Isomers

Molecular Shapes & Stereochemistry

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http://chemconnections.org/general/movies/Isomerism.MOV

Isomerism

• *Isomers*: two compounds with the same formulas but different arrangements of atoms.

- *Structural isomers have different connectivity of atoms*.
- *Geometrical isomers* and optical isomers are stereoisomers (i.e. have the same bonds, but different spatial arrangements of atoms).
- *Stereoisomers* have the same connectivity but different spatial arrangements of atoms.







Structural isomers have the same molecular formula but different arrangements of atoms (bond positions). Which of the following are structural isomers of each other?



A. 1 & 2
B. 2 & 3
C. 1 & 3
D. All of them are structural isomers

Geometric Stereoisomers: cis-trans

- To maintain orbital overlap in the pi bond, C=C double bonds cannot freely rotate.
- Although the two molecules below have the same connectivity, they are NOT identical.









trans



Geometrical (cis-trans) isomers have the same molecular formula and connected bond positions, but a different arrangement of atoms. Which two of the following are cis-trans geometrical isomers?



A. 1 & 2 B. 2 & 3 C. 1 & 3 D. All of them are cis-trans isomers

Chemical Communication

cis

http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html



http://www.learner.org/resources/series61.html

Pheromone Synthesis [20:40-23:51]

Chemical Communication Smell / Pheromones

http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html



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http://www.learner.org/resources/series61.html

Pheromone Synthesis [20:40-23:51]

Stereoisomers: Enantiomers Chirality & Carbon Atoms



Each carbon atom with four different substituents are chiral.

http://chemconnections.org/general/movies/Chirality.mov

Chirality







Chiral molecules have one or more carbons that have **4** different substituents. They have the same molecular formula and arrangements of atoms, but have stereoisomers ("enantiomers") that are non-superimposable mirror images of each other. Which of the following molecules is chiral?



Stereoisomerism

• Enantiomers are chiral:

i.e. They are non-superimposable mirror images.

- Most physical and chemical properties of enantiomers are identical.
- Therefore, enantiomers are very difficult to separate eg. Tartaric acid... Louis Pasteur:





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 Enantiomers can have very different physiological effects: eg. (+) and (-) carvone, Advil (ibuprofen) (thalidomide) Shapes & Interactions: Mirror Images & Smell What is the molecular formula of carvone?



http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html

Shapes & Interactions: Mirror Images & Smell What is the molecular formula of carvone?



http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html

Proteins & Small Molecules

The interaction of a large protein bio-polymer, acetylcholinesterase, with a relatively small molecule of acetylcholine. A general process similar to the way that scientists think we smell, which relates to many other physiological processes.



http://chemconnections.org/general/movies/richard.mpg



Thalidomide



Thalidomide was administered as a racemic mixture (50:50 mix of enantiomers) to stave off morning sickness during pregnancy.



From the late 1950s – early 1960s more than 10,000 children in 46 countries were born with deformities caused by one of the two enantiomers. 50% survived.





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The S-(-) enantiomer, which is on the left, caused the deformities. The severity and location of the deformities depended on when thalidomide was taken: On the 20th day of pregnancy it caused central brain damage in the fetus, on Day 21 it would damage the eyes, on Day 22 the ears and face, on Days 24-28 arm and leg damage would occur.

Thalidomide did not damage the fetus if taken after 42 days gestation.

Molecular Modeling Bonus

	Chem 106 / Dr. Rusay						
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Choose any biologically active molecule, pharmaceutical, natural product, etc. Using molview's search, find & open the file, use the Tool Menu to find the Embed URL



 $C_{20}H_{23}CIN_2O$

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