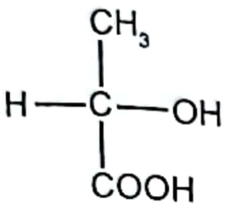
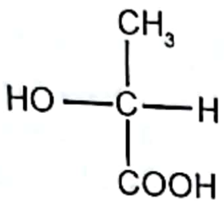
5.5 Optical isomerism :

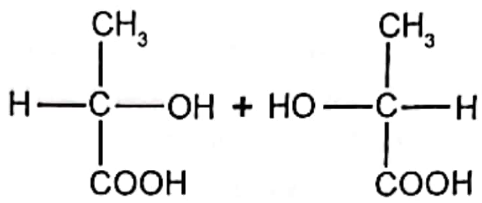
1. Lactic acid : Lactic acid contain one asymmetric carbon.The two stereo isomers of lactic acid forms non super impossible mirror images. Structure **I** is dextro rotatory and structure II is leavo rotatory. Dextro isomer rotate the plane polarised towards right, leavo isomer rotate the plane polarised towards left, thus the structures I and II are called enantiomers.d - lactic acid and l -lactic acid are optical active. But Racemic lactic acid is optical inactive due to external compensation.



d - Lactic acid (I)

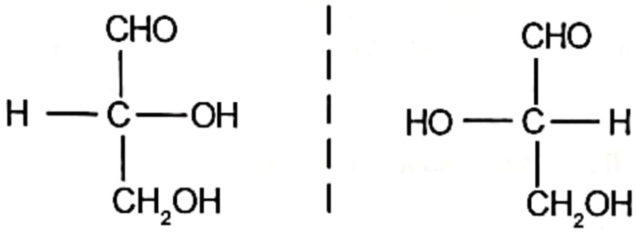


l - lactic acid(II)



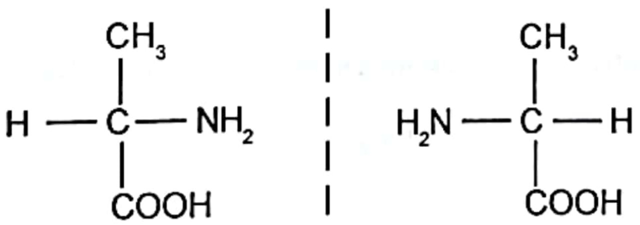
Racemic lactic acid

2. Glyceraldehyde : Glyceraldehyde contain one asymmetric carbon.The two stereo isomers of Glyceraldehyde forms non super impossible mirror images. Structure **I** is dextro rotatory and structure II is leavo rotatory. Dextro isomer rotate the plane polarised towards right, leavo isomer rotate the plane polarised towards left, thus the structures I and II are called enantiomers.



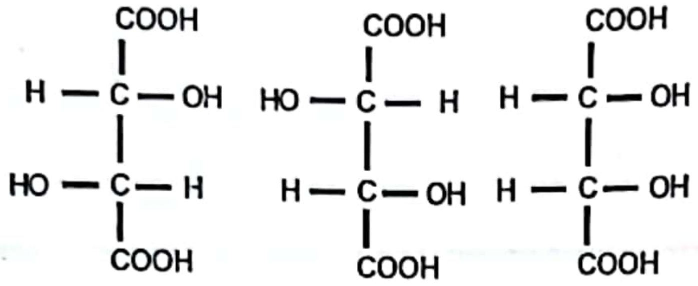
I II

3. Alanine: It is an α- amino acid. Alanine contain one asymmetric carbon.The two stereo isomers of Alanine forms non super impossible mirror images. Structure **I** is dextro rotatory and structure II is leavo rotatory.Dextro isomer rotate the plane polarised towards right, leavo isomer rotate the plane polarised towards left,thus the structures I and II are called enantiomers.

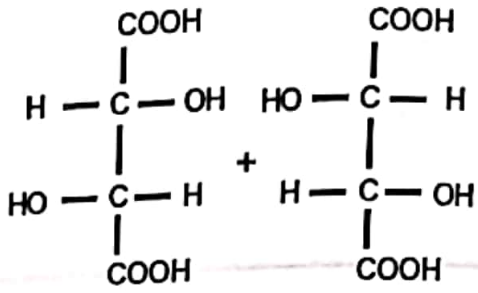


I II

4. Tartaric acid : It has Two same type of asymmetric carbon atoms and it has four isomeric forms .



d -Tartaric acid l - Tartaric acid m - Tartaric acid



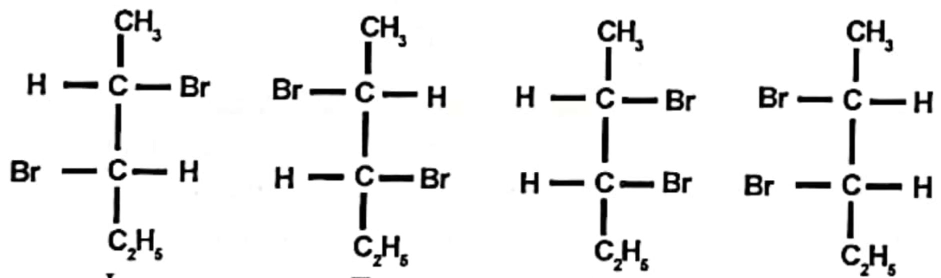
Racemic Tartaric acid

d -Tartaric acid and l -Tartaric acids are optical active . Meso tartaric acid is optical inactive due to internal compensation. Racemic tartaric acid is optical inactive due to external compensation. d -tartaric acid and l - tartaric acids are enantiomers, because they are non super impossible mirror images. d ,m and l, m Tartaric acids are Diastereomers.

5.6 Enantiomers and Diastereomers : The optical active substances exists in two or more isomeric forms, which have identical in chemical properties , physical properties except their action towards plane polarised light are called enantiomers. Enantiomers are defined as the stereo isomers which are the mirror images of one another and which rotates the plane polarised light equally but in opposite direction.**or** Non super impossible mirror images are called Enantiomers.

The isomers which does not appear as object mirror images are called diastereomers. Diastereomers differ in physical properties like solubility amd melting point

Eg : 2,3 - di bromo pentane. It has two dissimilar chiral carbons.



I II III IV

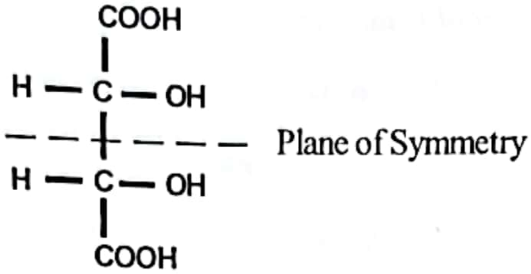
1. I ,II and III ,IV are Enantiomers as they are mirror images to each other.

2. I,III & I,IV & II,III & II,IV are Diastereomers as they are not mirror images to each other.

5.7 Meso compounds : Optical inactive compound with asymmetric carbon is known as Meso compound. These are the compounds which contain two or more chiral carbons and optically inactive due to the presence of plane of symmetry.

The optical inactivity of meso compounds is due to the internal compensation. i.e the optical rotation in half of the molecule is cancled by other half of the molecule in opposite direction. So, the specific rotation is zero.

Eg : Meso Tartaric Acid



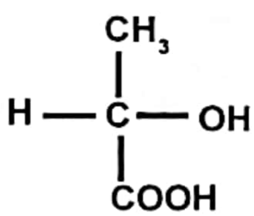
m - Tartaric Acid

5.8 Calculation of Number of Isomers :

Case (i) : If the compound can not be cut into two equal halfs.

1. Number of optical isomers = 2^n
2. Number of Enantiomers = $2^n / 2$
3. Number of Racemic mixtures = $2^n / 2$
4. Number of Meso compounds = 0
5. Number of configurational isomers = $2^n + 0$

Example : (Number of Asymmetric carbons = 1)



Lactic acid

1. Number of optical isomers = 2^n = $2^1 = 2$
2. Number of Enantiomers = $2^1 / 2 = 1$
3. Number of Racemic mixtures = $2^1 / 2 = 1$
4. Number of Meso compounds = 0
5. Number of configurational isomers = $2^1 + 0 = 2$

Case (ii) : If the compound can be cut into two equal halfs. If compound contain even number of Asymmetric carbons.

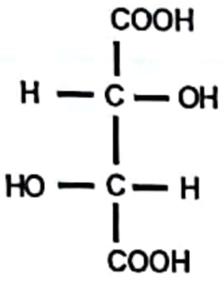
1. Number of optical isomers = 2^{n-1}
2. Number of Enantiomers = $2^{n-1} / 2$

3. Number of Racemic mixtures $= 2^{n-1} / 2$

4. Number of Meso compounds $= 2^{n-2/2}$

5. Number of configurational isomers $= 2^{n-1} + 2^{n-2/2}$

Example : (Number of Asymmetric carbons = 2)



Tartaric Acid

1. Number of optical isomers $= 2^{n-1} = 2^{2-1} = 2$
2. Number of Enantiomers $= 2^{n-1} / 2 = 2^{2-1}/ 2 = 1$
3. Number of Racemic mixtures $= 2^{n-1} / 2 = 2^{2-1}/ 2 = 1$
4. Number of Meso compounds $= 2^{n-2/2} = 2^{2-2/2} = 1$
5. Number of configurational isomers $= 2^{2-1} + 2^{2-2/2} = 3$

Case (iii) : If compound contain Odd number of Asymmetric carbons.

1. Number of optical isomers $= 2^{n-1} - 2^{n-1/2}$
2. Number of Enantiomers $= \frac{2^{n-1} - 2^{n-1/2}}{2}$
3. Number of Racemic mixtures $= \frac{2^{n-1} - 2^{n-1/2}}{2}$
4. Number of Meso compounds $= 2^{n-1/2}$
5. Number of configurational isomers $= 2^{n-1}$

Example : (Number of Asymmetric carbons = 3)

Tri Hydroxy Glutaric Acid

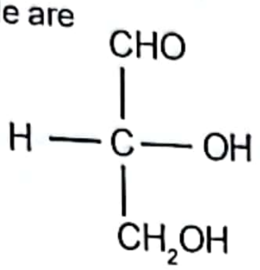
1. Number of optical isomers $= 2^{n-1} - 2^{n-1/2} = 2^{3-1} - 2^{3-1/2} = 4 - 2 = 2$
2. Number of Enantiomers $= \frac{2^{n-1} - 2^{n-1/2}}{2} = \frac{2^{3-1} - 2^{3-1/2}}{2} = 1$
3. Number of Racemic mixtures $= \frac{2^{n-1} - 2^{n-1/2}}{2} = \frac{2^{3-1} - 2^{3-1/2}}{2} = 1$
4. Number of Meso compounds $= 2^{n-1/2} = 2^{3-1/2} = 2^{2/2} = 1$
5. Number of configurational isomers $= 2^{n-1} = 2^{3-1} = 2^2 = 4$

5.9 Configurational isomerism : The special arrangement of groups or atoms around the asymmetric carbon is known as configuration. These are two types

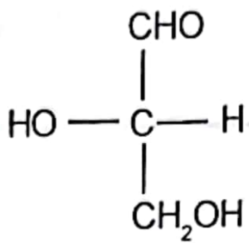
1. Relative configuration (D,L-notation)

2. Absolute configuration (R,S – configuration)

5.9.1 D , L - Notations (Relative configuration) : In This method Configuration for a compound is assign by comparing the configuration of Glyceraldehyde. In this the - OH group to the right on the chiral centre and is given by D - Configuration, the - OH group to the left on the chiral centre and is given by L - Configuration. Stereo isomers of Glyceraldehyde are

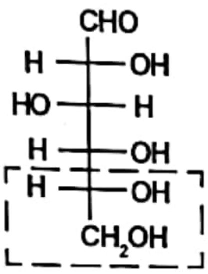


D (+) - Glyceraldehyde
- OH on Right side

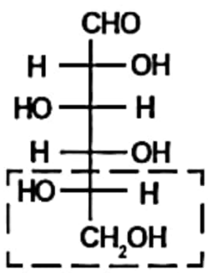


L (-) - Glyceraldehyde
- OH on Left side

The molecules that are chemically related to D - Glyceraldehyde are assigned the D - Configuration and those related to L - Glyceraldehyde are designated with L - Configuration. D, L - configurations have nothing to do with d , l notations.



D - (+) - Glucose



L - (-) - Glucose

5.9.2 Cahn - Ingold - Prelog R - S notational system : This notation has two steps

Step1: The priority order should be given to the 4 different atoms or groups attached to the chiral carbon by the below rules.

Sequence Rules: 1. The atom having highest atomic number is given the first priority and the atom with least atomic number has given the least priority

I	F	Cl	Br
①	④	③	②

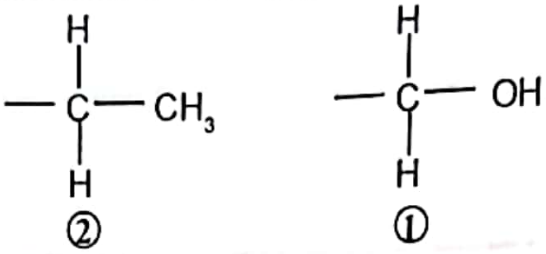
2. In case of isotopes priority is given basing on the mass number

Eg: priority order is $_1H^1 < {}_1H^2 < {}_1H^3$

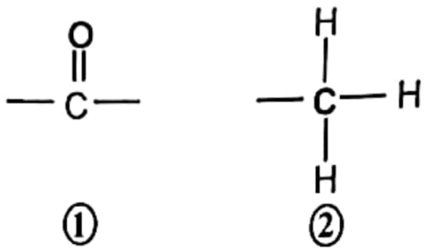
3. In case of groups priority given basing on the atomic number of key atom.

Eg: the priority order is $—OH > —NH_2 > —CH_3$

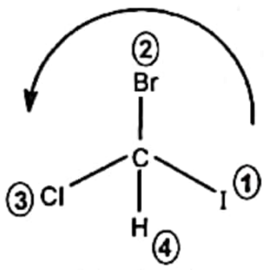
4. Priority cannot be given basing on the atomic number of key atom then priority is given basing on the atomic number of the next atom attached to the key atom.



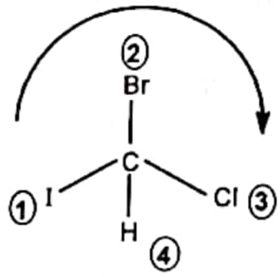
5. If the key atom with either double bond or triple bond consider that atom as two atoms or three atoms.



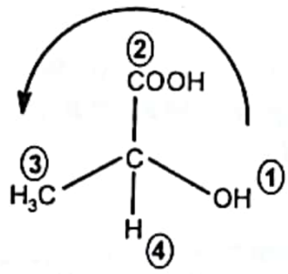
Step 2: After deciding the priority the tetrahedral carbon is oriented in such away that least priority group is directed away from the eye. After that when we move from first priority group to the least priority group in clock wise direction that is from left to right, then the notation is **R** (Latin Rectus) and if we move in anti – clock wise direction then its notation is **S** (Latin Siniste) .



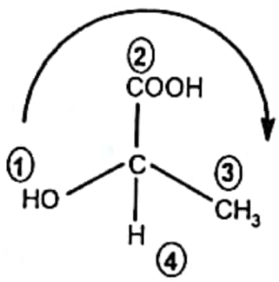
S - Configuration



R - Configuration



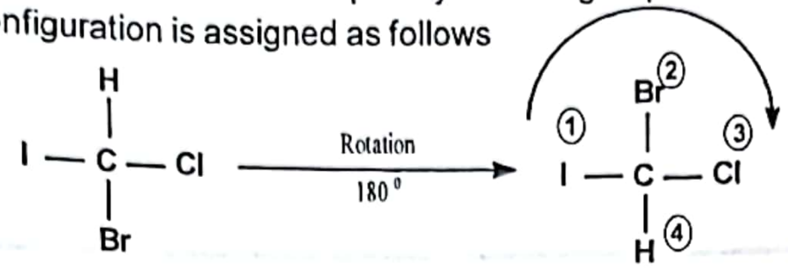
S - Configuration



R - Configuration

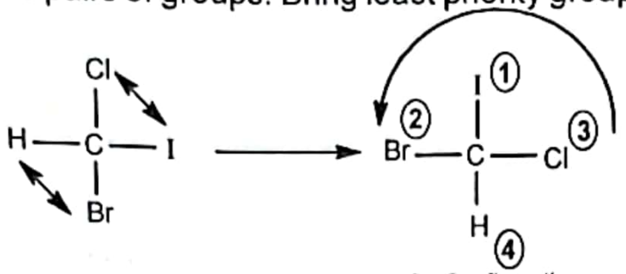
In this projection we have vertical lines and horizontal lines. The groups on vertical line pointed pointing away from the viewer and the group on the horizontal line pointing towards the viewers.

Case 1 : When the least priority group is at the top then the molecule has to be rotated to an angle 180°. So, that the least priority atom or group comes to the bottom and then configuration is assigned as follows



R - Configuration

Case 2 : If least priority group on horizontal line take opposite configuration. By doing mutual exchange of two pairs of groups. Bring least priority group on vertical line.



S - Configuration

5.12 E - Z notation : If there are four different groups present on C = C then we cannot call them as cis – trans isomers. For these compounds Z and E notation is introduced.These have similar rules as that of R-S notation. According to this " when atoms of higher atomic number are on the same side of the double bond , the double is said to be Z configuration. Z stands for the German word ' Zusammen ' which means " together ". When atoms of higher atomic number are on opposite sides of the double bond it is said to be E configuration. E stands for the German word ' Entgegen ' which means "opposite "

Step1 : priority order should be given to the four different atoms or groups attached to the chiral carbon by following below rules.

Rules: 1. The atom having highest atomic number is given the first priority and the atom with least atomic number has given the least priority

I	F	Cl	Br
①	④	③	②

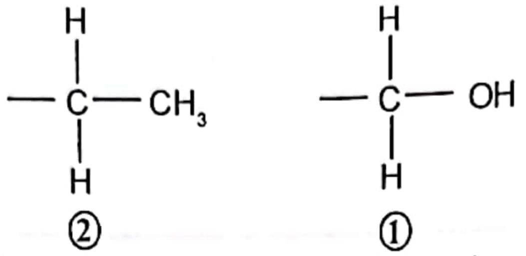
2. In case of isotopes priority is given basing on the mass number

Eg: priority order is $_1H^1 < {}_1H^2 < {}_1H^3$

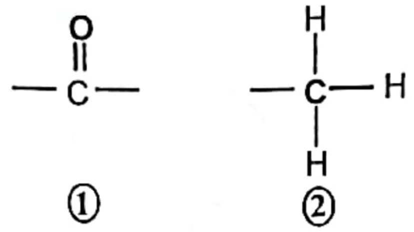
3. In case of groups priority given basing on the atomic number of key atom.

Eg: the priority order is $—OH > —NH_2 > —CH_3$

4. Priority cannot be given basing on the atomic number of key atom then priority is given basing on the atomic number of the next atom attached to the key atom.

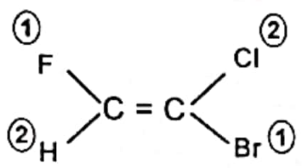


5. If the key atom with either double bond or triple bond consider that atom as two atoms or three atoms.

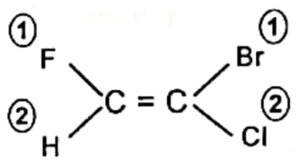


Step 2 : After deciding the priorities of two groups of highest priority on same side then the notation is **Z**, if two groups of highest priority on opposite side then the notation is **E.**

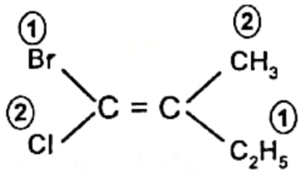
Eg :



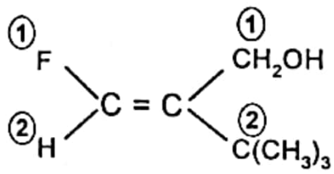
E - Notation



Z - Notation



E - Notation



Z - Notation