STEREOISOMERS OF CARBON COMPOUNDS

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Stereoisomers of Carbon Compounds

Stereochemistry: That part of the science which deals with structure in three dimensions

Isomers: Have same molecular formula, but different structures

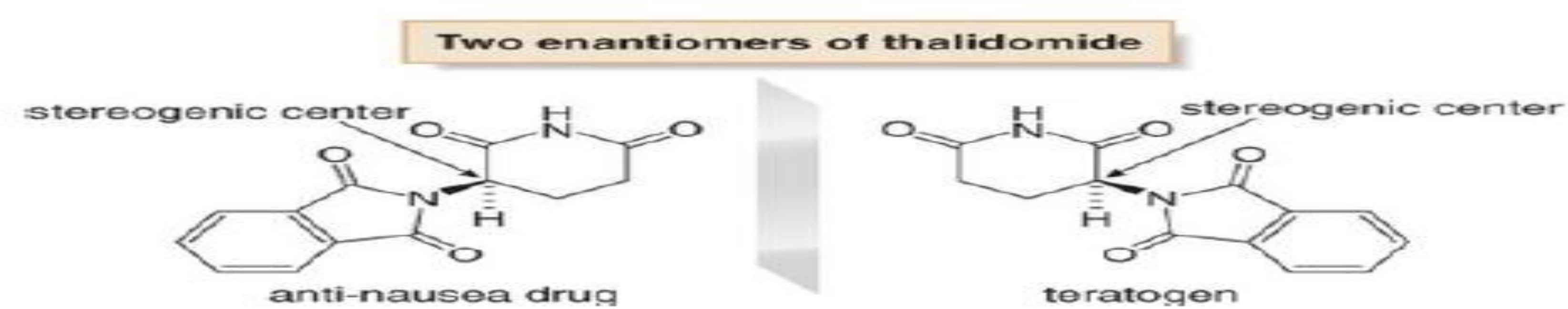
C_2H_6O → CH_3CH_2OH **alcohol**

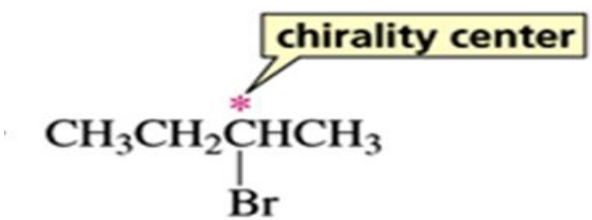
C_2H_6O → CH_3OCH_3 **ether**

Stereoisomers of Carbon Compounds

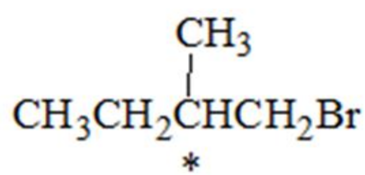
Chiral compounds: are optically active; they rotate the plane of polarized light.

Achiral compounds: do not rotate the plane of polarized light. They are optically inactive.

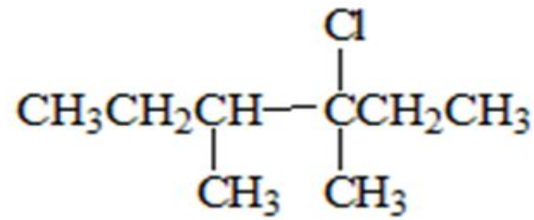




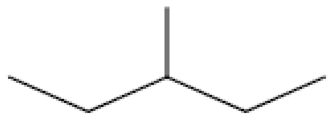
2-bromobutane

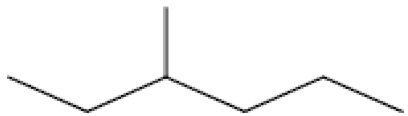


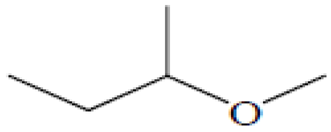
1-bromo-2-methylbutane

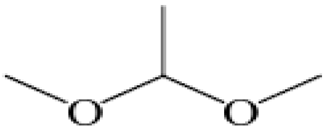


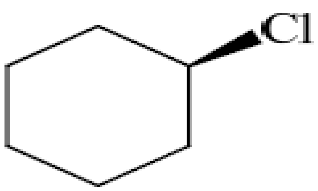
Stereoisomers of Carbon Compounds

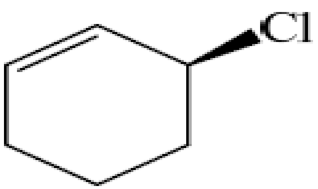


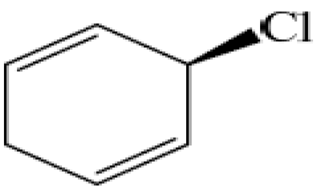


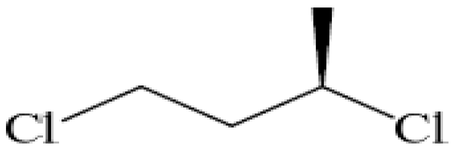


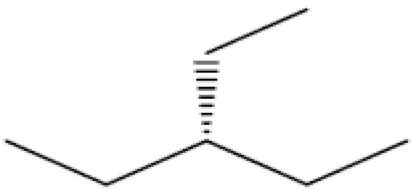


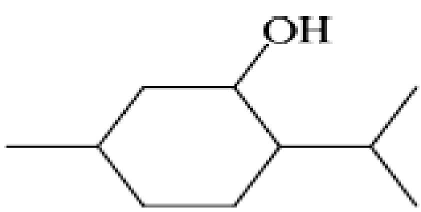


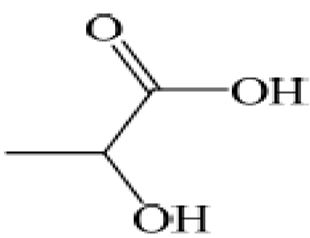


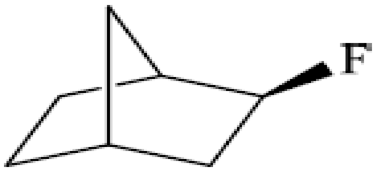








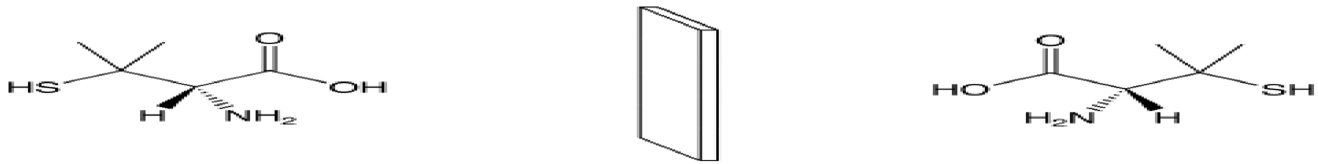




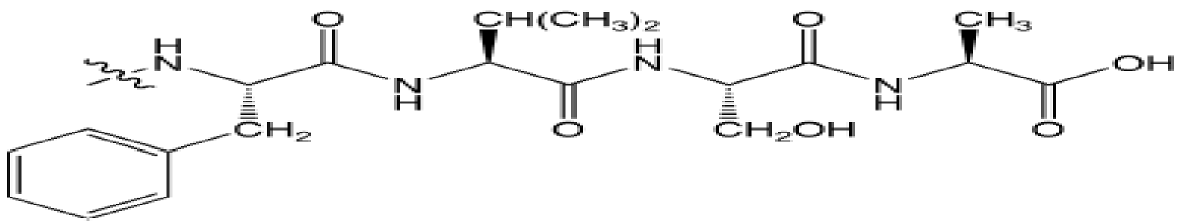
Stereoisomers of Carbon Compounds

Enantiomers, therefore have different physiological responses

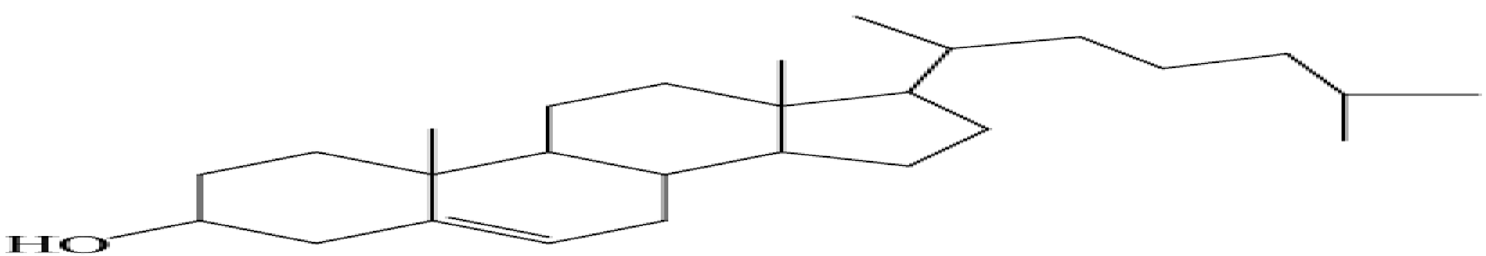
Consider Penicillamine



antiarthritic   toxic



Short peptide segment



CHOLESTEROL

Stereoisomers of Carbon Compounds

Optical Activity

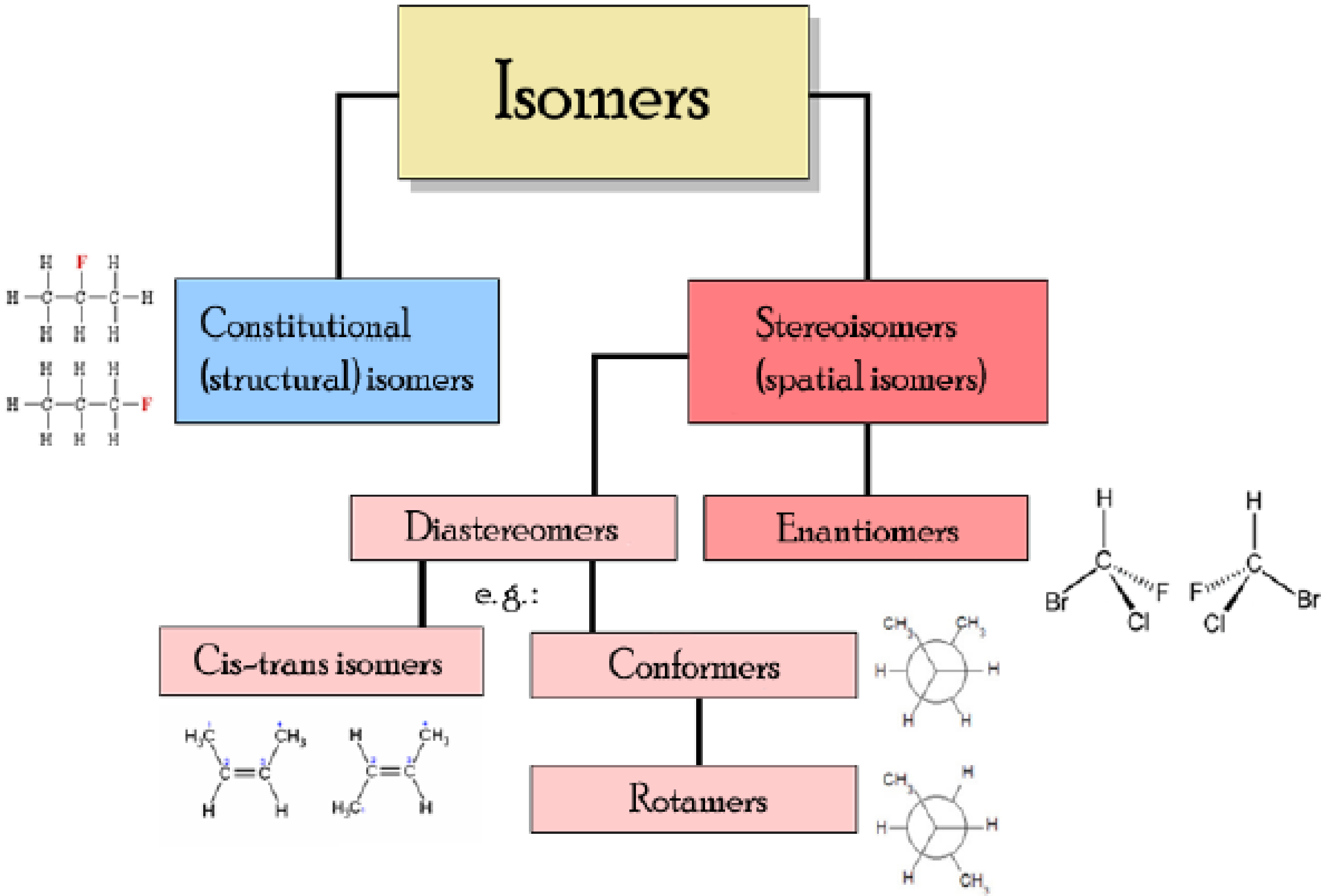
- ***Optically Active:*** compounds rotate plane polarized light. Chiral compounds (compounds not superimposable on their mirror objects) are expected to be optically active.
- ***Optically Inactive:*** compounds do not rotate plane polarized light. Achiral compounds are optically inactive.

Stereoisomers of Carbon Compounds

Summary of Isomerism Concepts

- Isomers, contain same atoms, same formula
  - Constitutional isomers, different connectivities, bonding.
  - Stereoisomers, same connectivity, different three dimensional orientation of bonds
    - Enantiomers, mirror objects
    - Diastereomers, not mirror objects

Stereoisomers of Carbon Compounds



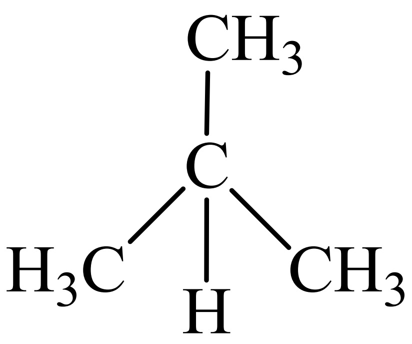
Stereoisomers of Carbon Compounds

Constitutional (*Structural*) *Isomers:* same molecular formula, different connectedness

Butane, a four-carbon molecule, is the simple alkane that has two structural isomers.

Ex.

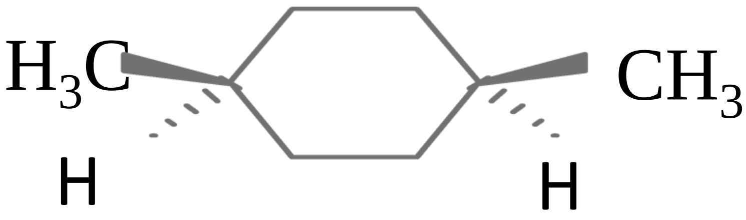
C_4H_{10} $CH_3CH_2CH_2CH_3$



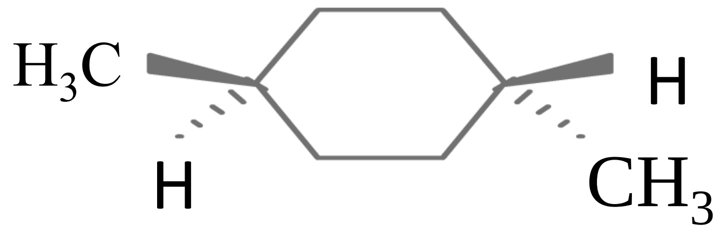
n-butane isobutane

Stereoisomers of Carbon Compounds

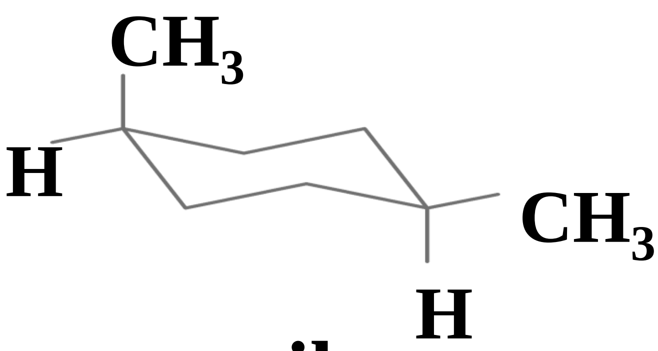
Stereoisomers ***:*** compounds with the same connectivity, different arrangement in space



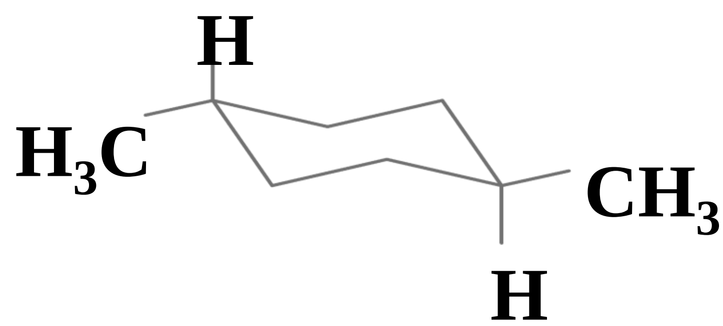
cis



trans

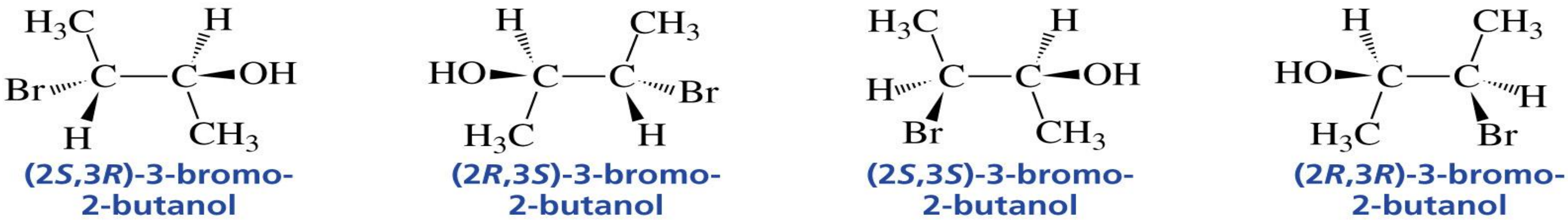


axil

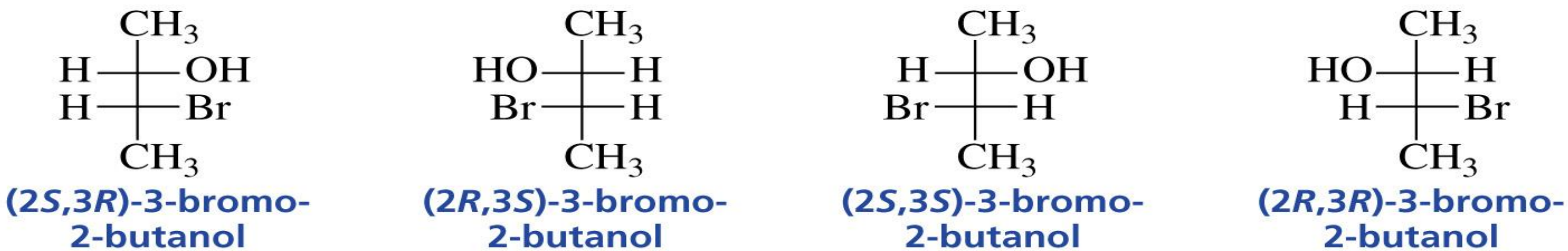


eq

Stereoisomers of Carbon Compounds



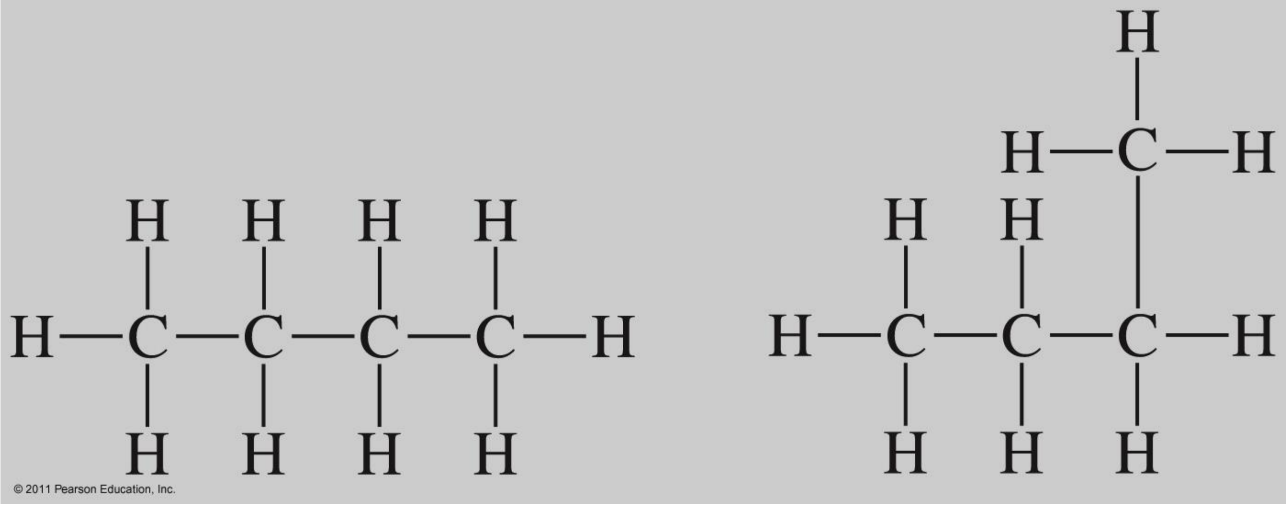
perspective formulas of the stereoisomers of 3-bromo-2-butanol



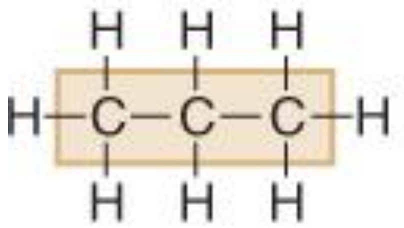
Fischer projections of the stereoisomers of 3-bromo-2-butanol

Stereoisomers of Carbon Compounds

Conformational isomers: are isomers that are not different compounds because they have different arrangements of the atoms of the compound. They are also known as *conformers*. ***Consider butane:*** The structure of butane can be represented as shown on the next slide.



Stereoisomers of Carbon Compounds



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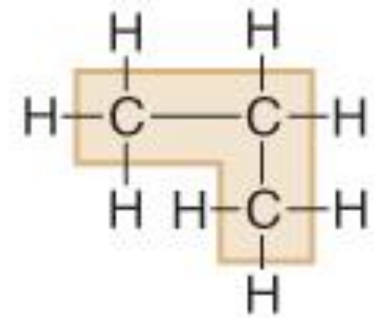
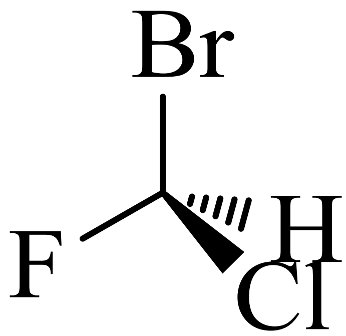
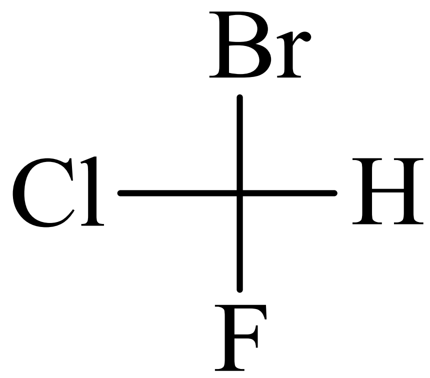
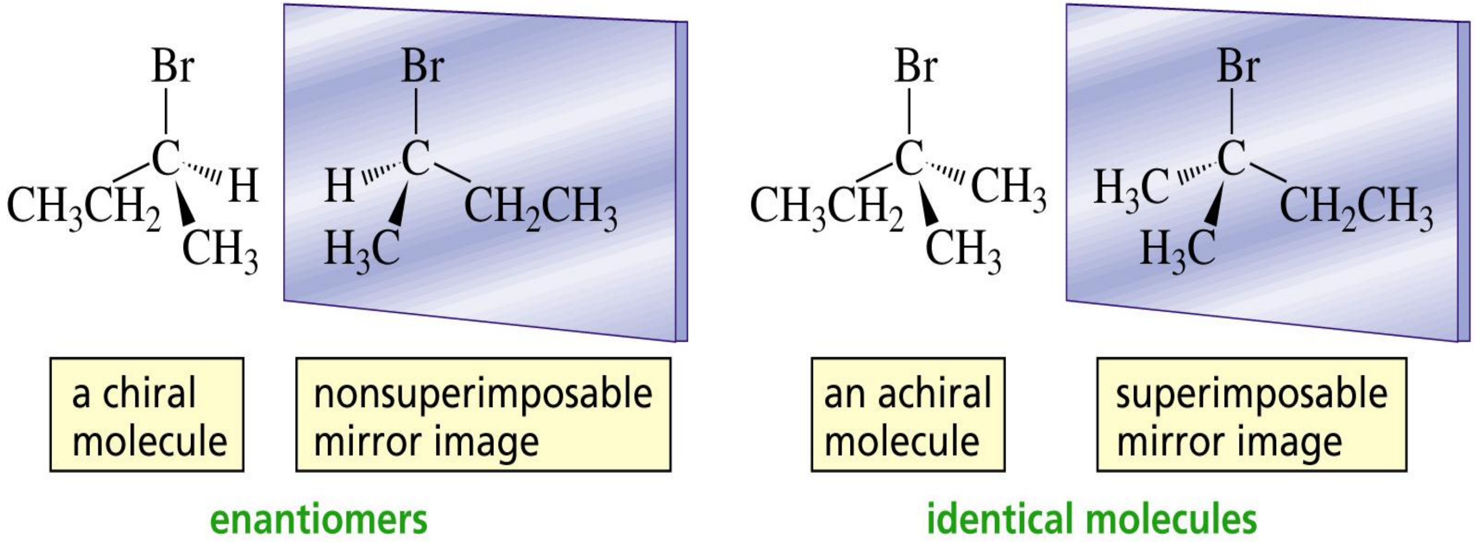


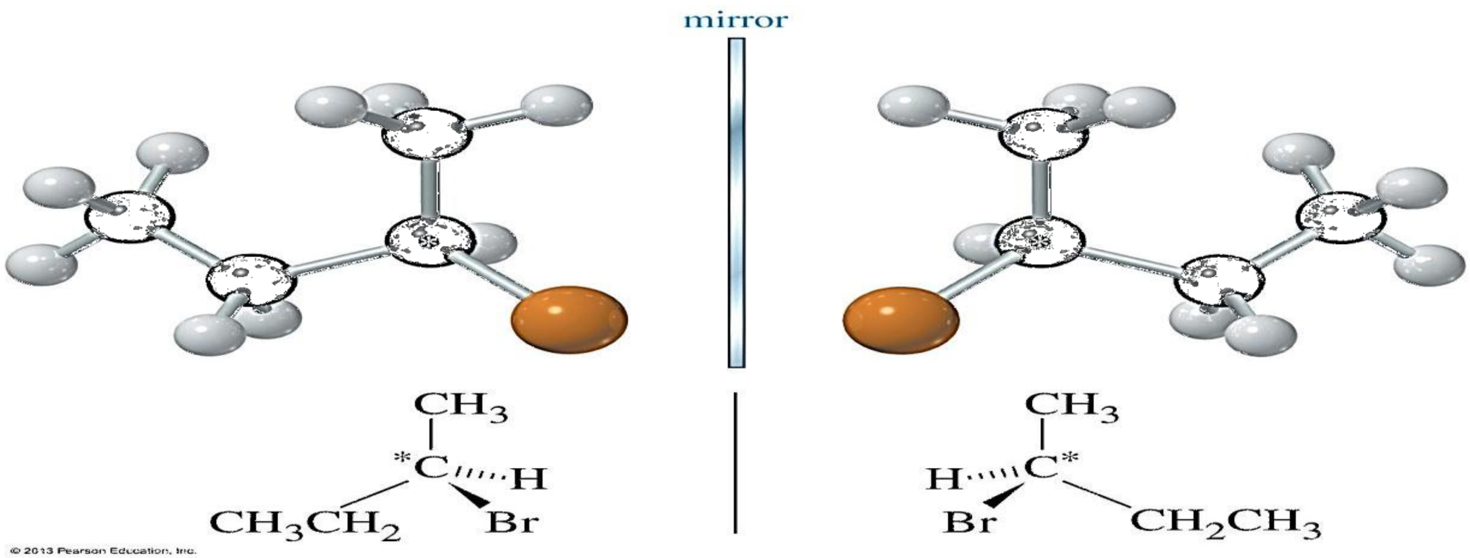
Configuration : the arrangement in space of the four different groups about a chiral center.





Stereoisomers of Carbon Compounds





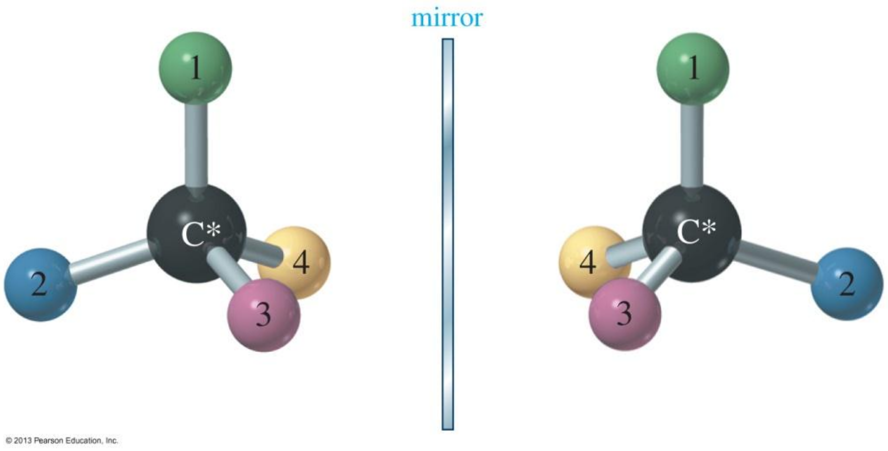
Stereoisomers of Carbon Compounds

Enantiomers : Compounds that are no superimposable mirror images. Any molecule that is chiral must have an enantiomer.

stereoisomers that are non-superimposable mirror images ; only properties that differ are direction (+ or -) of optical rotation

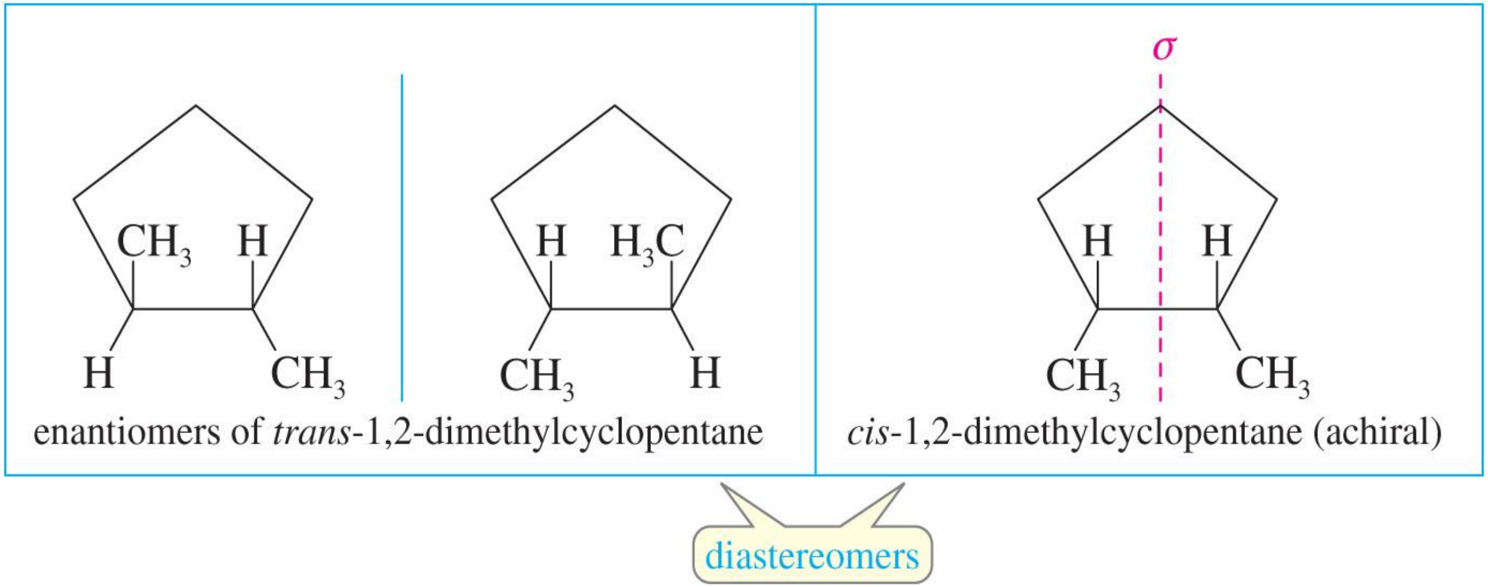
Stereoisomers of Carbon Compounds

- Also called *asymmetric carbon* atom.
- Carbon atom that is bonded to four different groups is chiral.
- Its mirror image will be a different compound (enantiomer).



Stereoisomers of Carbon Compounds

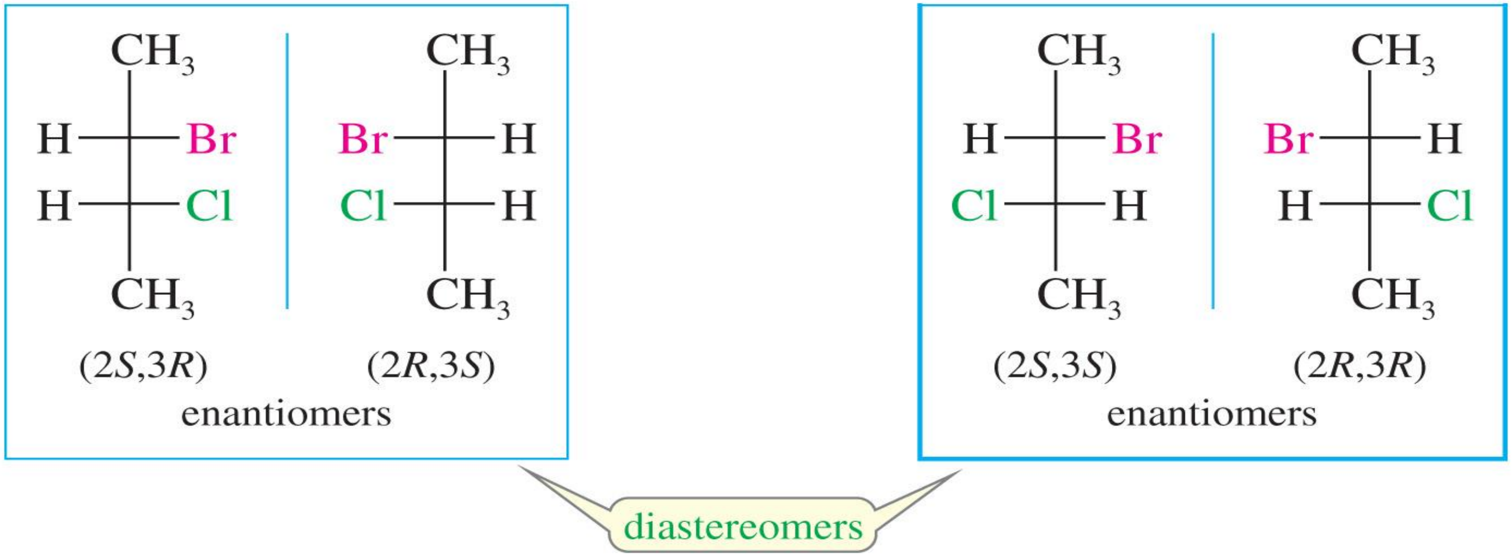
Diastereomers : stereoisomers that are not mirror images; different compounds with different physical properties.



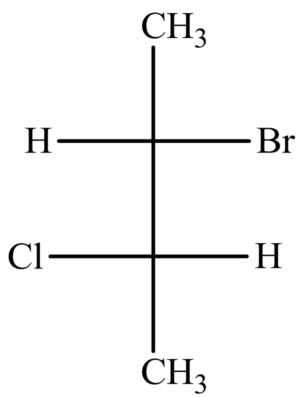
Stereoisomers of Carbon Compounds

Diastereomers

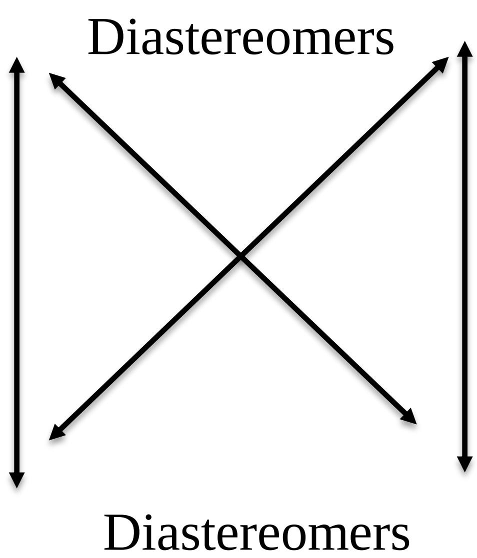
- Molecules with two or more chiral carbons.
- Stereoisomers that are not mirror images.

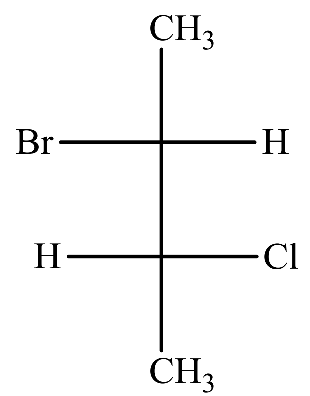


Stereoisomers of Carbon Compounds

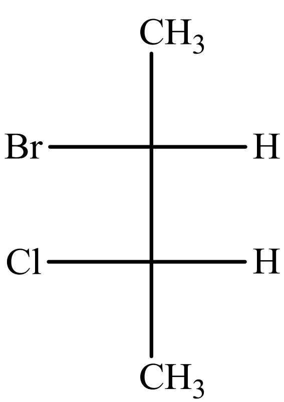


(*2S,3S*) 2-bromo-3-chlorobutane

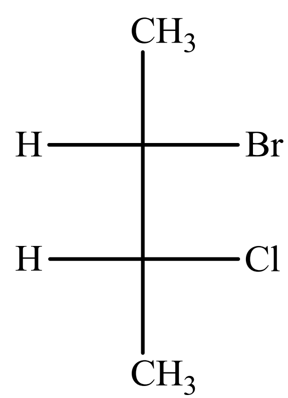




(*2R,3R*) 2-bromo-3-chlorobutane

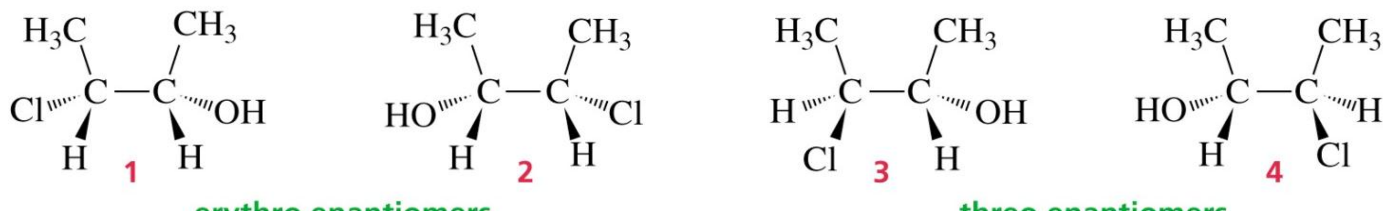


(*2R,3S*) 2-bromo-3-chlorobutane



(*2S,3R*) 2-bromo-3-chlorobutane

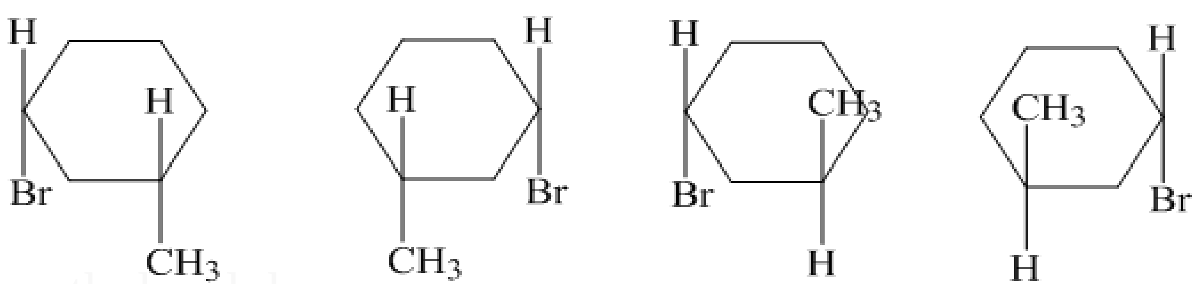
Stereoisomers of Carbon Compounds



3-chloro-2-butanol

1 2 3 4

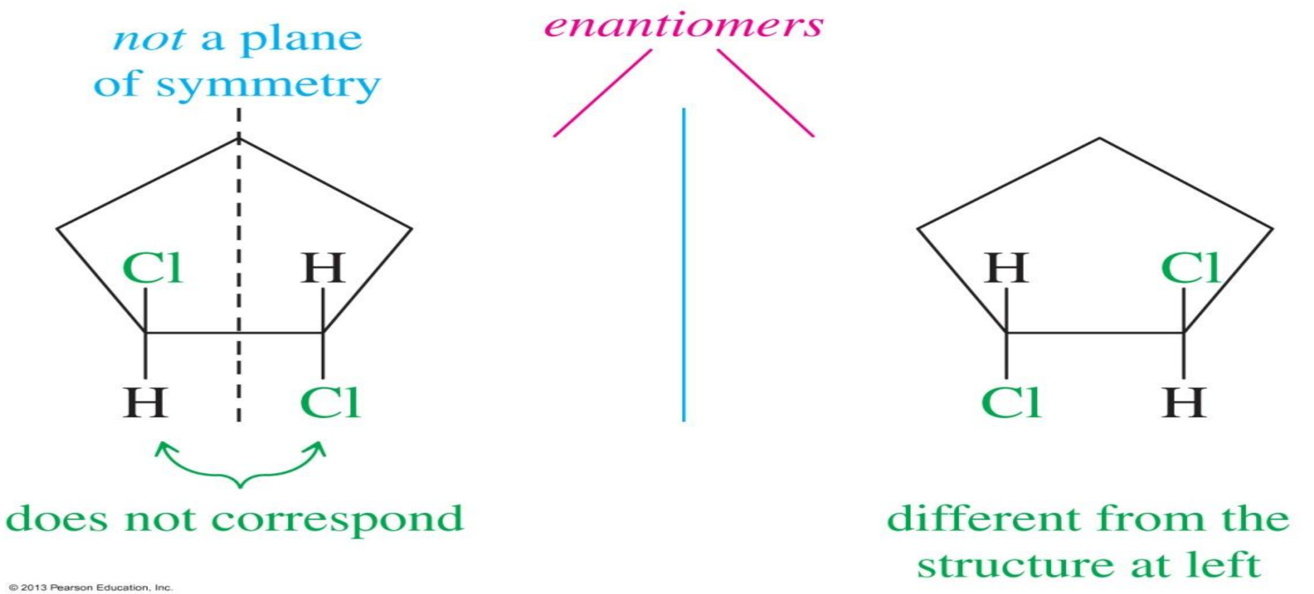
erythro enantiomers threo enantiomers

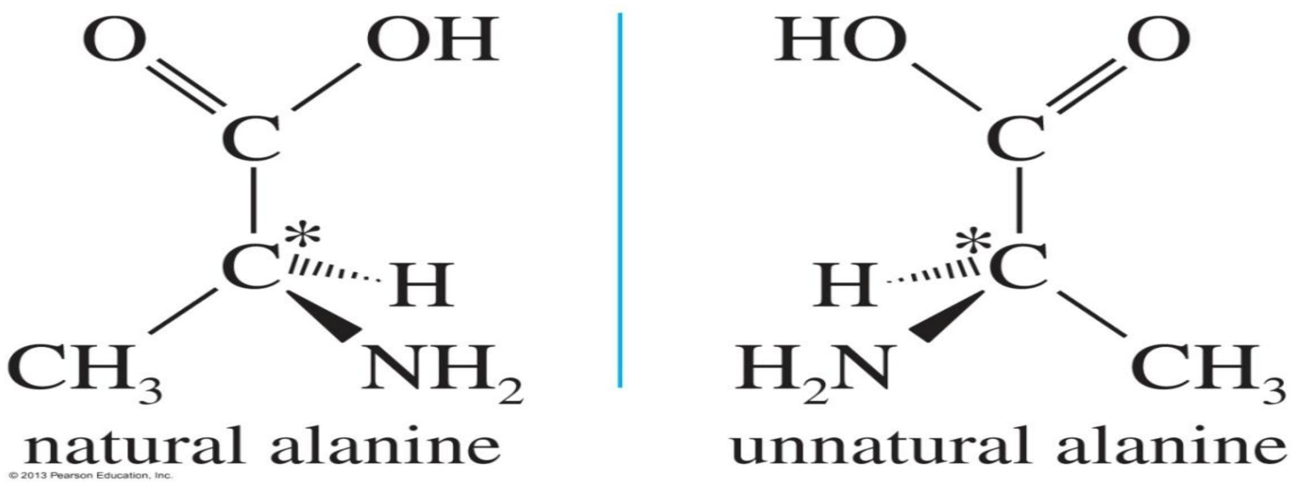


cis-1-bromo-3-methylcyclohexan

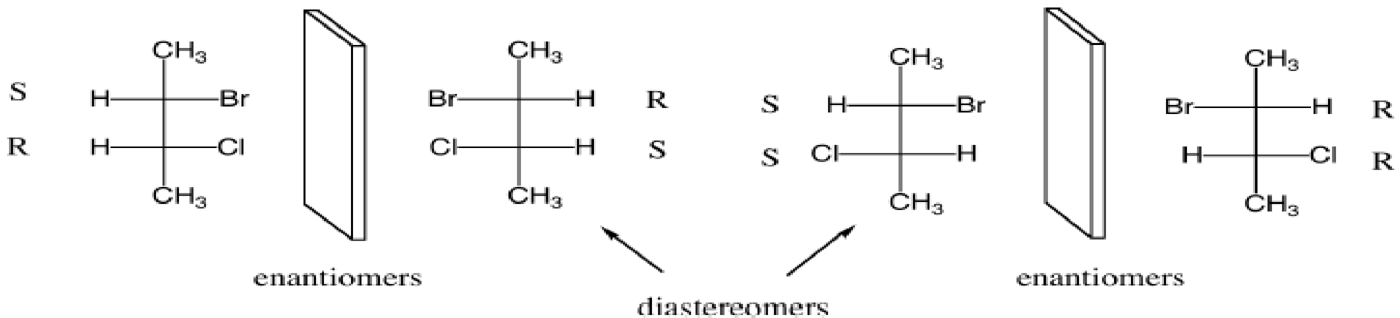
trans-1-bromo-3-methylcyclohexane

Stereoisomers of Carbon Compounds



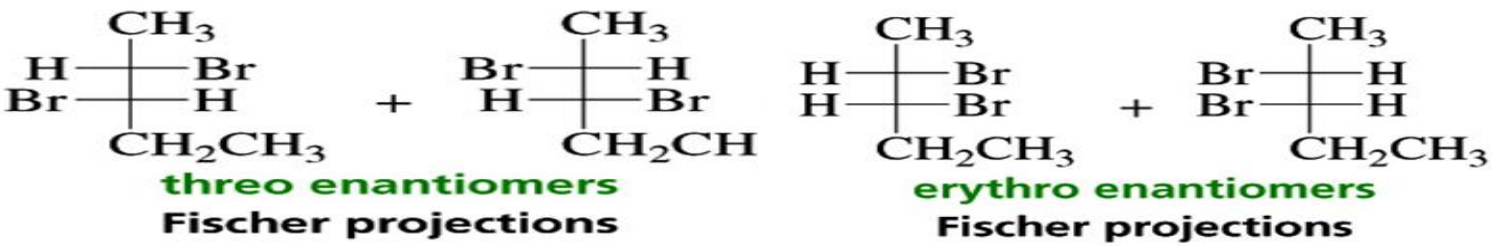


Stereoisomers of Carbon Compounds

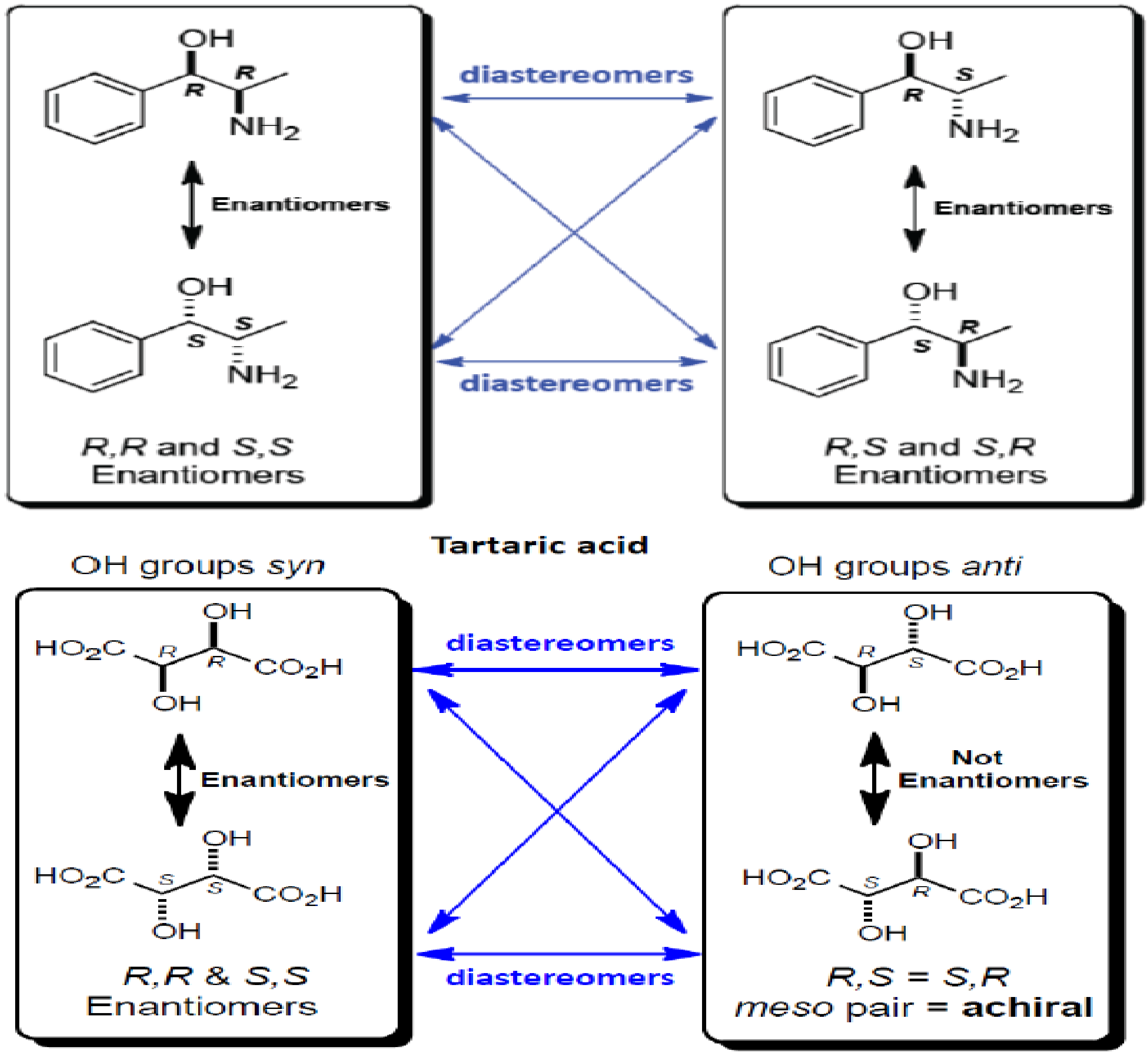


stereochemistry of the product

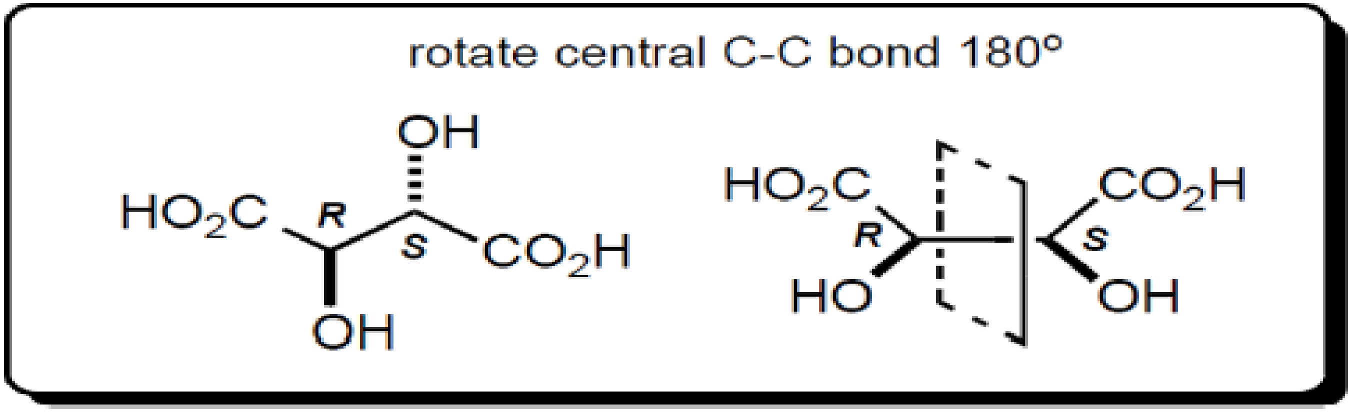
a pair of diastereomers



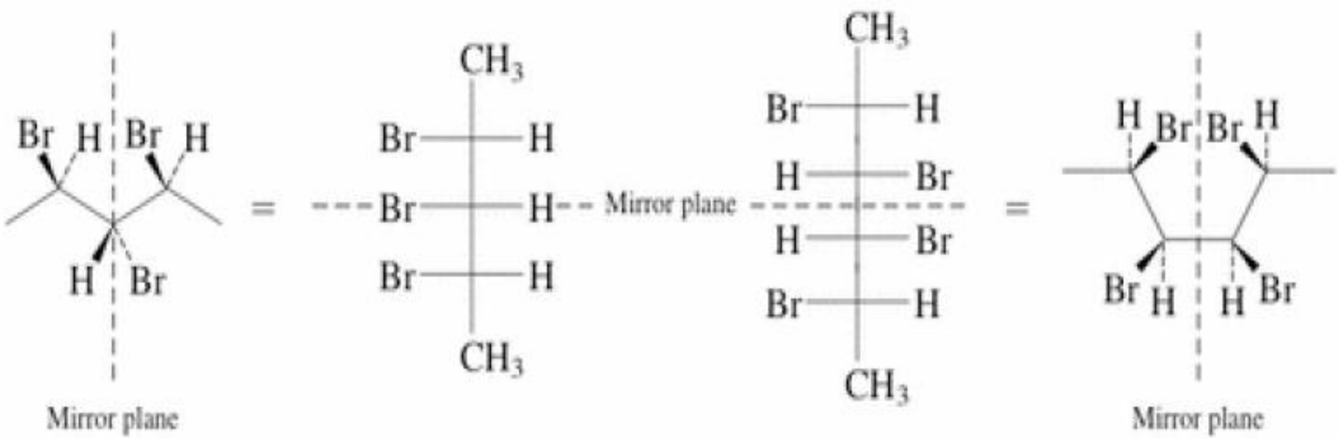
Stereoisomers of Carbon Compounds



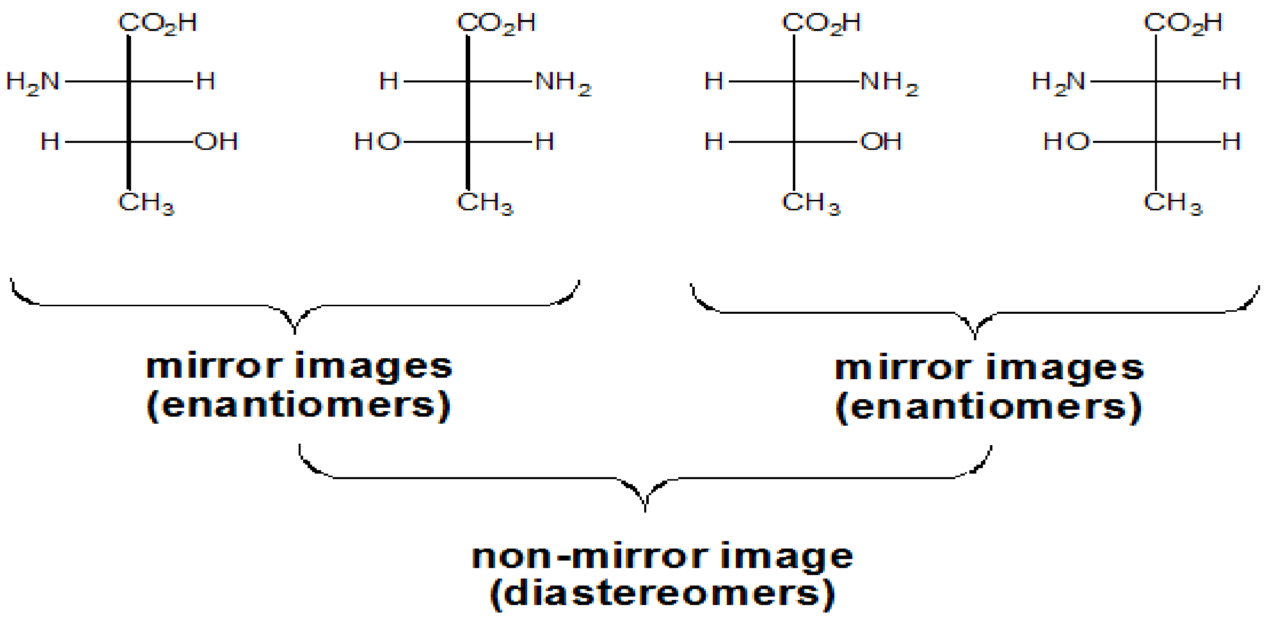
Stereoisomers of Carbon Compounds



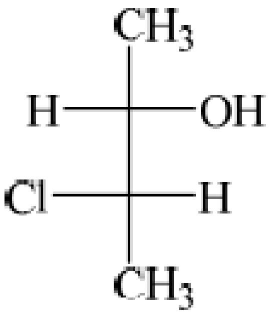
Meso Compounds with Multiple Stereocenters



Stereoisomers of Carbon Compounds



Stereoisomers of Carbon Compounds



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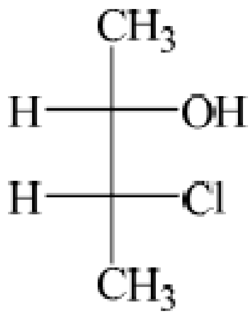

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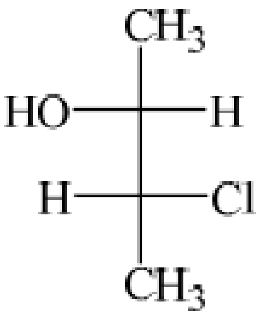

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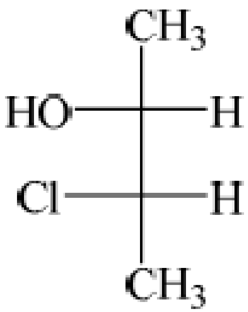

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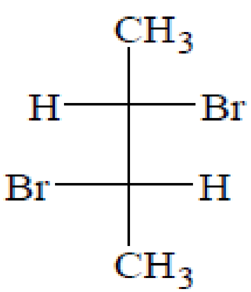
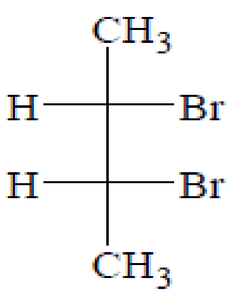
For example:



1



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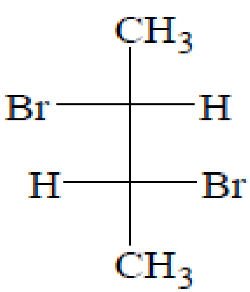

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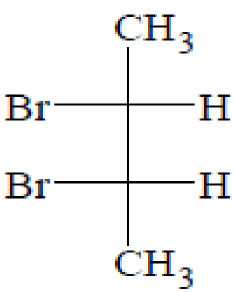

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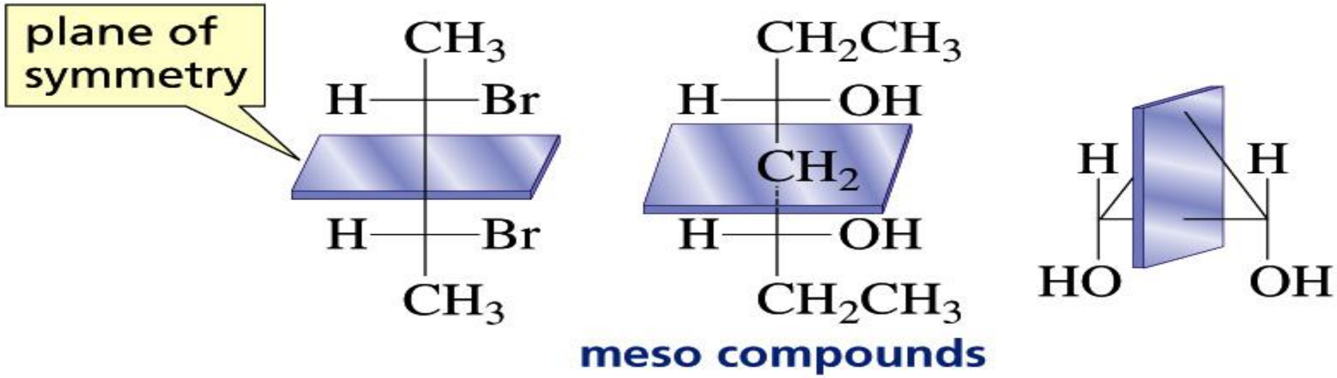
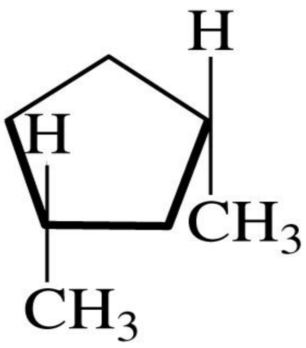
Stereoisomers of Carbon Compounds

Meso compounds: are achiral compounds that has multiple chiral centers. It is superimposed on its mirror image and is optically **inactive** despite its stereocenters.

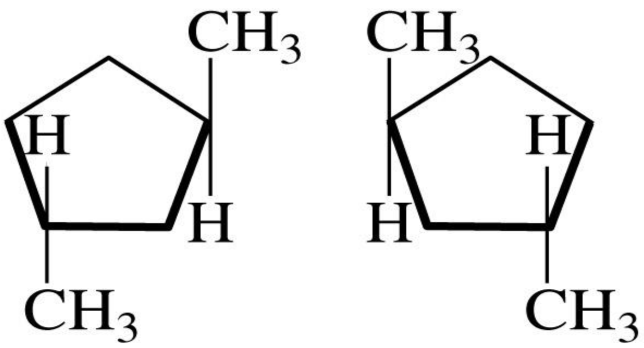


Stereoisomers of Carbon Compounds



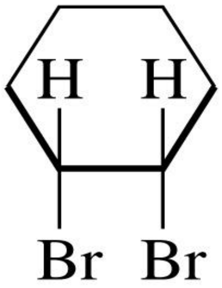
cis-1,3-dimethylcyclopentane

a meso compound



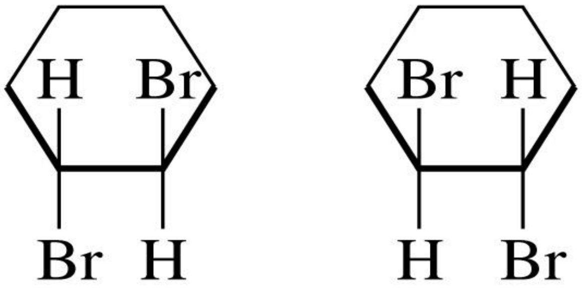
trans-1,3-dimethylcyclopentane

a pair of enantiomers



cis-1,2-dibromocyclohexane

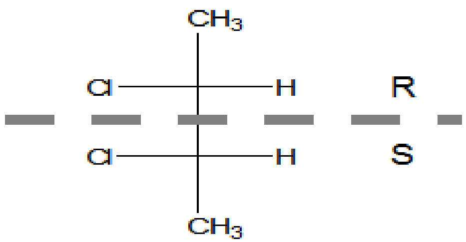
a meso compound



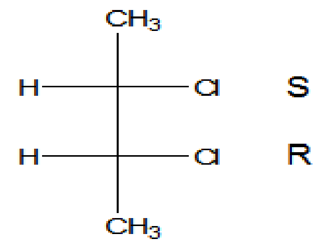
trans-1,2-dibromocyclohexane

a pair of enantiomers

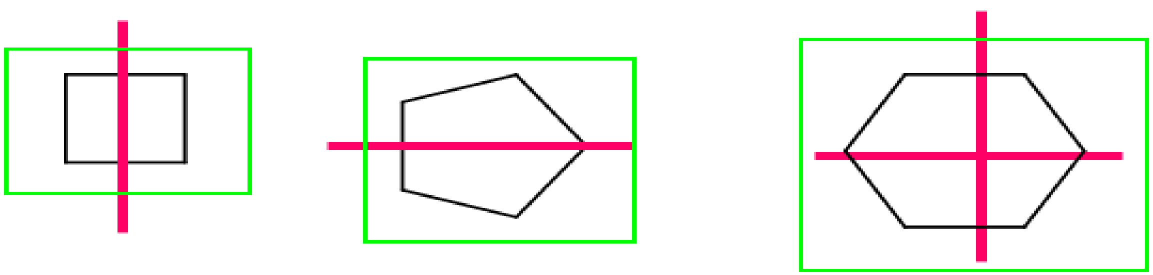
Stereoisomers of Carbon Compounds



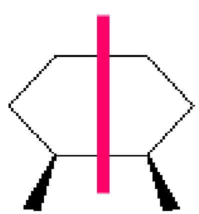
Meso



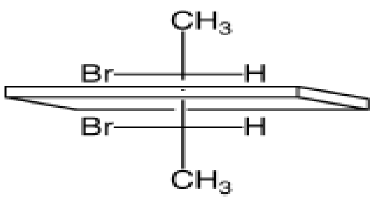
Can be superimposed by 180 deg rotation.



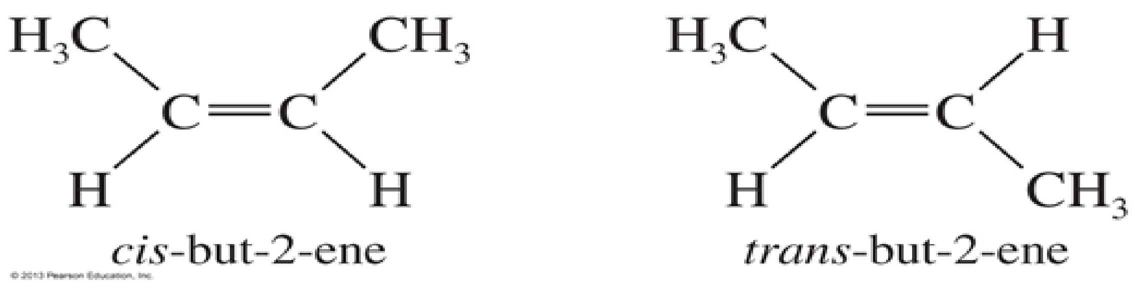
cis



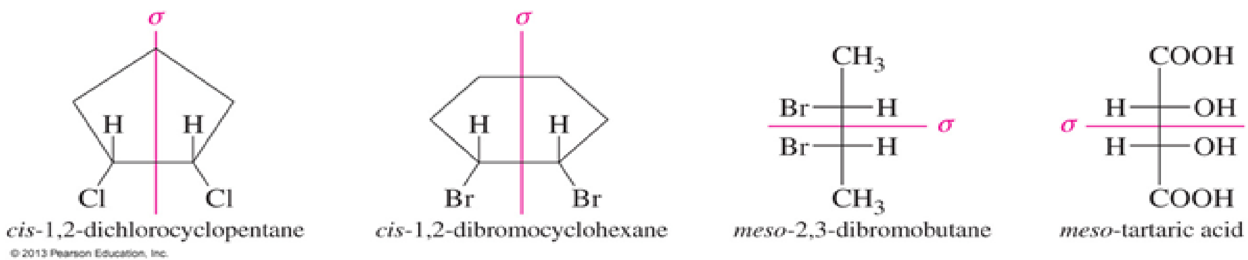
(1*S*,2*R*)-1,2-dimethylcyclohexane

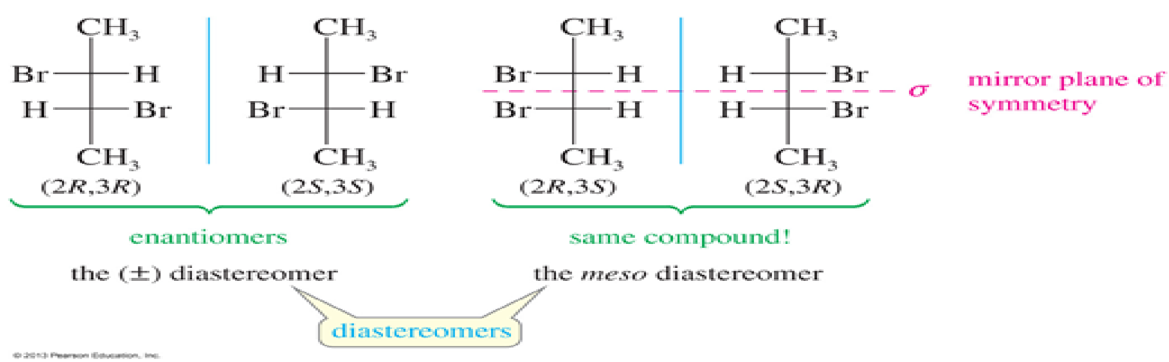


Stereoisomers of Carbon Compounds

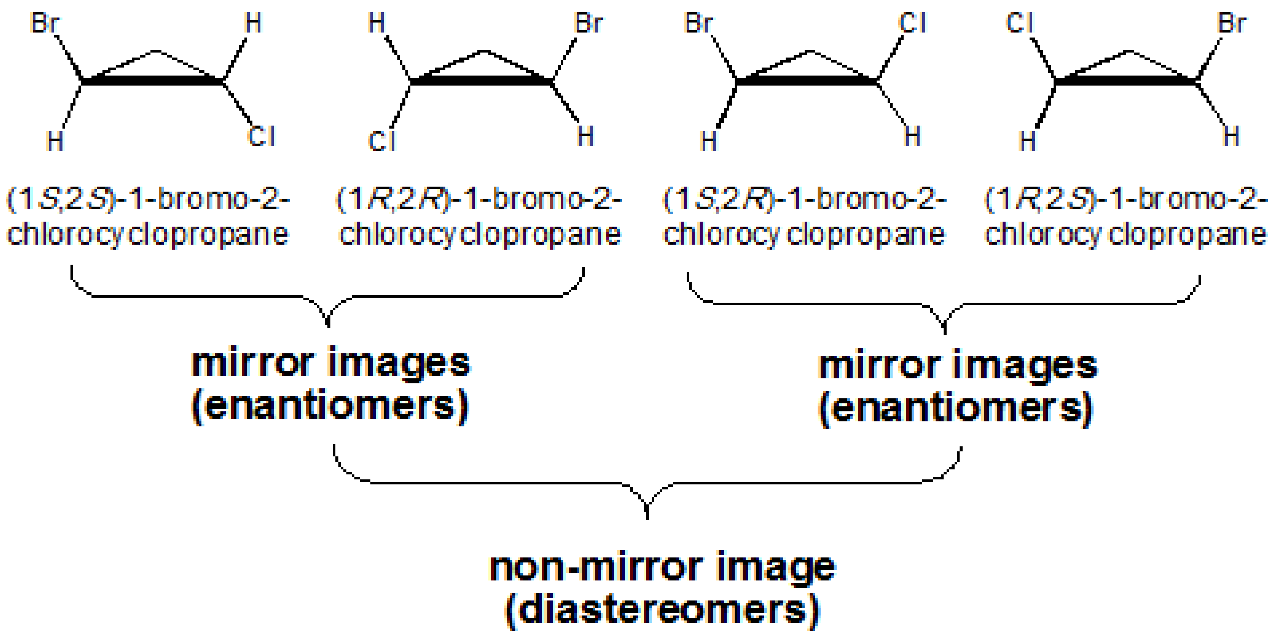


Meso Compounds





Stereoisomers of Carbon Compounds



7.11: Achiral Molecules with Two Chirality Centers

meso (achiral) chiral

Meso: molecules that contain chiral atoms but are achiral because they also possess a plane of symmetry.

Stereoisomers of Carbon Compounds

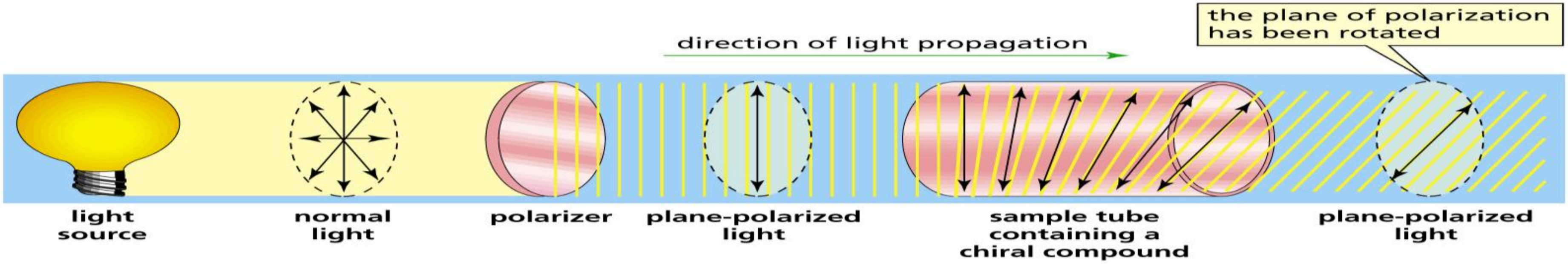
Polari meter – device that measures the optical rotation of the chiral compound

dextrorotatory : when the plane of polarized light is rotated in a clockwise direction when viewed through a Polari meter.

(+) or (*d*) do not confuse with D

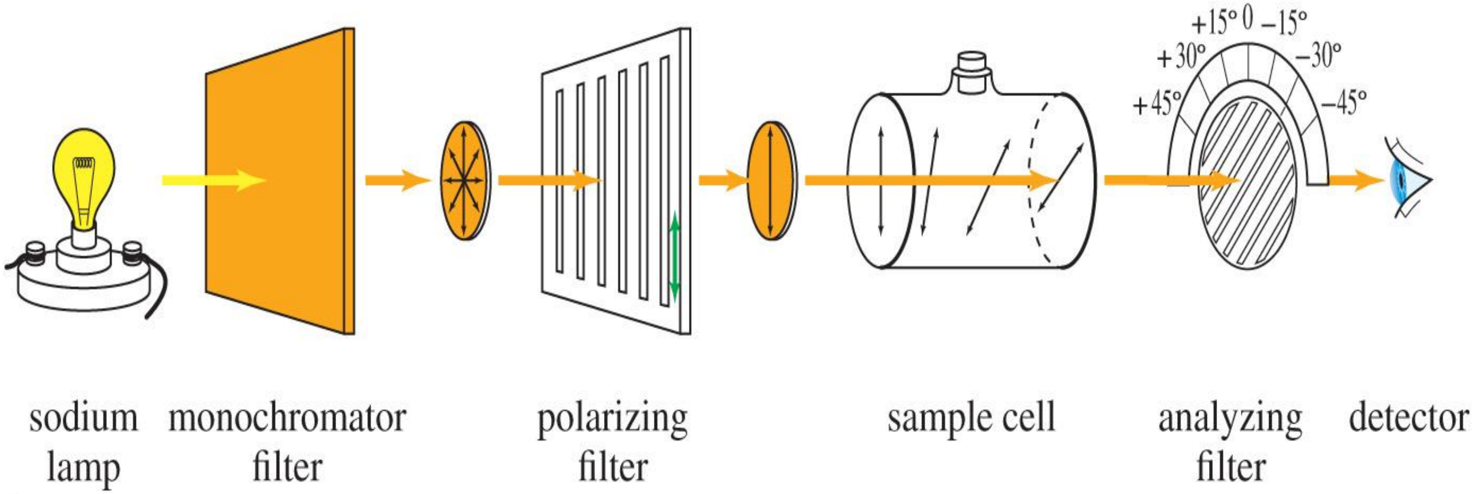
levorotatory : when the plane of polarized light is rotated in a counter-clockwise direction when viewed through a Polari meter.

(-) or (*l*) do not confuse with L



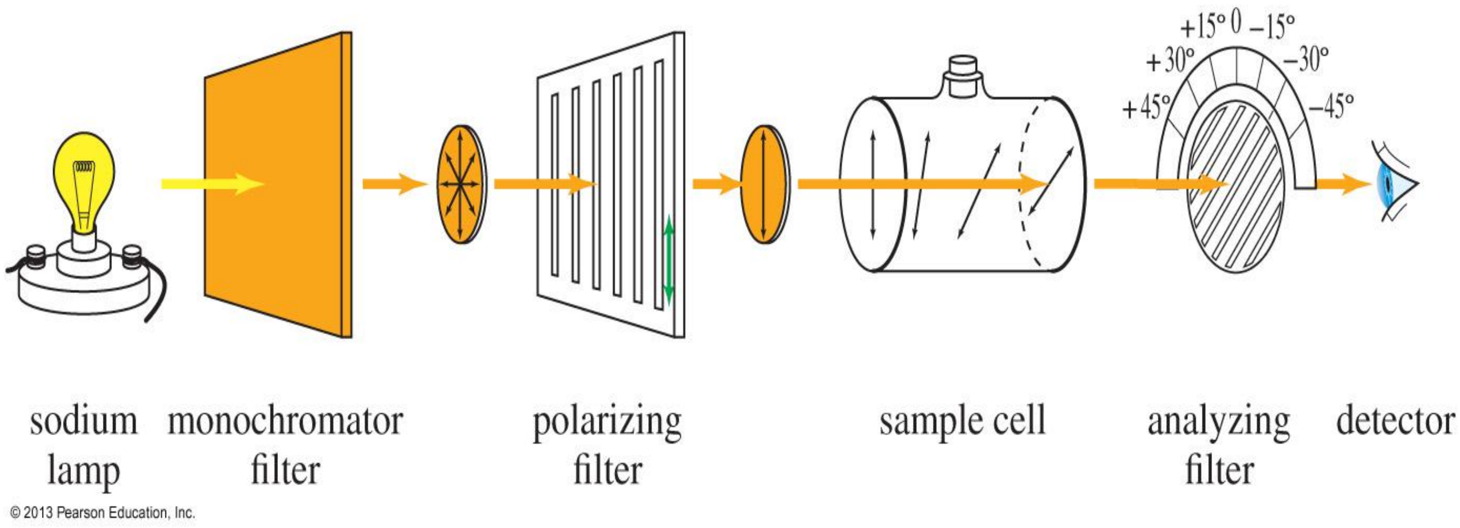
Optical Activity

Enantiomers rotate the plane of polarized light in opposite directions, but same number of degrees.



Stereoisomers of Carbon Compounds

Polari meter



Clockwise **Counterclockwise**

Dextrorotatory (+) **Levorotatory (-)**

Specific Rotation

Observed rotation depends on the length of the cell and concentration, as well as the strength of optical activity, temperature, and wavelength of light.

$$[\alpha] = \frac{\alpha\ (\text{observed})}{c \bullet l}$$

Where α (observed) is the rotation observed in the Polari meter, *c* is concentration in g/mL, and *l* is length of sample cell in decimeters.

Specific Rotation, [α]

$$[\alpha] = \alpha / cl$$

a = observed rotation

c = concentration in g/mL

l = length of tube in dm

Dextrorotary designated as *d* or (+), clockwise rotation

Levorotary designated as *l* or (-), counter-clockwise rotation

Solved Problem

When one of the enantiomers of 2-butanol is placed in a Polari meter, the observed rotation is 4.05° counterclockwise. The solution was made by diluting 6 g of 2-butanol to a total of 40 mL, and the solution was placed into a 200-mm Polari meter tube for the measurement. Determine the specific rotation for this enantiomer of 2-butanol.

Solution

Since it is levorotatory, this must be (–)-2-butanol The concentration is 6 g per 40 mL = 0.15 g/mL, and the path length is 200 mm = 2 dm. The specific rotation is

$$[a]_{D}^{25} = \frac{-4.05^{\circ}}{(0.15)(2)} = -13.5^{\circ}$$

Solved Problem

A sample of a compound A in chloroform (0.500 g/mL) at 25.0^{o}C shows a rotation of $^{+}2.5^{o}$ in a 1.0 decimeter cell. What is the specific rotation?

THANK YOU