Stereochemistry of Organic Molecule

الكيمياء والمجسمة للمركبات العضوية

Introduction

- The term *isomers* comes from the Greek words *isos* and *meros*, meaning “made of the same parts.” That is, isomers are compounds that are constructed from the same atoms (same molecular formula) but that still differ from each other.

مصطلح الأيزومرات يأتي من الكلمات اليونانية isos و meros، وتعني "مصنوعة من نفس الأجزاء". أي أن الأيزومرات عبارة عن مركبات مكونة من نفس الذرات (نفس الصيغة الجزيئية) ولكنها لا تزال تختلف عن بعضها البعض

Isomers

Different compounds with same molecular formula

جزيئات مختلفه لكن لها نفس التركيب الجزيئي

Constitutional isomers

Isomers whose atoms have a different connectivity

الجزيئات مختلفه في طريقه التوصيل

Stereoisomers

Isomers that have the same connectivity but that differ in the arrangement of their atoms in space

جزيئات لديها نفس طريقه التوصيل لكن تختلف في ترتيب الذرات في الفراغ

ايزومرات (Isomers)

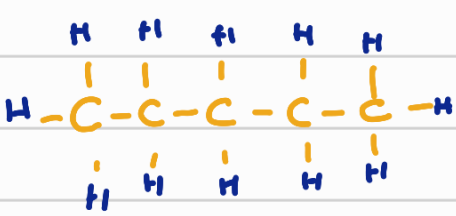
مركبات لها نفس الصيغة الجزيئية (نفس عدد الذرات)
لكن تختلف من حيث التركيب الجزيئي

Isomers

Constitutional isomer
ايزومرات بنائيه

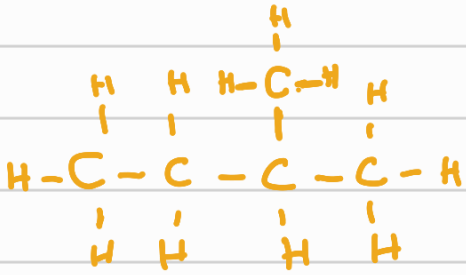
* لديها نفس عدد الذرات لكن الذرات موصوله بشكل مختلف

* لها اسم مختلف



C_5H_{12} *

Pantane



C_5H_{12}

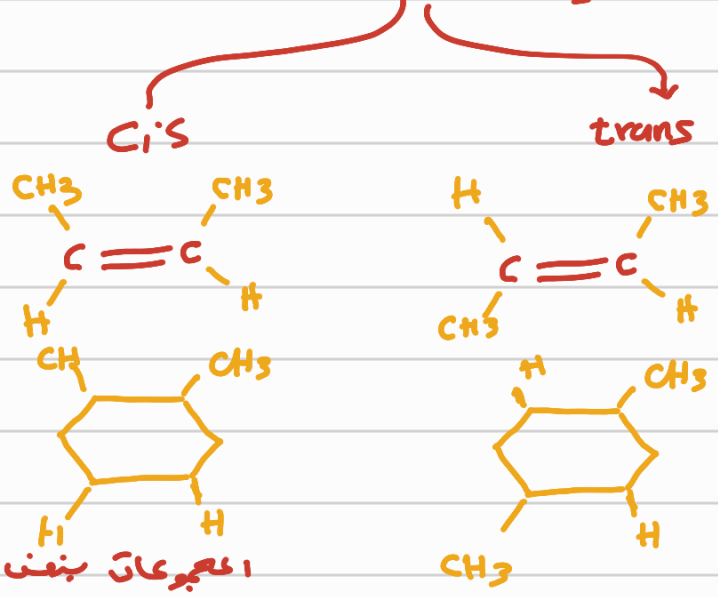
Methyl butane

(اختلف الشكل ، اختلف الطول ، اختلف الاسم)

Stereoisomer
ايزومرات فراغيه

هي جزيئات لها نفس الصيغة الجزيئية ونفس طريقة الوصلات لكن مختلفه في تركيبها الفضائي

تظهر في الجزيئات التي تحتوي حلقات او روابط ثنائية



* المجموعات بنفس الطرف cis

المجموعات على طرفي مختلفين trans

ايزومرات بنائيه

Constitutional Isomers

تختلف في ترتيب الروابط بين الذرات

- Constitutional (or structural) isomers differ in the order in which their atoms are bonded together.
- For example, there are three isomers of C_5H_{12}:

Pentane, methylbutane, and dimethylpropane.

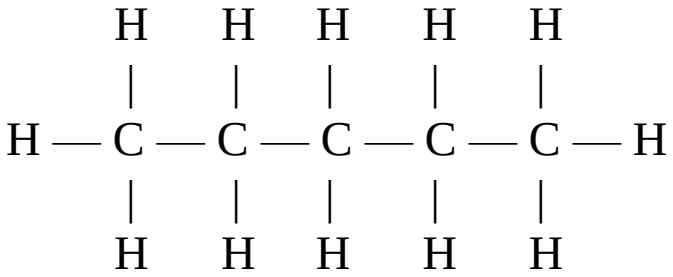
- These three isomers differ in the lengths of their base chain but not in the functional groups present (i.e., only alkyl groups are present in this case).

CH3

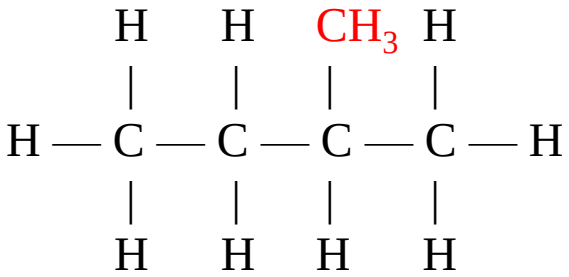
هذه الايزومرات تختلف بطول السلسلة الرئيسيه

Constitutional Isomers

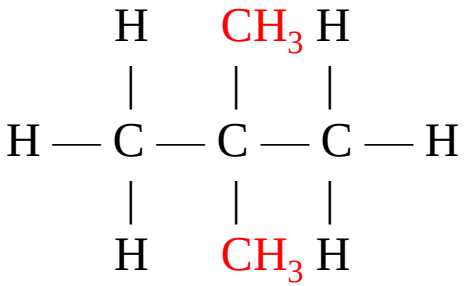
C_5H_{12} 3 ایزومرات د



Pentane, C_5H_{12}



Methylbutane, C_5H_{12}



Dimethylpropane, C_5H_{12}

Methyl: — CH_3

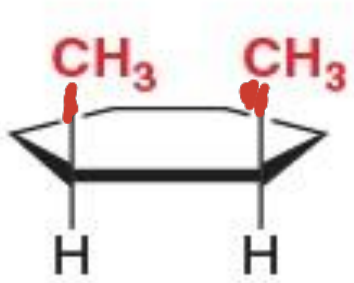
Stereoisomers

جزيئات لها نفس التركيب لكنها تختلف بالترتيب الفراغي للذرات

- Stereoisomers are compounds that have the same constitution but differ in the spatial arrangement of their atoms.
- The *cis* stereoisomer exhibits groups on the same side of the ring, while the *trans* stereoisomer exhibits groups on opposite sides of the ring.

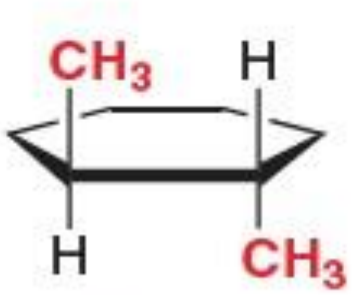
على نفس الطرف من الحلقة

على طرفين متعاكسين



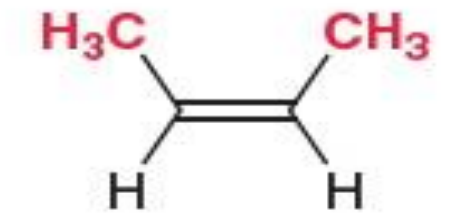
cis-
1,2-Dimethylcyclohexane

Cis-

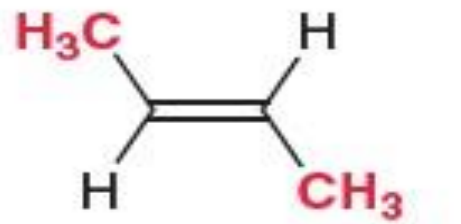


trans-
1,2-Dimethylcyclohexane

In addition to the examples above, the terms *cis* and *trans* are also used to describe stereoisomerism among double bonds:



cis-2-Butene
Boiling point = 4°C



trans-2-Butene
Boiling point = 1°C

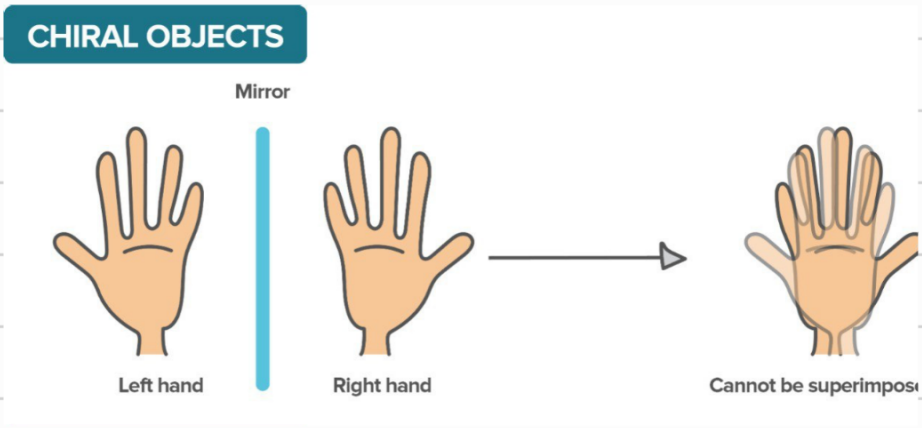
- The *cis* stereoisomer exhibits groups on the same side of the double bond, while the *trans* stereoisomer exhibits groups on opposite sides of the double bond. The two drawings above represent different compounds with different physical properties, because the double bond does not experience free rotation as single bonds do. Why not? Recall that a π bond is formed from the overlap of two *p* orbitals. Rotation about the C–C double bond would effectively destroy the overlap between the *p* orbitals. Therefore, the C–C double bond does not experience free rotation at room temperature.

Chirality

- Any object can be viewed in a mirror, revealing its mirror image. Take, for example, a pair of sunglasses. For many objects, like the sunglasses in Figure 5.3, the mirror image is identical to the actual object. The object and its mirror image are said to be **superimposable**.
- This is not the case if we remove one of the lenses (Figure 5.4). The object and its mirror image are now different. One pair is missing the right lens, while the other pair is missing the left lens. In this case, the object and its mirror image are *nonsuperimposable*.

FIGURE 5.3
An object that is superimposable on its mirror image.

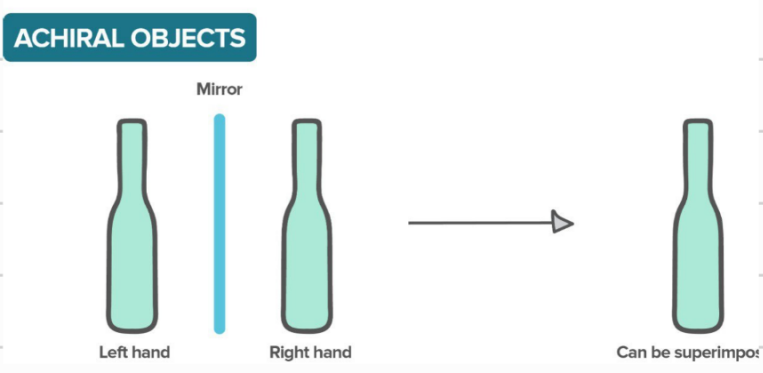
FIGURE 5.4
An object that is not superimposable on its mirror image.



Chiral

The mirror image is not Identical to the acual object

(Not superimposable)



AChiral

The mirror Image is Identical to the actual object

(superimposable)

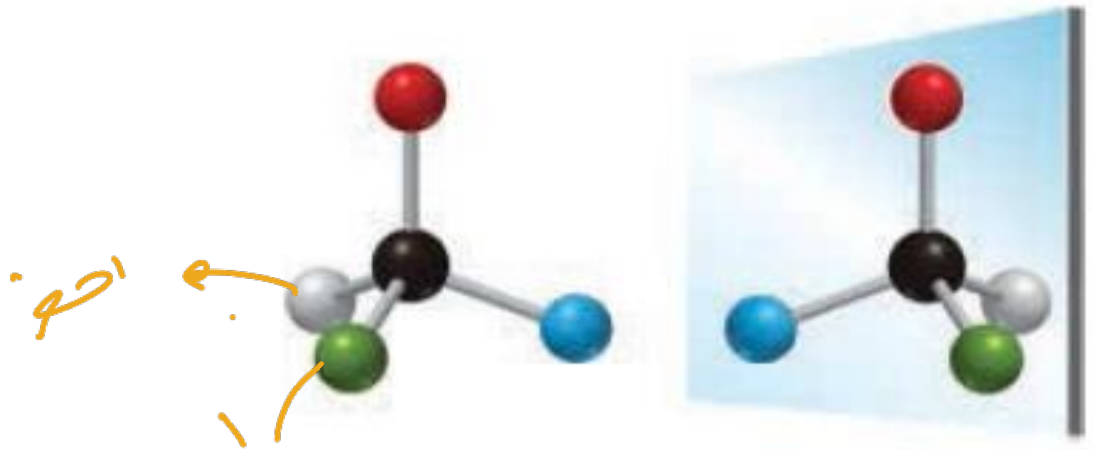
Chirality

- Many familiar objects, such as hands, are nonsuperimposable on their mirror images. A right hand and a left hand are mirror images of one another, but they are not identical; they are not superimposable on one another. A left hand will not fit into a right-handed glove, and a right hand will not fit into a left-handed glove.
- Objects that are not superimposable on their mirror images are called **chiral** objects, from the Greek word *cheir* (meaning "hand").
- All three-dimensional objects can be classified as either chiral or achiral.
- Molecules are three-dimensional objects and can therefore also be classified as either chiral or achiral. Chiral molecules are nonsuperimposable on their mirror images. Achiral molecules are superimposable on their mirror images.

Molecular Chirality

اشهر مثال على Chiral هي ارتباط ذره الكربون ٤ ذرات مختلفة

- The most common source of molecular chirality is the presence of a carbon atom bearing four different groups. There are two different ways to arrange four groups around a central carbon atom. These two arrangements are nonsuperimposable mirror images.



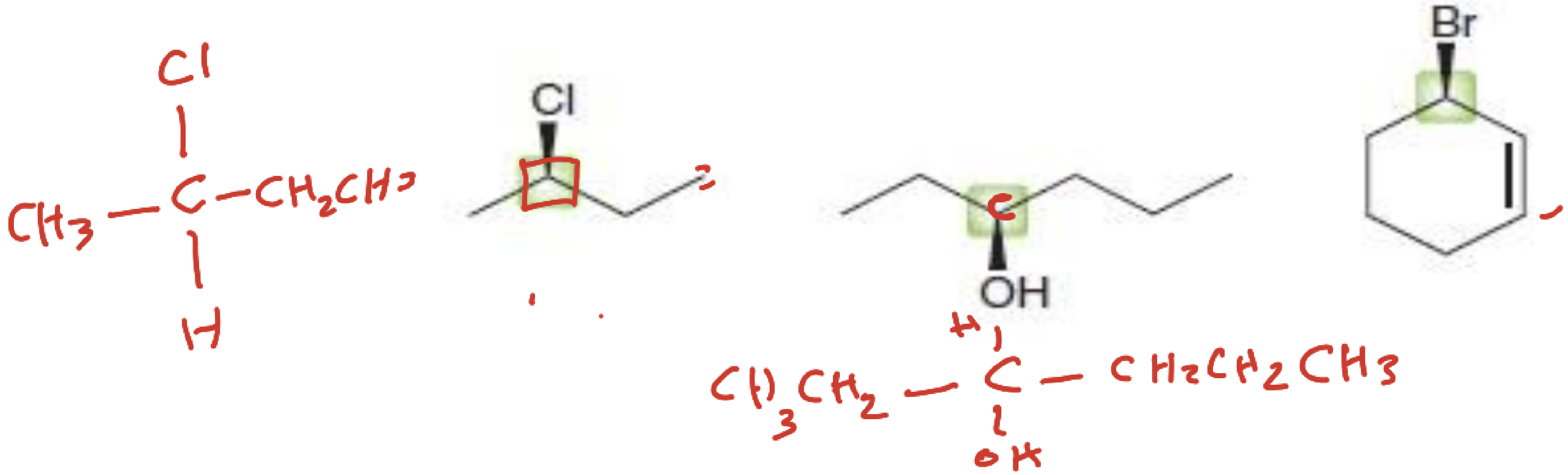
Chiral

هنالك طريقتين لترتيب الذرات حول الذره المركزيه بحيث لا تتطابق الاصلاع لهذه

Molecular Chirality

ذرة الكربون في جزيء (رباعي الاوجه) المرتبطة
بأربع اطراف مختلفة (chirality center)

- In 1996, the IUPAC recommended that a tetrahedral carbon bearing four different groups be called a **chirality center**. Despite this recommendation, organic chemists often use other more common terms, including *chiral center*, *stereocenter*, *stereogenic center*, or *asymmetric center*. Below are several examples of chiral centers:



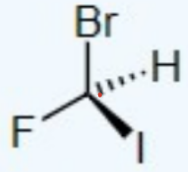
Enantiomers

المجزي و صورته بالمرآة
Enantiomers يسميان

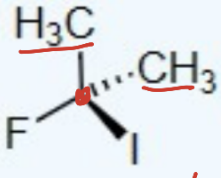
- When a compound is chiral, it will have one nonsuperimposable mirror image, called its **enantiomer** (from the Greek word meaning "opposite"). The compound and its mirror image are said to be a pair of enantiomers. The word "enantiomer" is used in speech in the same way that the word "twin" is used in speech. When two children are *a pair of twins*, each one is said to be *the twin of the other*. Similarly, when two compounds are *a pair of enantiomers*, each compound is said to be *the enantiomer of the other.* A chiral compound will have exactly one enantiomer, never more and never less.

كل مركب Chiral له enantiomer واحد

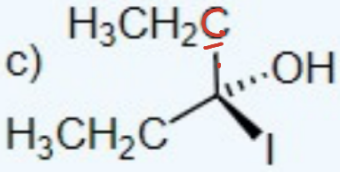
Identify the following molecules as chiral or achiral.

a) 

Chiral

b) 

achiral

c) 

AChiral

Answer

a) chiral (4 different groups off C)

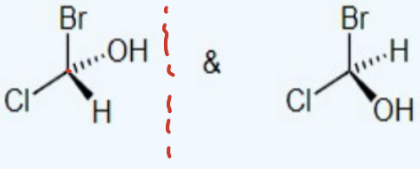
b) achiral (2 identical -CH_3 substituents off central C)

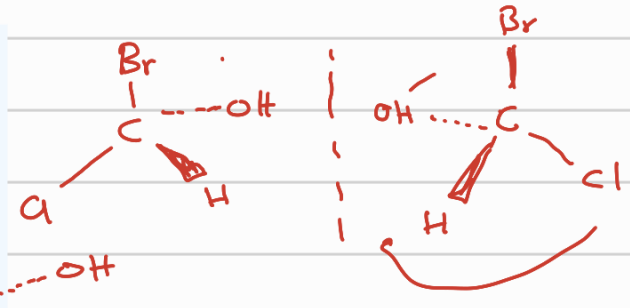
c) achiral (2 identical -CH_2CH_3 substituents off central C)

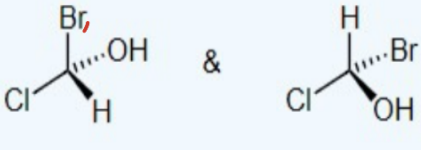
يجب ان تكون الجزيئ وصورته

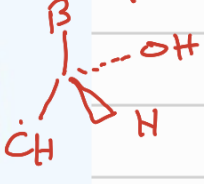
Determine if the following sets of compounds in each group are enantiomers or the same compound.

Image

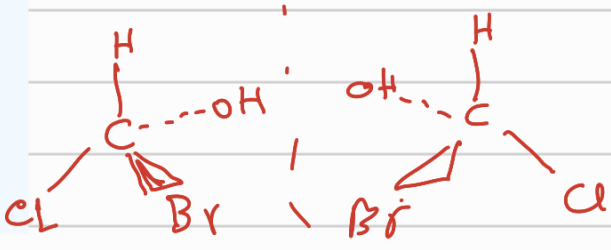
a) 



b) 



c) 



Answer

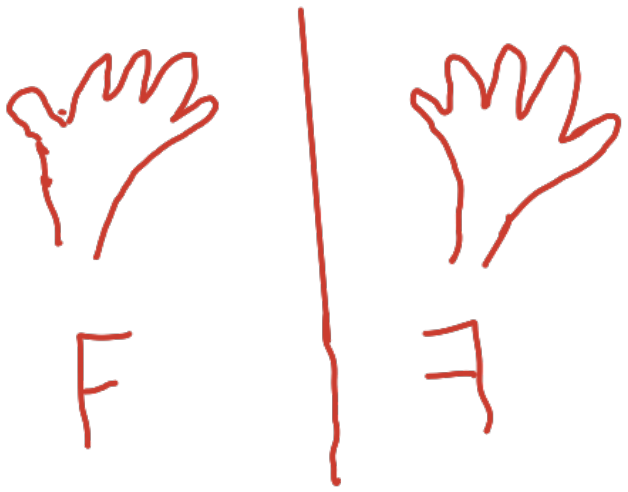
a) enantiomers – non superimposable mirror images

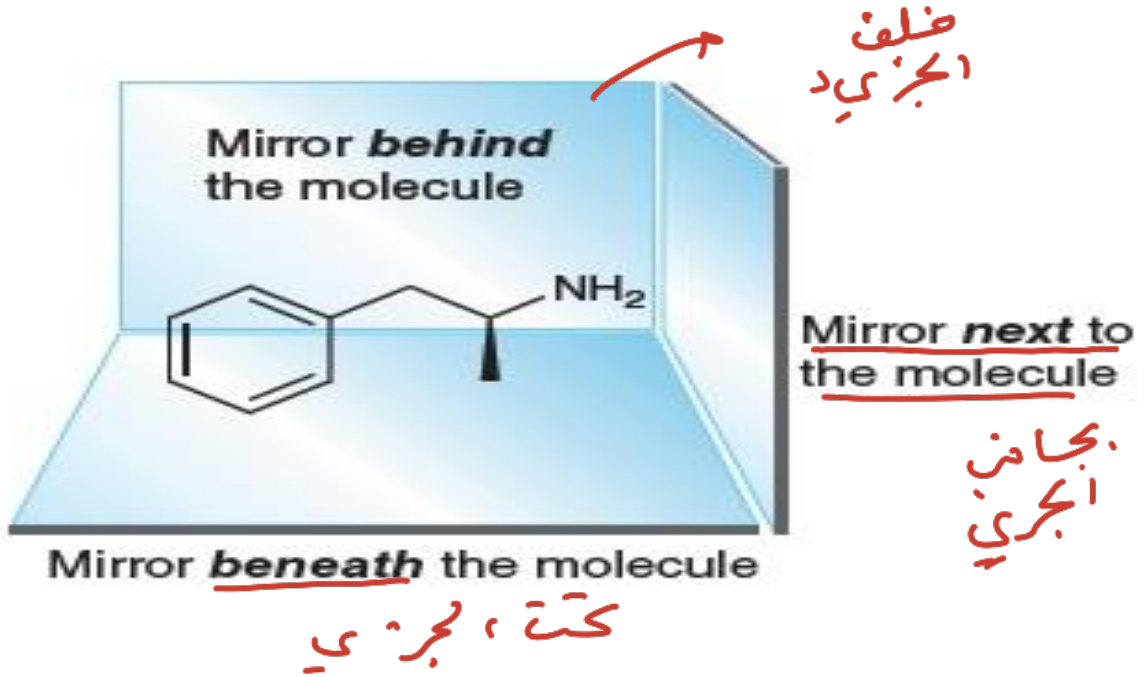
b) same compound – when you rotate the molecule on the right it is identical to the one on the left

c) enantiomers – non superimposable mirror images

Drawing an Enantiomer

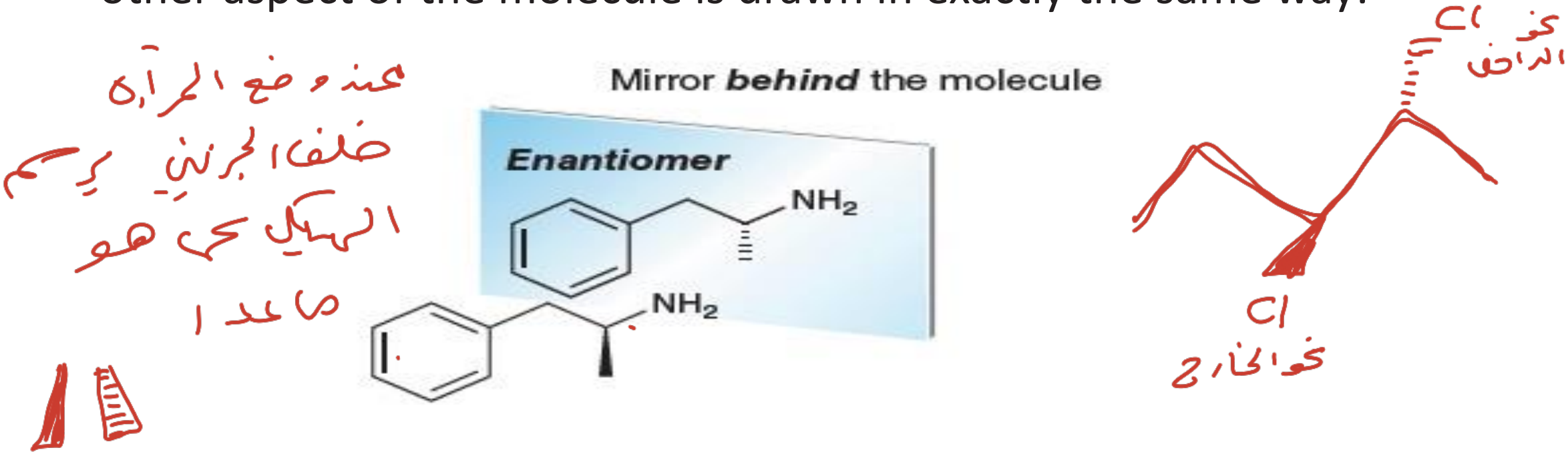
- Amphetamine is a prescription stimulant used in the treatment of ADHD (attention-deficit hyperactivity disorder) and chronic fatigue syndrome. During World War II it was used heavily by soldiers to reduce fatigue and increase alertness. Draw the enantiomer of amphetamine.





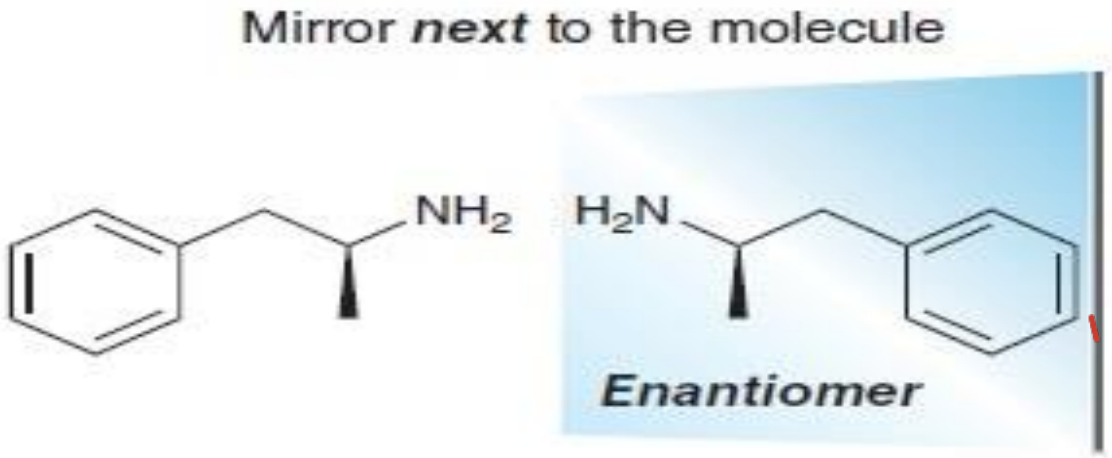
Drawing an Enantiomer

- It is easiest to place the mirror behind the molecule, because the skeleton of the molecule is drawn in exactly the same way except that *all dashes become wedges and all wedges become dashes.* Every other aspect of the molecule is drawn in exactly the same way:



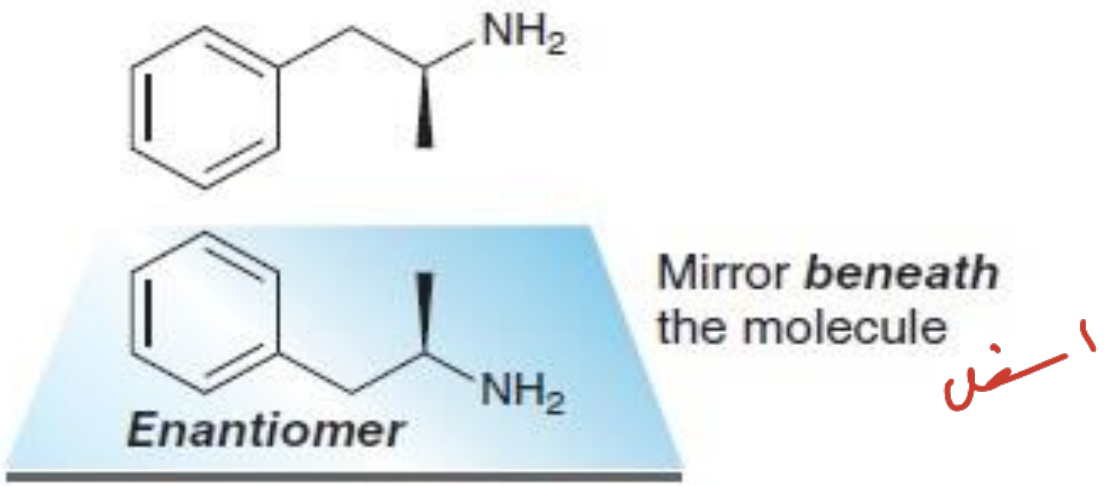
Drawing an Enantiomer

- The second way to draw an enantiomer is to place the mirror on the side of the molecule. When doing so, draw the mirror image of the skeleton, but all dashes remain dashes and all wedges remain wedges.



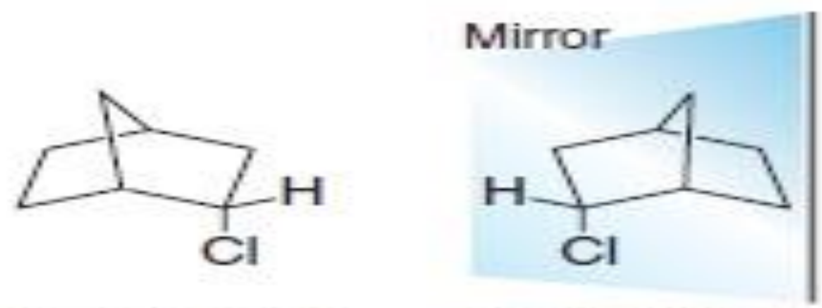
Drawing an Enantiomer

- Finally, we can place the mirror under the molecule. When doing so, draw the mirror image of the skeleton; once again, all dashes remain dashes and all wedges remain wedges:



Drawing an Enantiomer

- In general, it is easiest to use the first method. Simply redraw the compound, replacing all dashes with wedges and all wedges with dashes. However, this method will not work in all situations. In some molecular drawings, wedges and dashes are not drawn, because the three-dimensional geometry is implied by the drawing. This is the case for bicyclic compounds. When dealing with bicyclic compounds, it will be easier to use one of the other two methods (placing the mirror either on the side of the molecule or below the molecule).



Compound A Compound B

في حالات تكون الجزئ مرسوم
بطريقة تراعي الابعاد
لا يتم تحديد wedge و dashes
لا تنفع الطريقة الاولى لذلك
يتم استخدام الطرق الاخرى

Optical Activity

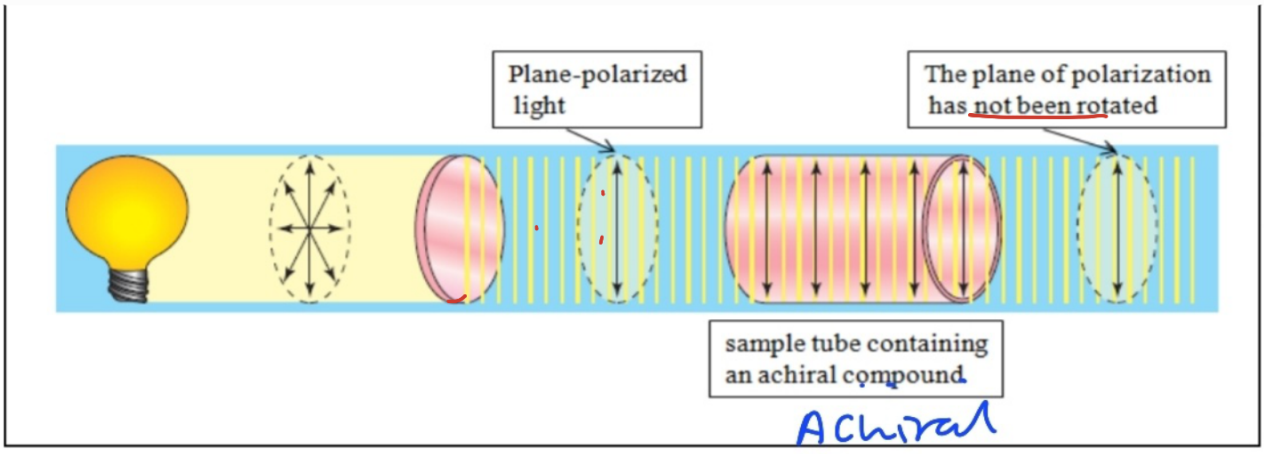
النشاط الضوئي

- In 1815, French scientist Jean Baptiste Biot was exploring the nature of light by passing plane-polarized light through various solutions of organic compounds. In so doing, he discovered that solutions of certain organic compounds (such as sugar) rotate the plane of plane-polarized light.
- These compounds were therefore said to be **optically active**. He also noted that only some organic compounds possess this quality. Compounds lacking this ability were said to be **optically inactive**.

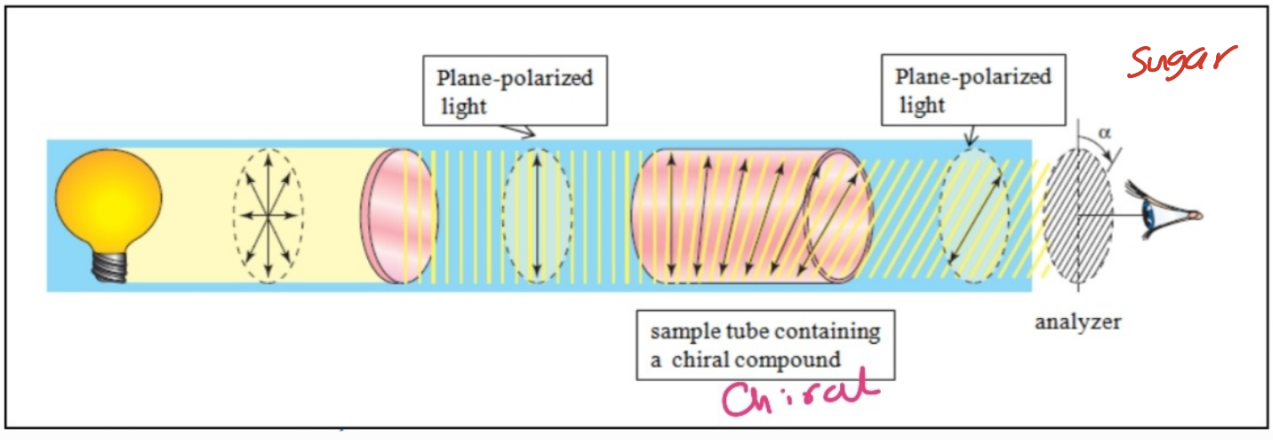
نشطه ضوئياً

غير نشطه ضوئياً

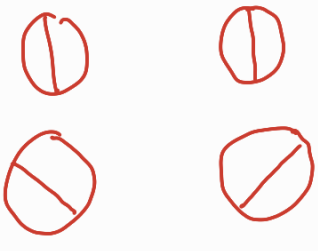
درس العالم ضوء مستقطب في مجموعه من السوائل (المضويه (مركبات مختلفه)
لاحظ ان بعض المركبات العضويه عاداره على تدوير محور الاستقطاب
وسمي هذا المحلول هذا نشيطه ضوئياً



عديمة النشاط الضوئي



نشطة ضوئيا



F 7

Enantomes

نشط ضوئي

Clockwise

D

Contor clockwise

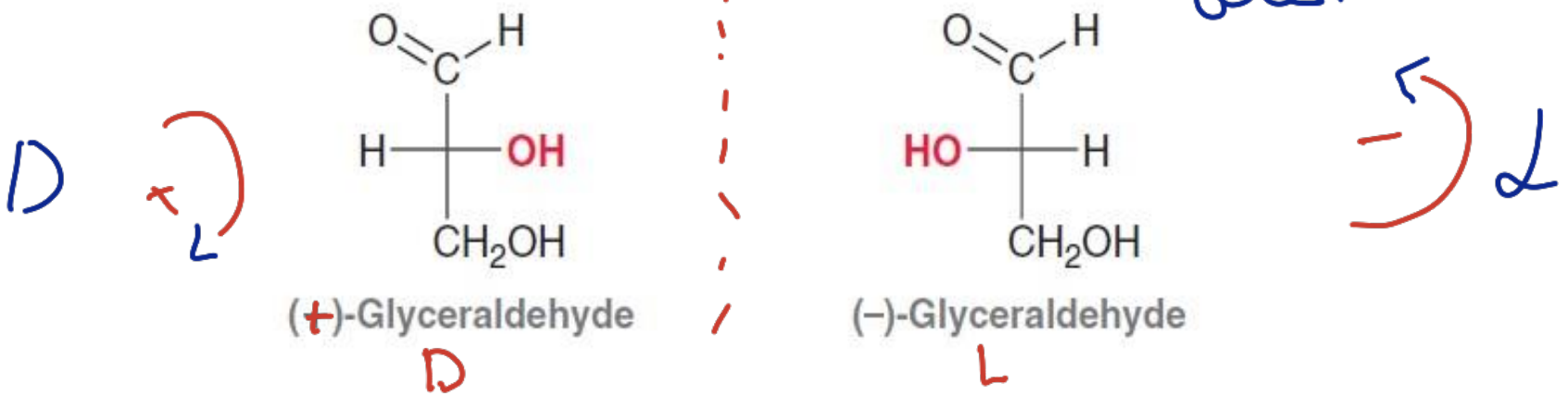
L

Source of Optical Activity

- In 1847, an explanation for the source of optical activity was proposed by French scientist Louis Pasteur. Pasteur's investigation of tartrate salts led him to the conclusion that optical activity is a direct consequence of chirality. That is, chiral compounds are optically active, while achiral compounds are not.
- Moreover, Pasteur noted that enantiomers (nonsuperimposable mirror images) will rotate the plane of plane-polarized light in equal amounts but in opposite directions.
- A compound exhibiting a positive rotation (+) (clockwise) is called **dextrorotatory**, while a compound exhibiting a negative rotation (–) (counterclockwise direction) is called **levorotatory**.

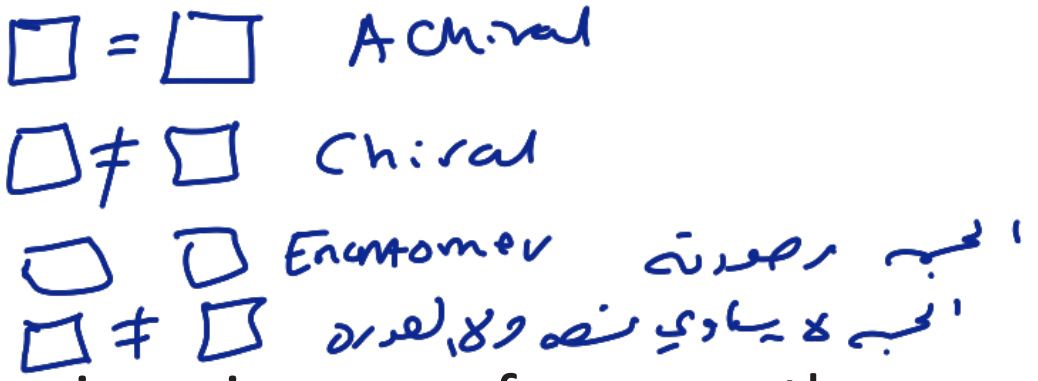
D and L Sugars

- Glyceraldehyde is one of the smallest compounds considered to be a carbohydrate. It has only one chiral center and therefore can exist as a pair of enantiomers.

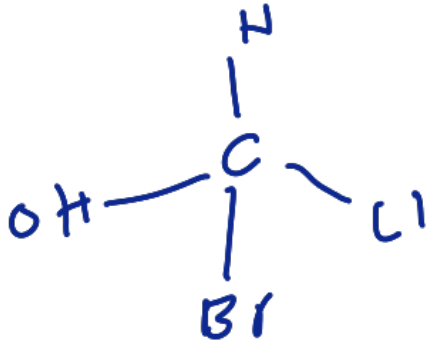


- Only (+) glyceraldehyde is abundant in nature, so glyceraldehyde obtained from natural sources is generally referred to as D-glyceraldehyde. Levorotatory or L-glyceraldehyde can be made in the laboratory, but it is generally not observed in nature.

Diastereomers



- Enantiomers are stereoisomers that are mirror images of one another, while **diastereomers** are stereoisomers that are not mirror images of one another. According to these definitions, we can understand why *cis-trans* isomers are said to be diastereomers, rather than enantiomers.
- An important difference between enantiomers and diastereomers is that enantiomers have the same physical properties, while diastereomers have different physical properties.

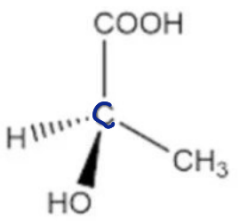


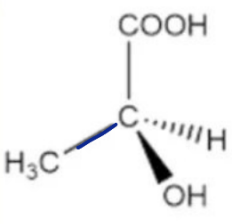
Diastereomers

Enantiomers Vs Diastereomers

The Chemistry Notes

Mirror Image

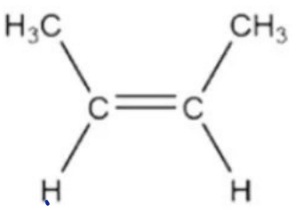


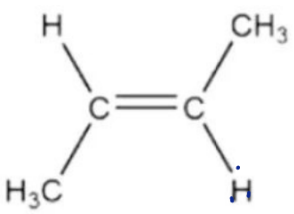


(-)-lactic acid (+)-lactic acid

الاول يتطابق مع الصورة

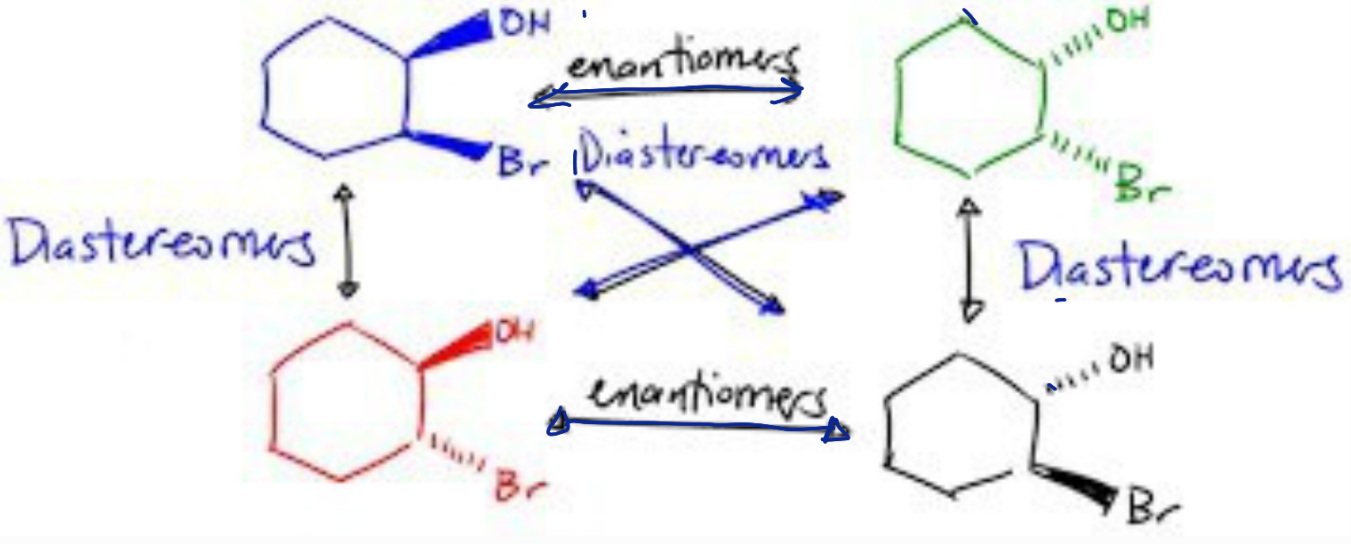
Enantiomers ✓





cis-but-2-ene trans-but-2-ene

Diastereomers ✓



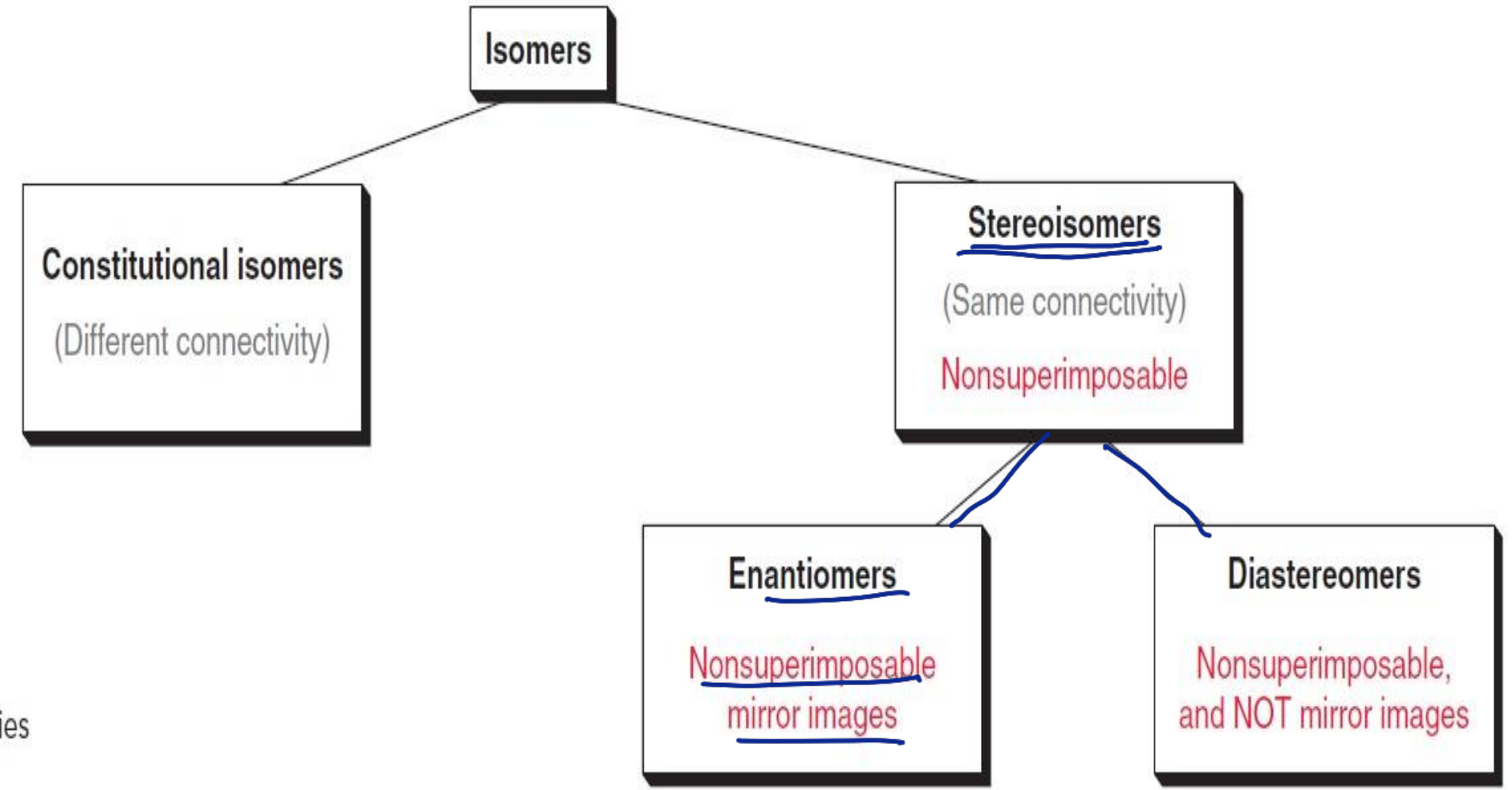


FIGURE 5.11
The main categories of stereoisomers.