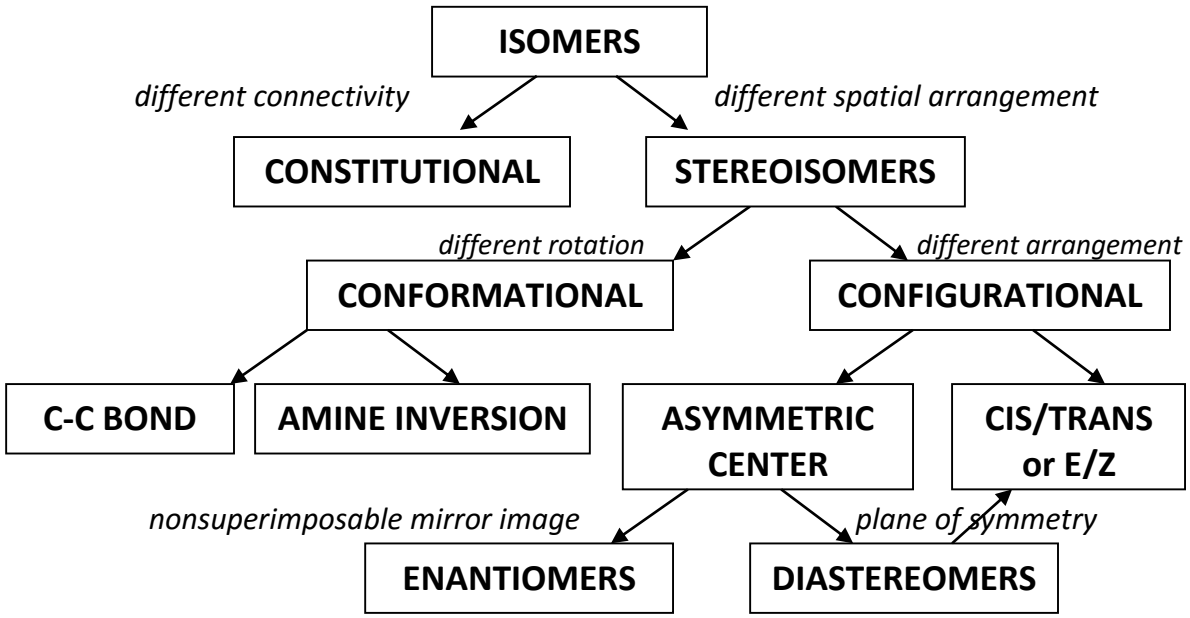
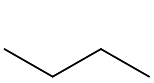
Isomerization in Organic Compounds

Chem12A, Organic Chemistry I

Isomers: same molecular formula but different…



CONSTITUTIONAL ISOMERS: different connectivity of atoms.



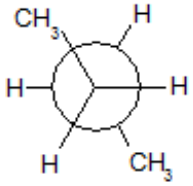
butane

2-methylpropane

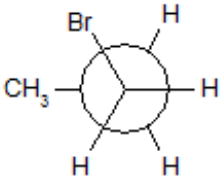
STEREOISOMERS: different three-dimensional rotation.

CONFORMATIONAL ISOMERS: different rotation around a bond or atom.

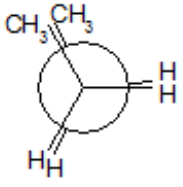
For C-C: around single bonds (sigma overlap) ONLY. Pi bonds restrict rotation.



anti

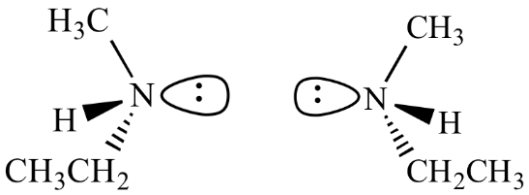


gauche



eclipsed

For Amine Inversion: The trigonal pyramidal structure around the N atom inverts the lone pair 180 degrees.



CONFIGURATIONAL ISOMERS: different spatial arrangement around an asymmetric center or locked atom.

Asymmetric center: an sp^3-hybridized carbon with four different substituents attached
Chiral: has a non-superimposable mirror image
Achiral: has no superimposable mirror image

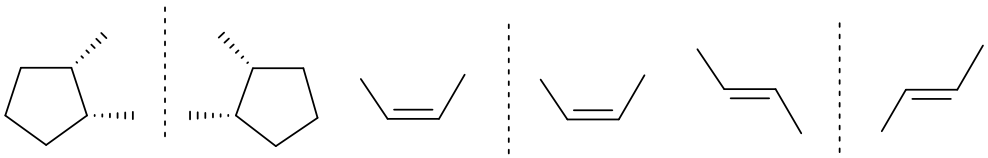
CIS-TRANS ISOMERS: different spatial arrangement around a locked atom (C=C or ring)
RINGS: **cis**: both up or both down, **trans**: one up and one down

cis isomer trans isomer

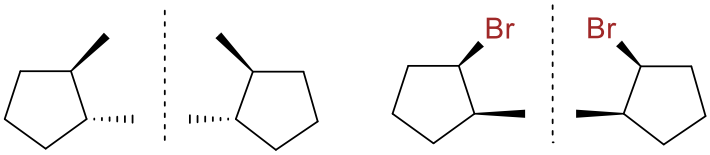
ALKENES: **cis/Z**: both up or both down from C=C, **trans/E**: one up and one down from C=C

cis isomer trans isomer

- If the molecule has an internal plane of symmetry, it is achiral and ONLY a cis-trans isomer.



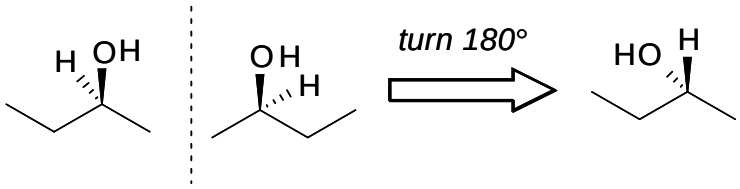
achiral



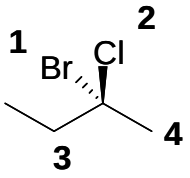
chiral

ENANTIOMERS: different orientation of the substituents around a stereocenter.

Enantiomers come in pairs (2 molecules) that are non-superimposable mirror images of one another.

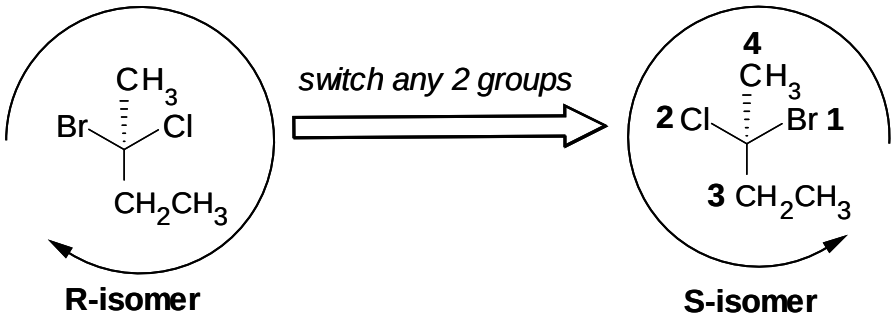


- Each of the groups around a stereocenter is assigned a priority (1-4, 1 being highest) based on the atomic number of the element directly attached to the stereocenter.
    - If two or more substituents have the same atom, travel down the chain until the first point of difference is reached.
    - Any hydrogen bonded to the stereocenter will *always be lowest* in priority.

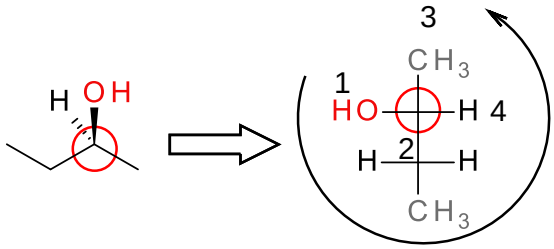


1.) --Br
2.) --Cl
3.) --CH_2CH_3
4.) --CH_3

- The molecule is oriented with the 4 group (lowest priority) pointing to the back.
    - If the numbers 1-3 are oriented *clockwise,* the molecule is the R-isomer.
    - If the numbers 1-3 are oriented *counterclockwise,* the molecule is the S-isomer.

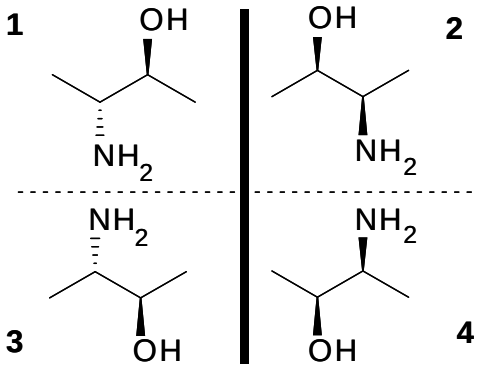


Fischer Projection: horizontal rows are wedges, vertical columns are dashes



Counterclockwise, but reverse since #4 is a wedge = **R-isomer**

DIASTEREOMERS: different orientation of groups around a stereocenter BUT are not non-superimposable mirror images (enantiomers).



1 and **2** are diastereomers.
1 and **3** are *enantiomers*.
1 and **4** are diastereomers.
2 and **3** are diastereomers.
2 and **4** are *enantiomers*.

Cyclic cis/trans without a plane of symmetry and meso compound are also diastereomers.