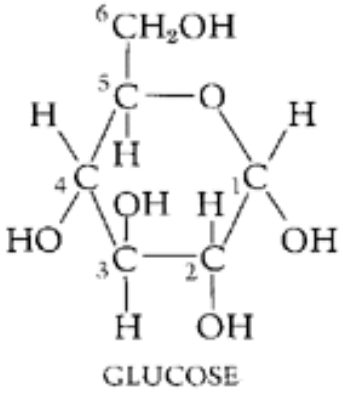
Isomers

SBI4U

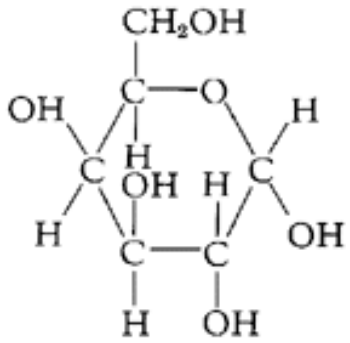
Isomers

- **Isomers** are compounds that have the same molecular formula but different structures and **<u>therefore different chemical properties.</u>**

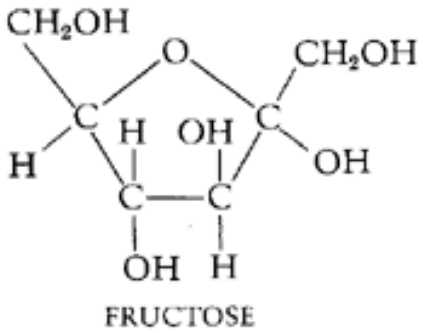
<u>You need to memorize these three molecules</u>



GLUCOSE



GALACTOSE

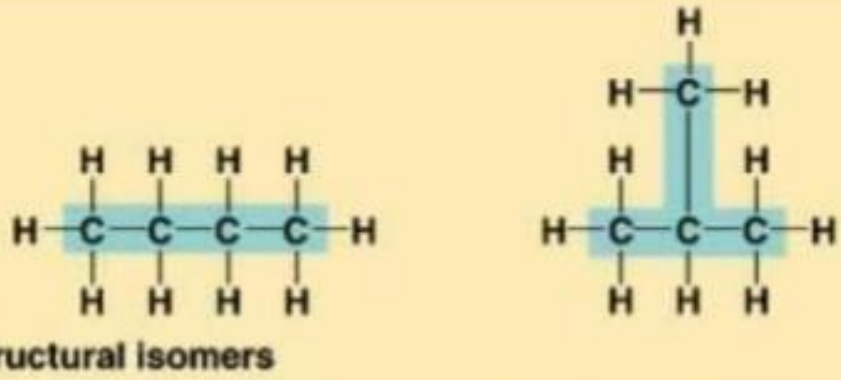


FRUCTOSE

All three molecules chemical formula is $C_6H_{12}O_6$

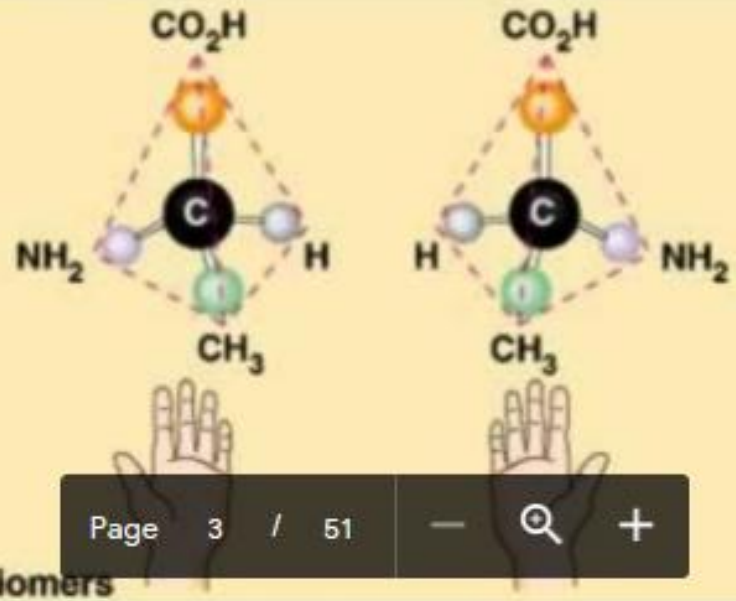
3 types of Isomers

- Structural isomers
- Geometric isomers
- Enantiomers



(a) Structural isomers

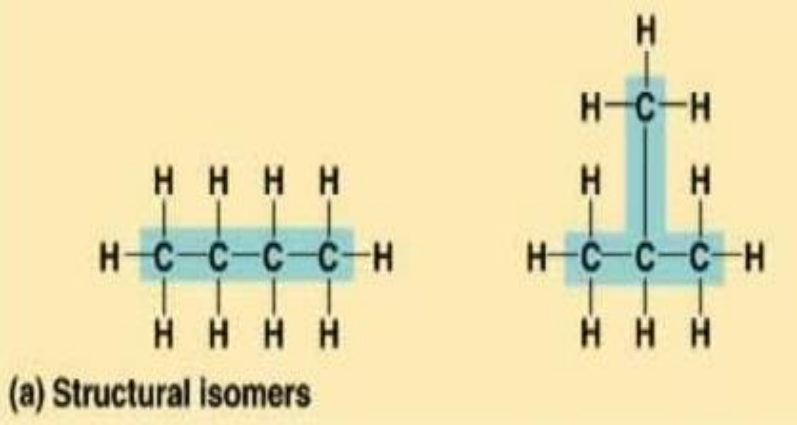
(b) Geometric isomers



(c) Enantiomers

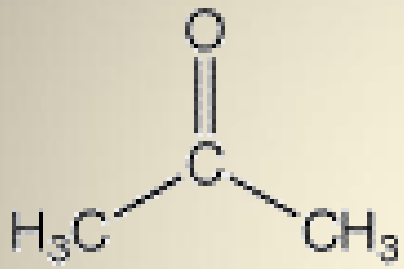
1. Structural Isomers

- Same KIND and AMOUNT of atoms (molecular formula) but the atoms have **different connectivity**



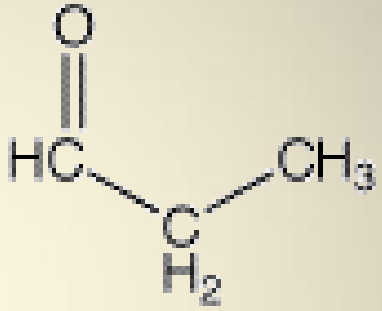
For example, butane and isobutane have the same molecular formula C_4H_{10}, but butane has a straight skeleton and isobutane has a branched skeleton.

Structural isomers usually have different physical and chemical properties



acetone
2-propanone

boiling point 56 °C
melting point -94 °C



propionaldehyde
propanal

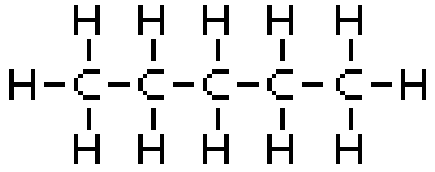
boiling point 48 °C
melting point -81 °C

Structural Isomer

- How many different structures can you make from C_5H_{12}?

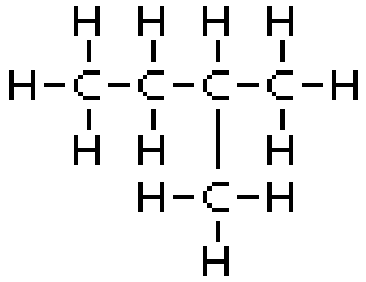
- How many structural isomers of $C_{20}H_{42}$

Isomers of pentane



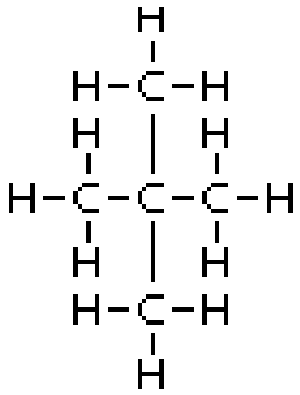
Pentane

36 °C (Boiling point)



Isopentane

28°C (Boiling point)



Neopentane

9.5 °C (Boiling point)

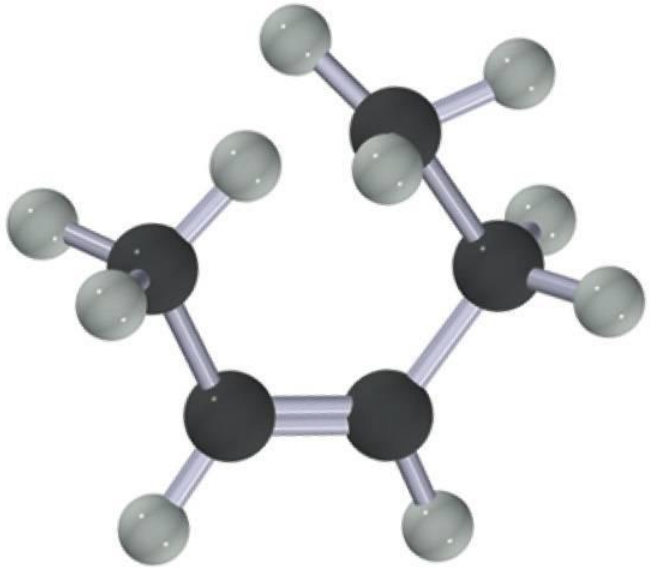
Structural Isomers

- C_5H_{12} 3
- $C_{20}H_{42}$ 366,319

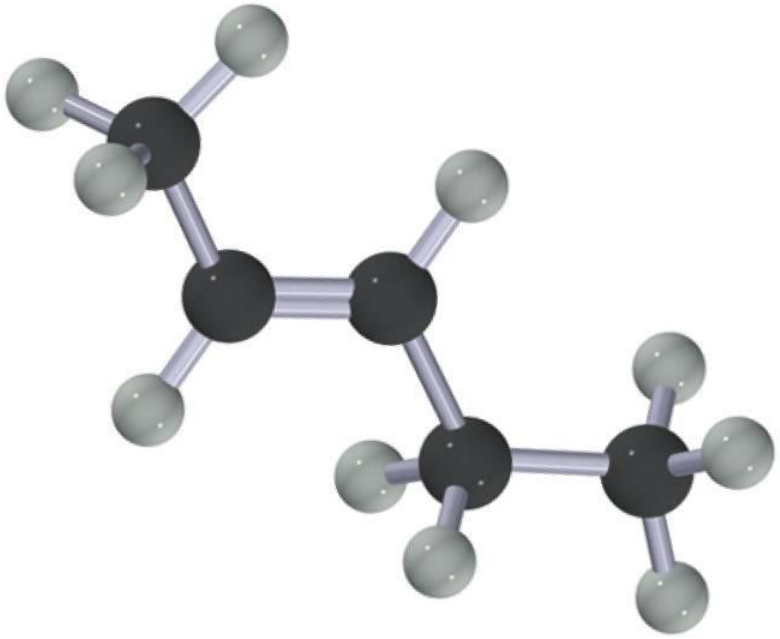
Structural isomers may also differ in the location of double bonds.

2. Geometric Isomers

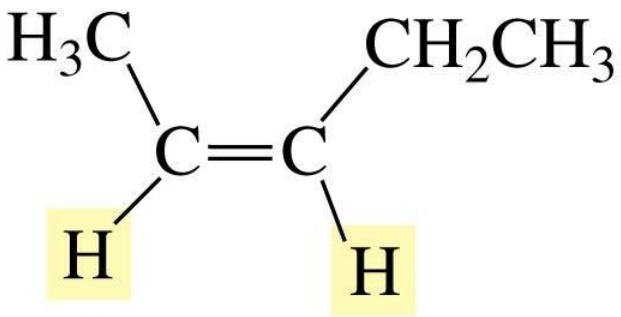
- **same molecular formula and the *SAME connectivity* but different spatial arrangements**
- Different arrangement around a carbon.
- Due to inflexibility of double bonds
- **Cis** (same side) and **trans** formation (across)



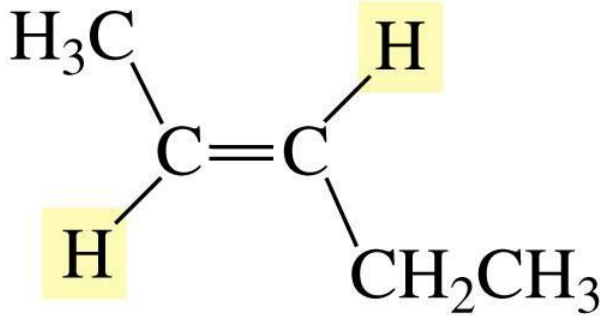
cis-2-pentene



trans-2-pentene



cis-2-pentene

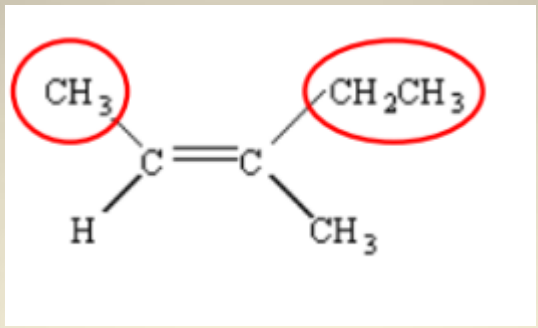


trans-2-pentene

To determine cis or trans conformations:

- Give each substituent group on each carbon of the double bond a priority
- Priority is given based on molecular mass of the group (i.e. the longer the carbon chain, the higher the priority)
- Classify cis or trans looking only the highest priority group on each carbon of the double bond

Example:



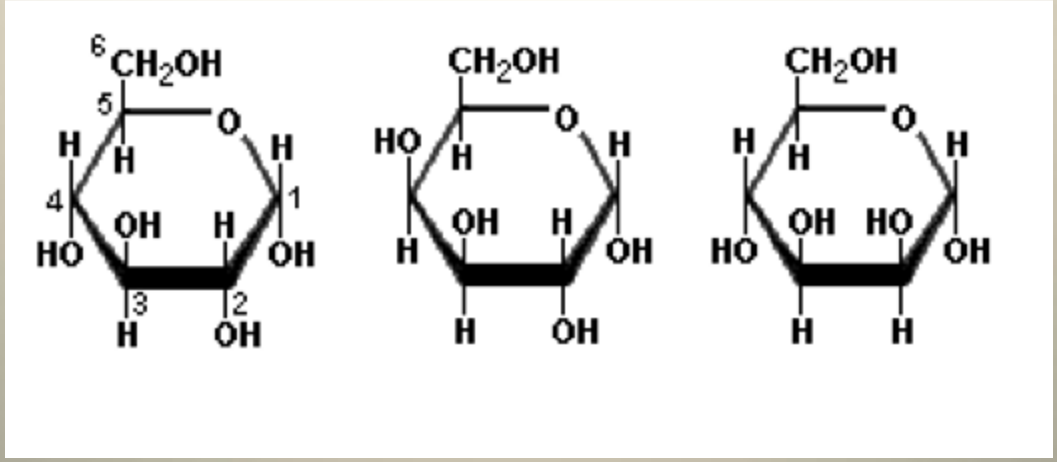
- Groups on the left of the double bond: methyl has higher priority than hydrogen

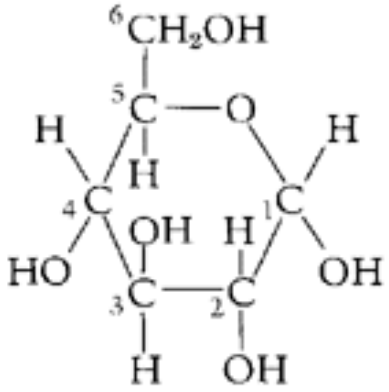
- Groups on the right of the double bond: ethyl has higher priority than methyl

- High priority groups are on the same side:

Therefore molecule is in a cis formation

- Another type of geometric isomer is found in ring structures and doesn't involve double bonds
- Due to the inflexible nature of the bonds that make up the ring





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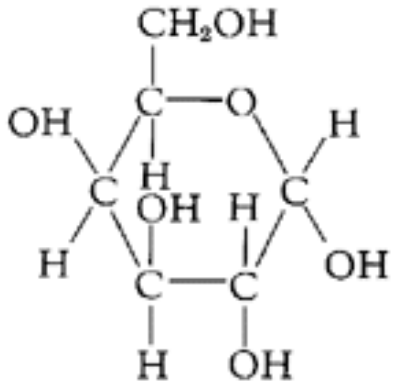

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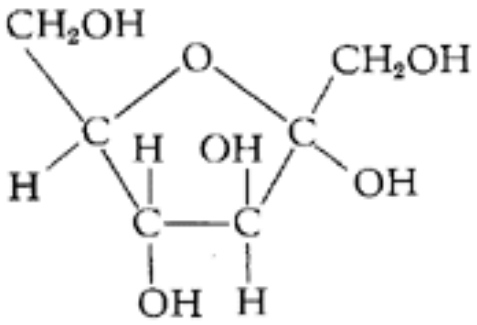


FRUCTOSE

Which are geometric isomers and which are structural isomers?

Summary of geometric isomers

SAME molecular formula and the SAME connectivity but different spatial arrangements

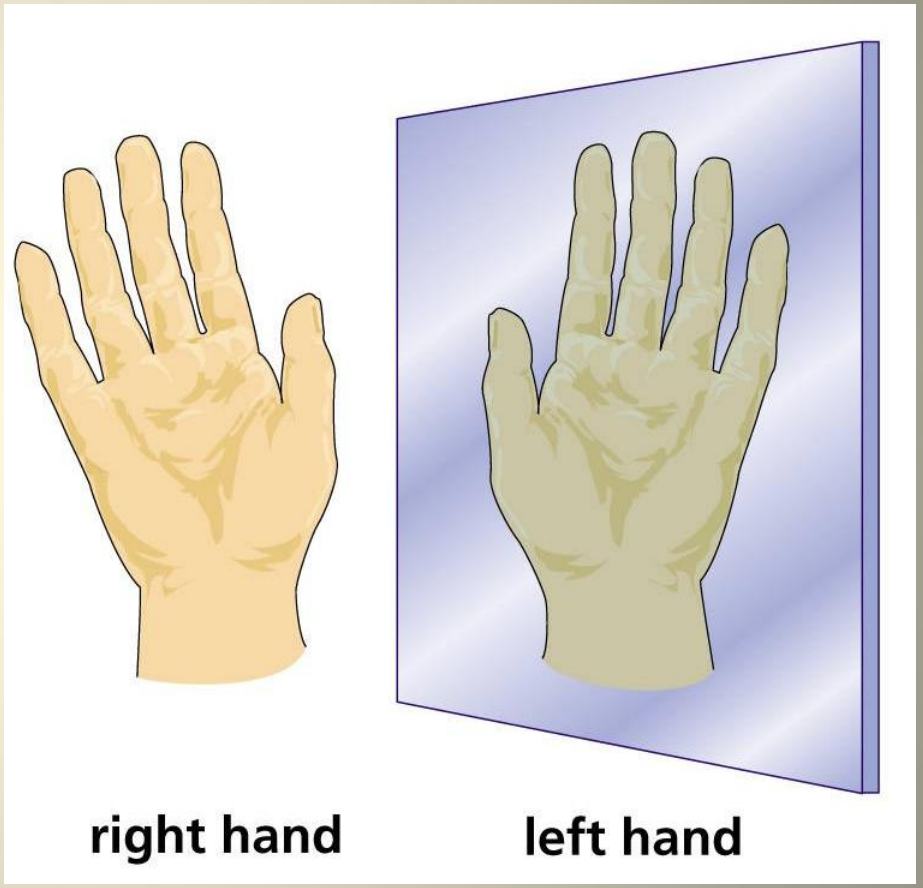
- Due to inflexibility of a bond (can't rotate):

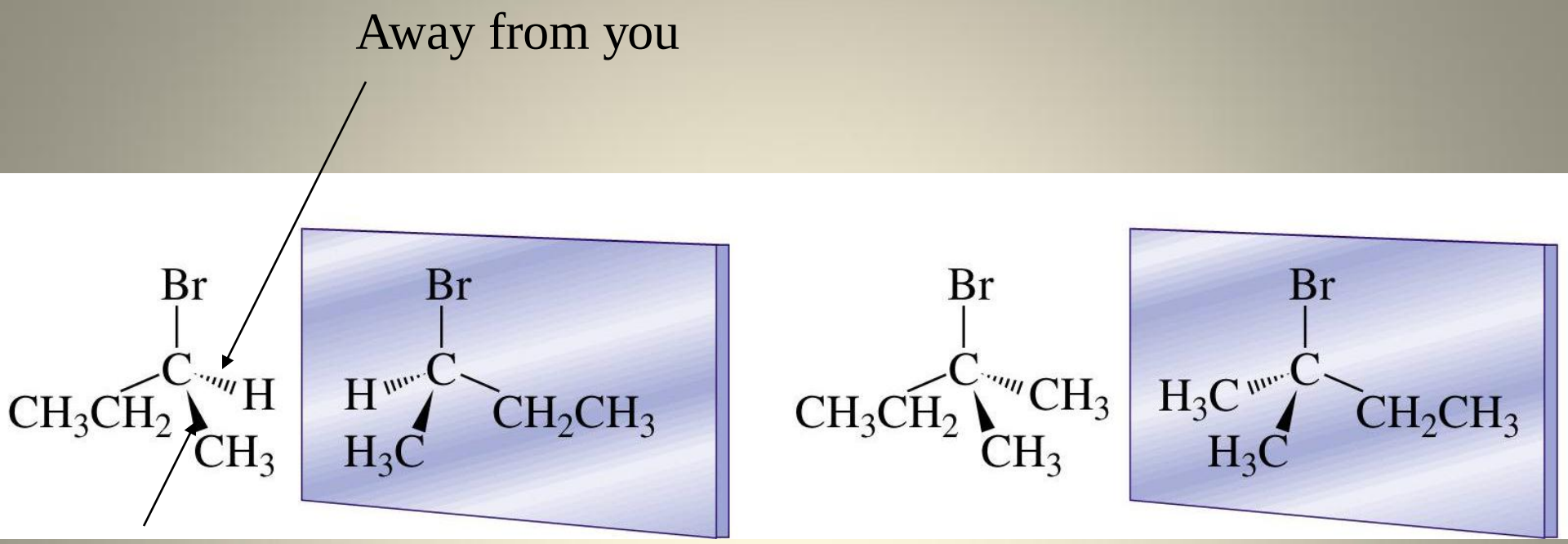
A. Double bonds
   - ❑ 2 substituent groups on each carbon of the double bond must be different
   - ❑ Classify as cis or trans based on priority of each substituent group.

B. Ring Formations

Enantiomer

- Molecules that are **mirror** images of each other
- Note: left and right hands are a pair of enantiomers (mirror images not identical)
- **Non-superimposable** mirror image
- Name other body parts that are enantiomers





a chiral molecule

nonsuperimposable mirror image

enantiomers

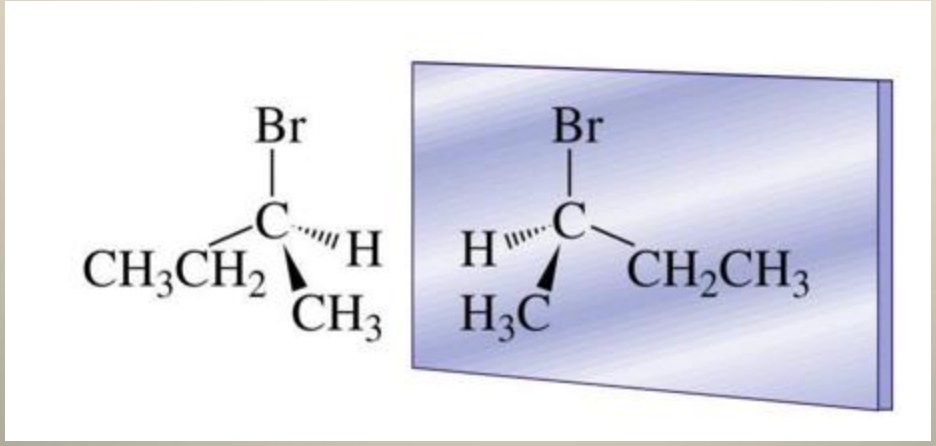
an achiral molecule

superimposable mirror image

identical molecules

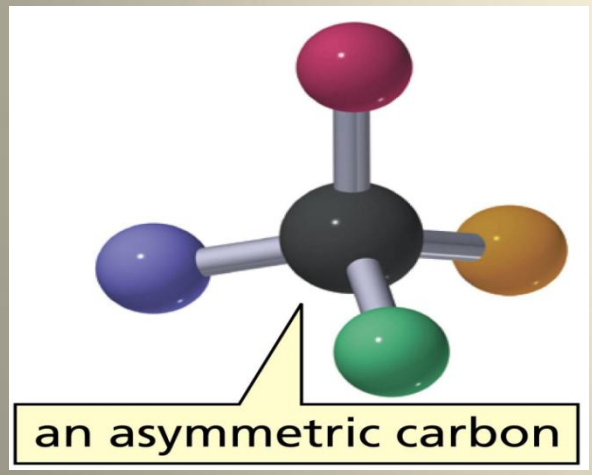
• Requirement: Enantiomers can only occur when each of the four groups attached to the central carbon atom are all different.

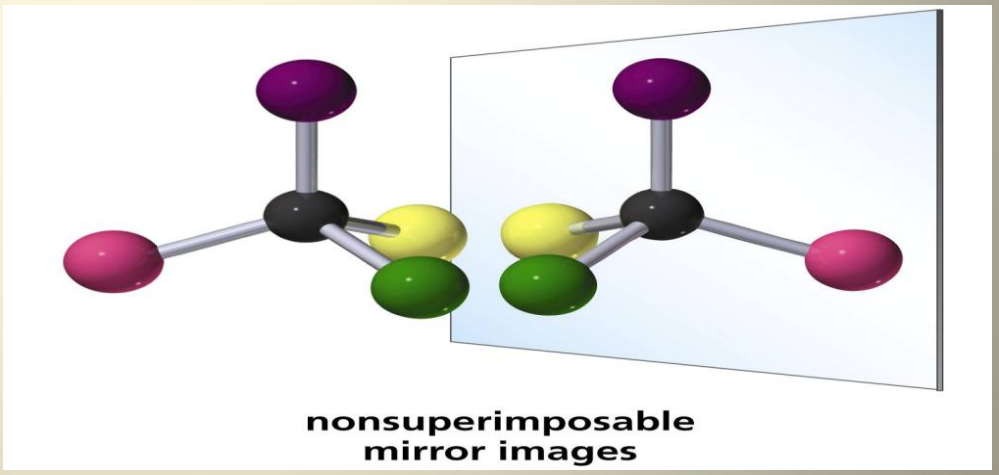
•The central carbon is known as a chiral carbon and the molecule is chiral



Chiral Molecules

- Asymmetric carbon: carbon with 4 different groups bonded to it
- No plane of symmetry
- Mirror image is non-superimposable

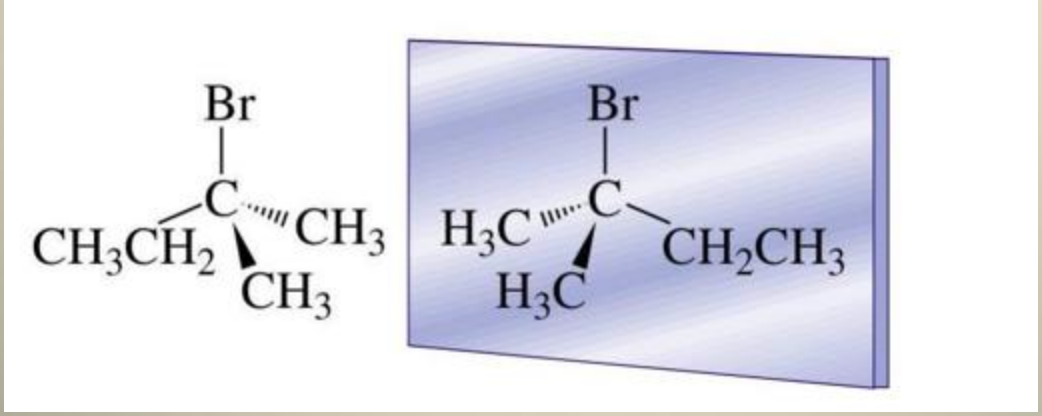




A molecule that can exist as a pair of enantiomers has the property of **chirality**

Achiral Molecules

- lacks chiral properties
- has a plane of symmetry
- Mirror image is superimposable (rotate the molecules to make them identical)

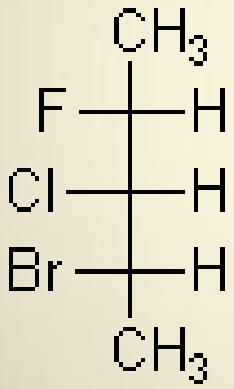


Enantiomer Rules

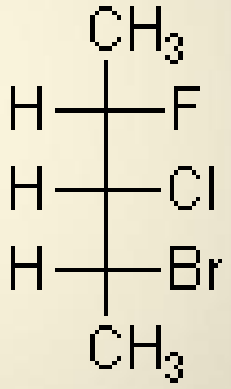
- Carbon must be chiral
- Mirror image

Is this a structural, geometric or enantiomer isomer?

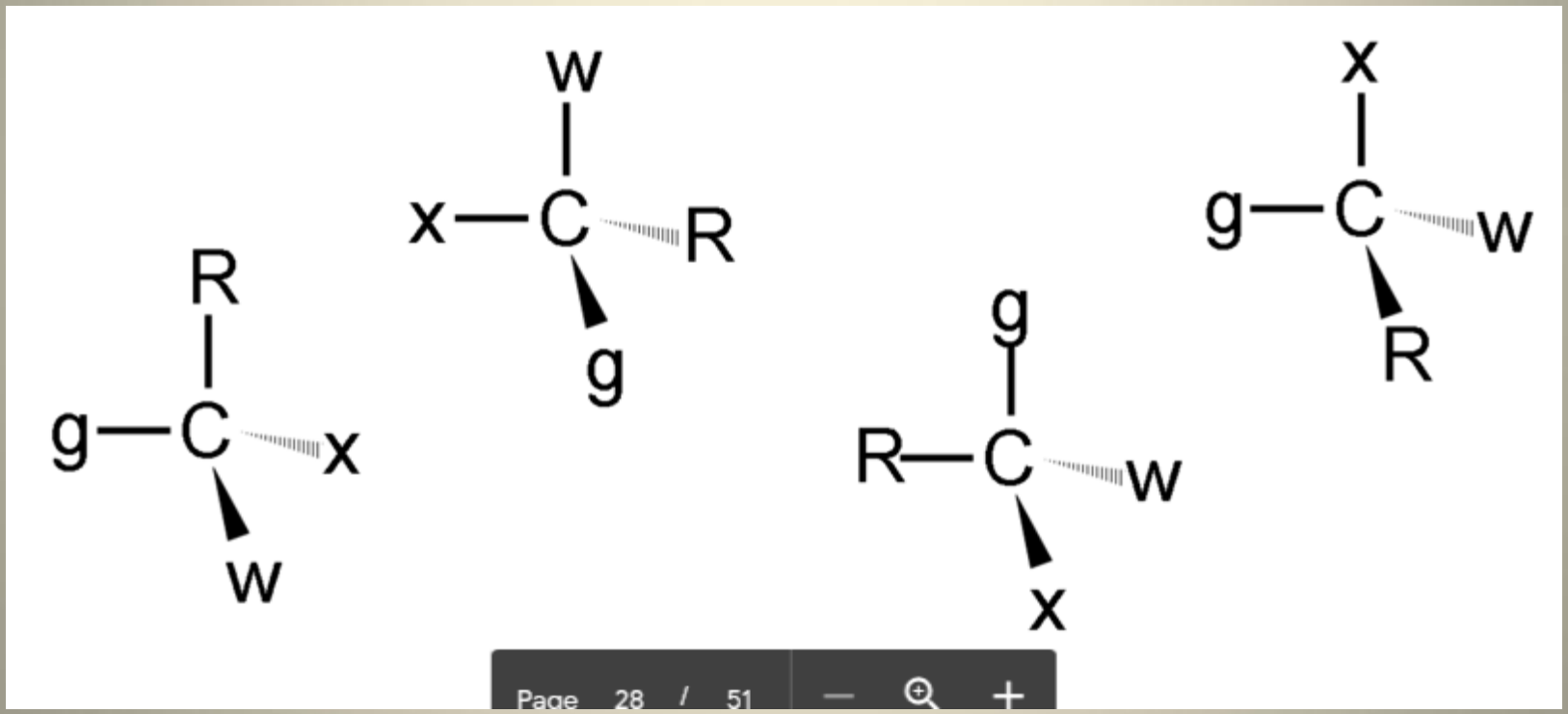
(E)



and



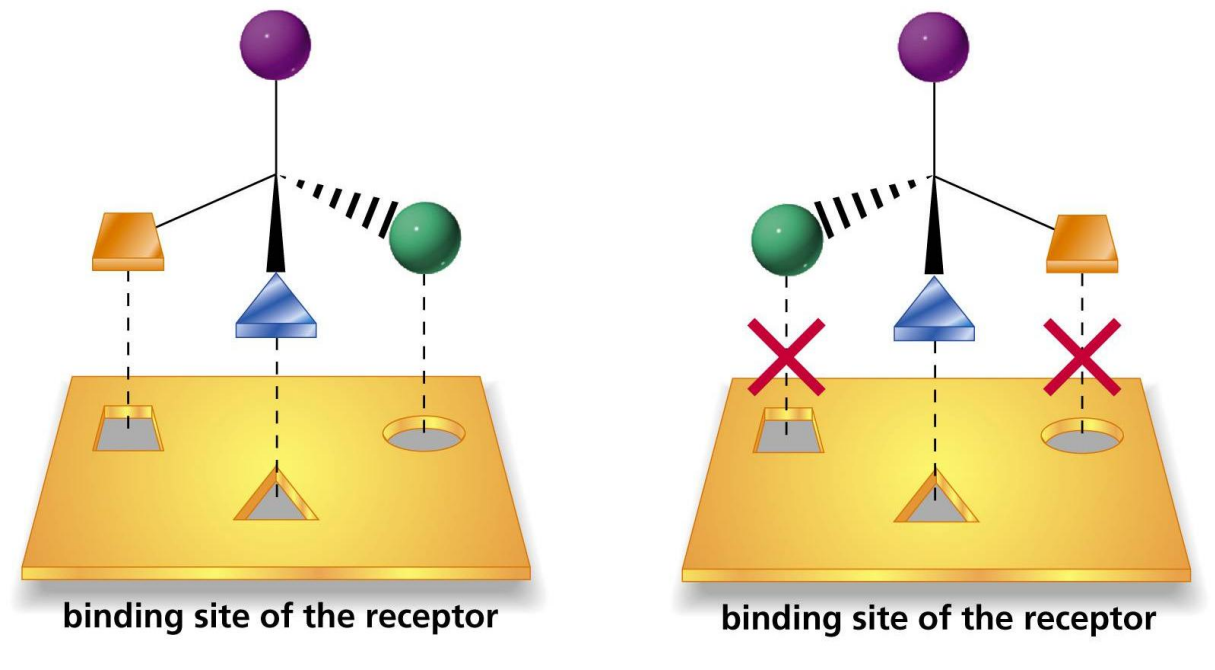
Which pairs are enantiomers?
Which pairs are identical?



Biological Application:

Enzymes are always chiral.

- Their binding sites are in a specific orientation that fits only one form of an enantiomer.
- Binding sites won't fit if the wrong enantiomer is present.

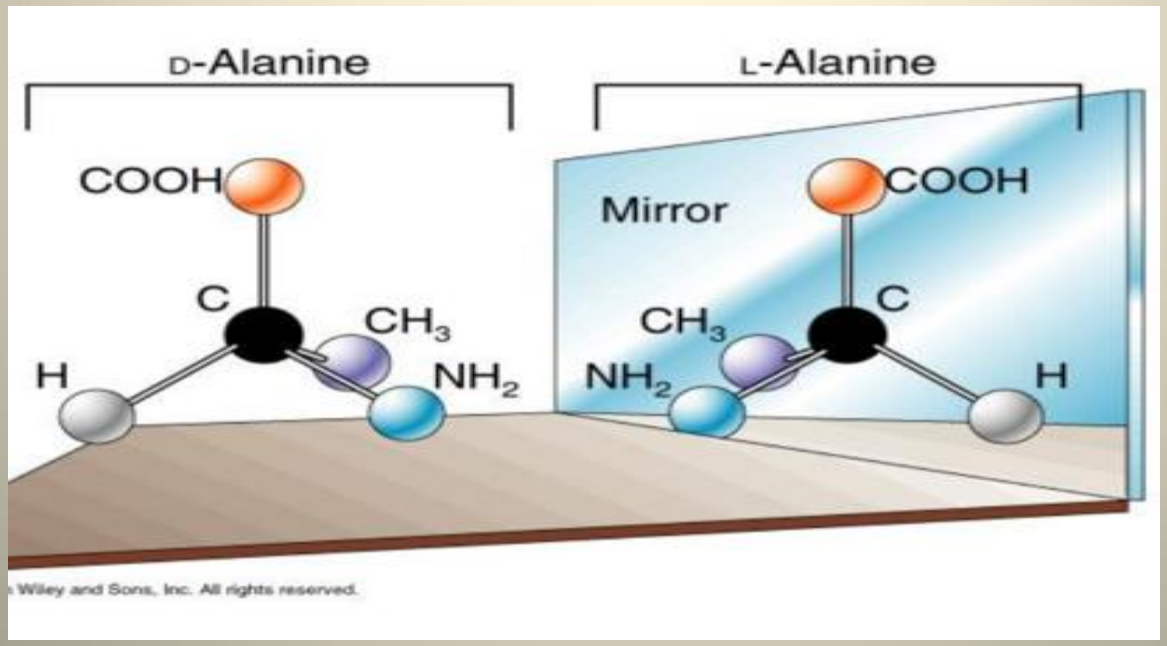


Analogy: A left hand will not fit into a right-handed glove

Biological Application:

Amino acids are building blocks of proteins

- Some amino acids can exist as enantiomers because of their chiralty
- Switching an enantiomer in a biological system can have detrimental effects



Racemic Mixture

- Racemic Mixture (racemate): A solution that contains equal quantities of both enantiomers

- Enantioenriched: A solution containing an excess of one enantiomer (compared to the other)

- Enantiomerically pure (entiopure): A solution containing only one enantiomer (absence of the other)
  Enantiomers can interconvert in vivo

Racemic Mixture: Thalidomide

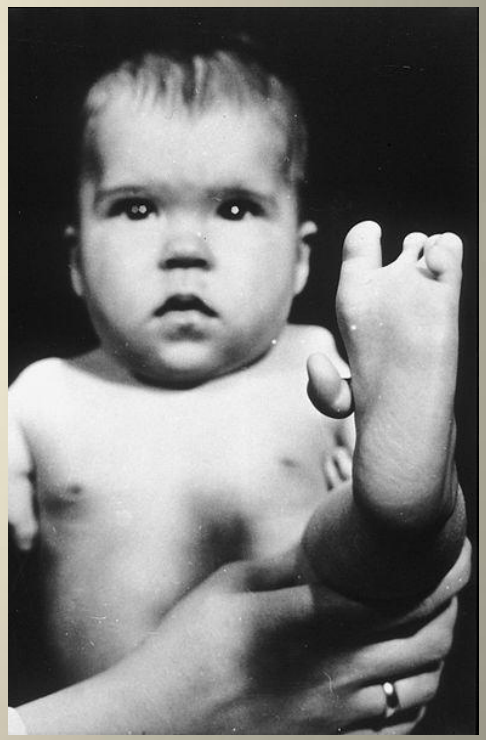
Even the subtle structural differences in two enantiomers have important functional significance because of emergent properties from the specific arrangements of atoms.

- A racemic drug given to pregnant women (in the 1960's) to combat morning sickness
- One of the thalidomide enantiomers worked as intended but the other caused birth defects (teratogen) and deat

Administering only one enantiomer will not prevent the teratogenic effect in humans.

- The body naturally creates the enantiomer.

Birth Defects



Other Enantiomers

- Other biological processes may be triggered by only one of the two possible enantiomers of a chiral molecule, often being unresponsive to the other enantiomer. For example, S-carvone ("left-handed") is the flavor of **caraway,** while R-carvone ("right-handed") is the flavor of **spearmint.**

Videoclips

- http://www.youtube.com/watch?v=MnD-nxtRouc
- http://www.youtube.com/watch?v=rT48OFFaDwE&feature=related

Things to keep in mind…

- Do the molecules have the same chemical formula?
  - If the formula is different, they are NOT isomers but completely different molecules
- Are the molecules identical?
  - If they are, they are NOT isomers.
- Are all the atoms connected in the same way to other atoms?
  - If not, they are STRUCTURAL isomers
- Look for an inflexible bond (double bond or ring) for geometric isomers
- Look for mirror images for enantiomers

- http://2.bp.blogspot.com/_K91FA3B4cpM/SJ_NUmBWWGI/AAAAAAAAACY/UzL8H8Q4oag/s400/ist2_1744503_frustration.jpg