STEREOCHEMISTRY

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For B.Sc. (I) Semester Students

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Stereochemistry deals with three dimensional representation of molecule in space.

The study of stereochemistry focuses on stereoisomers and spans the entire spectrum of Organic, Biological, Physical, and Supramolecular Chemistry.

Stereochemistry includes method for determining and describing these relationships; the effect on the physical or biological properties.

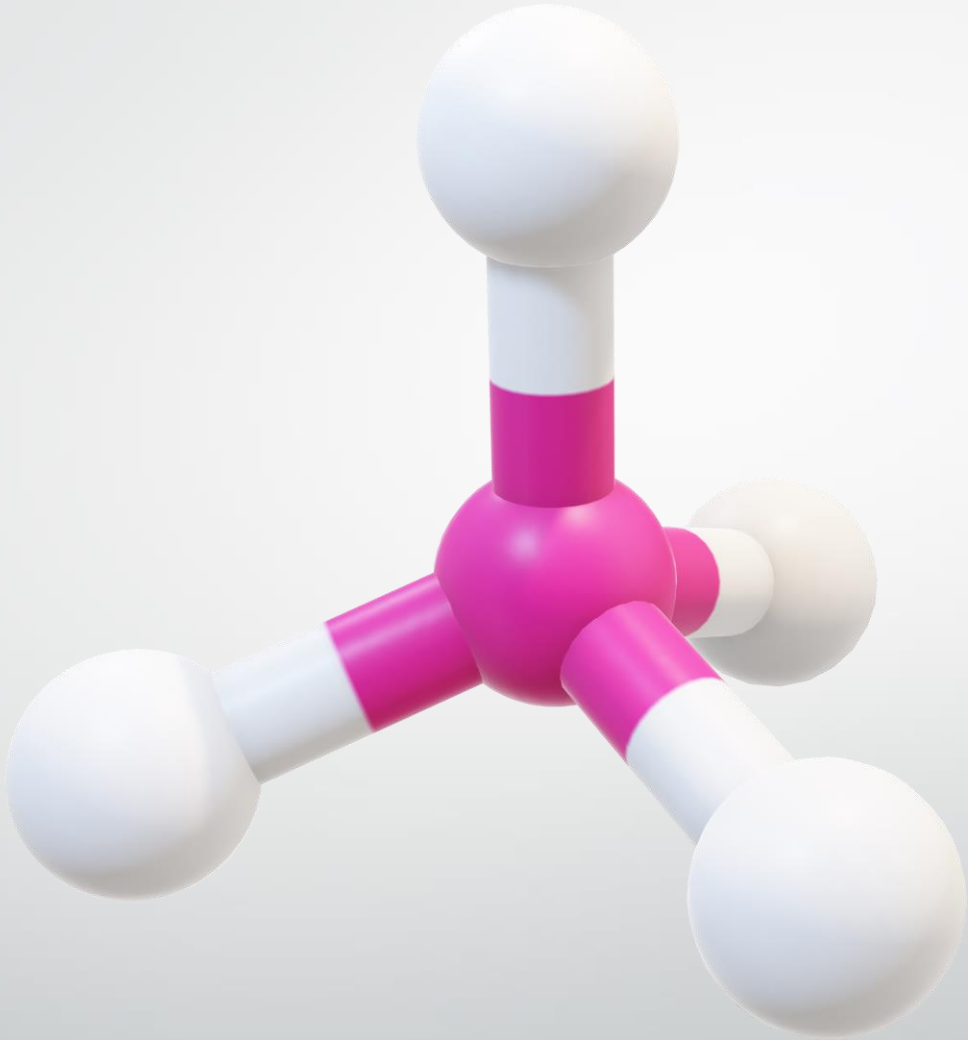
OBJECTIVES

- Classification of stereoisomers
- Recognize a stereo-genic centre in the molecular structure
- Various representation of three-dimensional molecules
- To be able to predict, identify and distinguish between enantiomers and diastereomers

Stereochemistry: Definition

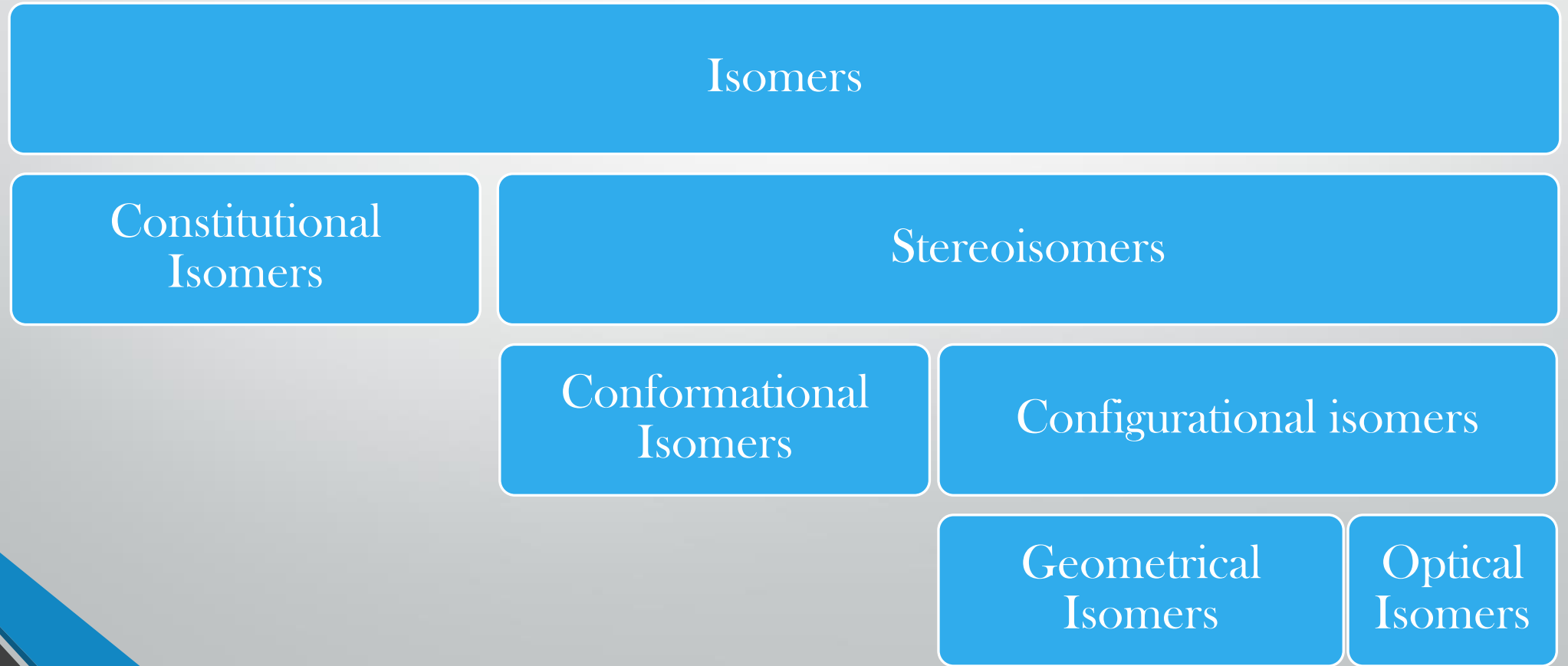
- The branch of chemistry which deals with three-dimensional structure of molecule and their effect on physical and chemical properties is known a stereochemistry

- To represent Organic molecule as three-dimensional object we need at least one sp3 hybridised carbon.



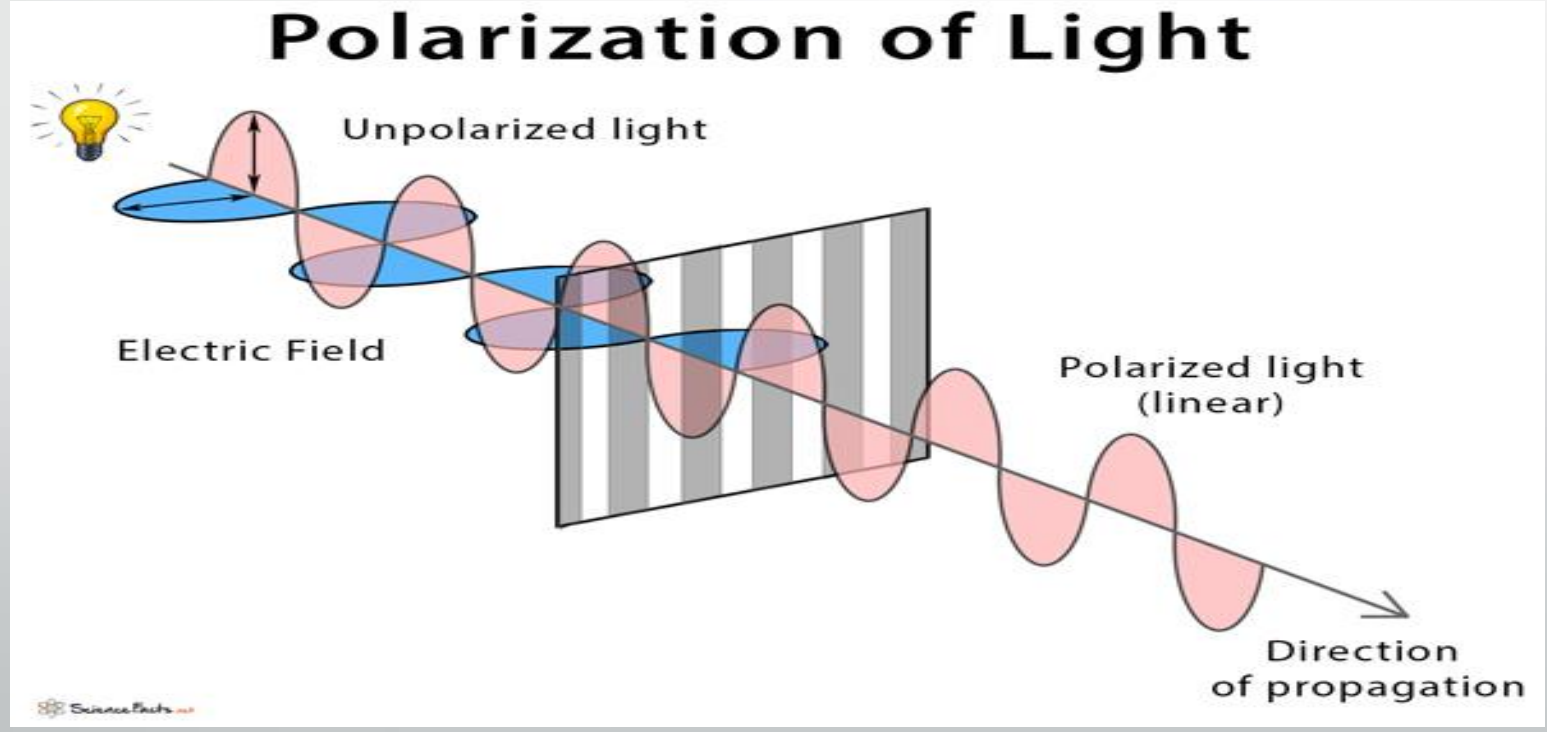
Isomers and their Classifications

- Different Compounds which have same molecular formula is known as isomer. (Obviously they are different from each others in any aspect)



Plane Polarised Light

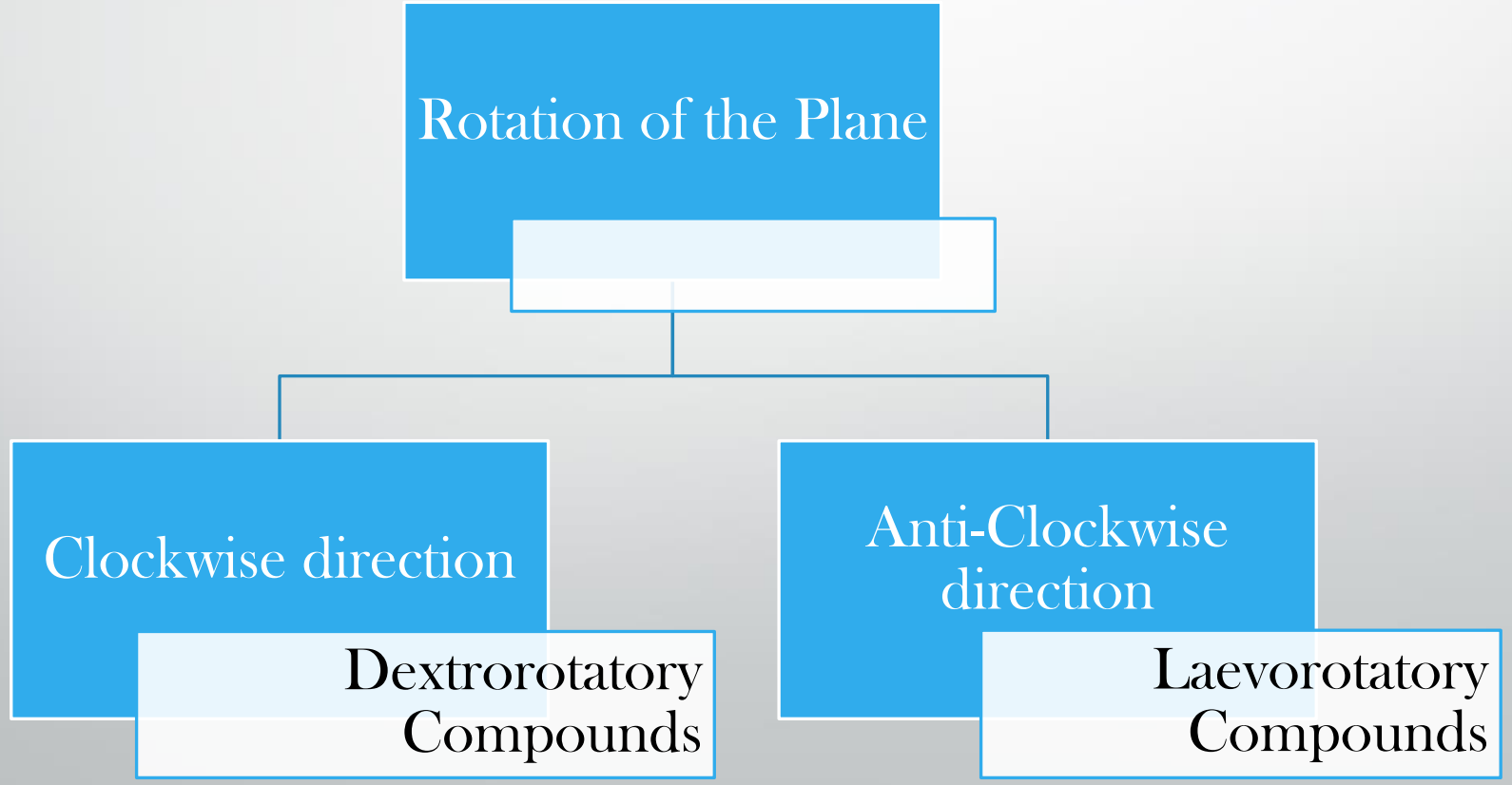
- When the light passes through the Nicol prism, the vibrations of the particles starts to occur in single plane. This type of light is termed is Plane Polarised Light.



Credit: https://www.sciencefacts.net/wp-content/uploads/2020/04/Polarization-of-Light.jpg

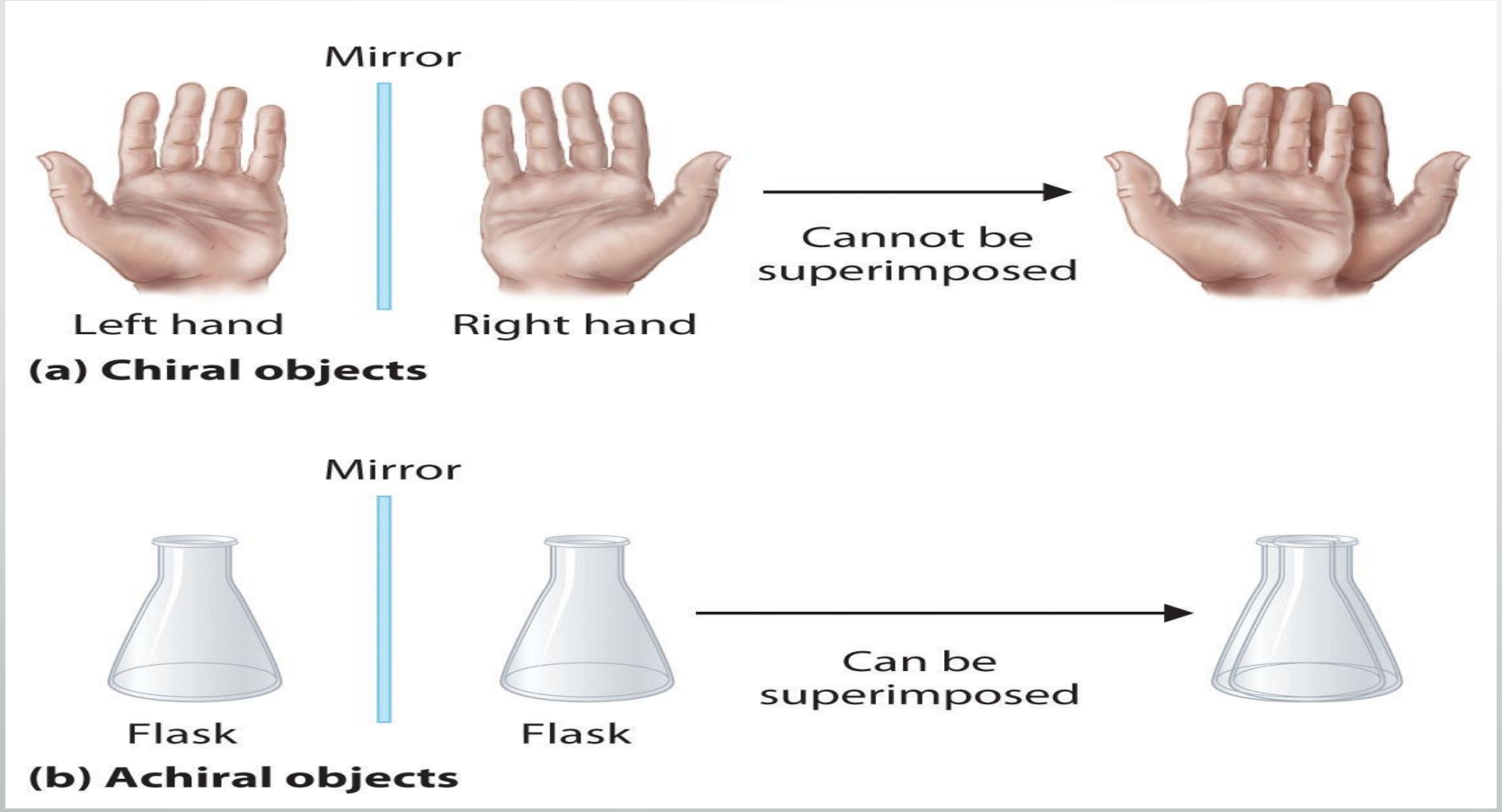
Optical Activity

- Compounds which have the tendency to rotate the plane of polarised light is known as Optically Active Compounds (Otherwise Inactive)



Chirality

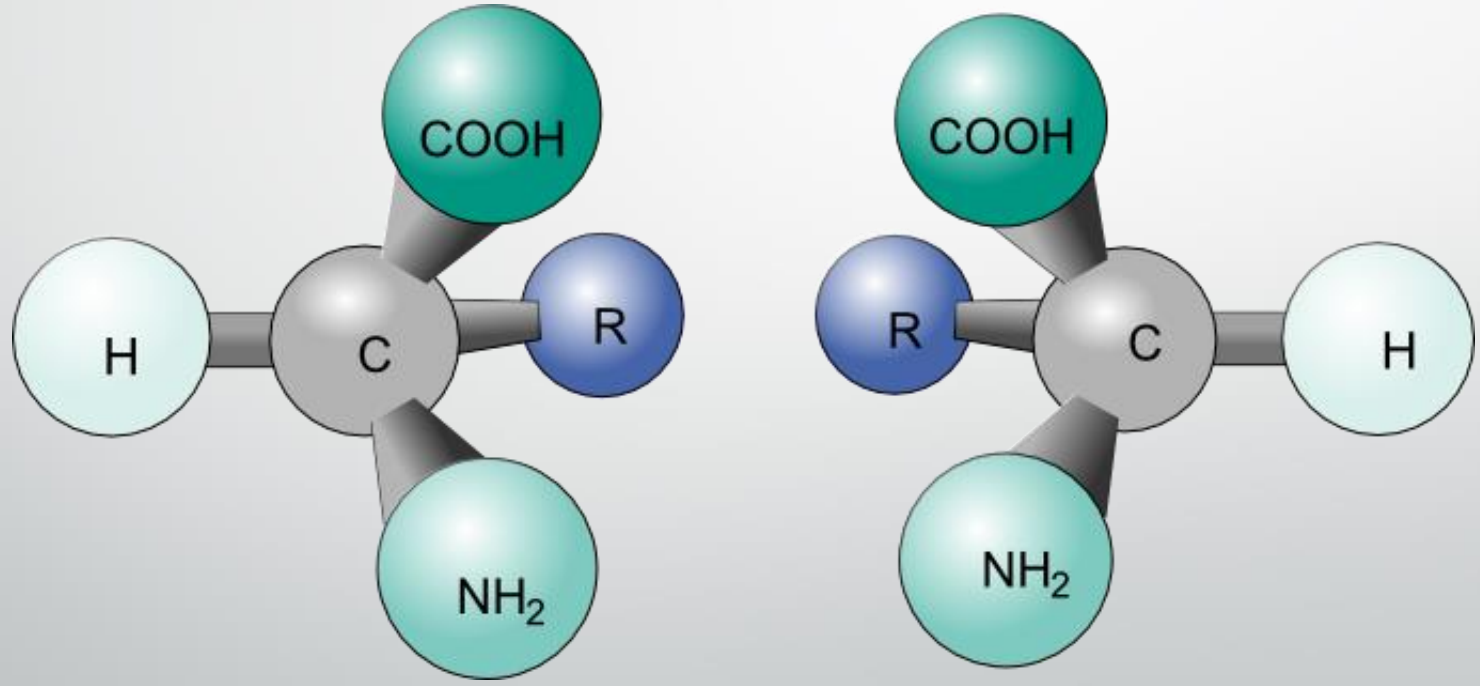
- An Object which is not superimposable upon its mirror image is known to be Chiral. The general property of 'handedness' is termed as chirality.



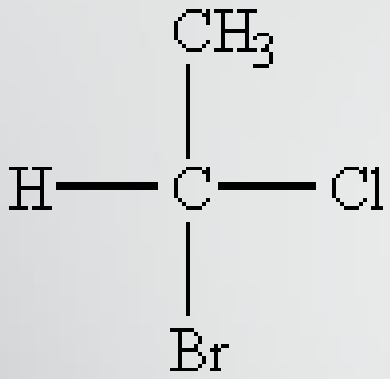
Credit : https://useruploads.socratic.org/ONCz1FXlS8LOON9FNTp5_122a3121b7268f235234e7a9091fc4ea.jpg

Asymmetric of Chiral Carbon

- A carbon atom bonded tetrahedrally to four different substituents is known as Asymmetric atom or Chiral atom.

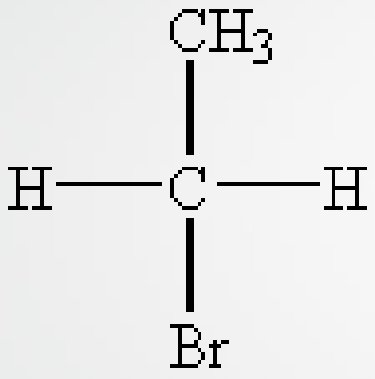


Credit: http://surl.li/gsacv



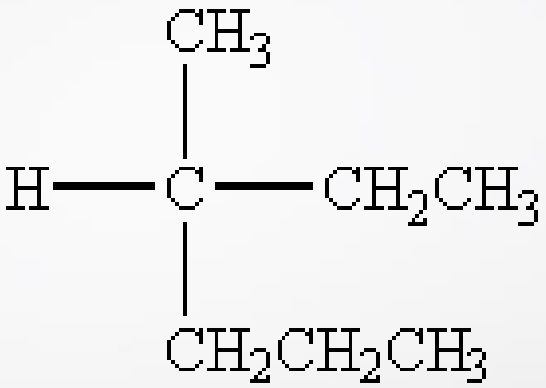
chiral

Has 4 differnt atoms bonded to the carbon



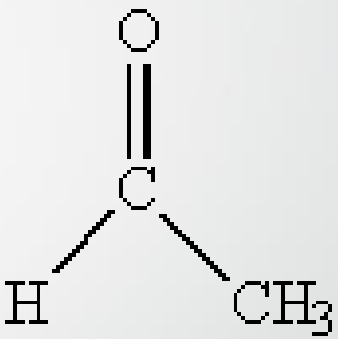
achiral

Does not have 4 different atoms or groups bonded to the carbon (2 hydrogens)



chiral

Has 4 differnt groups bonded to the carbon



achiral

Only has 3 atoms bonded to the carbon

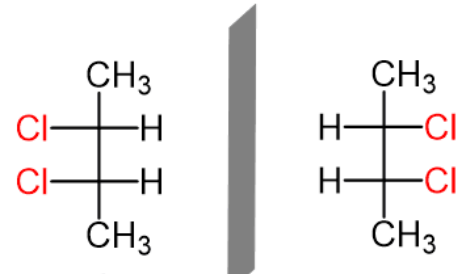
Credit : https://useruploads.socratic.org/ko6aEc68RpSSO3R5zE2I_Image12.gif

Meso Compounds

- If a molecule contains only one chiral centres it must be chiral. But molecules containing more than one chiral centres may or may not be chiral. Ex- Meso Compounds (superimposable to it's mirror image)

Meso compounds do not have enantiomers!

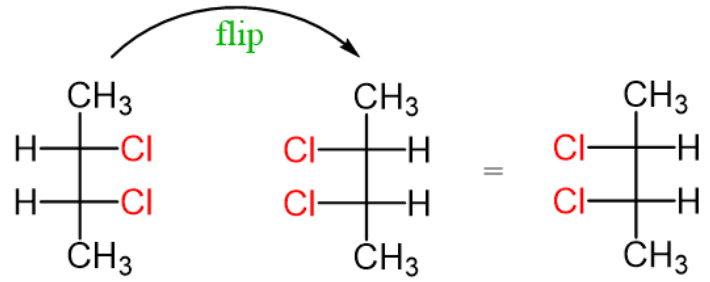
Step 1. Draw the mirror image



3

meso mirror image

Step 2. Flip the mirror image - it is the same compound



mirror image

3

mirror image is same as the molecule

i.e. they are superimposable

Credit : https://www.chemistrysteps.com/wp-content/uploads/2019/10/meso-compounds-do-not-have-enantiomers.png

Stereoisomers and their Classification

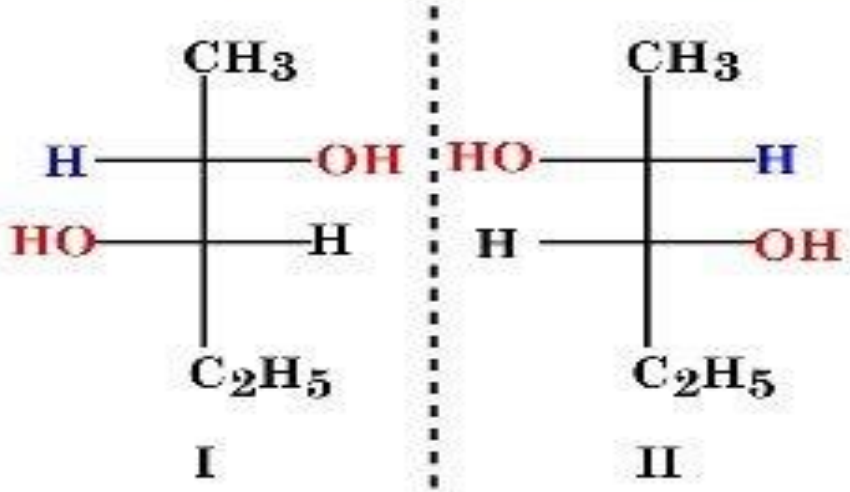
- Isomers having the same molecular formula but different spatial arrangement of their atoms is known as stereoisomers.

Enantiomers: Stereoisomers which are non superimposable mirror images of each others are called enantiomers. Chirality is the necessary and sufficient condition for the existence of enantiomers.

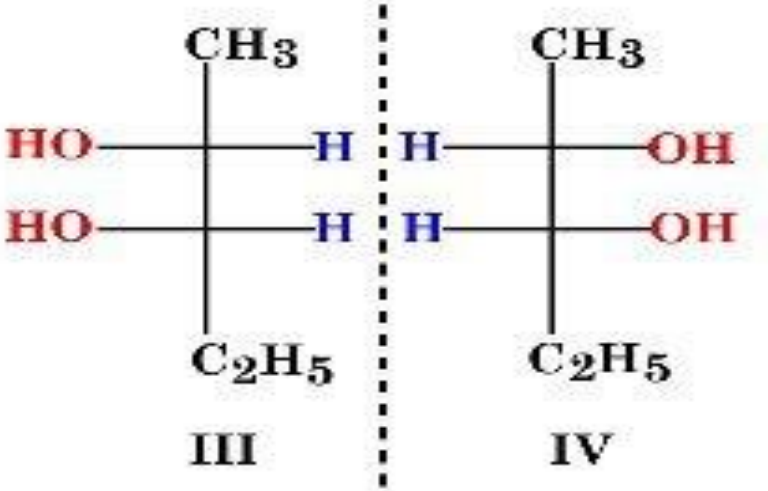
- Diastereomers: Stereoisomers that are not mirror images of each other are called diastereomers.

- **Geomatical Isomers**: Occurs as a result of restricted rotation about a bond. This is also called Cis-Trans, Syn-Anti Isomerism

Stereochemistry - Diastereomers



Compounds I and II are **enantiomers** of each other.

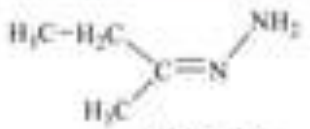


Compounds III and IV are **enantiomers** of each other.

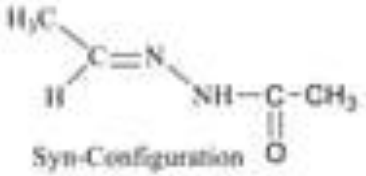
Compounds I and III are **diastereomers.**
Compounds I and IV are **diastereomers.**
Compounds II and III are **diastereomers.**
Compounds II and IV are **diastereomers.**

Credit : https://qph.cf2.quoracdn.net/main-qimg-f1b5d54c14f5276025dda2cfb41e58e9-lq

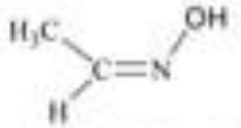
Examples of Syn-Anti Nomenclature



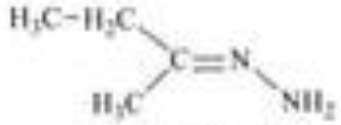
Methyl anti
OR
Ethyl syn



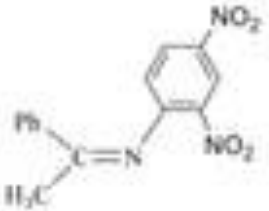
Syn-Configuration



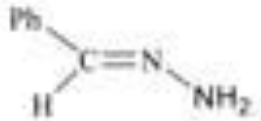
Anti-Configuration



Methyl syn
OR
Ethyl anti

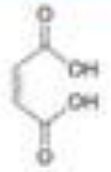


Methyl Anti-Configuration
OR
Phenyl Syn-Configuration

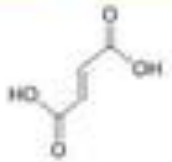


Syn-Configuration

Examples of Cis-Trans-Isomerism



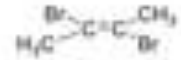
Maleic acid cis form



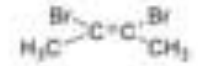
Fumaric acid trans form

Cis - cyclohexane-1,4-diol

Cis - cyclohexane-1,4-diol



trans-2,3-dibromobut-2-ene



cis-2,3-dibromobut-2-ene

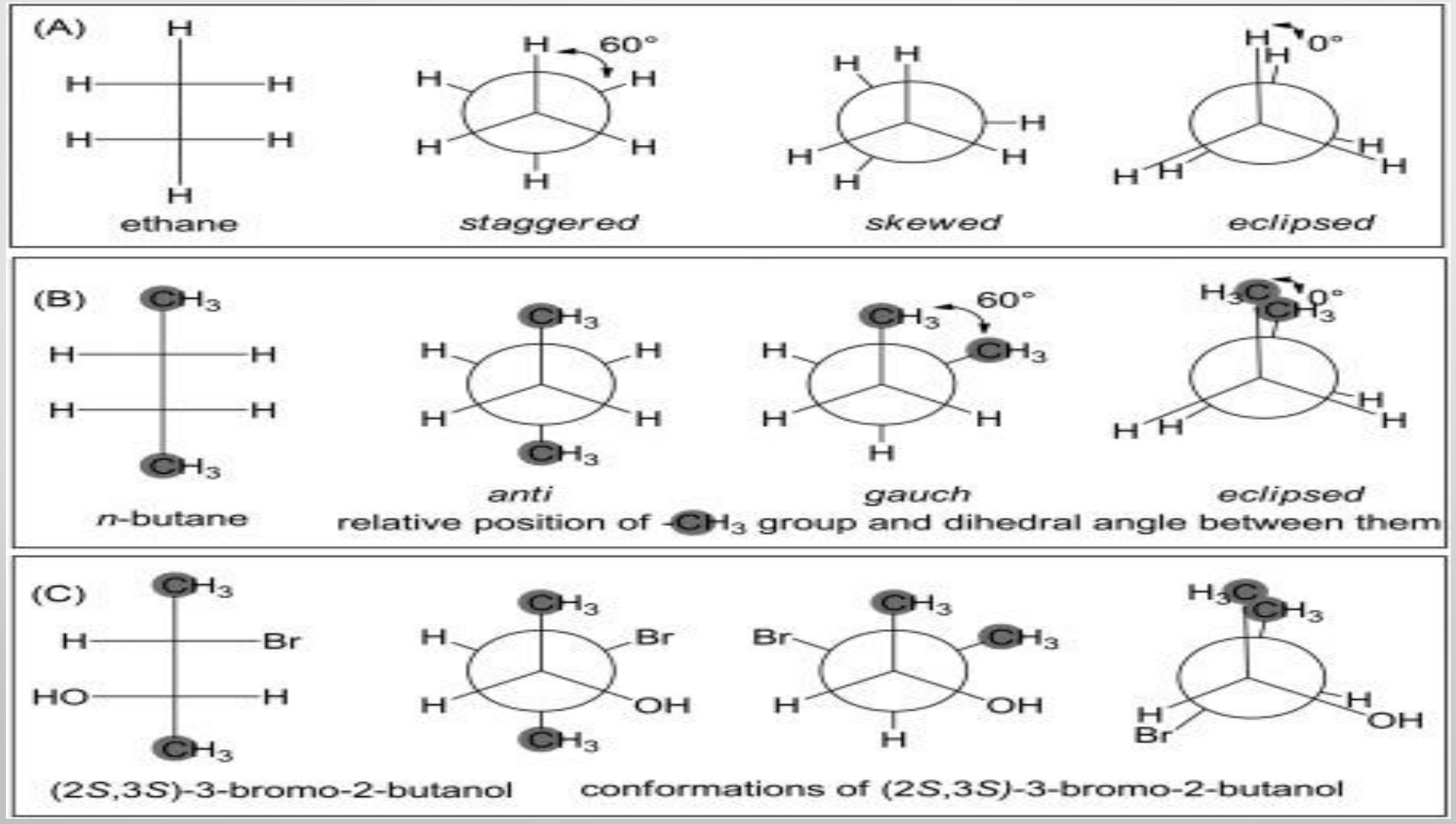
In case of cycloalkenes

cis-cyclodecene

trans-cyclodecene

Credit: https://image.slidesharecdn.com/

Conformational Isomers: Conformational Isomers are the isomers that can be converted into one another by a single bond.



Credit: https://ars.els-cdn.com/content/image/3-s2.0-B9780128210628000119-f01-07-9780128210628.jpg

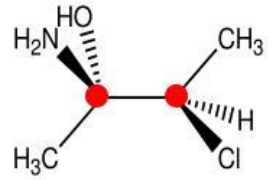
Flying Wedge Projection of Molecules

Master layout

wedge — Bond coming out of the plane

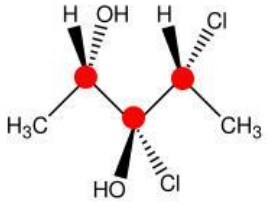
Bond on the plane

dash — Bond going in the plane



Beginner's level

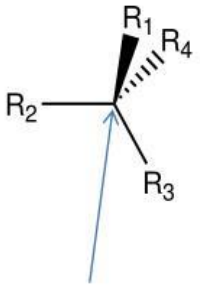
With two carbon center (red dots)



advance level

With three carbon center (red dots)

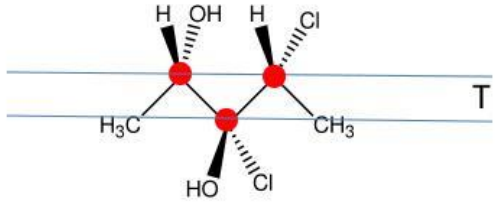
Wedge – dash representation



Carbon center

Here bond of $C\text{-}R_2$, $C\text{-}R_3$ are in the plane , while of $C\text{-}R_1$ is out of the plane and $C\text{-}R_4$ inside the plane, the bond $C\text{-}R_4$ is exactly behind the bond $C\text{-}R_1$, but to show the $C\text{-}R_4$ bond it is shown sideways

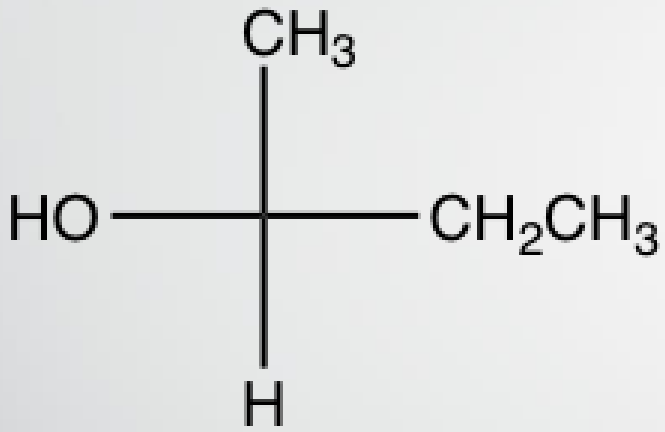
R_1 R_2 R_3 and R_4 are general notation for the atom



While looking the molecule from top or bottom the plane which is considered is of thickness T. In which the top layer passes through 2 carbon center and the lower layer through 1 carbon center

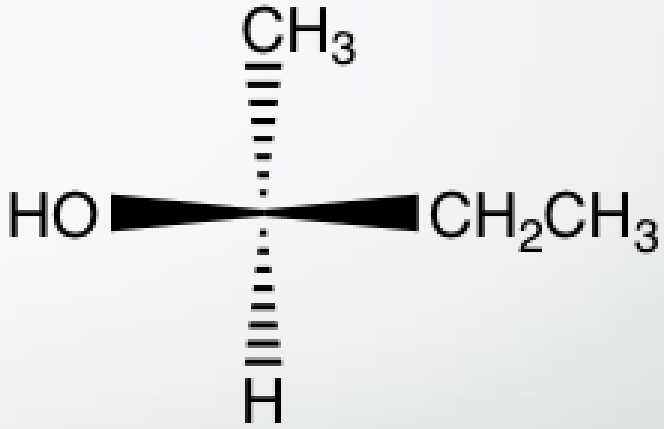
Credit : https://image2.slideserve.com/4049196/slide2-l.jpg

Fisher Projection of Molecules



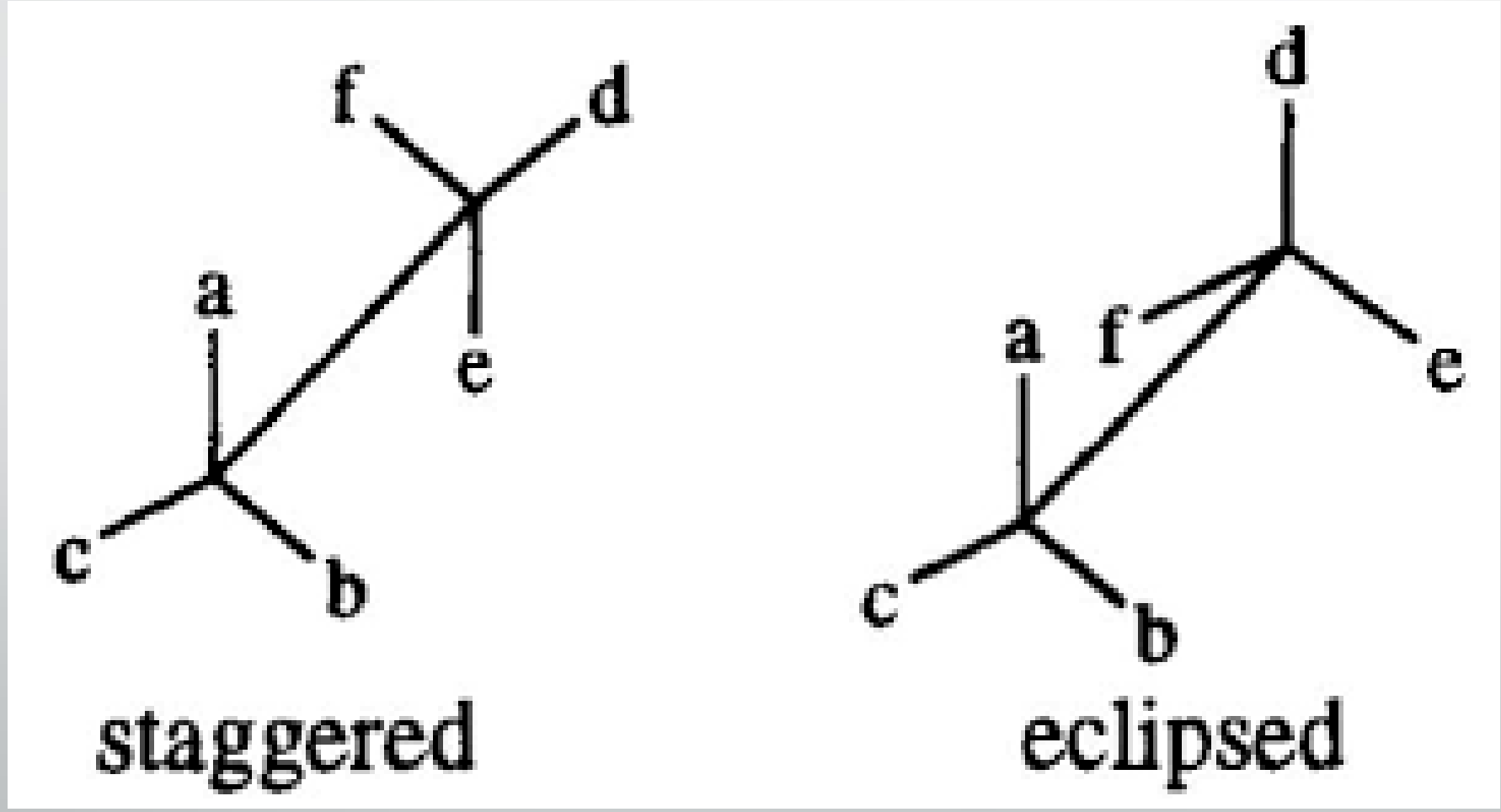
Fisher projection

equals to

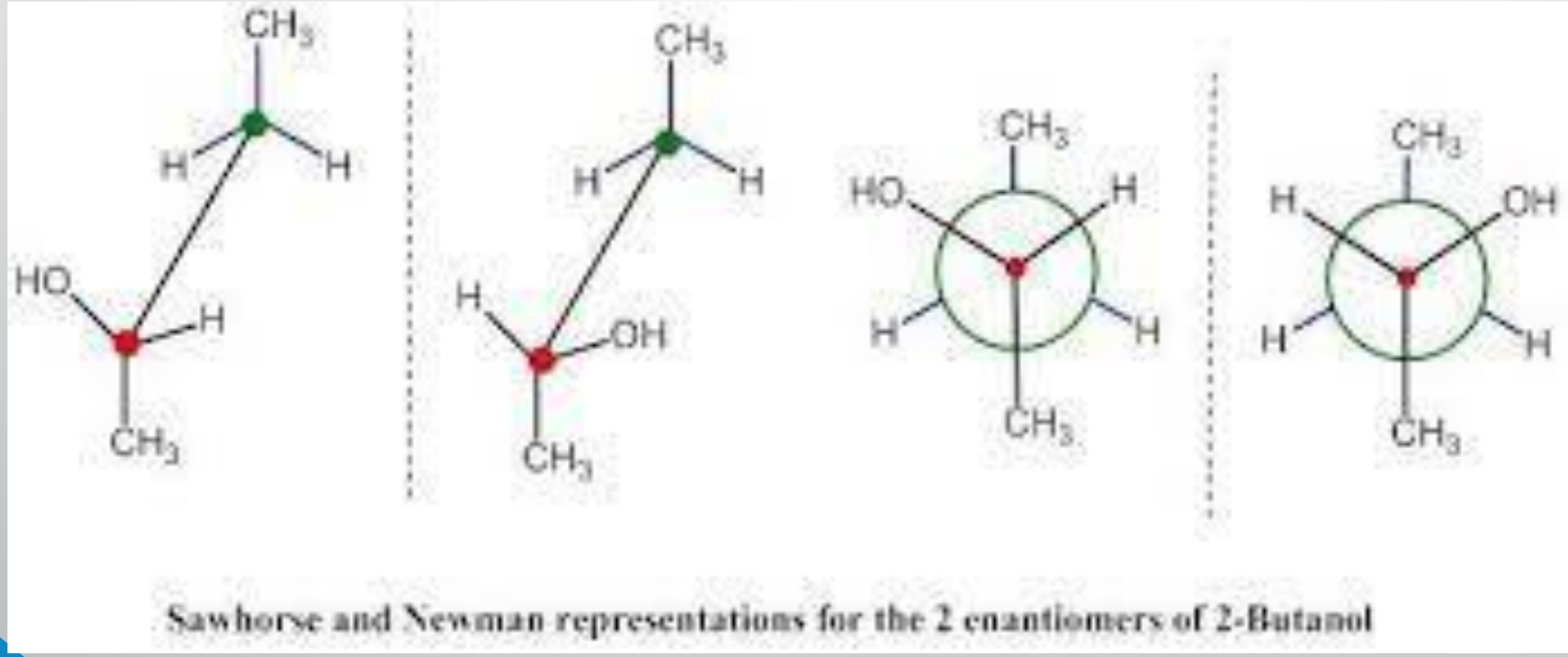


Perspective formula

Sawhorse Projection of Molecules



Newman Projection of Molecules



Sawhorse and Newman representations for the 2 enantiomers of 2-Butanol

Elements of Symmetry

- Elements of symmetry offers a simple device to decide whether a molecule is chiral or achiral.
- Whether it is superimposable on mirror image or Not
- When a molecule does not have a symmetry element: It is non superimposable on its mirror image and is chiral (Hence Optically Active)

Classification of Elements of Symmetry

Plane of Symmetry

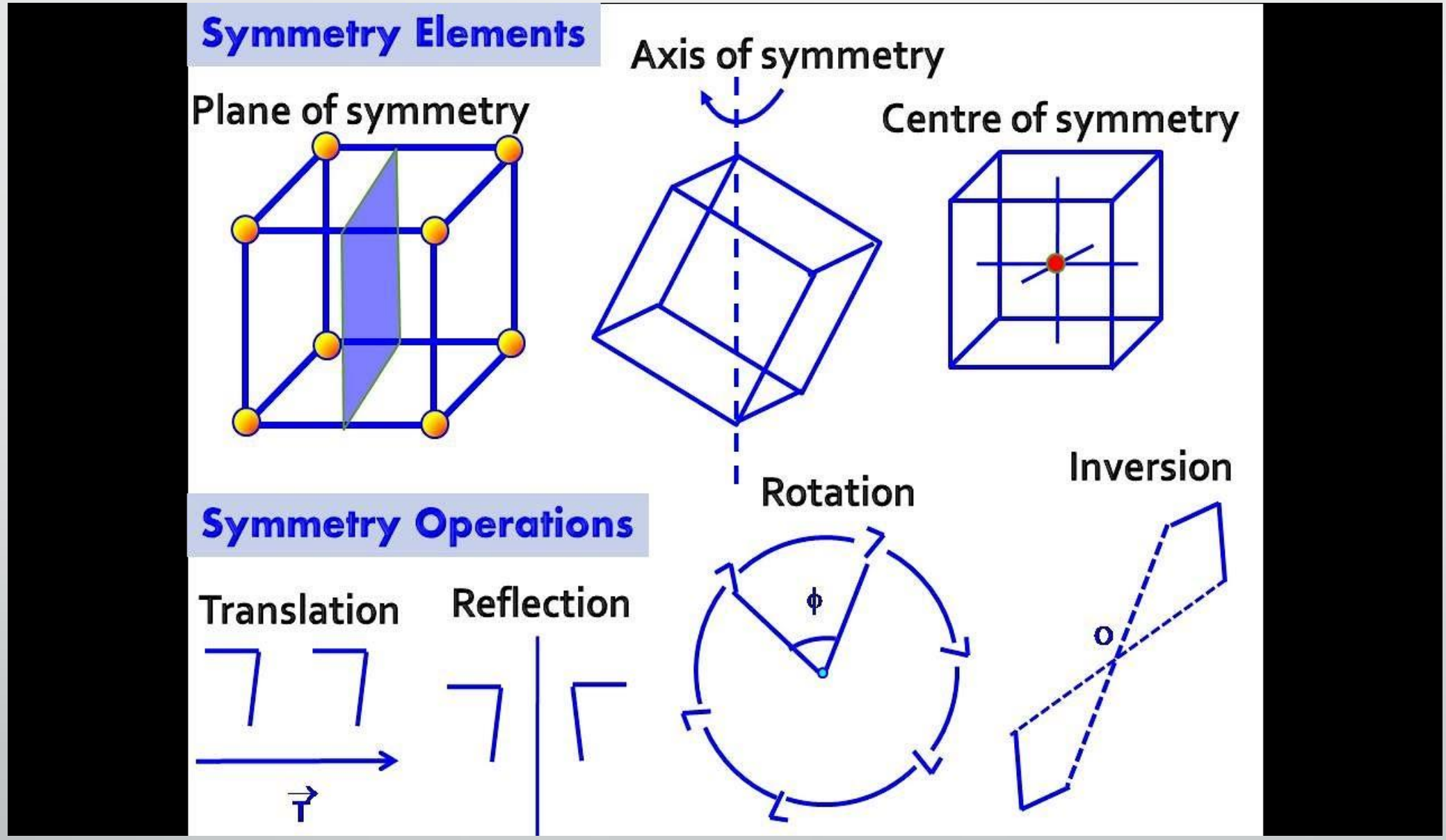
- Plane which divides a molecule into two equal halves

Centre of Symmetry

- If a line is drawn form any atom or group to this point and when extended to an equal distance beyond this point, meets the identical atom of group

Axis of Symmetry

- If when rotated through an angle about the axes and then followed by reflection in a plane perpendicular to the axis, the molecule is indistinguishable from the original molecule



Credit : https://i.ytimg.com/vi/Lwtz7hylnlU/maxresdefault.jpg

Reference Materials

1. Stereochemistry: Conformation and Mechanism, P.S. Kalsi.
2. Stereochemistry of Organic Compounds: Principles and Applications, D. Nasipuri.
3. Stereochemistry, D.G. Morris.
4. Theory of orientation and stereo-selection, Kenichi Fukui.
5. Organic Chemistry, 2nd edition, Clayden J., Greeves, N., & Warren.