Isomers

Molecular Shapes & Stereochemistry

Dr. Ron Rusay

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

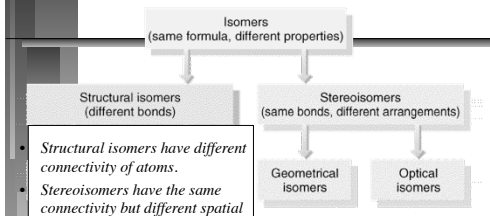
Isomerism

Isomerism

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

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

Isomerism



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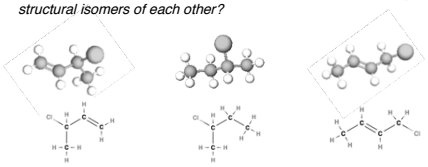
- *Stereoisomers have the same connectivity but different spatial arrangements of atoms.*
- *Geometrical isomers and Optical isomers are stereoisomers (i.e. have the same bonds, but different spatial arrangements of atoms).*

cis - trans

Enantiomers (Chiral: Non-superimposable Mirror Images)

Question

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



1 *2* *3*

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

Answer

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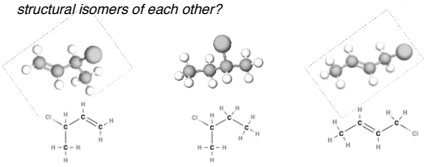

1 *2* *3*

A. 1 & 2
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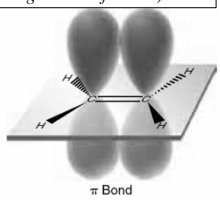
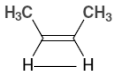
Geometric Stereoisomers: cis-trans

- *Geometrical isomers are stereoisomers (i.e. have the same bonds [connectivity], but different spatial arrangements of atoms).*

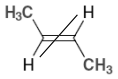
- *To maintain orbital overlap in the pi bond, C=C double bonds cannot freely rotate.*



- *Although the two molecules below have the same connectivity, they are NOT identical.*



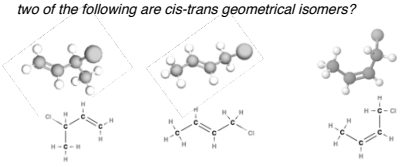
cis



trans

Question

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?



1 *2* *3*

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

Answer

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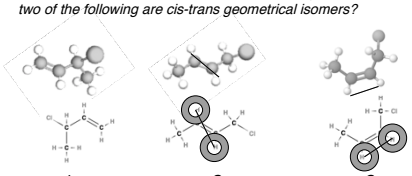

1 *2* ***trans*** *3* ***cis***

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

Chemical Communication

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

Pheromone Synthesis
[20:40-23:51]
http://www.learner.org/resources/series61.html

Chemical Communication

Smell / Pheromones

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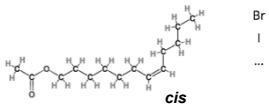
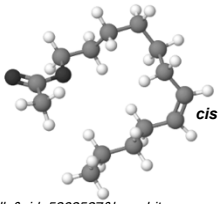


cis

S
F
Cl
Br
I
...



cis

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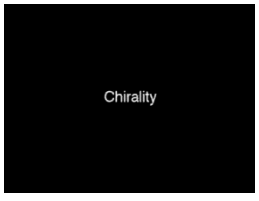
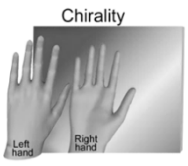
Pheromone Synthesis
[20:40-23:51]

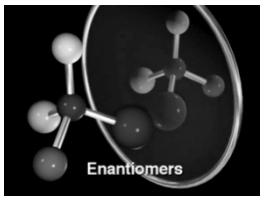
Stereoisomers: Enantiomers
Chirality & Carbon Atoms



Each carbon atom with four different substituents are chiral.

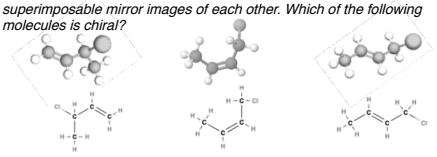
http://chemconnections.org/general/movies/Chirality.mov





Question

*Optical isomers, chiral molecules, can 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?*



1 *2* *3*

A. 1
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C. 3
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Answer

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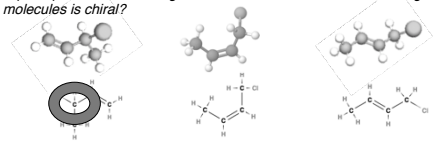

1 *2* *3*

A. 1
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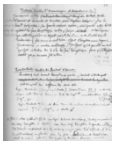
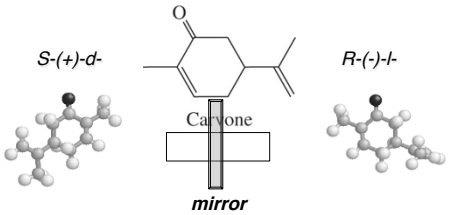
Stereoisomerism

- *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:



- *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?



S-(+)- caraway *R-(-)- spearmint*

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

Shapes & Interactions: Mirror Images & Smell
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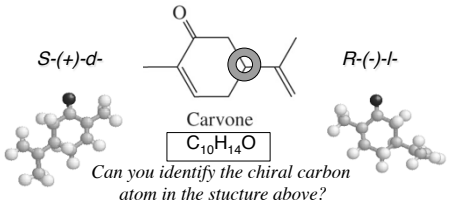

Can you identify the chiral carbon atom in the stucture above?

S-(+)- caraway *R-(-)- spearmint*

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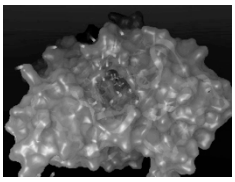
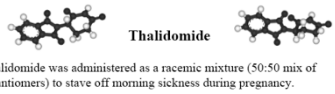
Proteins & Small Molecules

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.



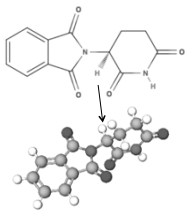
http://chemconnections.org/general/movies/richard.mpg



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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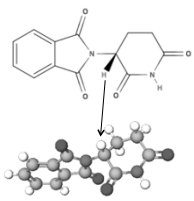


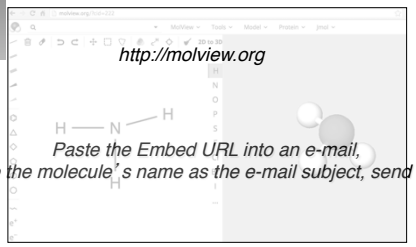
https://embed.molview.org/v1/?mode=balls&cid=75792&bg=white

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

Choose any biological molecule, pharmaceutical, natural product, etc.
Using molview's search, find & open the file, use the Tool Menu to find the Embed URL



http://molview.org

Paste the Embed URL into an e-mail,
Provide the molecule's name as the e-mail subject, send to Dr.R

http://molview.org

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Choose any biologically active molecule, pharmaceutical, natural product, etc.
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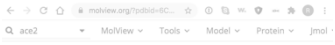
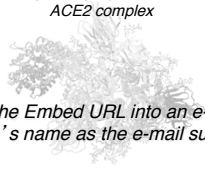


6CS2
SARS Spike Glycoprotein - human
ACE2 complex



Paste the Embed URL into an e-mail,
Provide the molecule's name as the e-mail subject, send to Dr.R