Chemistry-I
Module-5
Representations of 3 Dimensional Structures or Stereochemistry-1

31 March 2020

We can represent a compound's structure in three dimensions. In last lectures we were discussing about Compounds having same molecular formula but have different bonding connectivity. Here we are going to discuss a step ahead of that. Compounds, mainly organic compounds have same molecular formulae, have same bonding connectivity but they they have different structure in 3 dimension. Due to different 3D structure they have different physical and chemical properties. This branch of chemistry where we will try to understand 3-dimentional structure of compounds is called stereochemistry.

Here we have to represent all those three dimensional structures into two-dimension using some special techniques of drawing. These are standard and well accepted by scientists of all fields.

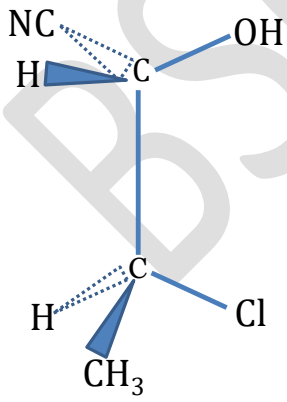
We can represent a chemical compound in following ways. Each of these is called projection formula. These are-

1) Flying-wedge projection formula
2) Fischer projection formula
3) Saw-horse projection formula
4) Newman projection formula

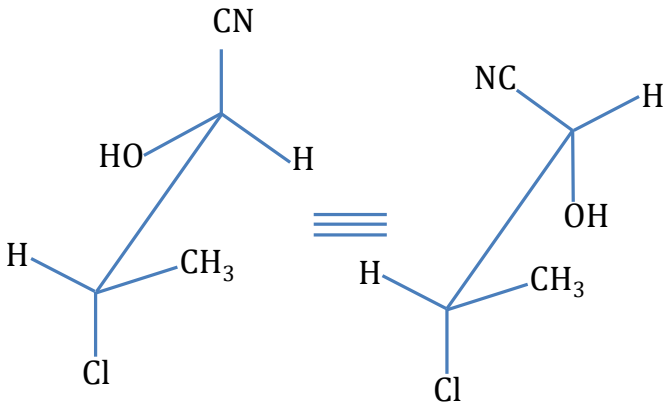
Let us take an example-

$CH_3CH(Cl)CH(OH)(CN)$

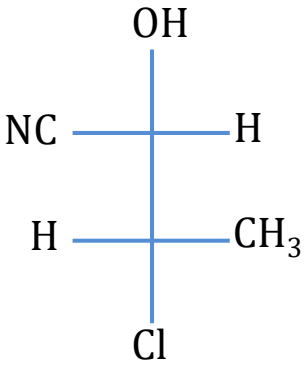
It has several isomers with several bonding connectivity. We will take one of them and represent them in all four projection formula.



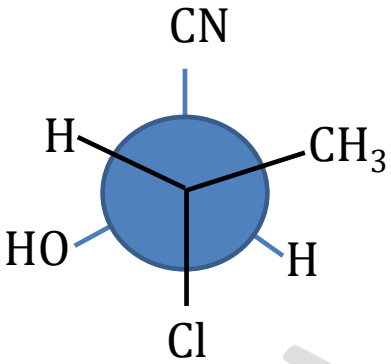
Flying-wedge projection



Saw-horse projection



Fischer projection



Newman projection

We can interconvert each structure into another.

In the next class we will discuss each projection and their inter conversion formula in detail.

That's all for today!

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1 April 2020 (updated on 8th April)

Detail discussion of the projection formulae

1. FLYING-WEDGE OR WEDGE-HASH PROJECTION FORMULA

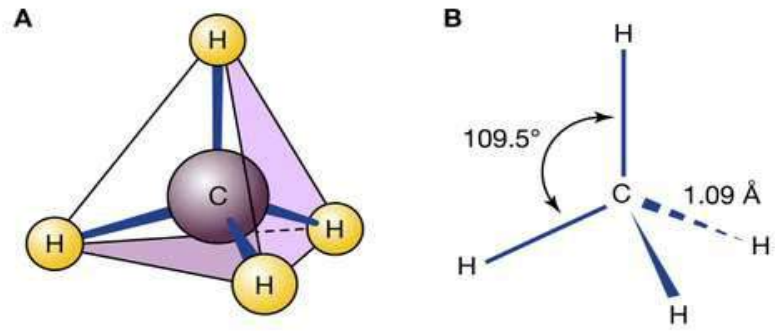
The Flying-Wedge projection is the most common three-dimensional representation of a three dimensional molecule on a two dimensional surface (paper). Tetrahedral structure (sp3 hybridized) needs to represent in 3D shape than sp^2 (e.g. alkenes) or sp systems (e.g. alkynes).

Wedge-hash (or wedge-dash) diagrams are usually drawn with two bonds in the plane of the page, one in front of the plane, and one behind the plane. This gives the molecule 3D perspective: we envisage the bold lines being closer to us and the hashes fading away in the background.

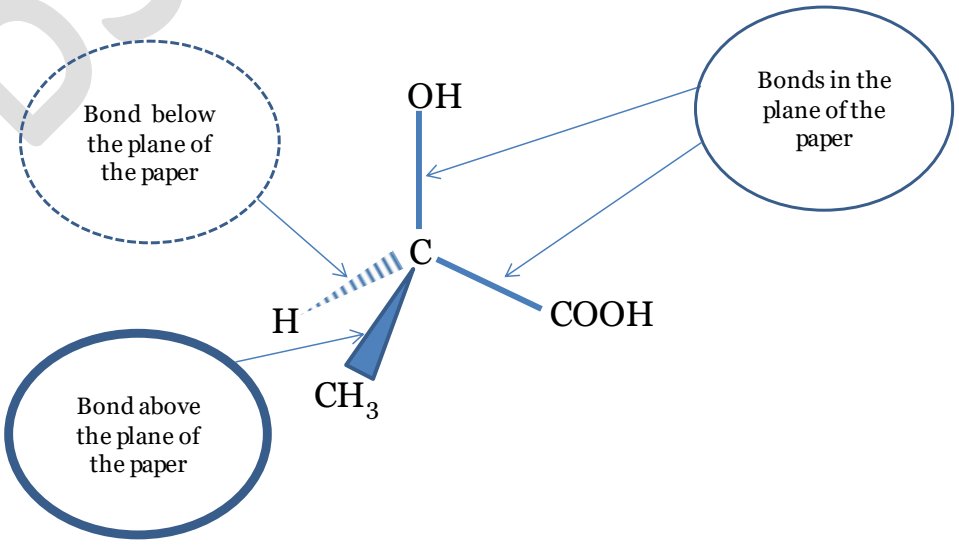
A solid Wedge ( ) represents a bond above the plane of the paper

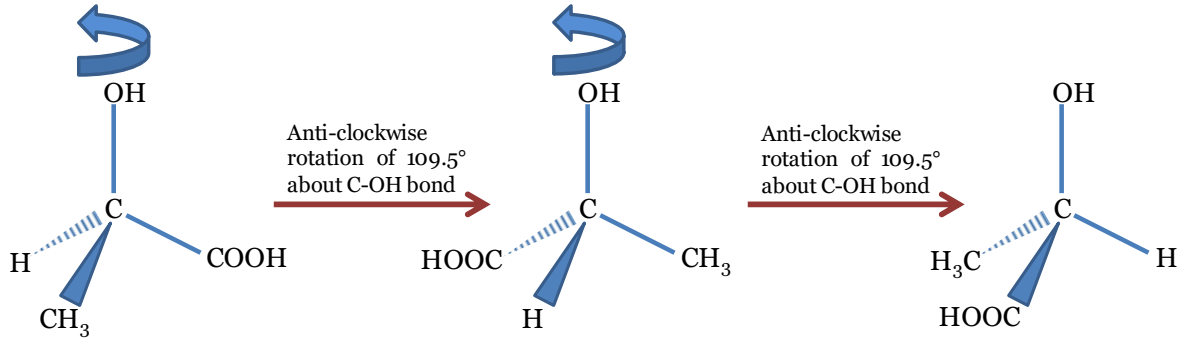
and a dashed wedge ( ) or a broken line (-----) represents a bond below the plane of the paper.

For example, methane (CH_4) has tetrahedral structure. It can be represent as follows-

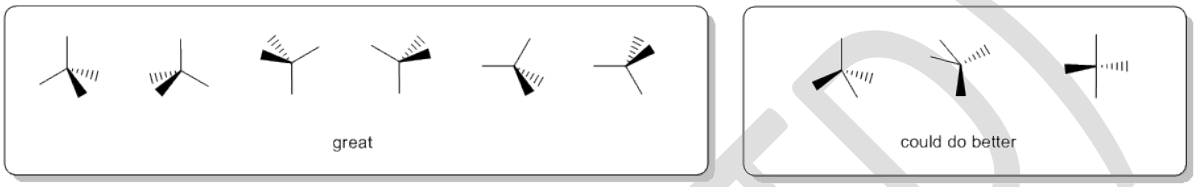


Flying wedge projection formula of (R)- Lactic acid can be shown as follows-





Above it is showing the rotation of the configuration to understand the 3D shape better.

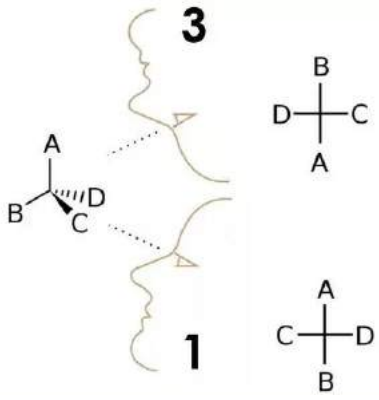


As a suggestion, they seem to be most effective when the "similar" pairs of bonds (2-in-plane, 2-out-of-plane) are next to each other, as shown in the left box above.

Remember that diagrams are being used to present the required information efficiently. Organic chemists use line diagrams to represent structures as part of the symbolic code because they are quicker and easier to draw as we can just leave out the C atoms and the H attached to those C atoms because we know to just assume that they are there. This idea also carries over into wedge-hash diagrams. A common scenario is shown below where the bond to an H has been omitted and it is assumed that we know that it is there.

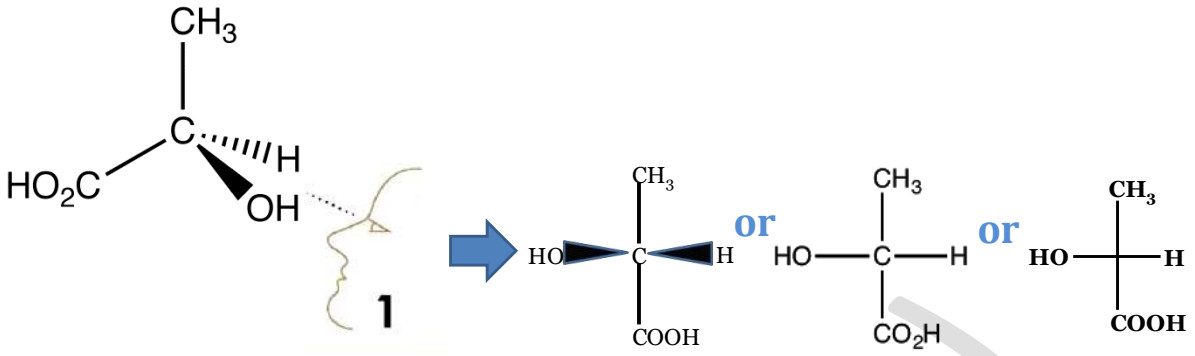
2. FISCHER PROJECTION FORMULA

The Fischer projection formula was devised by Emil Fischer in 1891.



In this projection formula the carbon chain is projected vertically. The horizontal bonds attached to a carbon are considered to be above the plane of the paper and towards the viewer

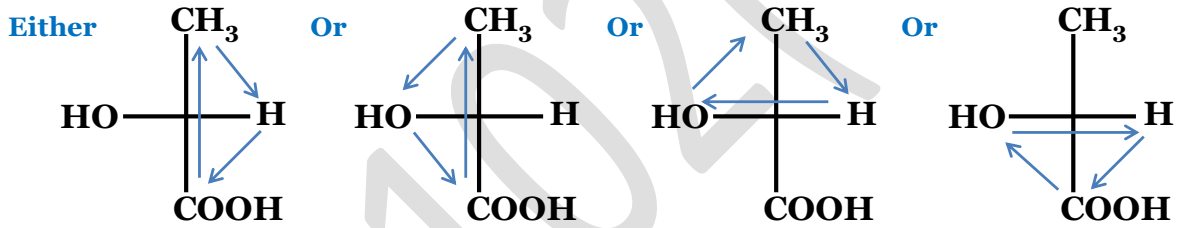
and the vertical bonds are considered to be below the plane of the paper and at the back of viewer.



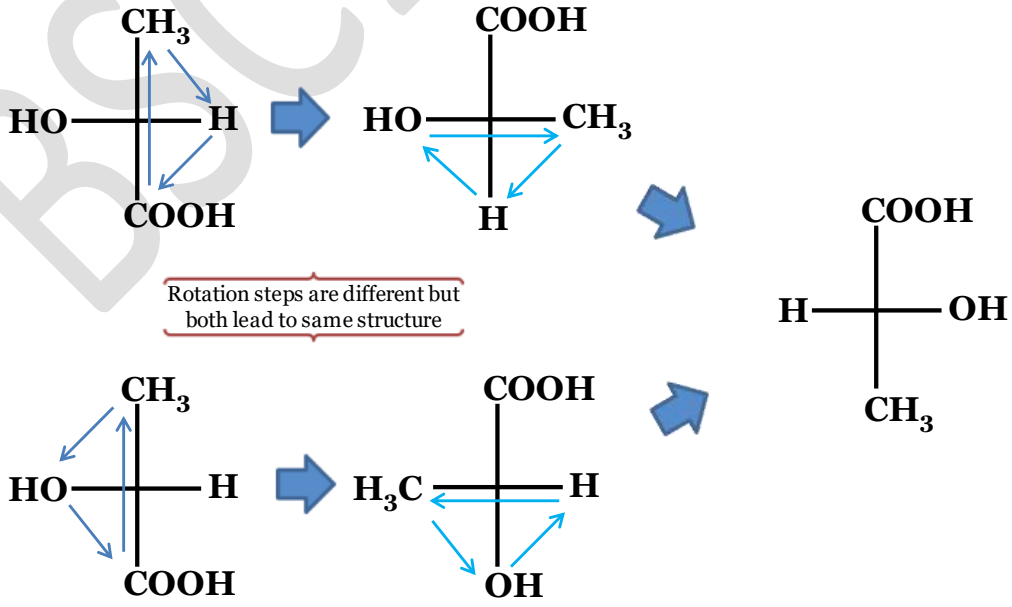
Extra Note:

Note that Fischer projections are typically drawn with the longest chain oriented vertically and with the more highly oxidised C (Carbon) at the top.

So the above structure of (R)- Lactic acid is not fully correct. We can rearrange the position of the groups. This rearrangement process should follow a rule. That rule to interchange or rearrange the groups is by completing the triangular motion of positions (clockwise or anti clockwise) as shown below.



We can choose any of these which will lead the configuration with more highly oxidised carbon at the top and the longest chain oriented vertically.



As this is a simple structure (with one chiral centre), we could just rotate the structure 180° keeping the entire structure in plane of paper.

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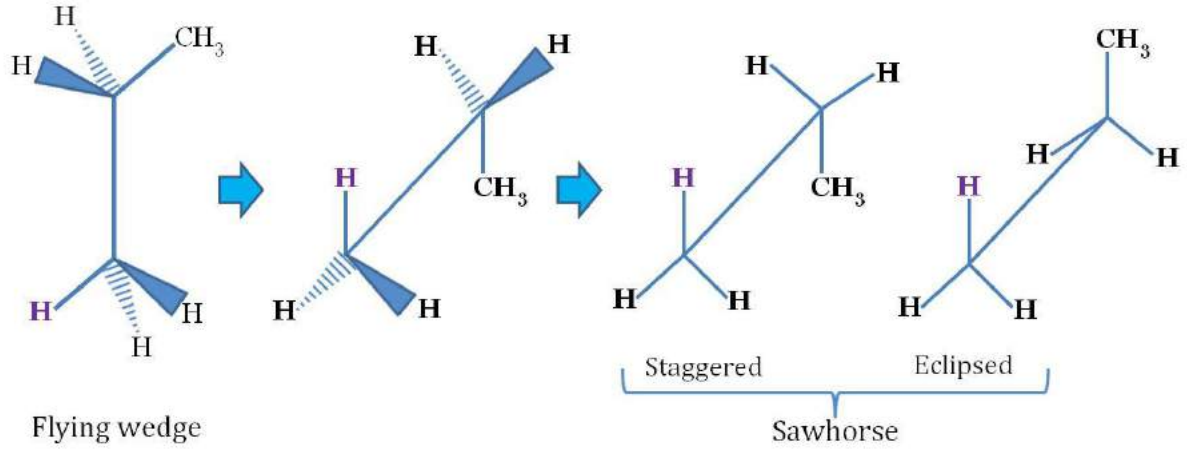
2 April 2020

Detail discussion of the projection formulae

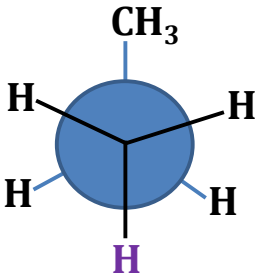
3. SAWHORSE PROJECTION FORMULA

In this representation, the molecule is viewed slightly from above and from the right and then projected on the paper. The bond between the two carbon atoms is drawn diagonally and of a relatively greater length for the sake of clarity. The lower left hand carbon is taken as the front carbon and the upper right hand carbon as the back carbon. All parallel bonds in sawhorse formula are Eclipsed and all anti parallel bonds are opposite or trans/anti to each other. The sawhorse presentation of Eclipsed and staggered conformations of propane are shown below.

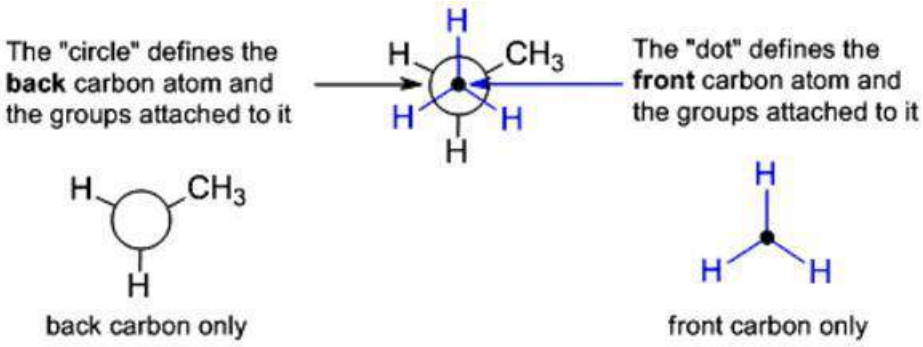
Sawhorse diagrams are similar to wedge-dash diagrams, but without trying to use "shading" to denote the perspective. The representation of propane shown below has been drawn so that we are looking at the molecule which is below us and to our left.



4. NEWMAN PROJECTION FORMULA



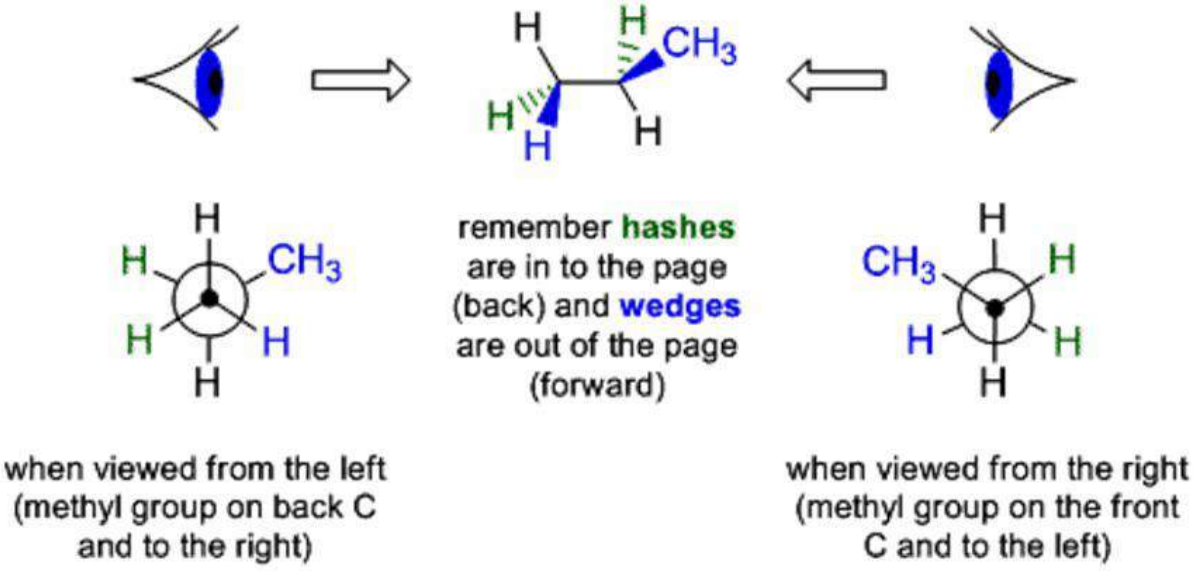
Newman projections are drawn by looking directly along a particular bond in the system (here a C-C bond) and arranging the substituents so that they are equally spaced around the atoms at each end of that bond. The protocol requires that the atoms within the central bond are shown as a dot and circle as defined below. Think of them as an end on view of a particular bond and the showing the arrangement of the groups around that bond.



In order to draw a Newman projection from a wedge-dash diagram, it is useful to imagine putting your "eye" in line with the central bond in order to look along it.

Let's work through an example, consider drawing a Newman projection by looking at the following wedge-dash diagram of propane from the left hand side.

- First draw the dot and circle to represent the front and back C respectively
- Since the front carbon atom has an **H** atom in the plane of the page pointing up we can add that first
- The back carbon atom has an **H** atom in the plane of the page pointing down
- Now add the other bonds to each C so that it is symmetrical
- The groups / bonds (**blue**) that were forward of the plane of the page in the original wedge-dash diagram are now to our right
- Those behind (**green**) the plane are now to our left



- Now you try the same thing, but looking from the right to generate the other Newman projection.

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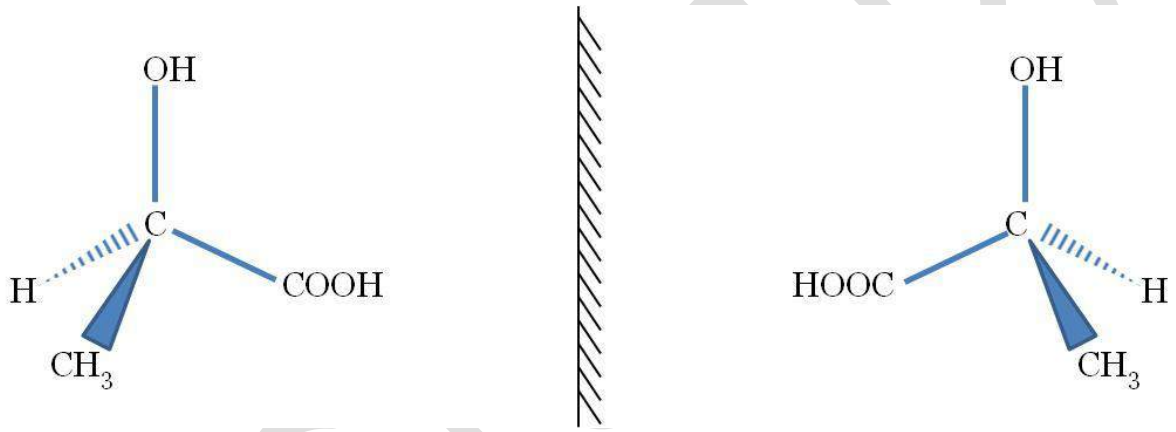
All the discussion we are doing is about organic molecules. Organic molecules and coordination complex molecules are not similar. Organic molecules have covalent character mostly, whereas inorganic complex salts (or simple salts) are ionic in nature. Properties of organic molecules are very much sensitive to three dimensional structures. I can give you an interesting example on that. Milk contains milk sugar, which is called (+)-lactose. The taste of (+)-lactose is sweet. But its mirror image structure compound, (-)-lactose is not sweet in taste and also harmful for our health. Is not it interesting? You may think that the following compounds are mirror image to each other and they are same. But it is not true.

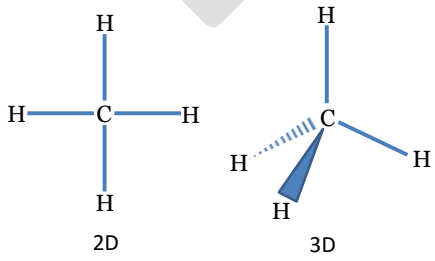


Now, we will enter little details of these three dimensional structures. Any three dimensional structure is described by configuration and conformation.

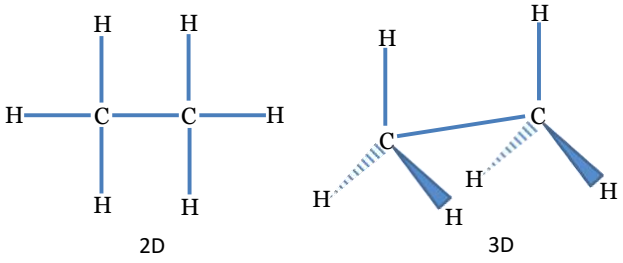
What is Configuration?

Configuration of an organic molecule represents an exact three dimensional arrangements of all the atoms in that molecule with respect to each other.

e.g.; methane (CH_4) and ethane (C_6H_6) have following configurations in three dimensions respectively.



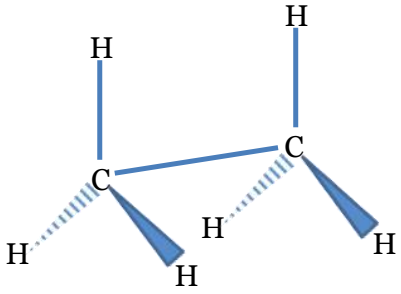
Methane (CH_4)



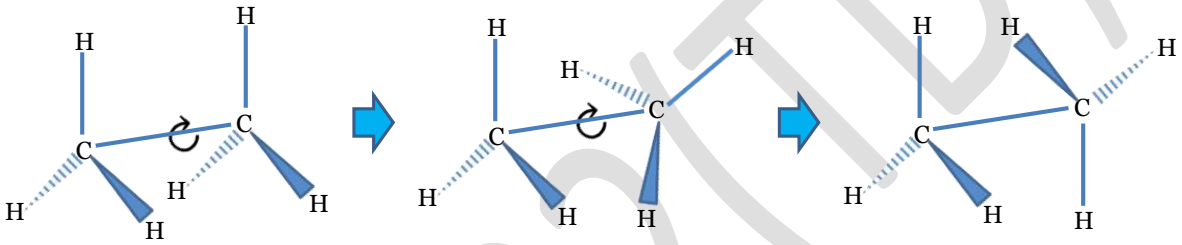
Ethane (C_2H_6)

Conformation: Conformation can be discussed only for those organic molecules which posses at least two carbon atoms are directly attached to each other.

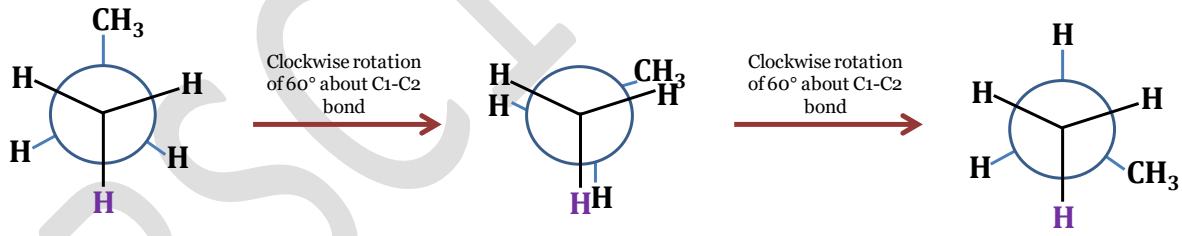
Let us take the example of ethane (C_2H_6).



It has been observed that the entire molecule of ethane can undergo different structural arrangements just by C-C single bond rotation.



These different structural arrangements which obtained as a result of free rotation around C-C single bond are called different conformations of that molecule. All these conformers have different energy to each other. It is easy to represent different conformers in Newman projection formula.



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5 April 2020

All the

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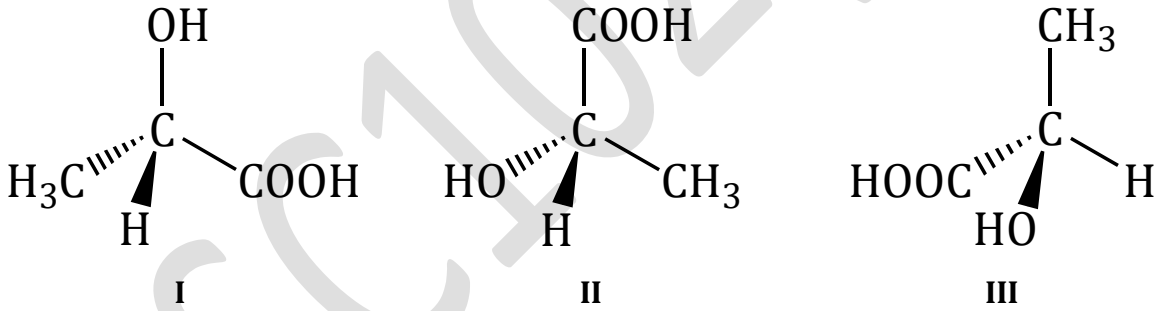
8 April 2020

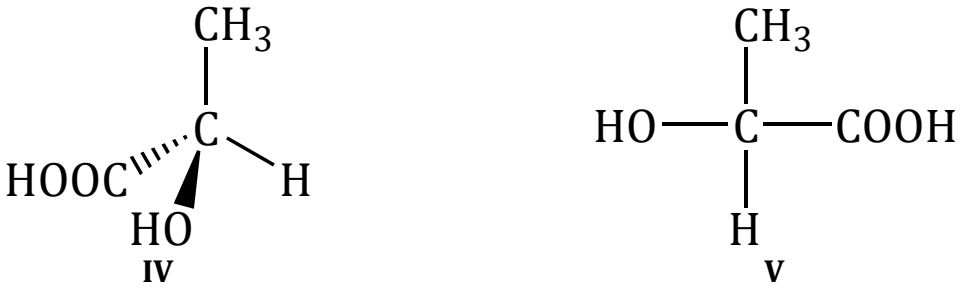
An absolute configuration refers to the relative arrangement of the atoms/groups of a molecule (mainly chiral) in three dimensions in precise way and its stereochemical description (e.g. R or S). Now how do you know that whether I, II, III are same or different molecules?



I **II** **III**

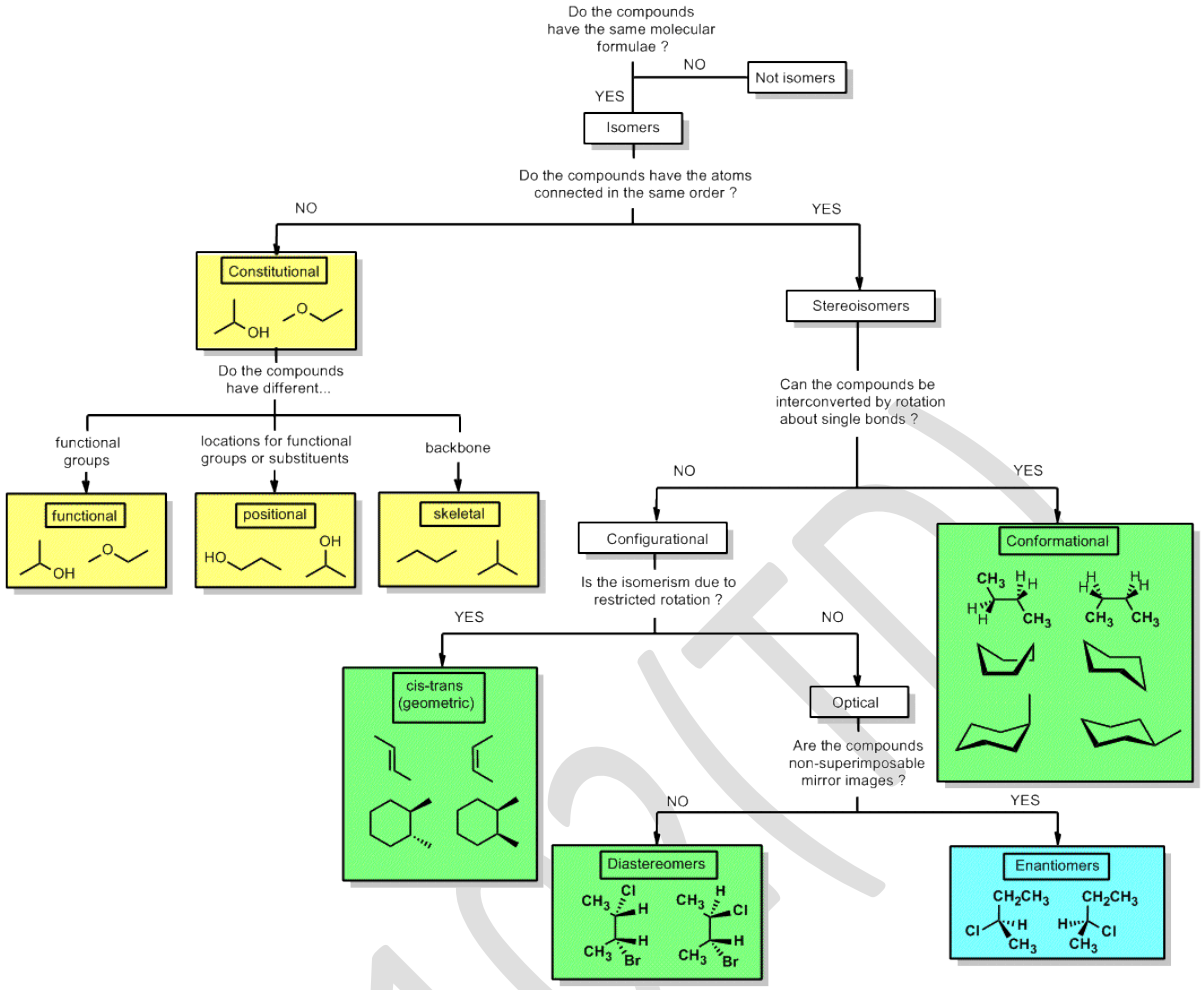
The answer is absolute configuration. Here, I and II are same molecule unlike III. Because when you will determine the stereochemical notation then you will find that I & II have 'S' and III has 'R' notation. We can view a molecule from different angles, but its absolute configuration will not change for that.

Again, what is the relation between IV and V? Their absolute configuration will help you for this.



IV **V**

Answer is they are enantiomer to each other.


Do the compounds have the same molecular formulae ?
NO
Not isomers
YES
Isomers
Do the compounds have the atoms connected in the same order ?
NO
YES
Constitutional
Stereoisomers
Do the compounds have different...
functional groups
locations for functional groups or substituents
backbone
functional
positional
skeletal
Can the compounds be interconverted by rotation about single bonds ?
NO
YES
Configurational
Conformational
Is the isomerism due to restricted rotation ?
YES
NO
cis-trans (geometric)
Optical
Are the compounds non-superimposable mirror images ?
NO
YES
Diastereomers
Enantiomers