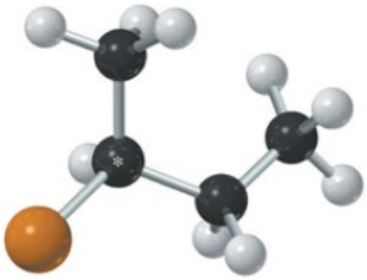
The Islamic University

Department of Pharmaceutical Chemistry

Title of the course: *Organic Chemistry* I

Level: 1st Class, 2nd Semester

Stereochemistry

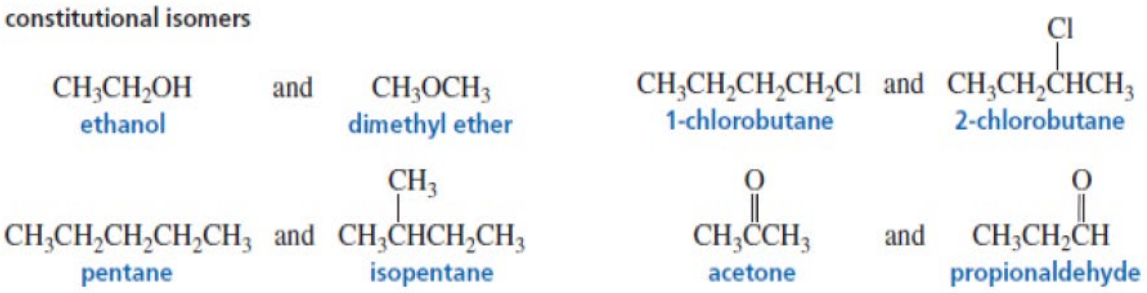


Dr.Tabarek Alnaqib

Stereochemistry: Branch of chemistry that involves the study of compounds in 3D.

Isomers: compounds that have the same molecular formula but differ in arrangement of atoms in space.

1-Constitutional isomers (structural isomers) : have the same molecular formula but different constitution(different connectivity).



2-Stereo isomers: same molecular formula and same constitution (same connectivity) but different spatial arrangement of atoms.

There are two types of stereoisomers:

1- Conformational

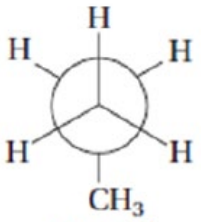
2- Configurational

A) Geometrical

B) Optical

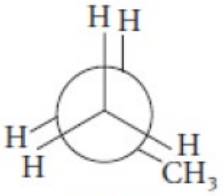
Conformational isomers: interconvertible by rotation about carbon-carbon single bond. two extreme conformation result—a *staggered conformation* and an *eclipsed conformation*.

Example 1: Draw the Newman projections for the staggered and eclipsed conformations of propane.



staggered

more stability



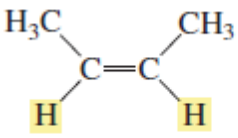
eclipsed

least stability

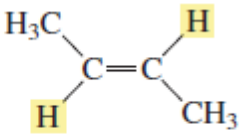
Configurational isomers: not interconvertible by rotation, only by breaking and making bonds. And divided to:

A- Geometric isomers: result from restricted rotation which can be caused either by a double bond or by a cyclic structure. As a result, 2 isomers cis (Z) -trans (E).

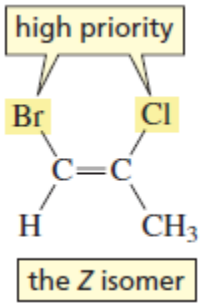
Priority rule: I > Br > Cl > F < O < N < C < H

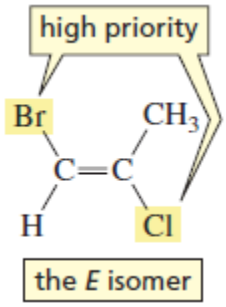


cis-2-butene



trans-2-butene





B- Optical isomers: compounds that rotates the plane of polarized light clockwise **dextrorotatory (+) d** or counterclockwise **levorotatory (-) l**. And divided into two types:

1- Enantiomers

2- Diastereomers

the optical activity of these compounds measured by instrument called

Polarimeter.

Chirality and optical activity

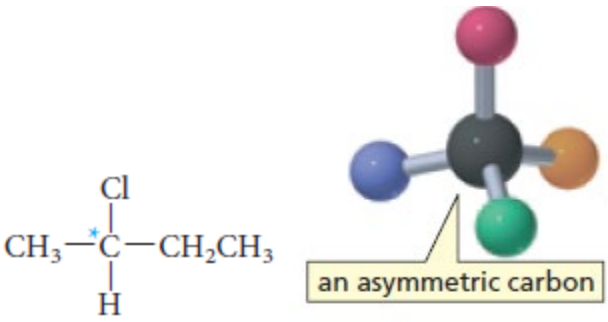
All three-dimensional objects can be classified as either chiral or achiral.

Chiral compound: structure is not superimposable on their mirror image.

Achiral compound: structure is superimposable on their mirror images.

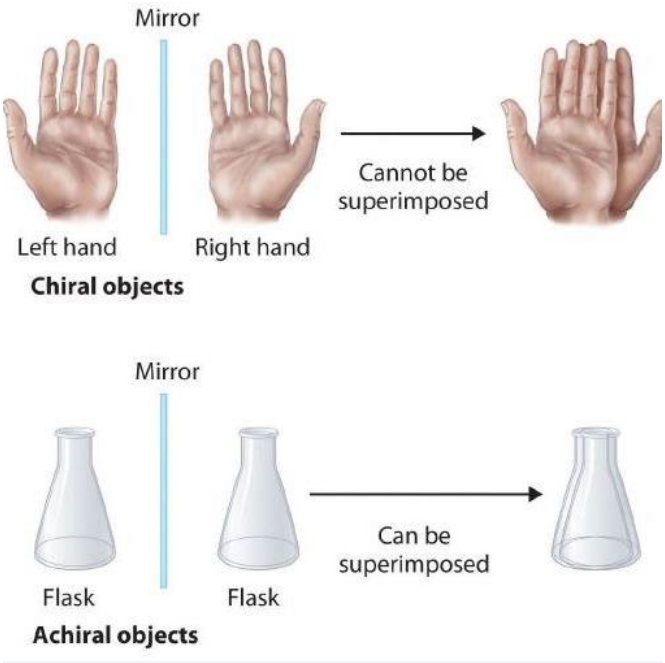
Organic compounds become (chiral) optically active if:

1- Contain **chiral carbon (stereogenic center)**: tetrahedral (sp3) carbon with 4 different groups (asymmetric).

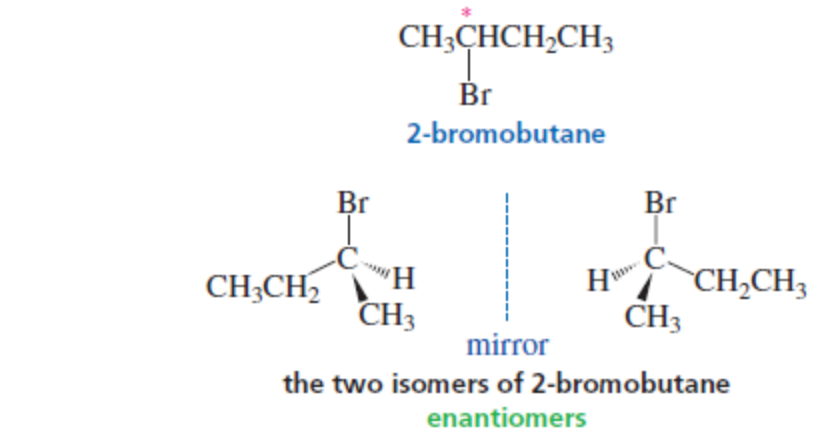


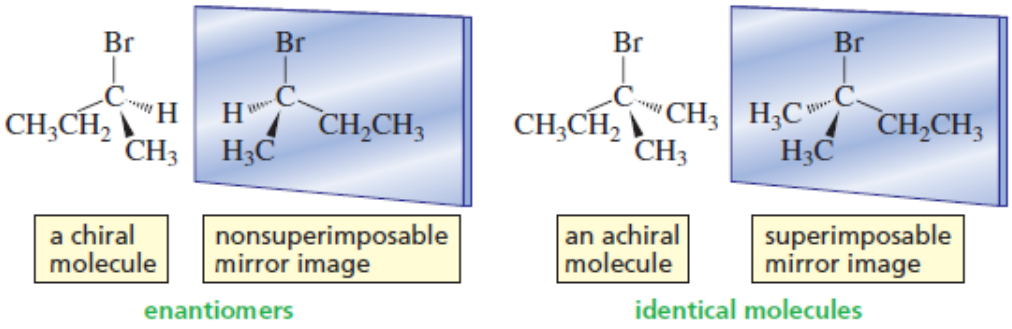
2- Have no elements of symmetry (plane of symmetry and center of symmetry)

3- Mirror image and non-superimposable



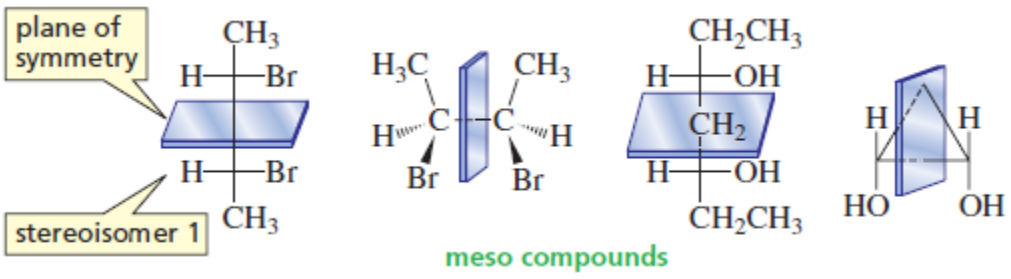
Enantiomers: an optically active compounds that rotate the plane of polarized light in equal angel but opposite direction. have same physical properties but differ in pharmacological actions.



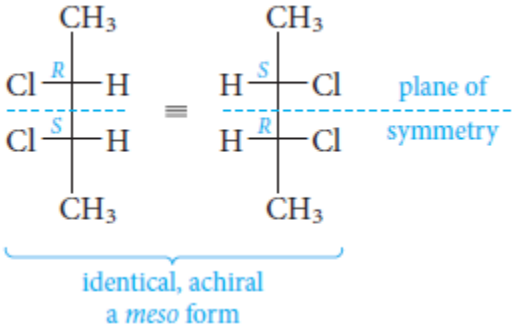


Element of symmetry:

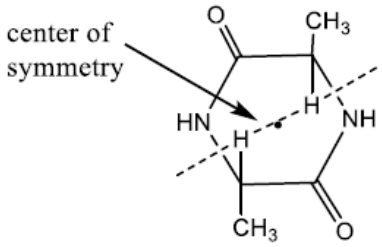
1-Plane of symmetry: is a plane that passes through a molecule in such a way that what is on one side of the plane is the exact reflection of what is on the other side.



Meso compound: optically inactive compound and have plane of symmetry.



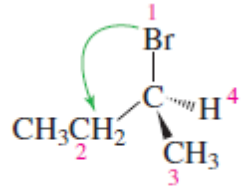
2-Center of symmetry: the point in the center of molecule to which a line can be drawn from any atom such that when extended an equal distance pass the center , the line meet another atom of the same kind.



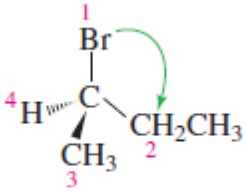
Racemic mixture (±) : A mixture of equal amounts of two enantiomers (R,S), do not rotate the plane of polarized light and optically inactive. **(+)** enantiomers cancel the optical activity of **(-)** enantiomer.

Naming enantiomers (R, S) system

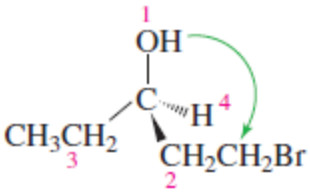
R and S can be used to describe the configuration of a chiral center.



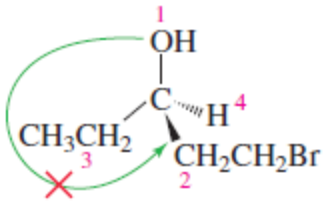
(*S*)-2-bromobutane

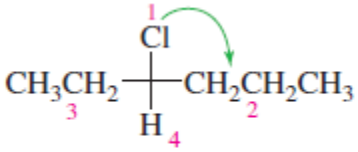


(*R*)-2-bromobutane

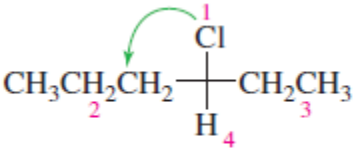


(*R*)-1-bromo-3-pentanol



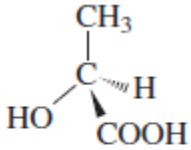


(*R*)-3-chlorohexane

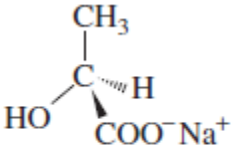


(*S*)-3-chlorohexane

We can tell by looking at the structure of a compound whether it has the ***R*** or the ***S*** configuration, but the only way we can tell whether a compound is **dextrorotary (+)** or **levorotary** (-) is to put the compound in a **polarimeter.**

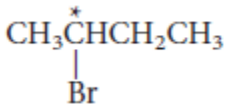


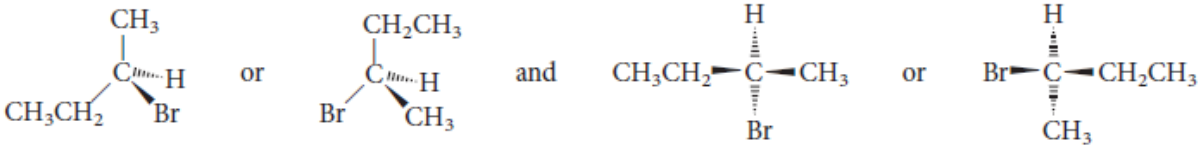
(*S*)-(+)-lactic acid



(*S*)-(–)-sodium lactate

Example 2: Draw the structure of (*R*)-2-bromobutane

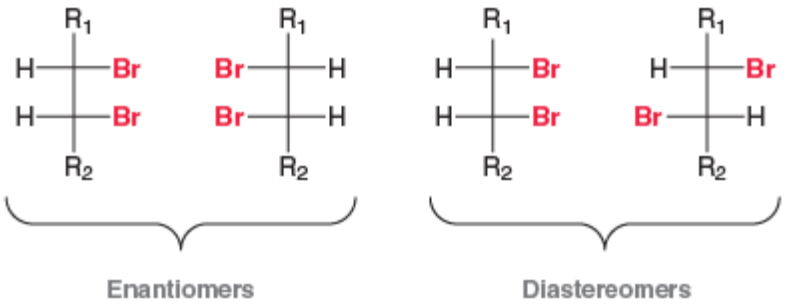




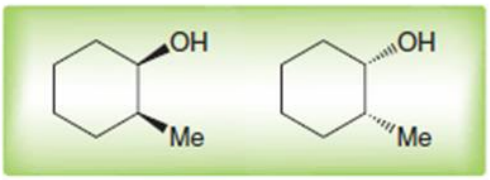
Enantiomers	Diastereomers
Isomers are non-Superimposable on their mirror image	Isomers are Superimposable on their mirror image
Opposite configuration on all chirality center.	Opposite configuration on some chirality center.
Have the same physical and chemical properties	Have the same physical and chemical properties

The possible optical isomers = 2^n

n= number of chiral carbon:

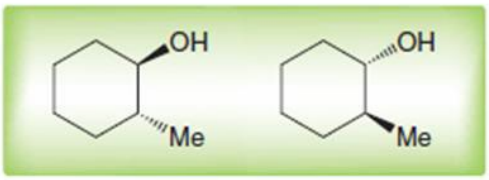


A pair of enantiomers



1*R*, 2*S* 1*S*, 2*R*

A pair of enantiomers



1*R*, 2*R* 1*S*, 2*S*