STEREOCHEMISTRY

Representation of molecules:

Generally molecules have a definite geometry in three dimensional spaces. It is very difficult and inconvenient to represent the three dimensional molecules in two dimensions of paper and blackboard. Therefore, several two-dimensional projection formulas have been developed to represent molecules having three-dimensional structures.

Formulas used to represent molecules having three-dimensional structures on a two-dimensional surface (paper or blackboard) are called projection formulas.

The important projection formulas that are used to represent chiral or achiral molecule are (i) flying-wedge formula (representation) (ii) Newman projection formula, (iii) sawhorse projection formula, (iv) Fischer projection formula, and (v) zigzag projection formula.

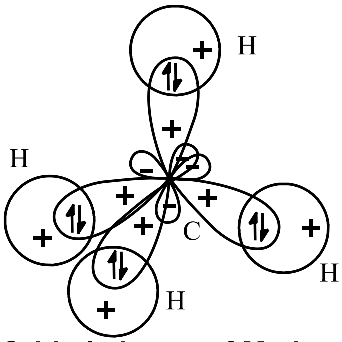
Orbital picture and structure of some simple organic molecules

Methane (CH_4)

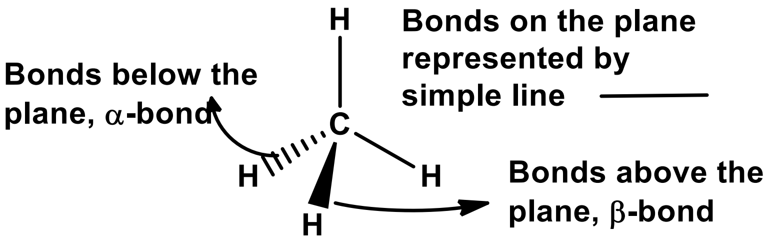
(i) All bonds are σ-bonds, central C-atom has 4 pair valence electrons in methane (4 electrons form C-atom and 4 electrons form four H-atoms)

(ii) The central C-atom is sp^3 hybridised.

(iii) The orbitals are directed in three dimensional spaces. So two orbitals remain on the plane of the paper, one above and another beyond the plane.



Orbital picture of Methane

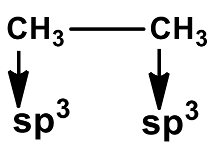


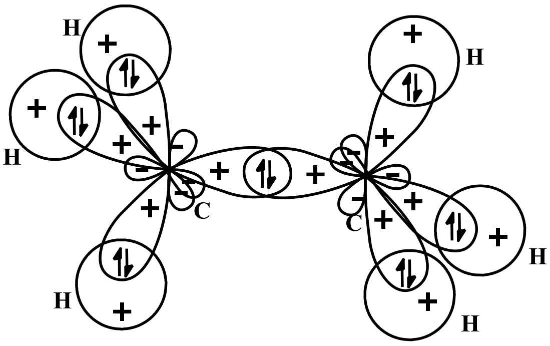
Structure of Methane

(iv) The bonds on the plane is depicted by simple line(—), above the plane by bold line (▬ or ▬) and below the plane by (''''''''||| or ------ line)

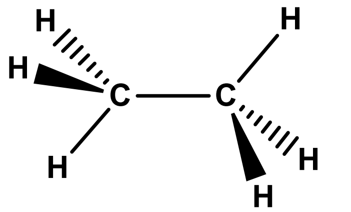
(v) above the plane bond (▬ or ▬) is called **β-bond** and below the plane is called (''''''''||| or ------ line) **α-bond**.

Ethane ($H_3C—CH_3$)





Orbital picture of Ethane

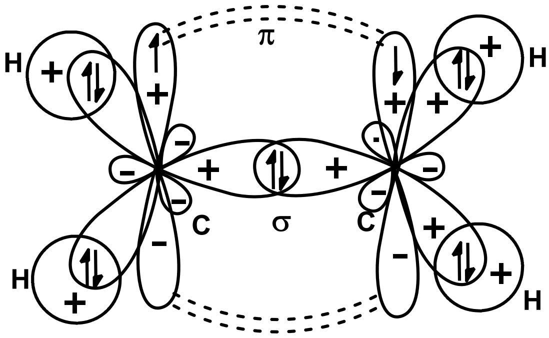


Structure of Ethane

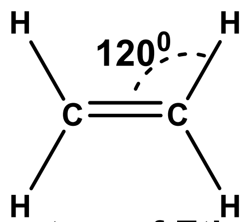
Ethylene ($H_2C{=}CH_2$):

(i) The two C─atoms are bonded together by **one σ-bond** and **one π-bond** so they are sp^2 hybridised.

(ii) The molecule is planar; all atoms remain in a plane.



Orbital picture of Ethylene

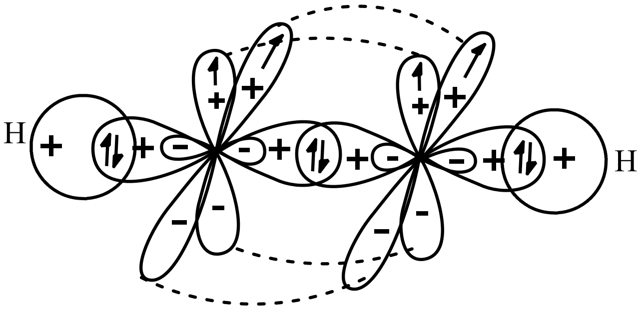


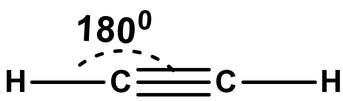
Structure of Ethylene
The molecule is planar
due to sp^2 hybridisation

Acetylene: (H─C≡C─H):

(i) The two carbon atoms are joined by **one σ-bond and two π-bonds**, so they are **sp-hybridised.**

(ii) The molecule is linear.





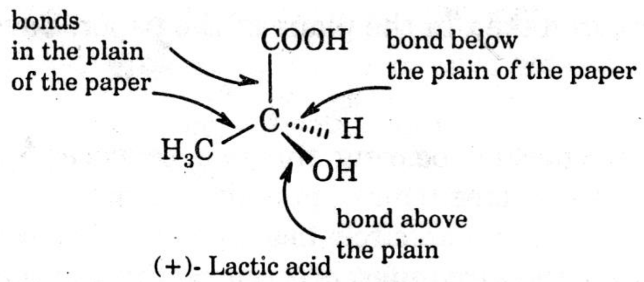
Structure of Acetylene

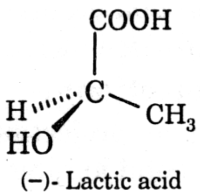
Flying wedge formula or three-dimensional representation:

In this representation :

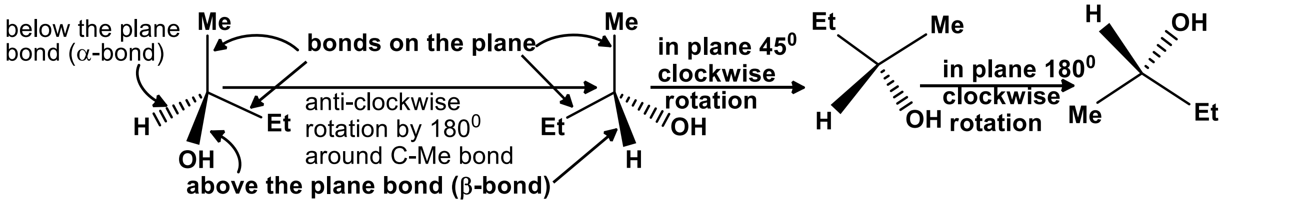
1. generally the C—C—C chain is drown on the plane of the paper
2. the molecule is viewed perpendicular to the C—C—C chain.
3. bonds lying on the plane of the paper are represented by **normal lines (—)**
4. bond above the plane (of paper) is usually shown by **solid wedge** (▬) is known as **β-bond**
5. bond below the plane (of paper) is usually shown by **hashed wedge (''''''''') or a broken line (- - -)** is known as **α-bond.**

Example:

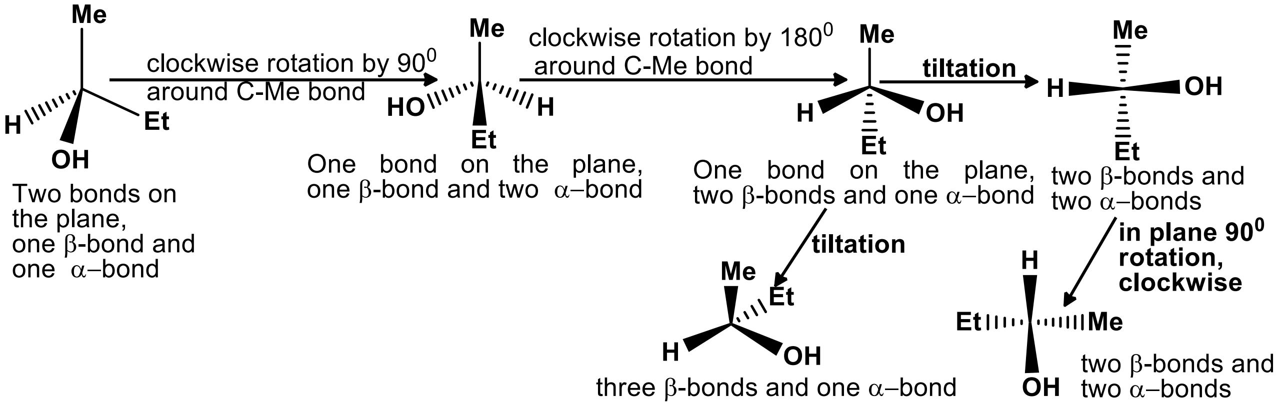




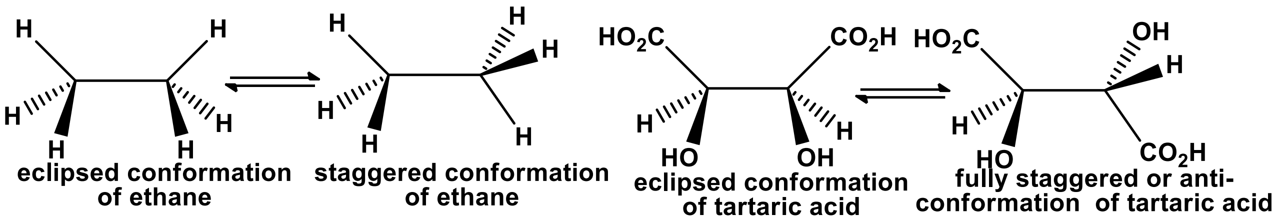
The different three dimensional orientations of bonds attached with the (central) key carbon atom of a tetrahedral molecule are as follows—



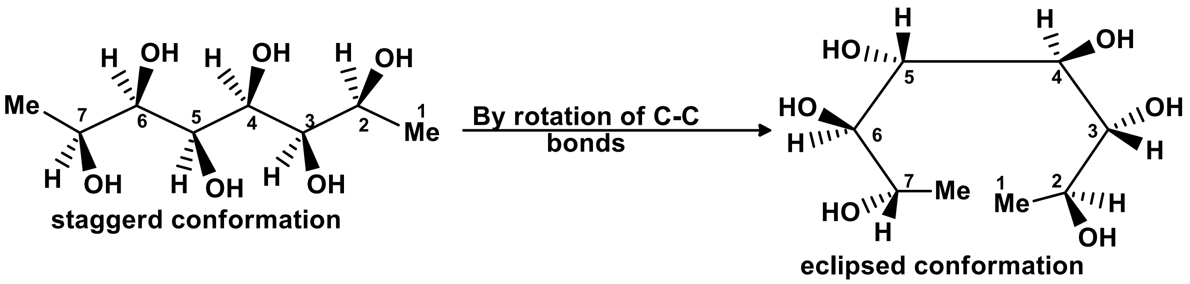
Two bonds on the plane (of paper), one bond above the plane (β–bond) and other below the plane α–bond)



Two carbon system:

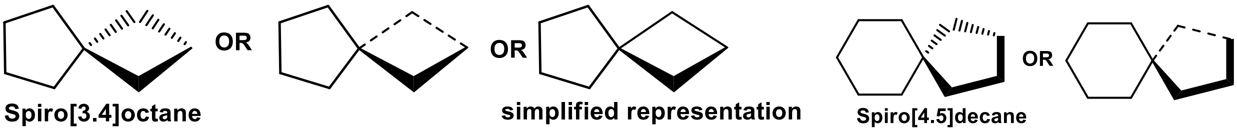


Multi carbon chain system:



6. In case of ring compound, the ring is drawn on the plane of the paper and the α-and β-bonds are drawn by hashed wedge and solid wedge respectively

7. In case of spiro compound, the two perpendicular rings are joined with a sp3 carbon atom so one ring is drawn on the plane of the paper and other is represented by solid and hashed wedge.

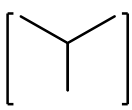
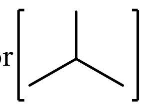


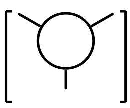
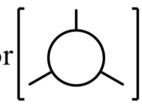
Newman projection formula:

1. This formula represents the relative position of groups of two adjacent carbon in two dimensional plane.

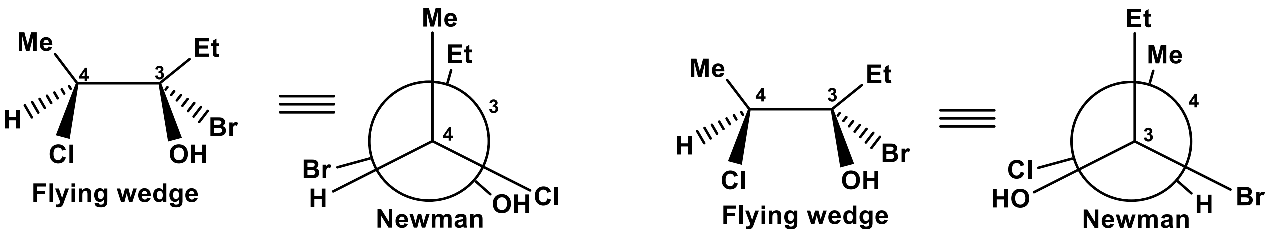
2. The molecule is viewed along the C—C bond (joining the key atoms) from one end of the molecule.

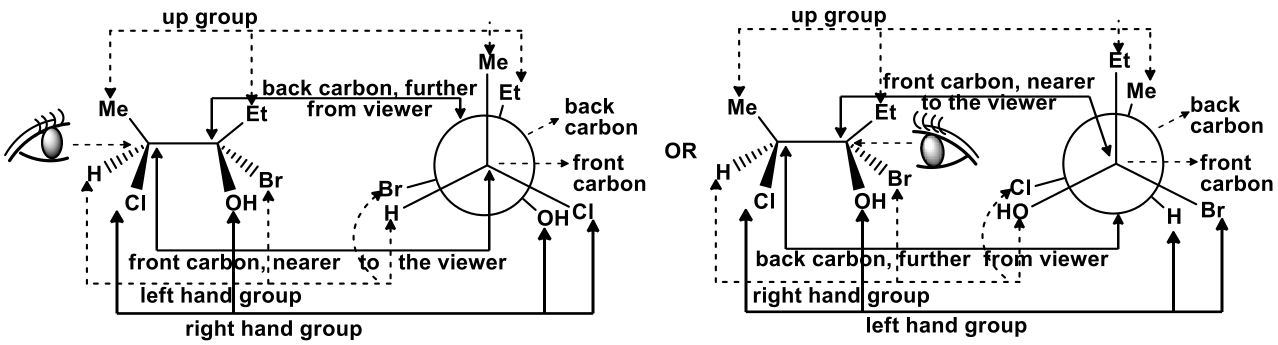
3. The back carbon atom is represented by a **circle** and the front carbon atom is depicted by a **point** at the centre of the circle.

4. The three bonds attached to the front carbon appear like  or 
The angle between two bonds is 120^0

5. The three bonds attached to the back carbon appear like  or 
The angle between two bonds is 120^0

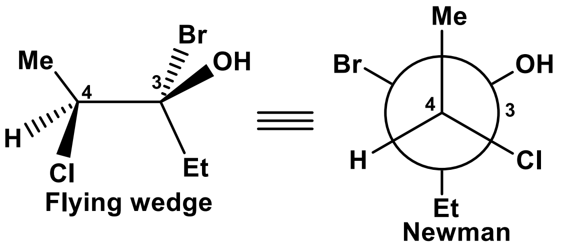
6. It is a graphic three dimensional perspective picture.



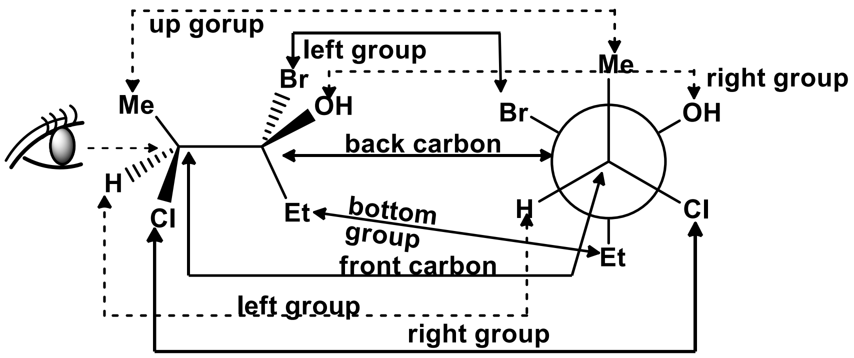


From the above correlation, we can interconvert (eclipsed conformation) Flying wedge to Newman projection formula and vice-versa.

In case of staggered conformation the following correlation can be made—



Staggered confromation



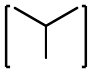
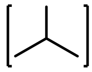
Sawhorse formula:

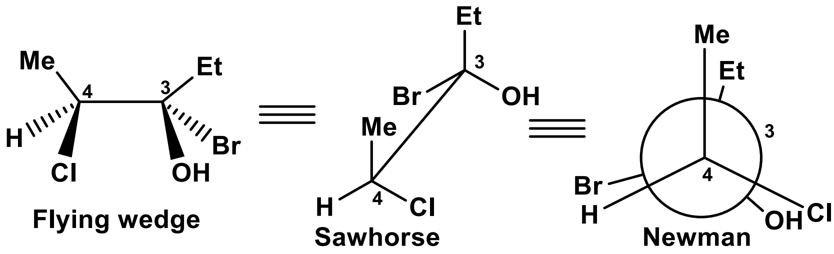
1. The molecule is viewed **laterally**.

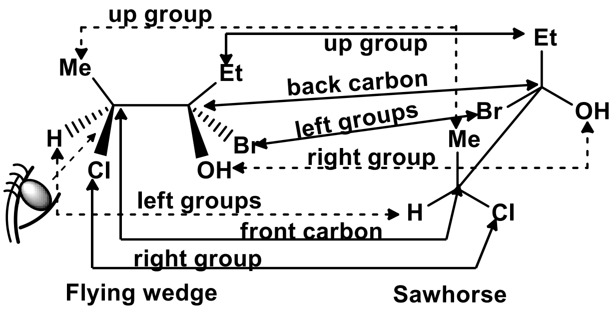
2. The molecule is kept in a **tilted manner** so that the midpoint of the bond joining the key (carbon) atoms lie on the projection plane (plane of the paper).

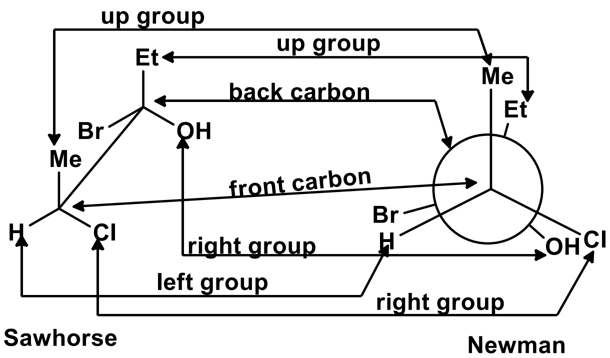
One half around the midpoint lies above and the other half below the plane of projection in oblique fashion.

3. The projection of the central bond generally (but not always) makes an angle of ~22.5° with the horizontal line.

4. The three bonds attached to the front and back carbon appear like  or 
The angle between two bonds is 120^0



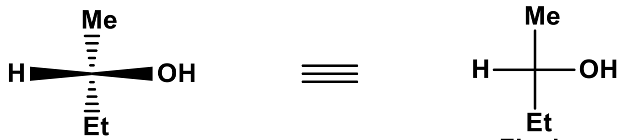




From the above correlation, we can interconvert Flying wedge to sawhorse to Newman projection and vice-versa.

Fischer projection formula:

1. It is a two dimensional projection of a particularly oriented three dimensional arrangement. The particular three dimensional arrangements is as follows—



Three dimensional Flying wedge formula, where two horizontal bonds are above the plane (β-bonds) and two vertical bonds are below the plane (α-bonds)

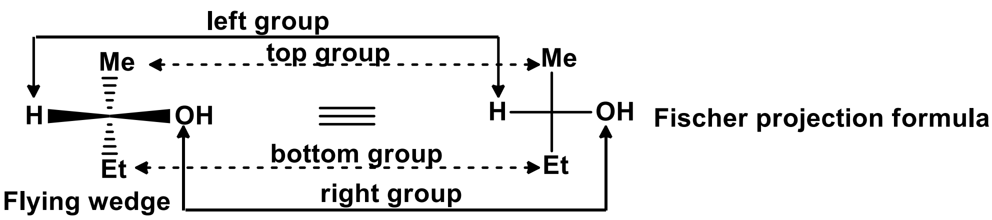
Fischer projection formula

2. The four single bonds around the central atom are represented as a large 'plus' (+) sign.

3. The vertical (top and bottom) bonds represent bonds **below the plane** of paper (away from the viewer)

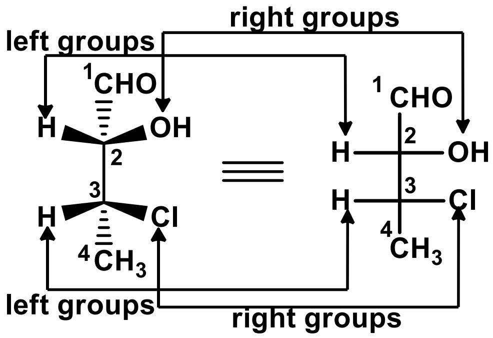
4. The horizontal bonds represent **above the plane** of paper (towards the viewer).

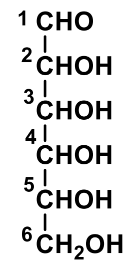
5. The central atom is placed on the projection plane (plane of paper).



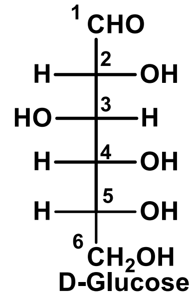
6. In case of multi carbon compounds, the main C—C chain is represented by a vertical line from top to bottom. Horizontal lines represent bonds pointing towards the viewer. The key carbon atoms lie at the point of intersection (junction) of vertical and horizontal lines.

7. Fischer projection always represents **eclipsed conformation** of the molecule.





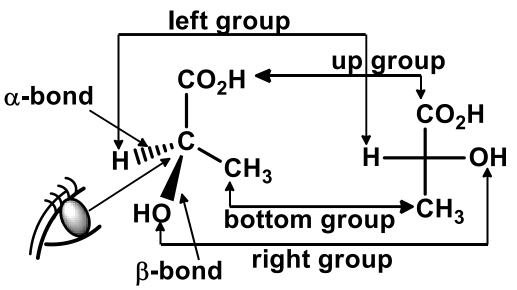
Gross formula of glucose

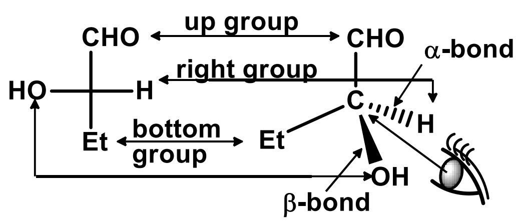


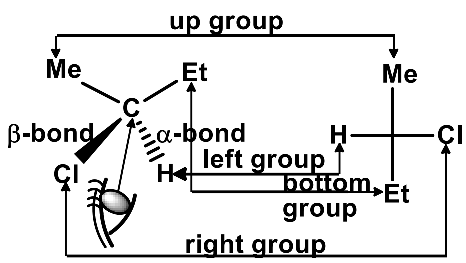
D-Glucose (Fischer projection)

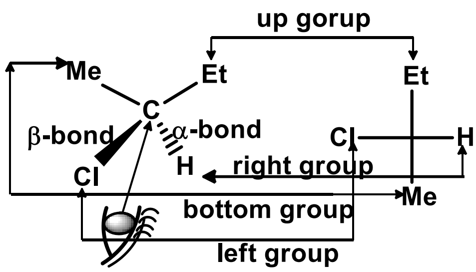
Simplified method for Flying wedge to Fischer inter conversion:

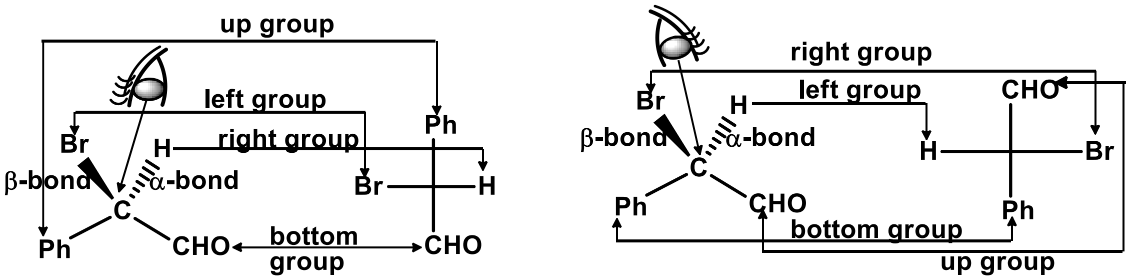
1. Look at the key (central) carbon atom in between α- and β- bond if there is one α– and one β–bond write the left, right, up and down groups what you are observing, to the Fischer projection formula.



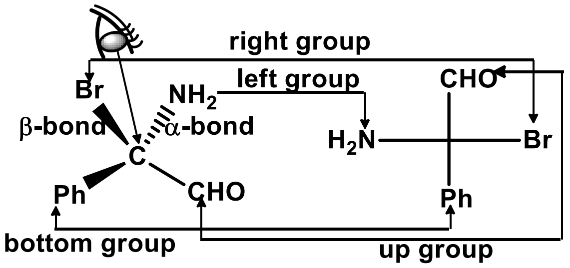


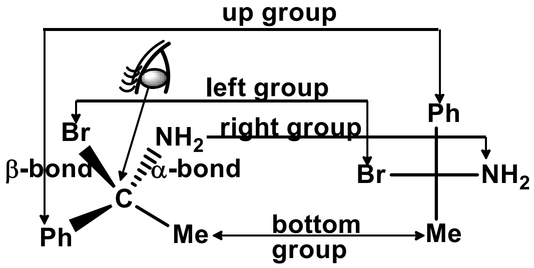




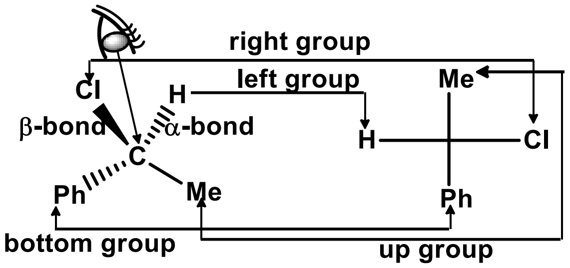


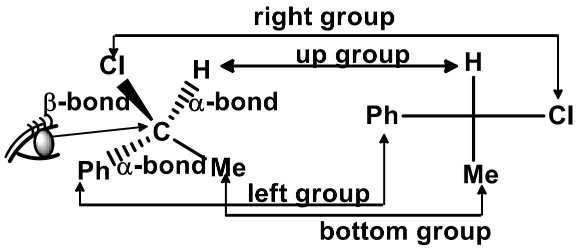
For molecule with two β- bonds:



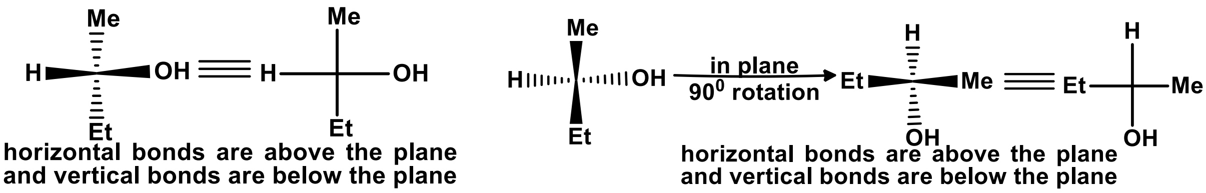


For molecule with two α-bonds:

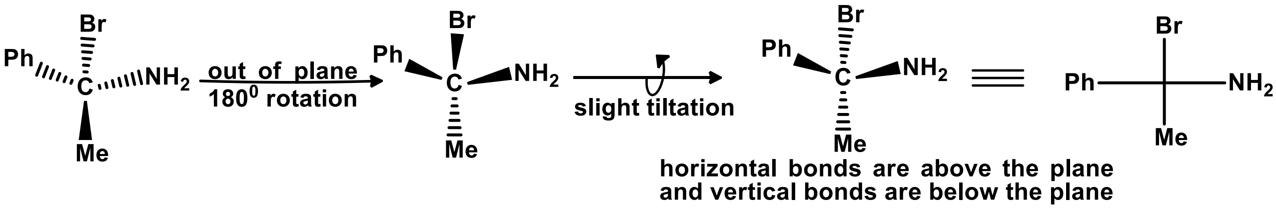




For molecule with two β-and two α-bonds:

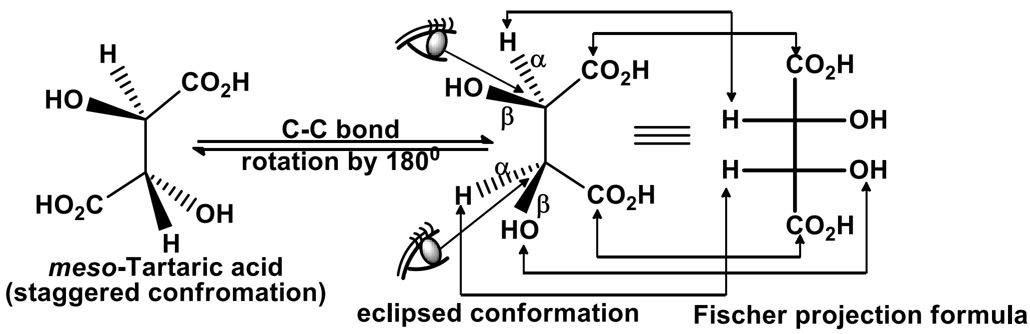


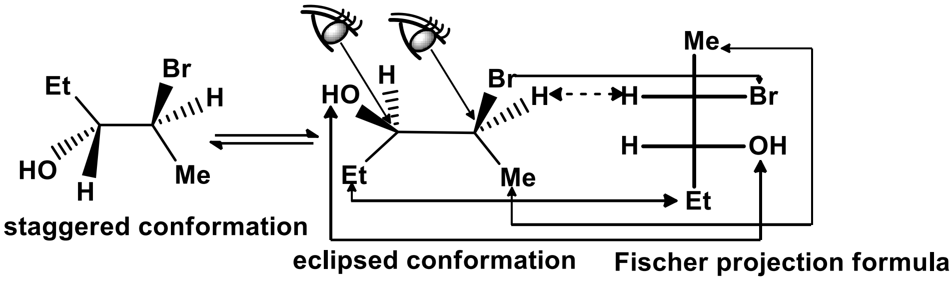
For molecule with three β-or three α-bonds:

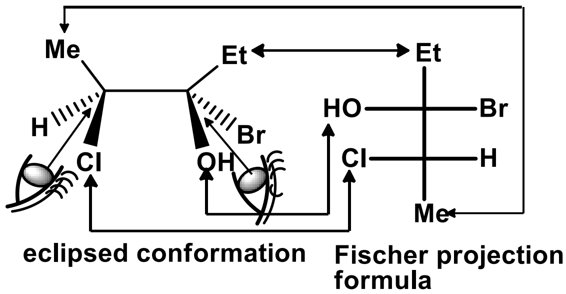


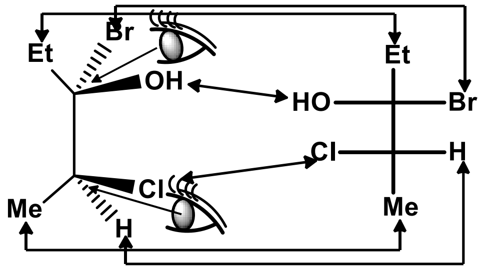
In the reverse way we can convert the Fischer projection to flying wedge formula.

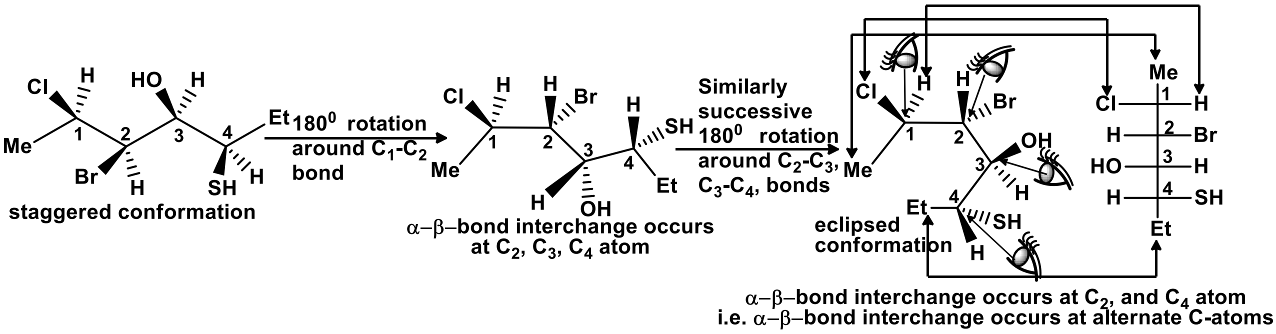
2. Fischer projection formula always represents the eclipsed conformation of the molecule. So first we should convert a staggered conformation to eclipsed by C—C bond rotation and then we should look at each key carbon centre one by one and write accordingly in Fischer projection formula.





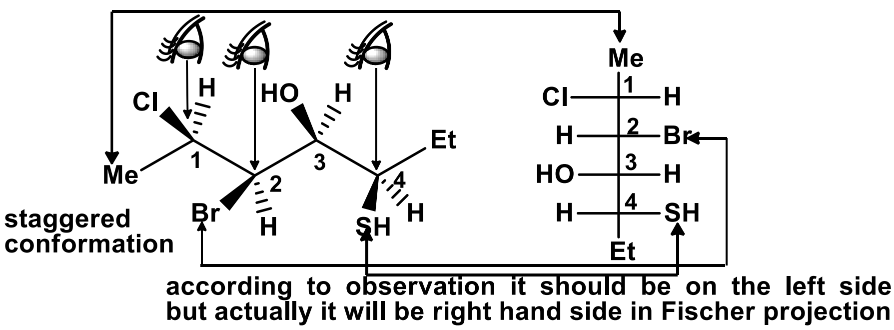




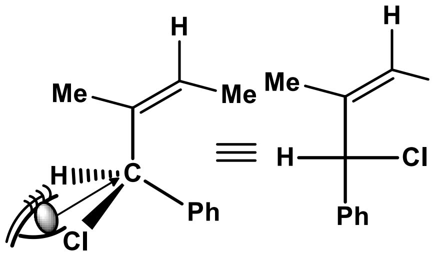


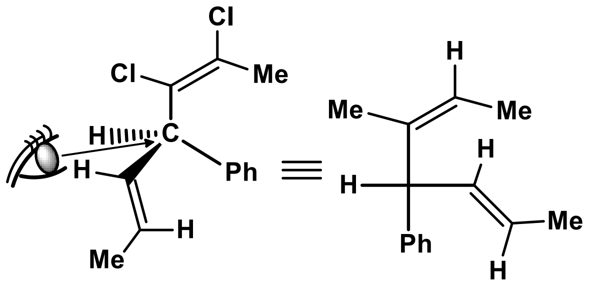
It is found that during transformation of a staggered conformation to eclipsed conformation the α– and β-bonds are interchanged at alternate C-atoms. If this α– β-bond interchange occurs at C_2 then it will also occurs at C_4, C_6, C_8 ….. etc.

So we can directly convert a staggered flying wedge formula to Fischer projection formula without converting it to eclipsed conformation. In this case we will write the opposite groups in left and right group in Fischer projection formula at alternate C-atom.

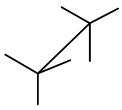


Fischer projection with groups with C=C



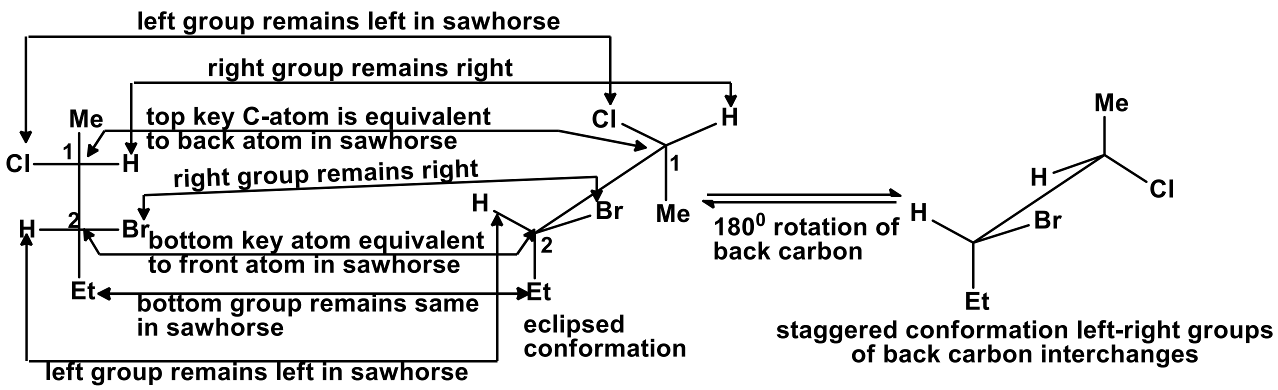


Fischer to sawhorse interconversion an vice-versa:

1. As Fischer projection always represents the eclipsed conformation so first draw the bonds in sawhorse as the following (Y—Y) from 

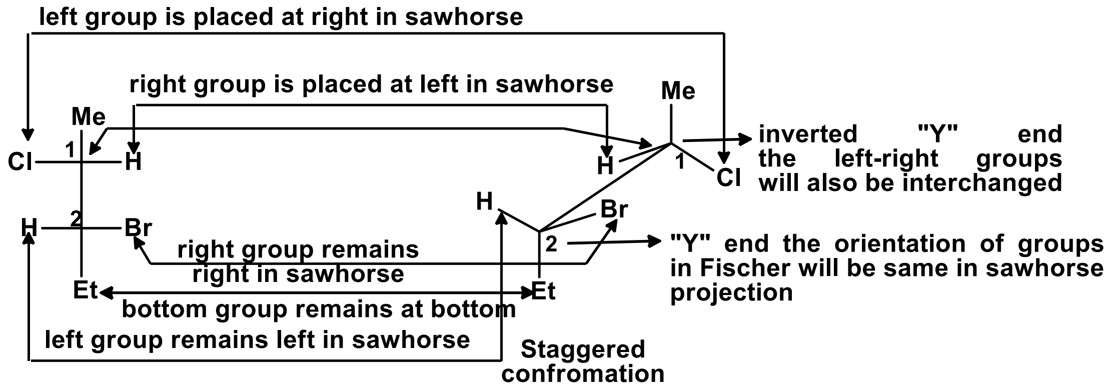
2. The bottom key carbon of Fischer projection is represented by the front carbon atom in sawhorse projection and the top carbon is equivalent to the back carbon in sawhorse.

3. The left right bonds Fischer projection remains same (left, right) in sawhorse projection.

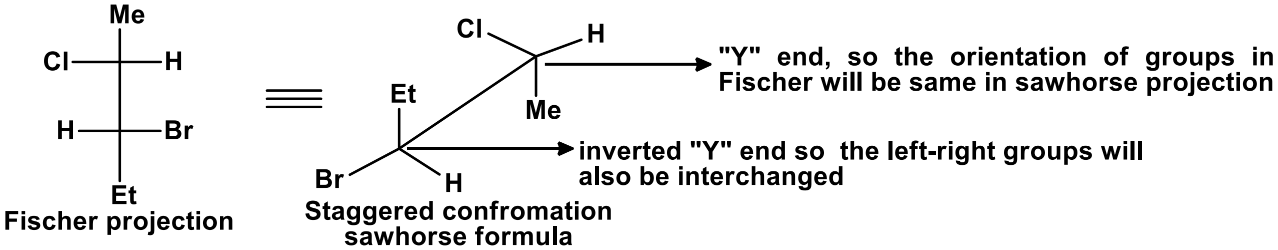


4. We can convert the Fischer projection to staggered form of sawhorse in that case one end group will be (Y) form and other end group will be inverted (Y) i.e. 

During conversion from Fischer to sawhorse, the left-right group of the "Y" end will remain same but in inverted "Y" end will be reverse i.e left group of Fischer projection will be right group in sawhorse and the right group will be left in sawhorse.



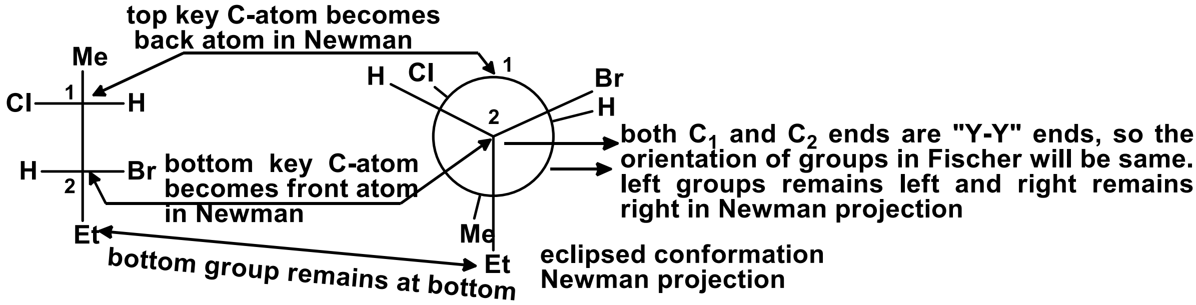
By the same way—



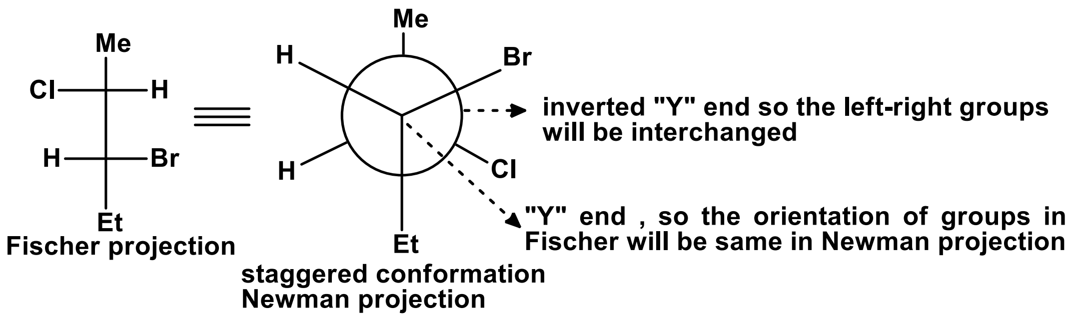
By the reverse way we can convert sawhorse formula to Fischer projection formula.

Fischer projection to Newman projection formula:

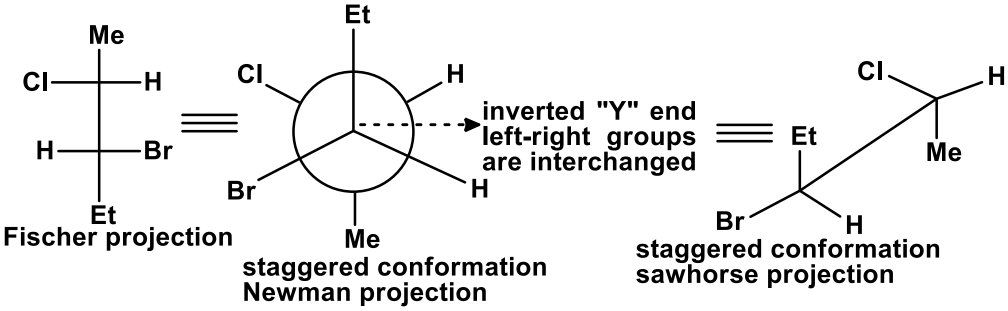
1. Fischer projection to Newman inter conversion follows the same procedure as Fischer to sawhorse.



We can convert Fischer to Newman projection in staggered conformation directly—

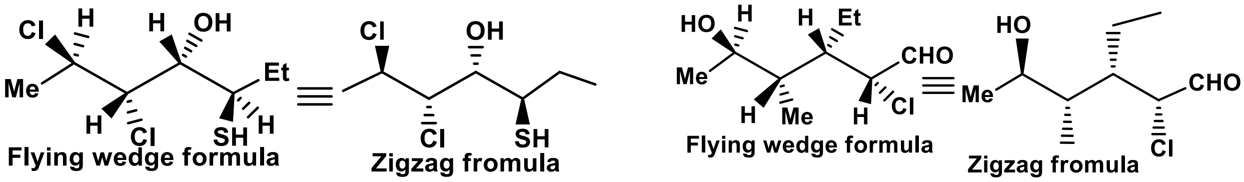


In the reverse procedure we can convert Newman to Fischer projection.



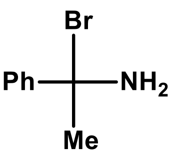
Zigzag formula:

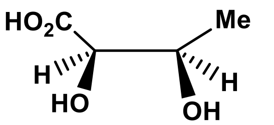
1. It is applicable for compound containing two or more carbon centres
2. It is always shown in staggered conformation.
3. The C—C chain is placed in the plane of the paper.
4. The H-atoms are assumed to be in the structure but is not drawn in the formula
5. The bonds above and below the plane are shown by solid wedge and hashed wedge respectively.
6. The C-atoms in C—C chain are not shown, each junction of bonds and end of bond represents carbon atoms with requisite number of H atoms attached with them.

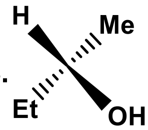


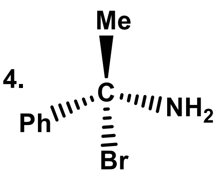
Problems: Representation of molecules:

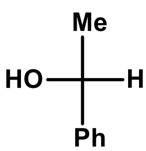
Write the Flying wedge, Fischer projection, Newman projection and sawhorse projection formula of the following molecules (whatever it is applicable)

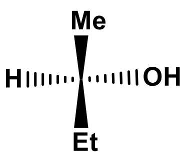
1. 

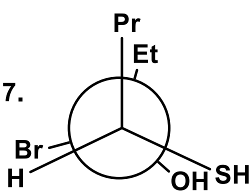
2. 

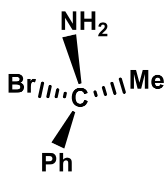
3. 

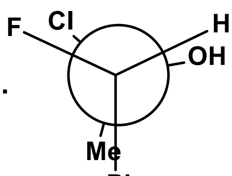
4. 

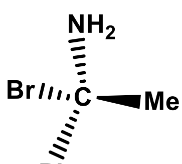
5. 

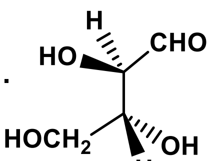
6. 

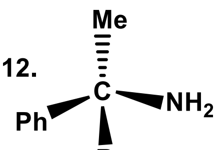
7. 

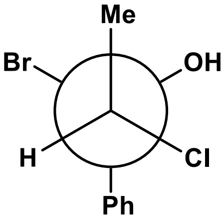
8. 

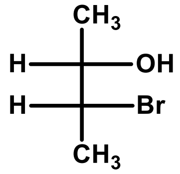
9. 

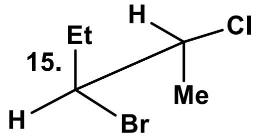
10. 

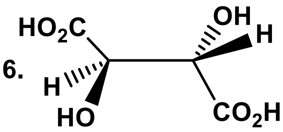
11. 

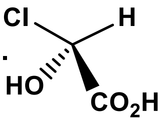
12. 

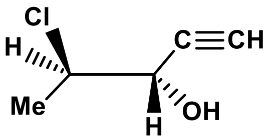
13. 

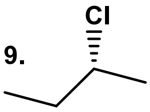
14. 

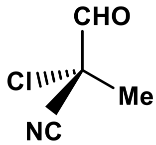
15. 

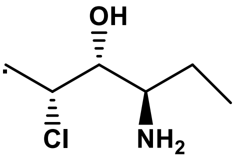
16. 

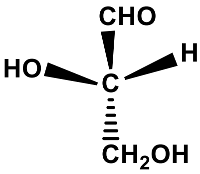
17. 

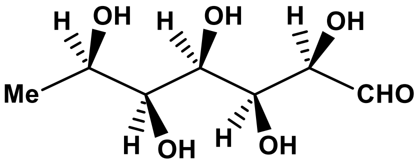
18. 

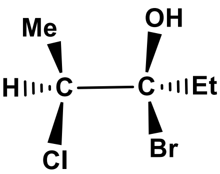
19. 

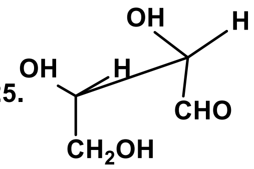
20. 

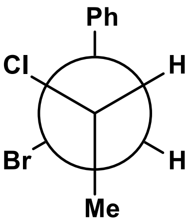
21. 

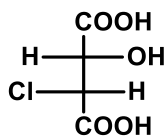
22. 

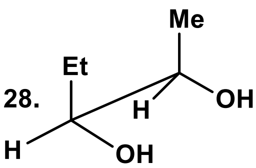
23. 

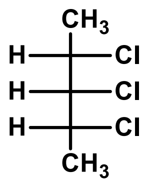
24. 

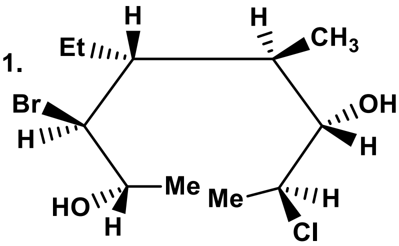
25. 

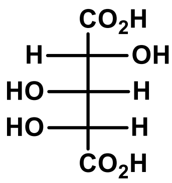
26. 

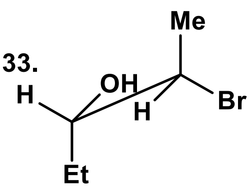
27. 

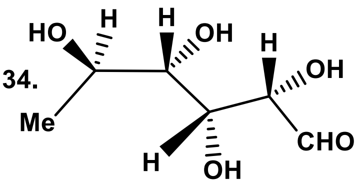
28. 

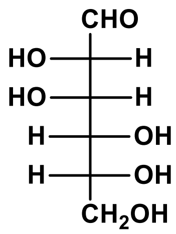
30. 

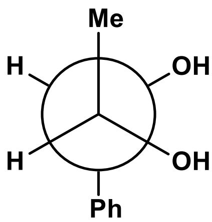
31. 

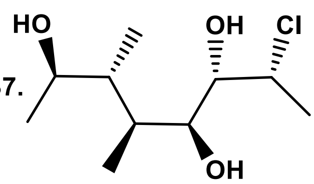
32. 

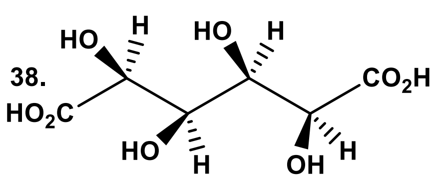
33. 

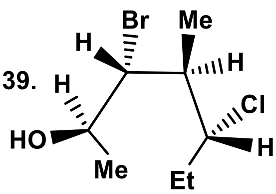
34. 

35. 

36. 

37. 

38. 

39. 

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