

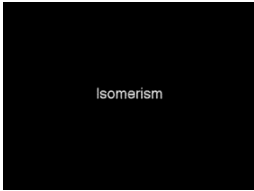
# Isomers

## Molecular Shapes & Stereochemistry

Dr. Ron Rusay

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# Isomerism

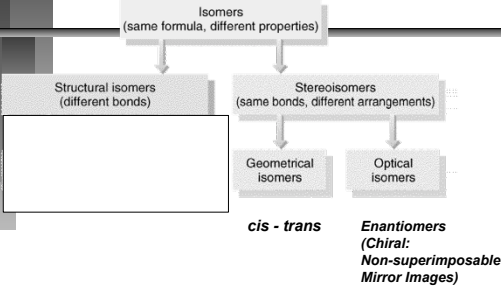


<http://chemconnections.org/general/movies/Isomerism.MOV>

## Isomerism

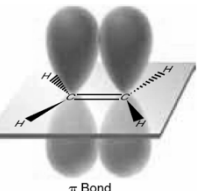
- Isomers: two compounds with the same formulas but different arrangements of atoms.
- Structural isomers have different connectivity of atoms.
- Geometrical isomers and optical isomers are stereoisomers (i.e. have the same bonds, but different spatial arrangements of atoms).
- Stereoisomers have the same connectivity but different spatial arrangements of atoms.

## Isomerism

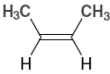


## Stereoisomers: cis-trans

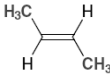
- To maintain orbital overlap in the pi bond, C=C double bonds cannot freely rotate.
- Although the two molecules below have the same connectivity, they are NOT identical.



π Bond




cis




trans

## Chemical Communication



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



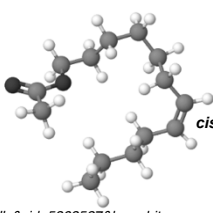
<http://www.learner.org/resources/series61.html>  
Pheromone Synthesis  
[20:40-23:51]

### Chemical Communication

Smell / Pheromones

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

S  
F  
Cl  
Br  
I  
...



**cis**

<https://embed.molview.org/v1/?mode=balls&cid=5363527&bg=white>  
<http://www.learner.org/resources/series61.html>

**Pheromone Synthesis**  
 [20:40-23:51]

### Molecular Modeling

Bonus

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. Contact your assigned group members. Be sure you have an e-mail that includes their e-mail addresses. Your group is to complete the table below and all of the questions that follow. Discuss the overall workload with your group and develop a plan to distribute the workload, coordinate the results, and have each member create this information in a pdf.

**Computers & Internet available in PS 110, if needed**

<http://molview.org>

Compound	$(EN_1 - EN_2)$	$(EN_1 + EN_2)$	Bonding Type
HF			
HCl			
HBr			

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

### Stereoisomers: Enantiomers

#### Chirality & Carbon Atoms

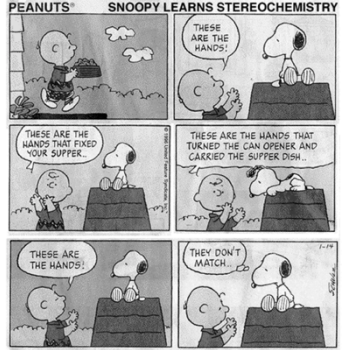
Chirality

Each carbon atom with four different substituents are chiral.


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

### Chirality

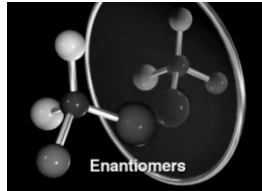
PEANUTS® SNOOPY LEARNS STEREOCHEMISTRY



### Chirality



Left hand Right hand


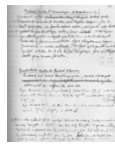


**Enantiomers**

### Stereoisomerism

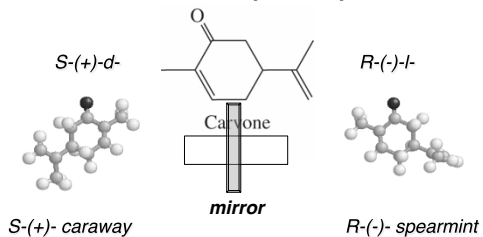
- Enantiomers are chiral: i.e. They are non-superimposable mirror images.
- Most physical and chemical properties of enantiomers are identical.
- Therefore, enantiomers are very difficult to separate eg. Tartaric acid...

Louis Pasteur:

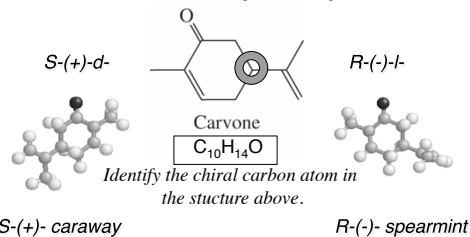
- Enantiomers can have very different physiological effects: eg. (+) and (-) carvone, Advil (ibuprofen) ..... (thalidomide)

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



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

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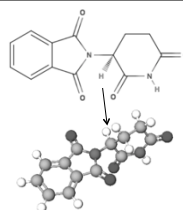
<http://chemconnections.org/organic/chem226/Labs/Smell/ChemComm.html>



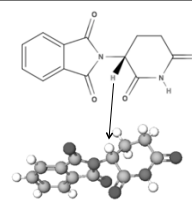
Thalidomide was administered as a racemic mixture (50:50 mix of enantiomers) to stave off morning sickness during pregnancy.



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.



<https://embed.molview.org/v1/?mode=balls&cid=92142&bg=white>



<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.