Elements of Symmetry

- Plane of symmetry (σ)
- Centre of symmetry (i)
- Proper Axis of Symmetry (C_n)
- Alternating Axis of Symmetry (S_n)

R and S Nomenclature

* R S system specifies the absolute configuration of asymmetric molecules.
* This system was Introduced by Cahn, Ingold and Prelog system.
* The symbol R and S stands for
  R → Rectus
  S → Sinister

Sequence Rule

The four groups attached to the asymmetric Carbon atom are assigned priority in accordance with the sequence rule

After assigning the group of atoms the molecule is rotated in such a way the lowest priority directed away from the viewer.

Higher the atomic Number of the atom attached higher is the priority

(eg) Cl, Br, I, F

17 35 53 9

Priority order I > Br > Cl > F.

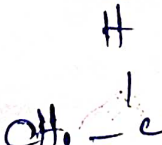
b). Cl, I, H, SO_3H (Sulphur)

17 53 1 16

I > Cl > SO_3H > H

II) If the atomic Number of two atoms of the same element (Isotopes) attached to the asymmetric carbon atom is same, the atom higher mass has the higher priority.

for (eg)



d-deutroethyl bromide

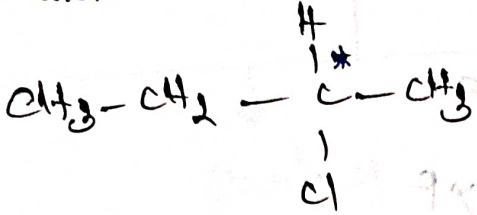
H D Br CH_3

1 2 35 6

^1H and ^2D are Isotopes.

Br > C > D > H

(iii) If the atom attached to the asymmetric Carbon atom are same then it is determined by the next atom.



Secondary butyl chloride

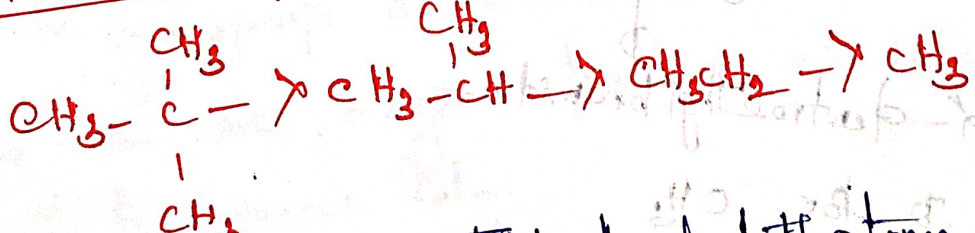
Cl CH_3 H C_2H_5

1 2 3 4

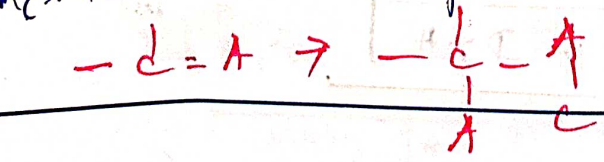
ethyl has the higher priority then methyl because the ethyl Group has carbon and hydrogen [C, H, H] whereas methyl Group has only hydrogen [H, H, H] Carbon has priority over hydrogen.

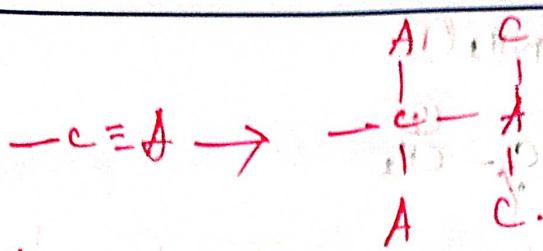
Priority order. $Cl > C_2H_5 > CH_3 > H$

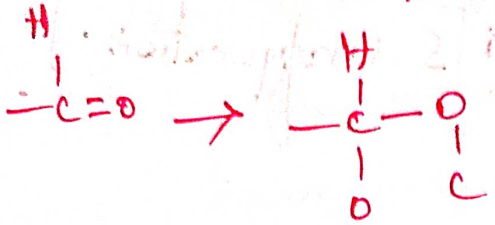
In General priority order

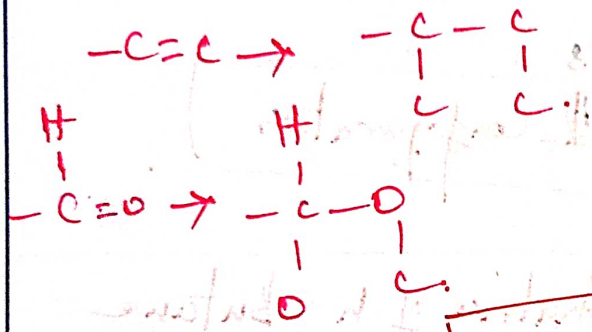


(iv) In case of double or Triple bonds both atoms are considered to be duplicated or Tripleated





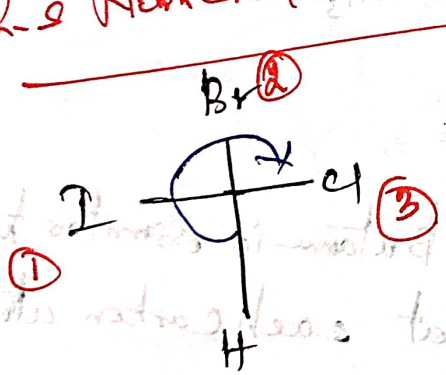




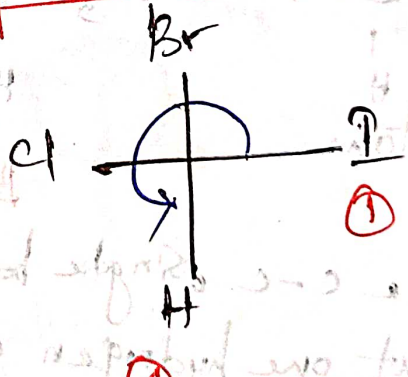
The priority order OH > CHO > CH_2OH > H

2.2 Nomenclature of Compounds

(1)

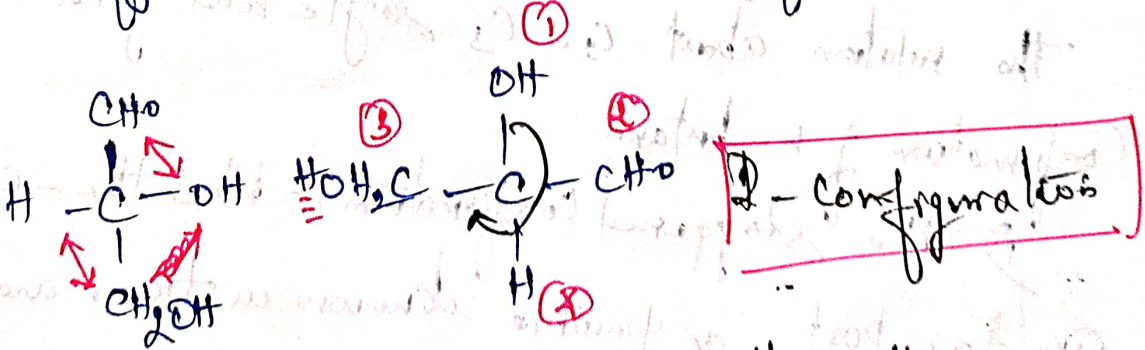


2- Configuration



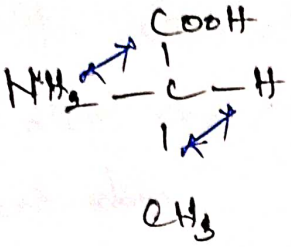
S- Configuration

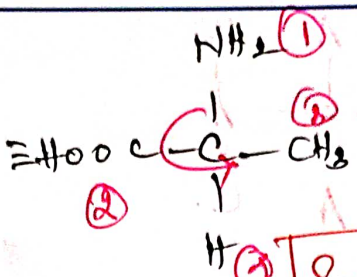
(2)



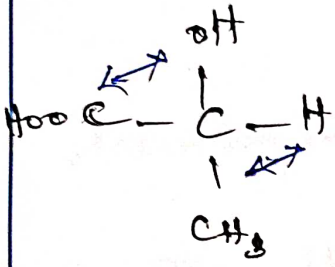
Priority order OH > CHO > CH_2OH > H

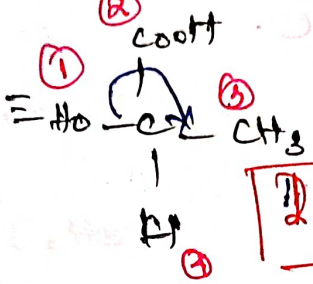
(8)





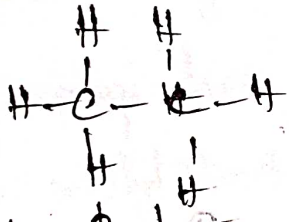
S-Configuration.



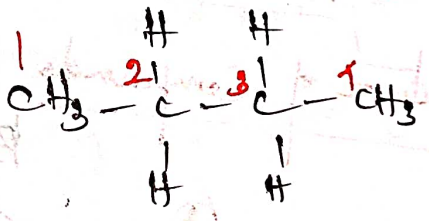


R-configuration

Conformation analysis of n-Butane



n-Butane



Butane

The middle C-C single bond in Butane is similar to ethane but one hydrogen atom at each carbon atom is replaced by methyl group (CH_3)

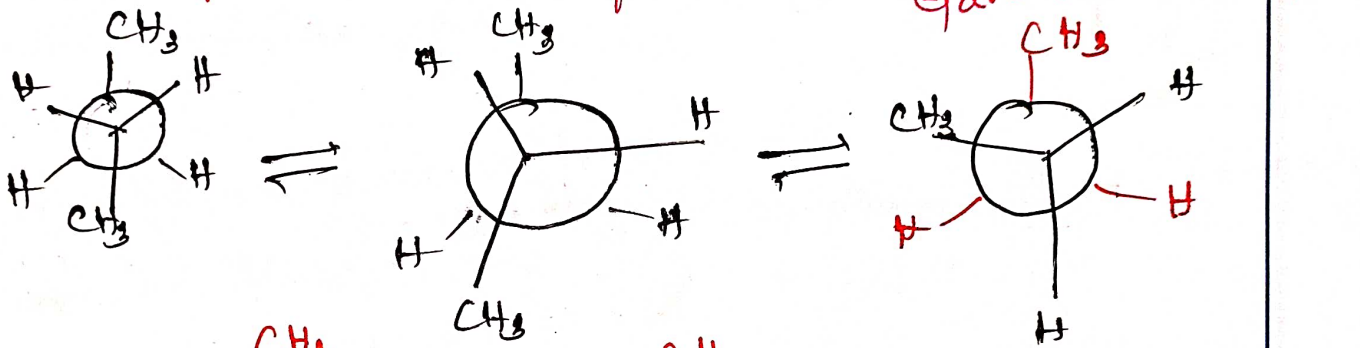
The rotation about C_2-C_3 single bond gives many Conformation of n-butane

1) The staggered conformation in which the $-CH_3$ groups are far part as possible known as trans and are more Conformation. It is the most stable conformation

2) Staggered Conformation known as the Gauche Conformation starting at 60°.

3) The other possible Conformation are eclipsed Conformation in which eclipsing occurs between hydrogen atom and methyl group.

Anti staggered-1 Eclipsed-2 Gauche staggered-3



Eclipsed-4 Gauche staggered-5 Eclipsed-6