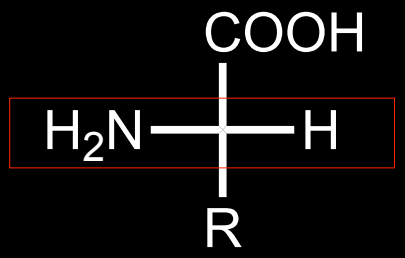
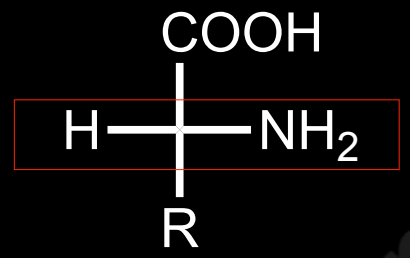
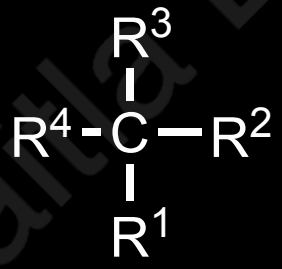
Configuration



L-amino acid



D-amino acid

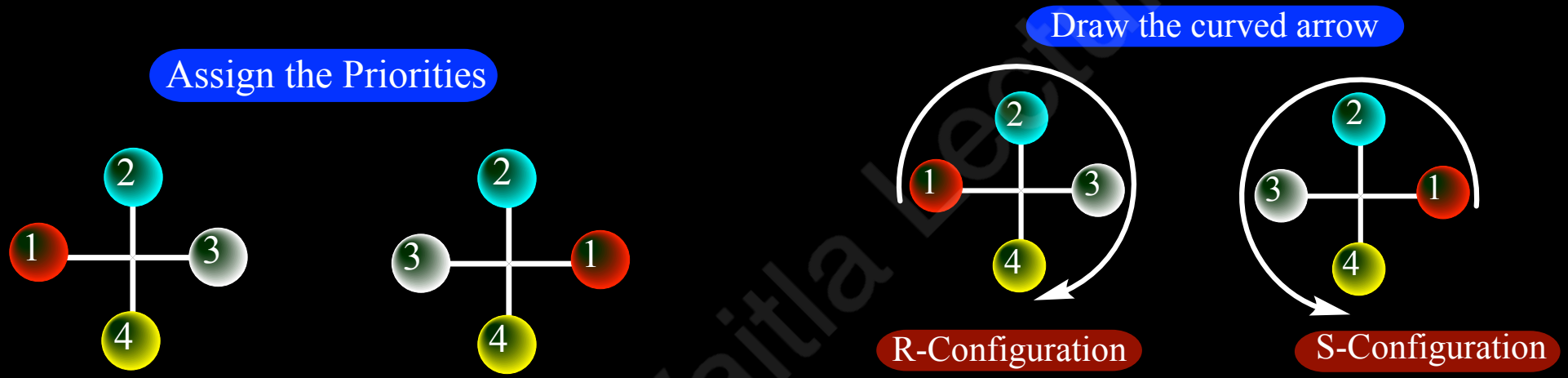


How to explain the configuration of this molecule?

Absolute configuration

To name the enantiomers of a compound unambiguously, their names must include the "handedness" of the molecule. The method for this is formally known as R/S nomenclature.

The method of unambiguously assigning the handedness of molecules was originated by three chemists: R.S. Cahn, C. Ingold, and V. Prelog and, as such, is also often called the Cahn-Ingold-Prelog rules.



* a curved arrow is drawn from the highest priority (1) substituent to the lowest priority (4) substituent

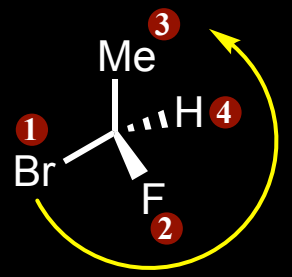
- If the arrow points in a counterclockwise direction the configuration at stereocenter is considered S ("Sinister" → Latin= "left").
- the arrow points clockwise,(Right when leaving the 12 o' clock position) then the stereocenter is labeled R ("Rectus" → Latin= "right").

R,S - Nomenclature

☆ Rule-1:

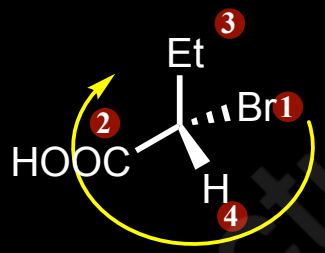
☞ The higher the atomic number, the higher the priority.

$I > Br > Cl > S > F > O > N > {}^{13}C > {}^{12}C > Li > {}^{3}H > {}^{2}H > {}^{1}H$



anti clockwise

S-Configuration



clockwise

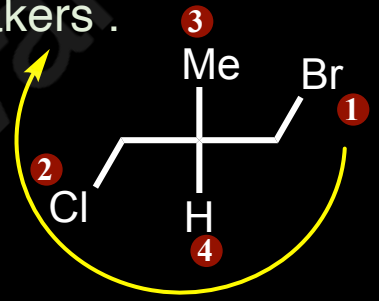
S-Configuration

Note:
4th Group is towards observer

☞ Orient the chiral centre such that the 4th priority substituent is pointing away from the viewer.

☆ Rule-2:

☞ In case of ties, use the next atoms along the chain of each group as tiebreakers .



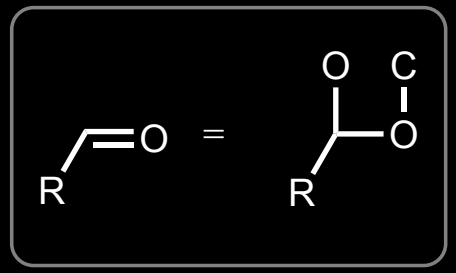
clockwise

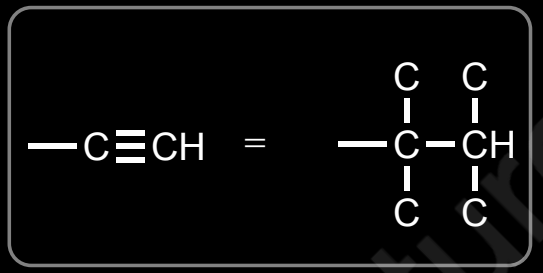
R-Configuration

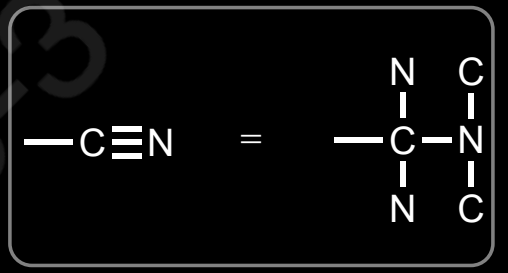
R,S - Nomenclature

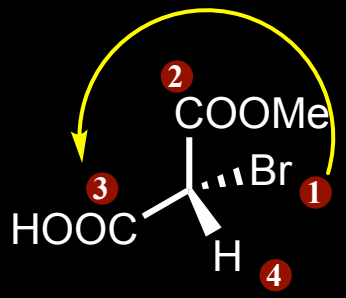
☆ Rule-3:

☞ Treat double and triple bonds as if each were a bond to a separate atom. For this method, imagine that each pi bond is broken and the atoms at both ends duplicated. (Phantom atom concept)





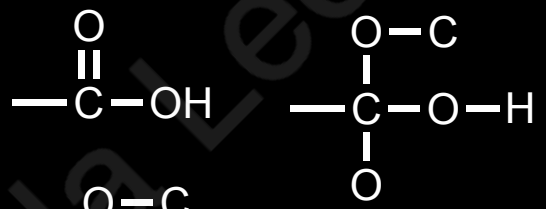




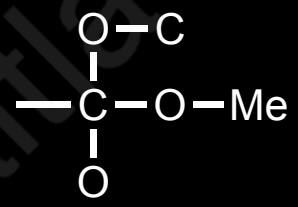
anti clockwise

R-Configuration

-COOH



-COOMe

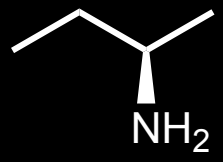


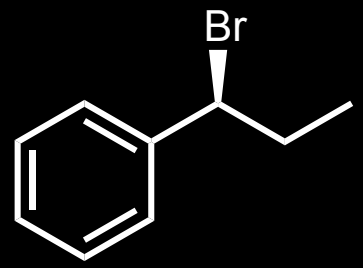
Note:

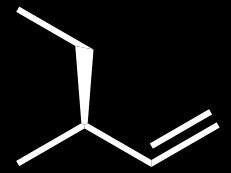
4th Group is towards observer

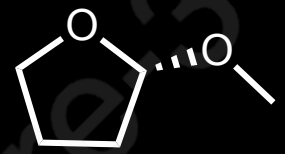
R,S - Nomenclature

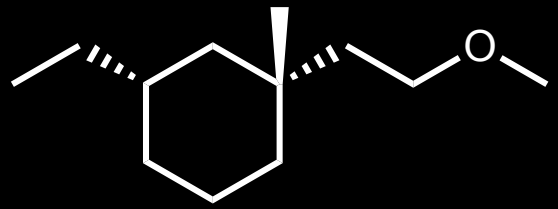
☆ Question: Identify the absolute configuration for the following molecules

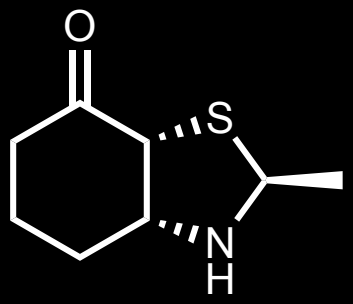


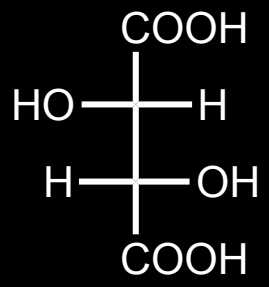


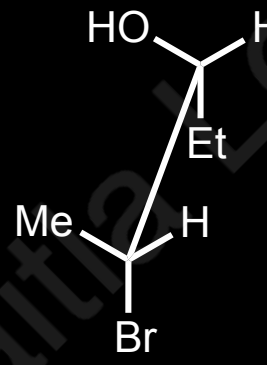


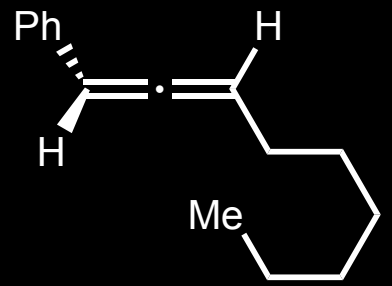












$[\alpha]_D$ = -248.4°

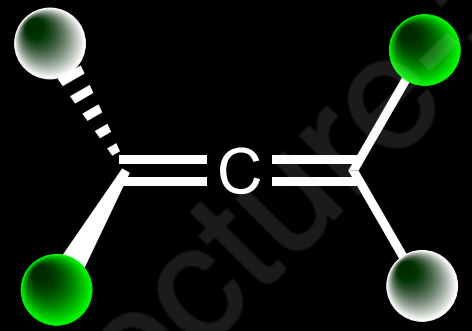
☞ Stereogenic unit is a unit in a molecule which is responsible for stereoisomerization or stereomer generation.

☞ Stereogenic unit can be either point, axis, plane, or helicity.

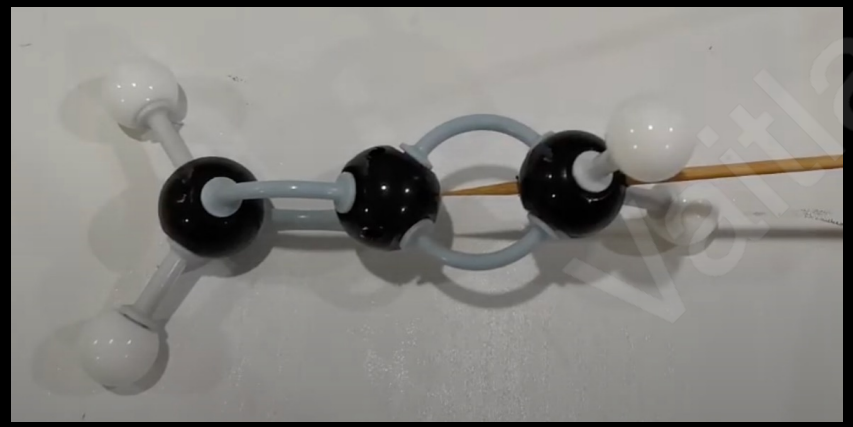
Axial chirality

Molecule does not possess a chiral center but contain chiral axis

Chiral axis: An axis about which a set of substituents is held in a spatial arrangement that is not superposable on its mirror image.

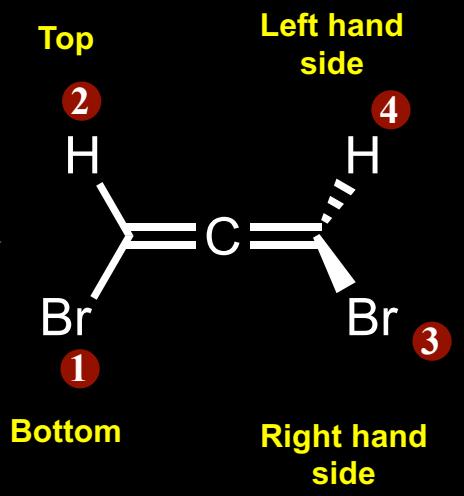


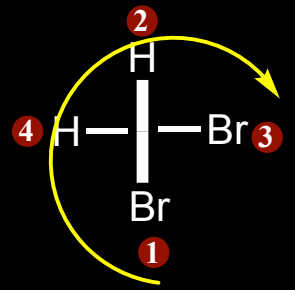
Allenes



R,S - Nomenclature

Look from this side



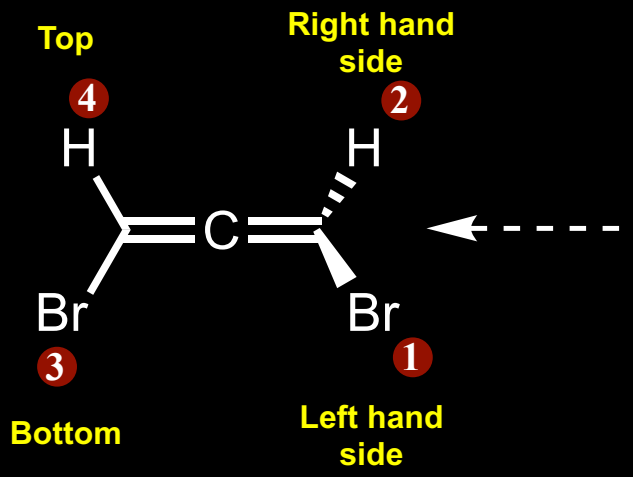


clockwise

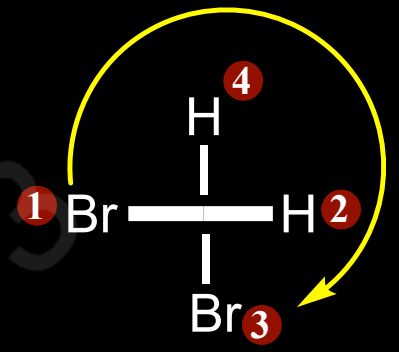
R-Configuration

Note:
Dont think about 4th group
(weather it is in horzontal/vertical line)

R,S - Nomenclature



Look from this side

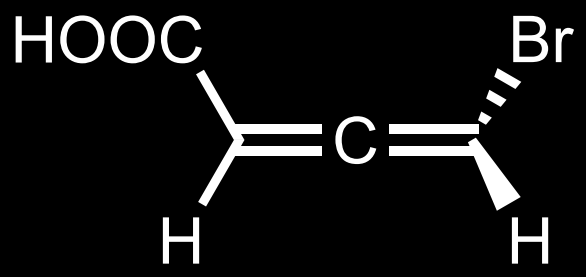


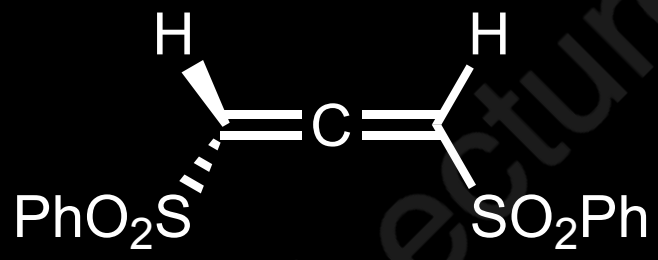
clockwise

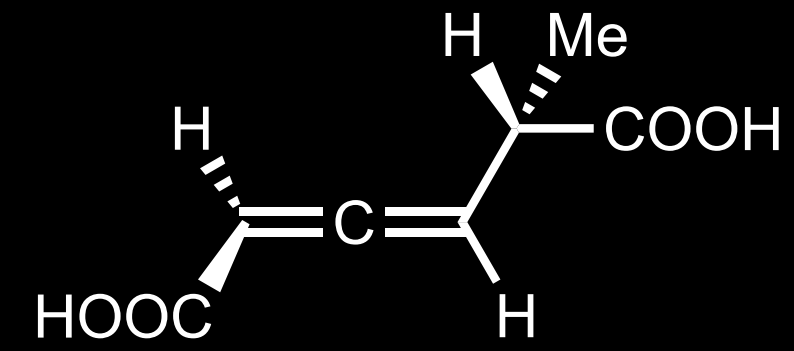
R-Configuration

R,S - Nomenclature

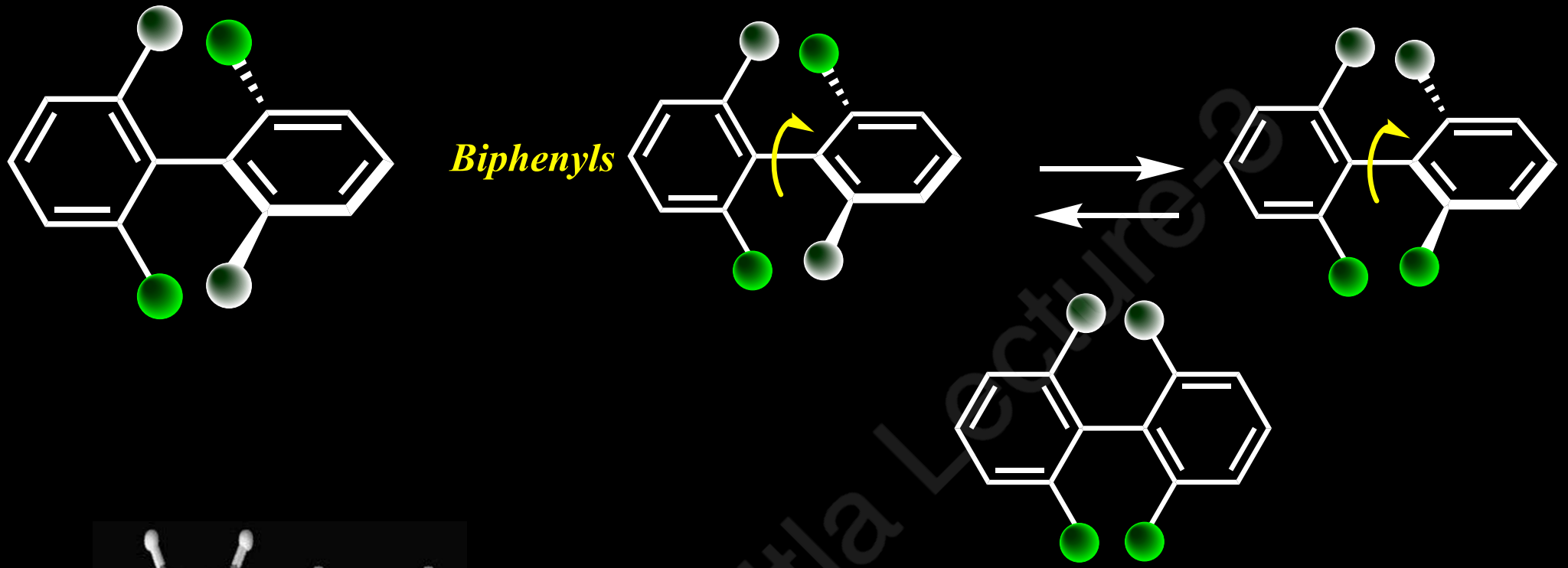
☆ Question: Identify the absolute configuration for the following molecules

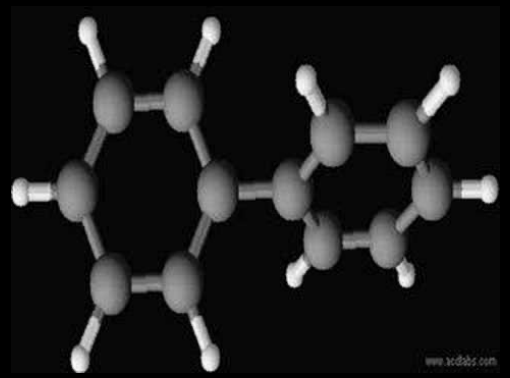


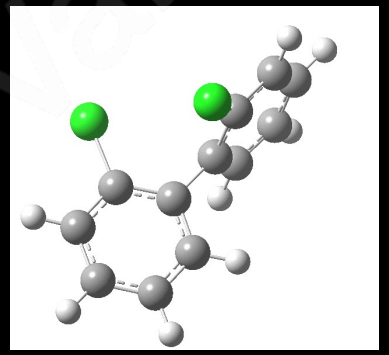




when the substituents are small in size

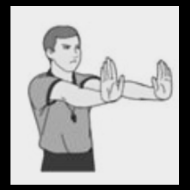


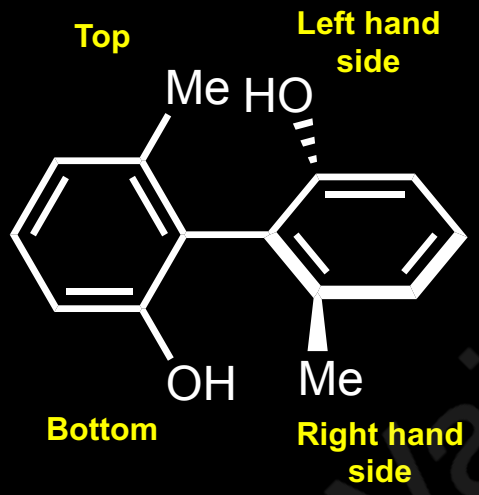


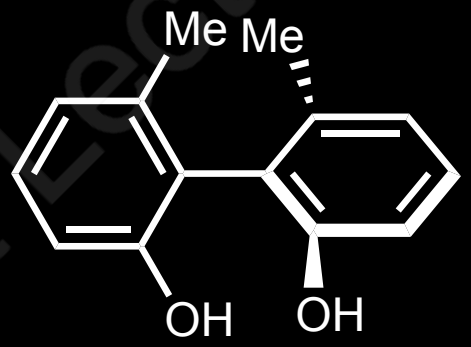


R,S - Nomenclature

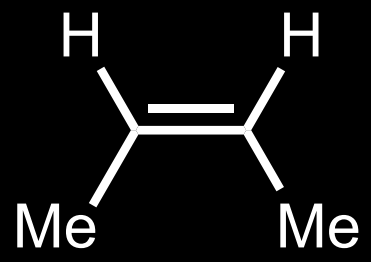
☆ Question: Identify the absolute configuration for the following molecules



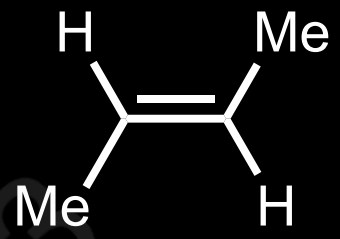




Geometrical Isomerism



cis

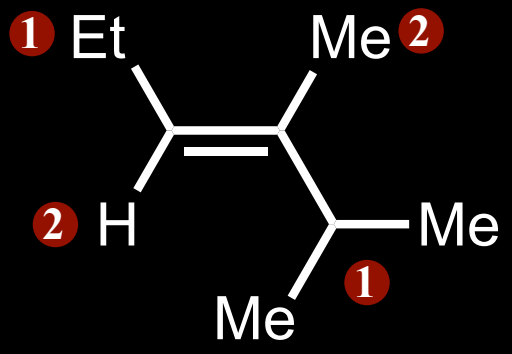


trans

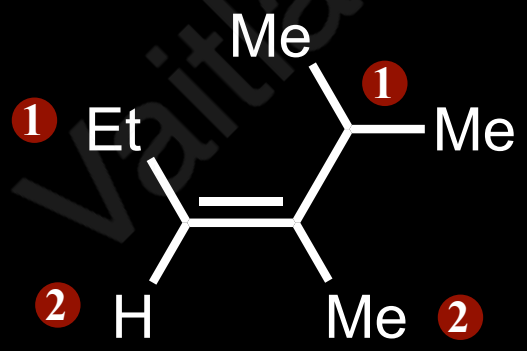
☞ Each carbon in the π– bond is attached to two substituents. For each carbon, these two substituents are ranked (1 or 2) according to the atomic numbers of the atom directly attached to the carbon.

☞ If both substituents ranked 1 are on the same side of the π– bond, the bond is given the descriptor ***Z***

☞ If both substituents ranked 1 are on the opposite side of the pi bond, the bond is given the descriptor ***E***



E



Z