4 Types of Isomers

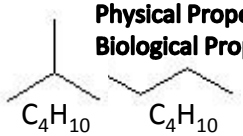
1. Structural Isomers/(Constitutional)
2. Geometric Isomers/(Cis/Trans)
3. Optical Isomers
    A. Enantiomers
    B. Diastereomers

4 Types of Isomers

Isomers

Constitutional/(Structural)

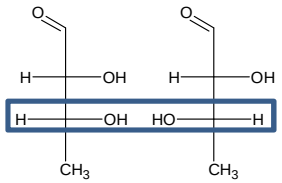
Same – Formula
Diff. – Structure
Chemical Properties
Physical Properties
Biological Properties



Stereoisomer/(Geometric)

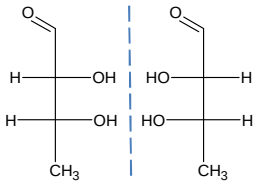
Diastereomers

Same – Formula
Structure
Diff. – Geometry
Chemical Properties
Physical Properties
Biological Properties



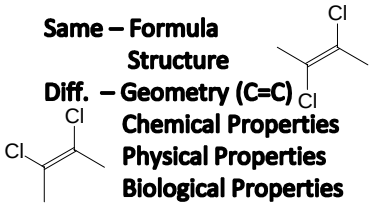
Enantiomers

Same – Formula
Structure
Chemical Properties
Physical Properties
Diff. – Geometry
Optical Rotation
Biological Properties



Geometric/Cis-Trans

Same – Formula
Structure
Diff. – Geometry (C=C)
Chemical Properties
Physical Properties
Biological Properties



Structural Isomers

Same

- Chemical Formula

Different

- Structure
- Chemical Properties
- Physical Properties
- Biological Properties

Example

C_4H_{10}

C_4H_{10}

Geometric Isomers

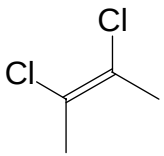
Same

- Chemical Formula
- Structure

Different

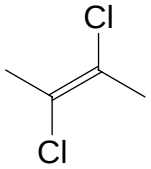
- Geometry (around C=C)
- Chemical Properties
- Physical Properties
- Biological Properties

Example



$C_4H_6Cl_2$

Cis-2,2-dichloro-2-butene



$C_4H_6Cl_2$

Trans-2,2-dichloro-2-butene

Optical Isomers
(Enantiomers)

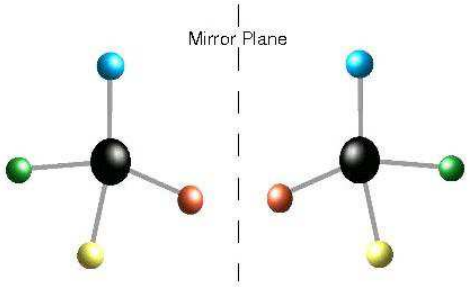
Definition: Chiral molecules that are mirror images of each other.

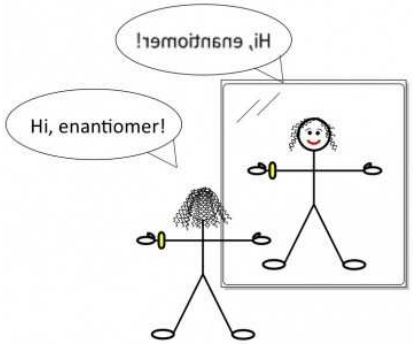
Same

- Chemical Formula
- Structure
- Chemical Properties
- Physical Properties

Different

- Geometry – stereoisomers that are mirror images
- Optical Rotation
- Biological Properties





Optical Isomers
(Diastereomers)

Definition:

Chiral molecules that are not enantiomers of each other.

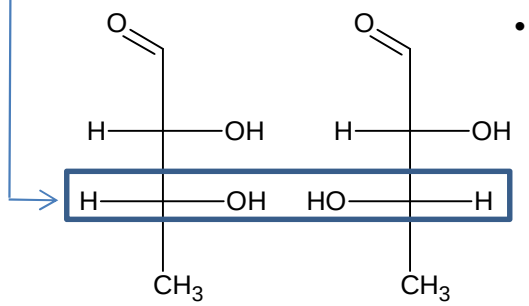
Differ in the orientation around one chiral carbon.

Same

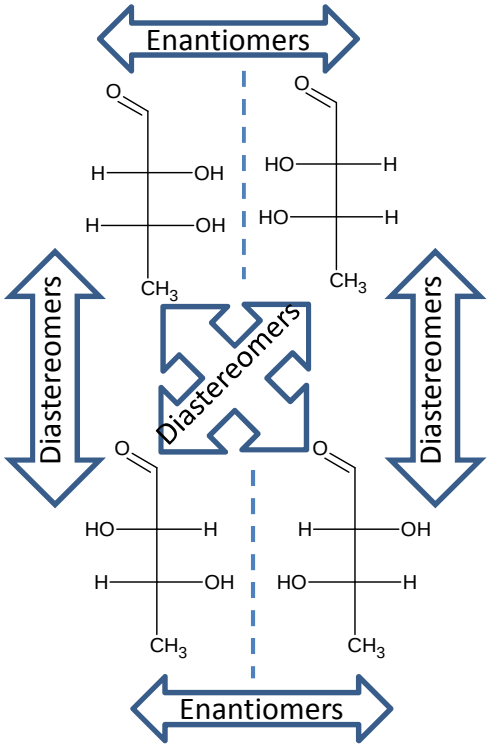
- Chemical Formula
- Structure

Different

- Geometry – stereoisomers that are not enantiomers
- Chemical Properties
- Physical Properties
- Optical Rotation
- Biological Properties



Enantiomers
vs.
Diastereomers


Enantiomers
Diastereomers
Diastereomers
Diastereomers
Enantiomers

Plane Polarized Light

Light normally oscillates/vibrates in every direction:

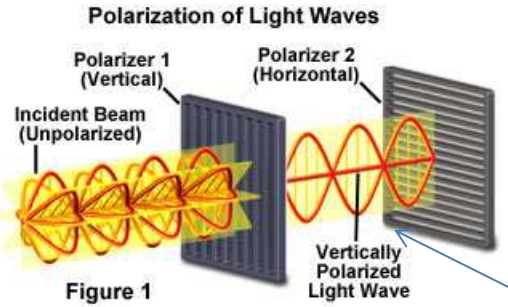
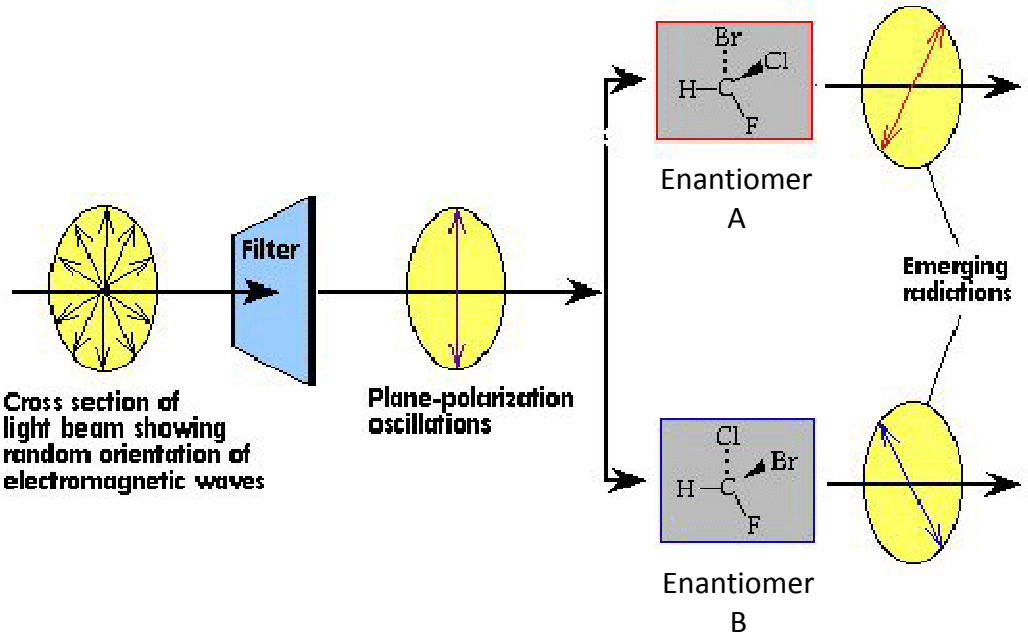


Figure 1

Plane Polarized Light oscillates/vibrates in only one direction:

Plane Polarized Light can interact with molecules:

Optical Rotation of Plane Polarized Light


Br
Cl
H
C
F
Enantiomer
A
Filter
Emerging
radiations
Cross section of
light beam showing
random orientation of
electromagnetic waves
Plane-polarization
oscillations
Cl
Br
H
C
F
Enantiomer
B

Chiral Molecules

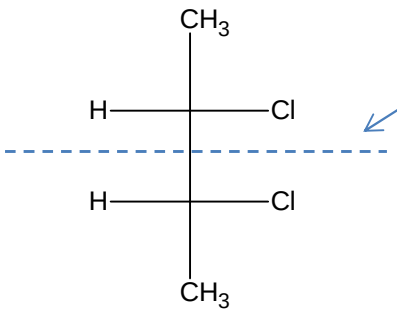
Definition:
Molecules that lack a plane of symmetry, and therefore have non-superimposable mirror images. Can rotate plane polarized light.

Requirements:
Carbon atoms with 4 bonds to different groups.
No additional plane of symmetry.

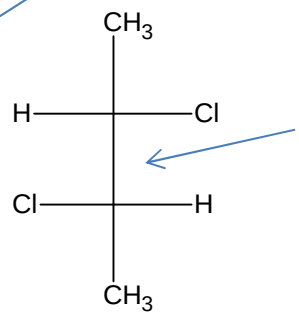
Important:
Chiral molecules that are enantiomers have the same physical and chemical properties but different biological properties.

Achiral Molecules

- Molecules that possess chiral carbons but have an additional plane of symmetry
- They do not rotate plane polarized light.
- Meso compounds are achiral.



Achiral/Meso



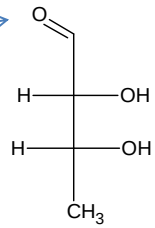
Chiral

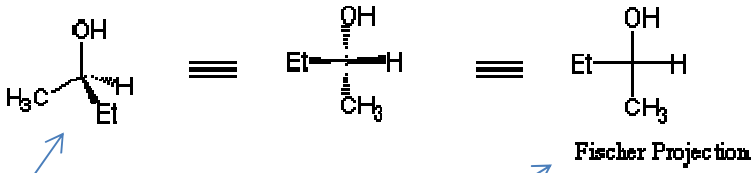
No Plane of Symmetry

Fischer Projections

Method for drawing chiral molecules in 2D.

- Always draw the most oxidized group at the top
- The carbon backbone is drawn top-bottom
- Swaps are allowed only for horizontal atoms
    - Odd number of swaps = diff. molecule
    - Even number of swaps = same molecule





3D View showing tetrahedral shape

2D Representation of a 3D shape

Dextrorotatory and Levorotatory

Dextrorotatory

- Rotates light clockwise
- (+)

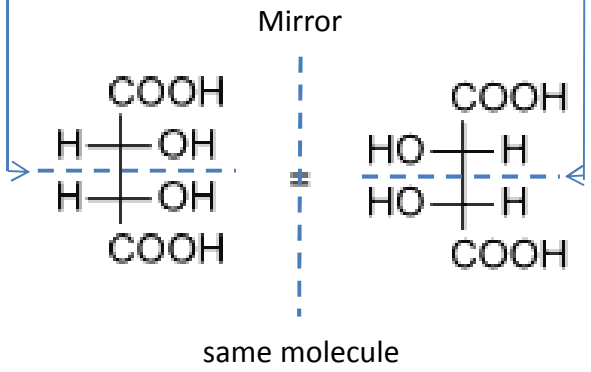
Levorotatory

- Rotates light counter clockwise
- (-)

Meso Compounds

Definition:
Meso compounds have 2 (or more) chiral atoms, but do not rotate plane polarized light due to have an extra plane of symmetry

- Extra plane of symmetry
- Mirror image = same molecule
- Does not rotate plane polarized light



Number of Stereoisomer

Maximum number of stereoisomers

2^n

n = number of chiral carbons

- $2^2 = 4$
- $2^3 = 8$
- $2^4 = 16$

- Meso compounds decrease the number of isomers formed

Racemic Mixtures

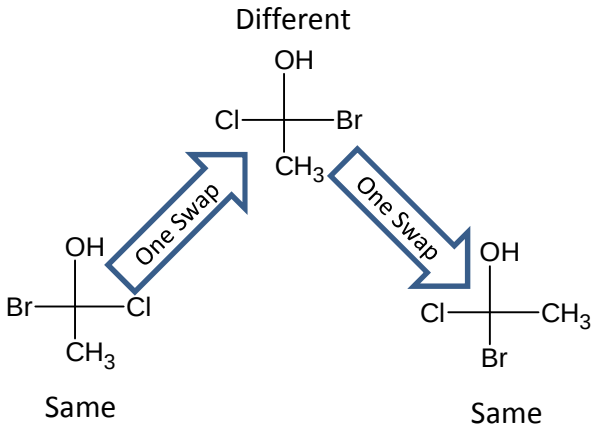
Definition:
A mixture of equal amounts of two enantiomers

- Does not rotate plane polarized light (the 2 enantiomers cancel each other out)

Same/Different

Two Fischer projections:

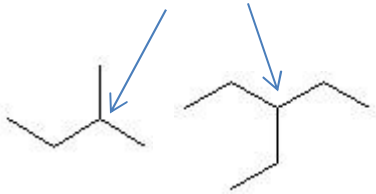
- Even # swaps = same molecule
- Odd # swaps = different molecule

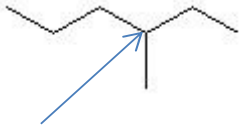


Identifying Chiral Carbons

Definition: Chiral carbons are bonded to 4 different groups of atoms

- no C=C or C≡C
- watch out for same groups like methyl/ethyl





chiral 4 different groups

- H
- methyl
- ethyl
- propyl