

Stereochemistry



Cahn-Ingold-Prelog priority rules

This is a system for the naming of stereoisomers of a molecule

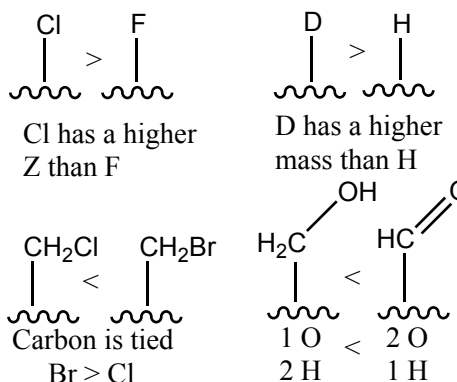
Naming molecules using CIP uses three steps:

1. Identify all stereocenters and double bonds
2. Assign priorities* to each of the groups at the stereocenters or on the double bond
3. Assign R/S or E/Z descriptors

*Assignment of priorities

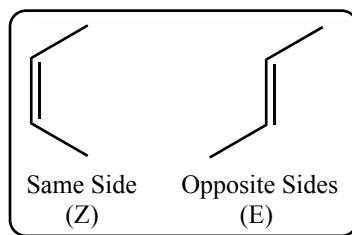
- i. Compare the atomic numbers of all atoms directly attached to the stereocenter
(The higher atomic number has higher priority)
- ii. If there is a tie, compare all atoms bound to each and assign priority. Continue until the first difference.
- iii. For isotopes higher atomic mass is higher priority and for double bonds, count the bound atom twice

Priority Examples



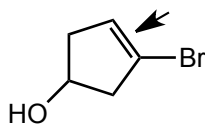
E vs Z notation

Because an alkene cannot rotate about its double bond, two groups on different carbons of the alkenecan either be on the same side of the double bond or on opposite sides of the double bond. These are named Z and E respectively.

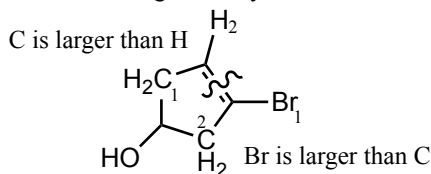


Note: If the alkene is disubstituted, then cis/trans notation may be used in place of E/Z. But, if there are three or more substituents E/Z notation **MUST** be used.

1. Identify double bond

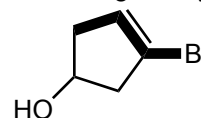


2. Assign Priority



3. Denote E or Z

Since the two, number 1, priority atoms are trans to each other the alkene has E geometry



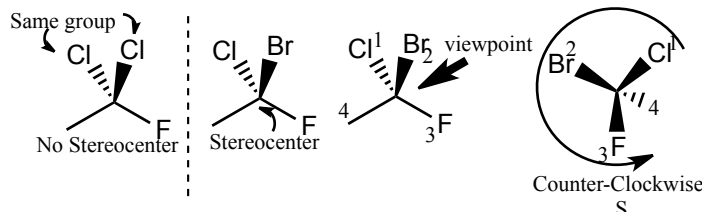
R vs S notation

In order to be a stereocenter, the sp^3 hybridized center must have 4 different groups attached to it.

When all groups are assigned correct priority, arrange the molecule so the lowest priority group is in the back and the three others are facing you. (Do not be confused if the lowest priority group is not already facing back. Build A Model).

Counting atoms prioritized 1, 2, 3 will go in a circle either clockwise (R) or counter-clockwise (S).

Group 4 is usually hydrogen but it does not have to be. Build a model to help with the 3-D orientation.



1. Assign Priority

2. Reorient group 4 back

3. Assign R or S

