Stereochemistry

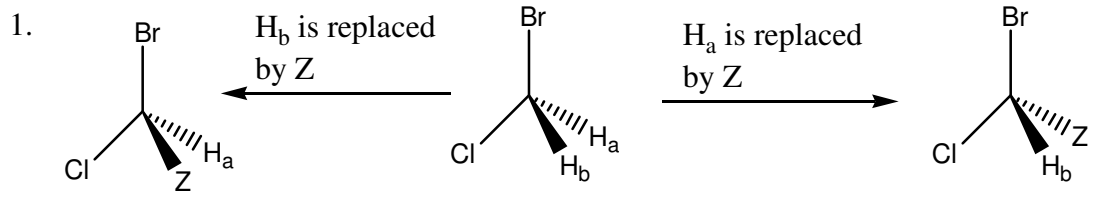
Pro-stereogenic centre:

Pro-R and pro-S descriptors:

In stereochemistry, prochiral molecules are those that can be converted from achiral to chiral in a single step. Enantiotopic or diastereotopic pair of atoms or groups on a prochiral centre in a molecule is designated as pro-R and pro-S if replacement of one of them by an achiral ligand with higher priority than the other in the sense of CIP rule, without disturbing the priority of remaining ligands, convert the prochiral centre into the chiral centre with R and S absolute configuration respectively.

Examples:

1.



Priority order
Br>Cl>Z>H_a

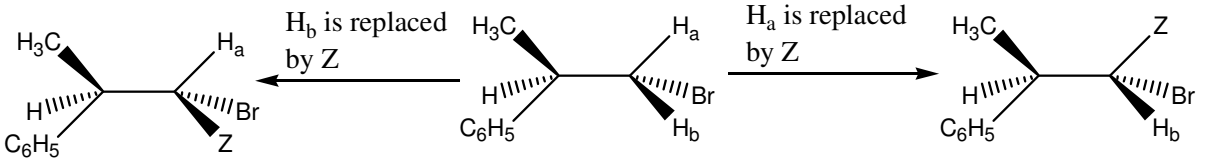
'S' isomer

Priority order
Br>Cl>Z>H_b

'R' isomer

Therefore H_a is pro-R and H_b is pro-S

2.



Priority order
Br>$CH(C_6H_5)CH_3$>Z>H_a

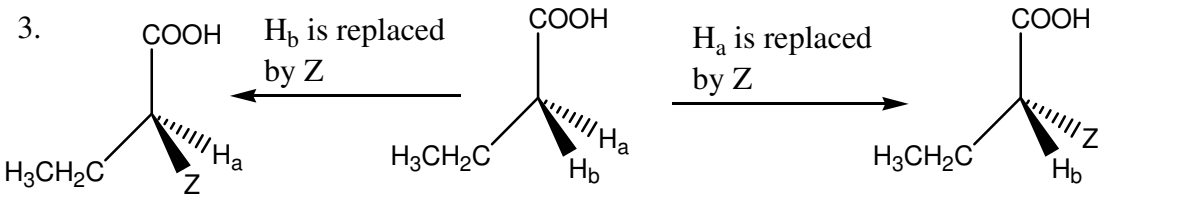
'R' isomer

Therefore H_a is pro-S and H_b is pro-R

Priority order
Br>$CH(C_6H_5)CH_3$>Z>H_b

'S' isomer

3.



Priority order is
COOH>Et>Z>H_a

'S' isomer

Priority order is
COOH>Et>Z>H_b

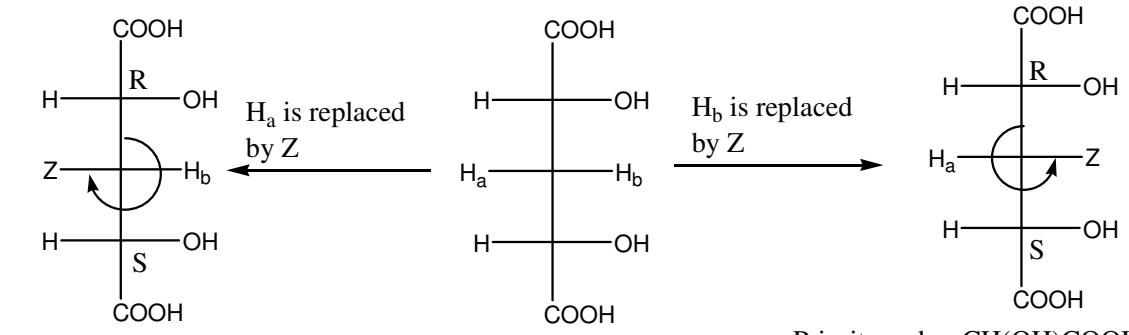
'R' isomer

Therefore H_a is Pro-R and H_b is Pro-S

Pro-r and pro-s descriptors:

The above concept can also be used for the centre which will be pseudoasymmetric centre after replacement with non equivalent ligand. For that case the designation will be pro-r and pro-s.

Example:



Priority order: CH(OH)COOH (R)> CH(OH)COOH (S)Z>H_b

's' isomer

Priority order: CH(OH)COOH (R)> CH(OH)COOH (S)Z>H_a

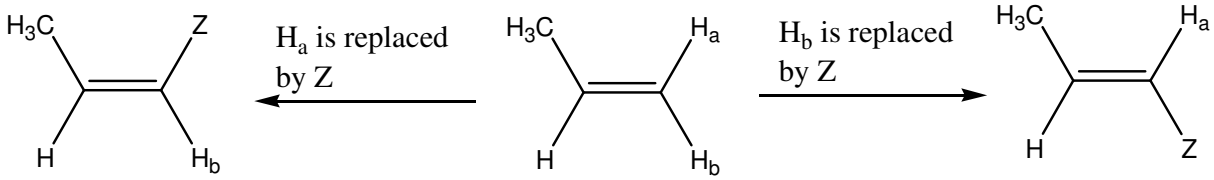
'r' isomer

Therefore H_a is pro-s and H_b is pro-r

Pro-E and pro-Z descriptors:

This above concept can also be used for the molecule which will show E/Z isomerism after replacement with non equivalent ligand. For that case the designation will be pro-E and pro-Z.

Example:



Z-isomer

E-isomer

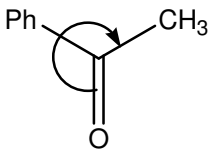
Therefore H_a is pro-Z and H_b is pro-E

Re/Si descriptors:

A trigonal planar sp^2-hybridized atom can be converted to a chiral centre when a substituent is added to the Re or Si face of the molecule. A face is labeled Re if, when looking at that face, the substituents at the trigonal atom are arranged in decreasing CIP priority order in a clockwise direction, and Si if the priorities decrease in counter-clockwise direction; note that the designation of the resulting chiral centre as S or R depends on the priority of the incoming group.

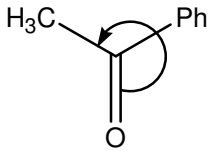
Examples:

1. Two faces of acetophenone are



Priority order of the groups is
O>Ph>CH_3

Re face

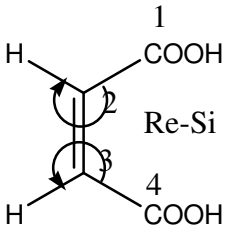


Priority order of the groups is
O>Ph>CH_3

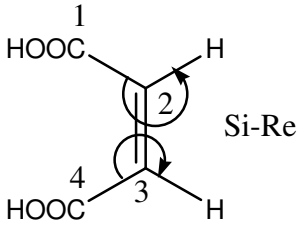
Si face

These two faces of the molecule are enantiotopic faces since separate addition of a non identical group at the carbon centre in these two faces produces two enantiomers.

2. Two faces of maleic acid are given below

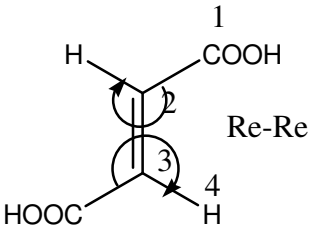


Prioroty order at C_2 and C_3 are
COOH>=CHCOOH>H
Thus C_2 is Re and C_3 is Si
Therefore this face is Re-Si

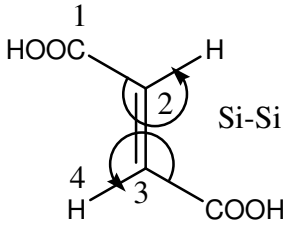


Prioroty order at C_2 and C_3 are
COOH>=CHCOOH>H
Thus C_2 is Si and C_3 is Re
Therefore this face is Si-Re

3. Two faces of fumaric acid are given below



Prioroty order at C_2 and C_3 are
COOH>=CHCOOH>H
Thus C_2 and C_3 both are Re
Therefore this face is Re-Re



Prioroty order at C_2 and C_3 are
COOH>=CHCOOH>H
Thus C_2 and C_3 both are Si
Therefore this face is Si-Si