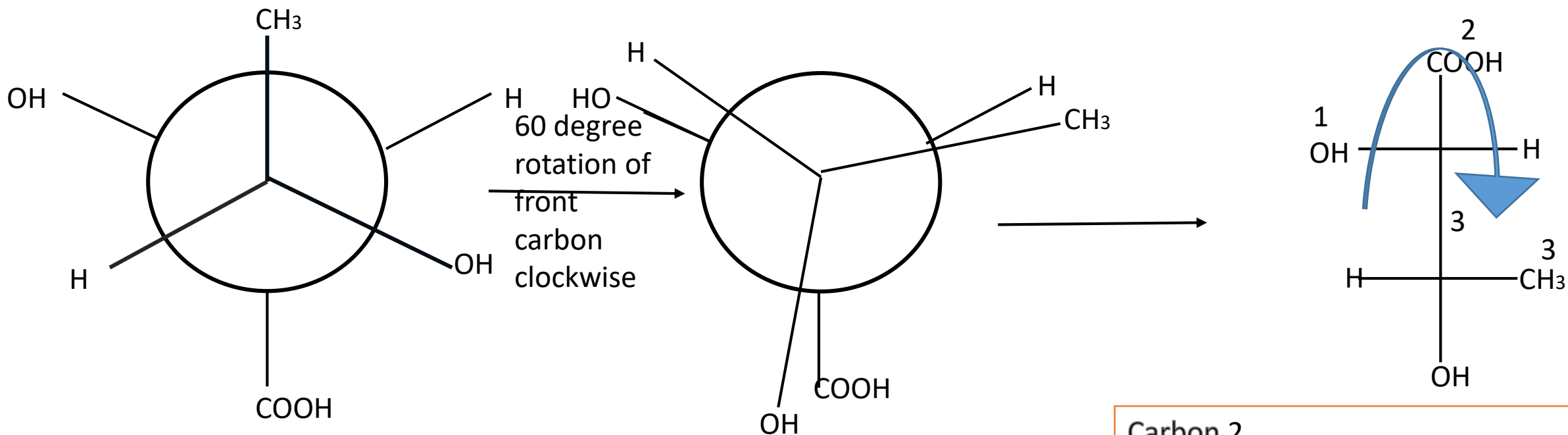
H-atom is on horizontal line

Anticlockwise from front, so clockwise from back

Notation R

2(R), 3(R) – dihydroxy butanoic acid

4. Assigning R, S Notation to Newman Projection formula

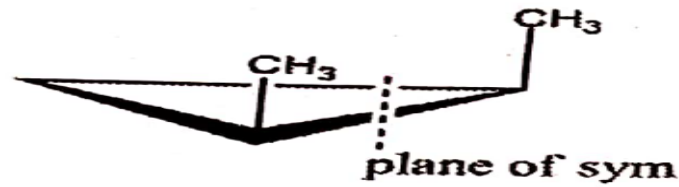


Carbon 2
H-atom is on horizontal line clockwise from front, so anticlockwise from back
Notation S

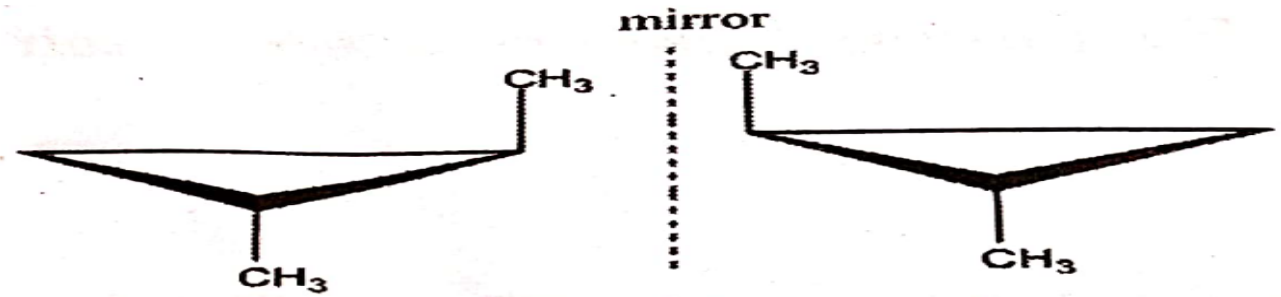
Carbon 3
H-atom is on horizontal line clockwise from front, so anticlockwise from back
Notation S

2(S), 3(S)-dihydroxybutanoic acid

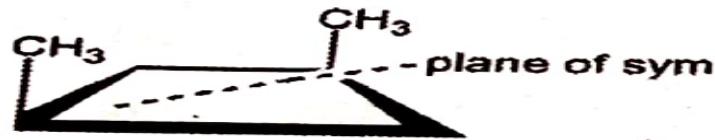
Optical Isomerism in Substituted Rings



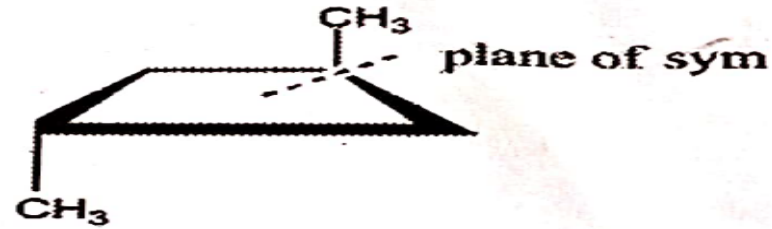
**(cis)-1,2-dimethylcyclopropane
optically inactive**



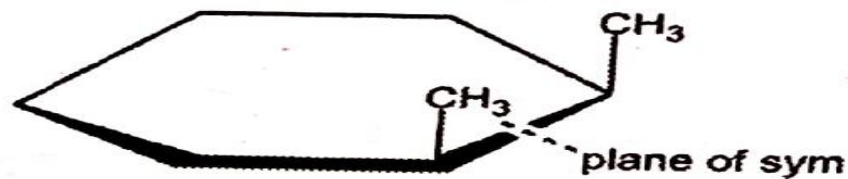
**(trans)-1,2-dimethylcyclopropane
optically active (enantiomers)**



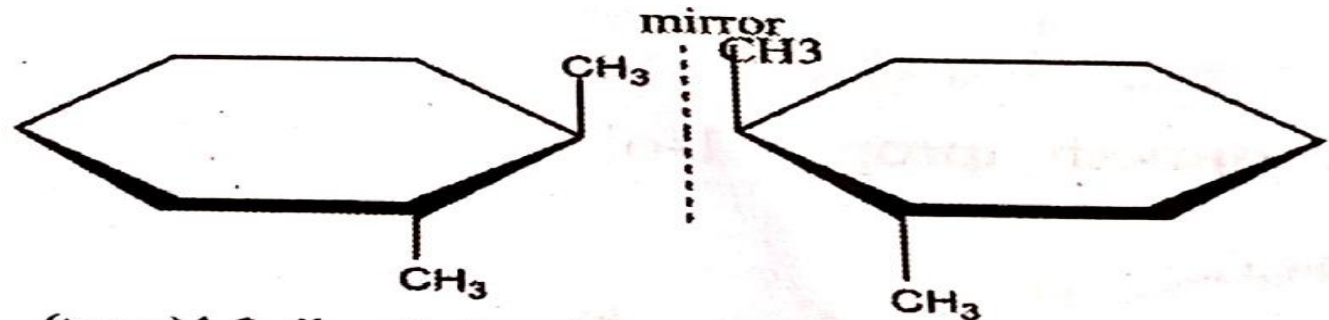
**(cis)-1,3-dimethylcyclobutane
optically inactive**



**(trans)-1,2-dimethylcyclobutane
optically inactive**



(cis)-1,2-dimethylcyclohexane

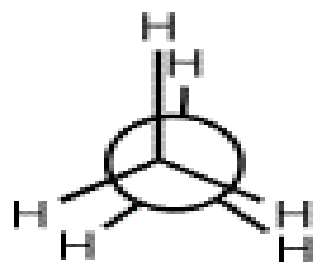


(trans)-1,2-dimethylcyclohexane-optically active

The different spacial arrangement of atoms that results from the rotation of groups about a c-c bond is called conformational isomers or rotational isomers. The energy difference between two extreme conformations is very small, thus rapid interconversions takes place at room temperature. Low energy conformer is more populated than high energy conformer at room temperature.

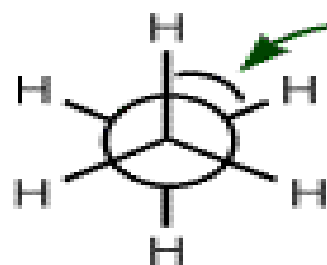
CONFORMATIONAL ANALYSIS OF ETHANE

ECLIPSED CONFORMATION



least stable

STAGGERED CONFORMATION



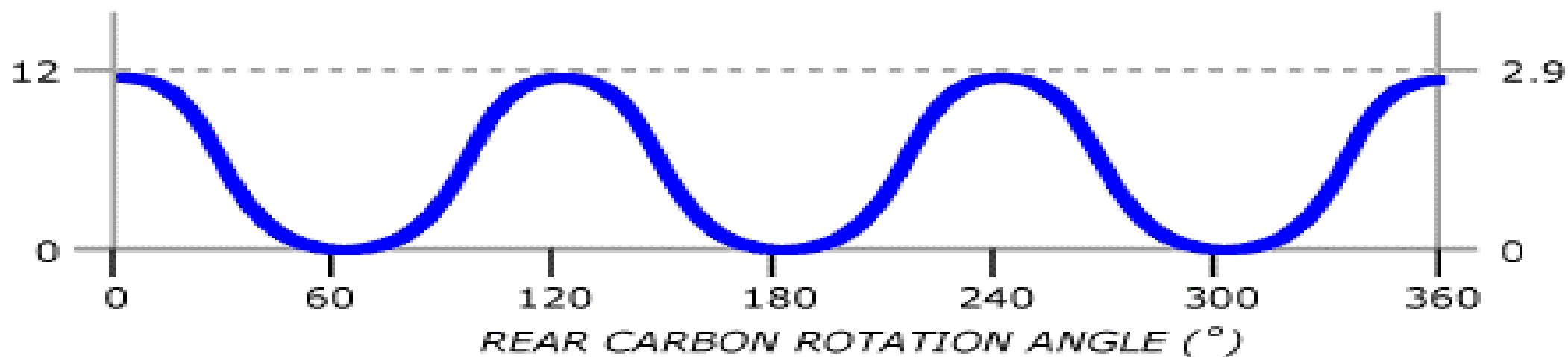
most stable

dihedral angle

**A Newman
projection**

ENERGY (kJ/mol)

kcal/mol



CONFORMATIONS OF BUTANE

