Symmetry, Stereochemistry and Applications
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Lecture - 10
Conformations and Configurations

Welcome back to the course entitled Symmetry, Stereochemistry and Applications. In the initial few lectures, we have discussed about nomenclature of organic compounds, symmetry elements and point groups that can be derived for different small organic and organometallic, complexes. So, with that brief introduction to the molecules and symmetry nomenclature, today, we would like to start discussing about the second part of the course where we will talk about the conformational analysis of organic molecules.

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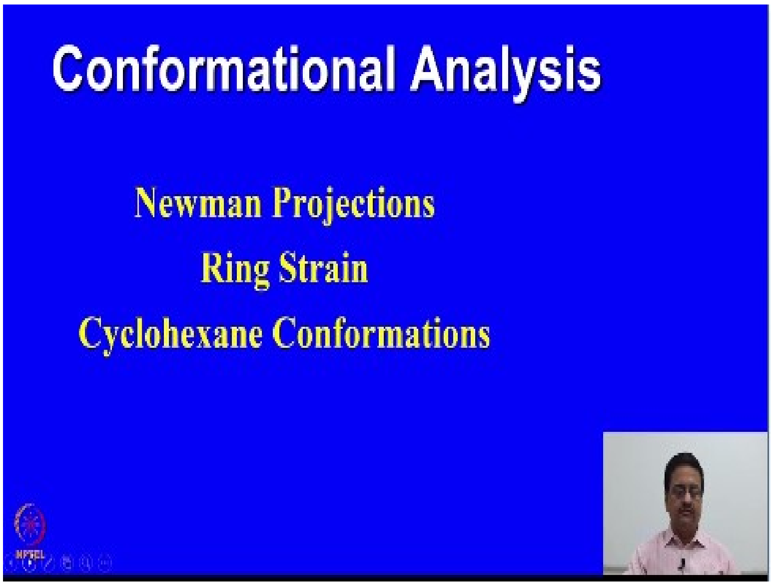

Conformational Analysis

Newman Projections

Ring Strain

Cyclohexane Conformations

So, here in this series of lectures, we will talk about Newman Projections, Ring Strain and Cyclohexane conformations in next few lectures.

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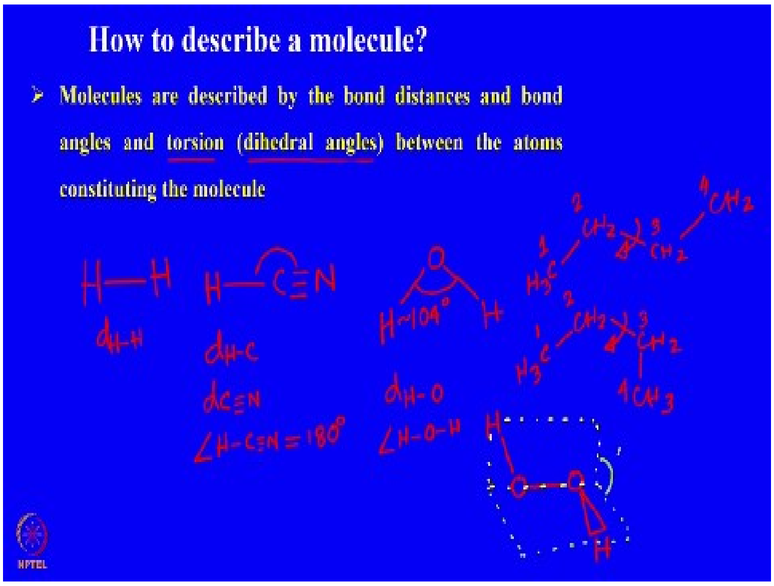

How to describe a molecule?

- Molecules are described by the bond distances and bond angles and torsion (dihedral angles) between the atoms constituting the molecule

So, the first question that we would like to address is how to describe a molecule. Molecules are generally described by the bond distance and bond angles and torsion angles that is the dihedral angles between the constituting atoms in the molecule and once you know the bond angles, bond lengths and torsion angles of a molecule, then we would also like to know how those atoms are oriented in space to know about their stereochemistry.

So, for example, for simple molecules like hydrogen, which is, which we all know that is a linear molecule so, for a simple molecule like hydrogen, it is sufficient to know the distance between the 2 hydrogen atoms. That is the bond length between the two hydrogen atoms. Then if we think of having a linear molecule like HCN, which is written like this. We have a single bond and a triple bond in this molecule.

So, we need to define or know the distance between the hydrogen and carbon. And we need to know the distance between the carbon and the triple bonded nitrogen. And also, we need to know the angle between hydrogen, carbon and nitrogen. Then only, we may be able to say that this molecule is linear if this angle is 180 degree. We have a simple molecule, which we all know is water, is also a triatomic molecule.

So, here what we need to know are the distances of hydrogen to oxygen and the angle H O H that is this angle, which spectroscopic data we know is about 104 degree. Then the concept of torsion angle or dihydral angle comes when there are 4 atoms connected in a sequence. So, for example, one can draw a butane like this and the same molecule like this. What is the difference? The difference is the torsional angle about this bond.

So, the angle between the planes formed by the atoms 1, 2 and 3 and 2, 3 and 4. So, the angle between the plane formed by atom 1, 2, 3 and the plane formed by 2, 3, 4 is called the torsion angle. How to understand this torsion angle easily is to draw a molecule which we all know is hydrogen peroxide. So, in hydrogen peroxide if we draw the 3 atoms, 1 hydrogen and 2 oxygens like this and the fourth hydrogen, fourth atom or the second hydrogen is coming here.

So, the way we have drawn it is those oxygens and this hydrogen is in the plane of the projection and the other hydrogen along with the 2 oxygen is above the plane of the projection like that. So, the angle between these 2 planes is the dihedral angle in this particular molecule that is the angle about this O O bond. So, when we have a molecule which has more bonds, so, you have more number of different bond angles and then you have more number of different torsion angles.

So, to describe a molecule one has to know all the possible bond lengths, bond angles and torsion angles.

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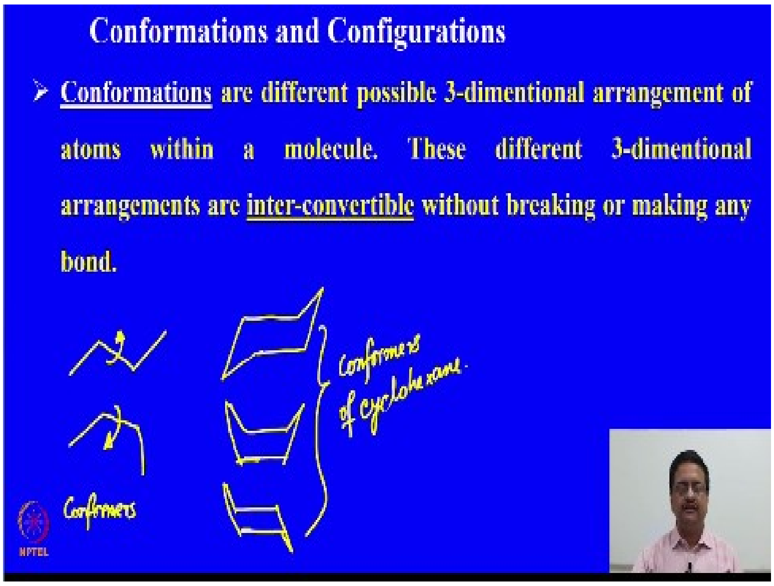

Conformations and Configurations

- Conformations are different possible 3-dimentional arrangement of atoms within a molecule. These different 3-dimentional arrangements are inter-convertible without breaking or making any bond.

So, when we try to write or draw the molecule in a two dimensional plane, we would like to know how those atoms are oriented in 3 dimension. We need to understand the difference between conformations and configurations. Conformations are different possible 3 dimensional arrangements of atoms within a molecule. These different 3 dimensional arrangements are inter-convertible without breaking or making any bond. So, what do we mean by that?

I will again take the example of butane. The way I had initially drawn are 2 different ways either this or that. So, the torsion angle about this and the torsion angle about that bond are different in these 2 different ways of representation and these are called the conformers. Conformers that means they are related by in an angle twist and one can be easily inter-converted to the other without breaking or making any bond.

Some other examples are the examples of cyclohexane, which will be the part of our discussion towards the next few lectures in this course. So, one can draw cyclohexane like that. One can draw a cyclohexane molecule like this and one can draw the cyclohexane also like that. So, these are different conformers of cyclohexane. These different forms can be inter-changed by bending or twisting the molecule.

And these conformers are temperature dependent. At lower temperature, the conformation which has lower energy is more stable and at higher energy, we start seeing different conformations of a given molecule.

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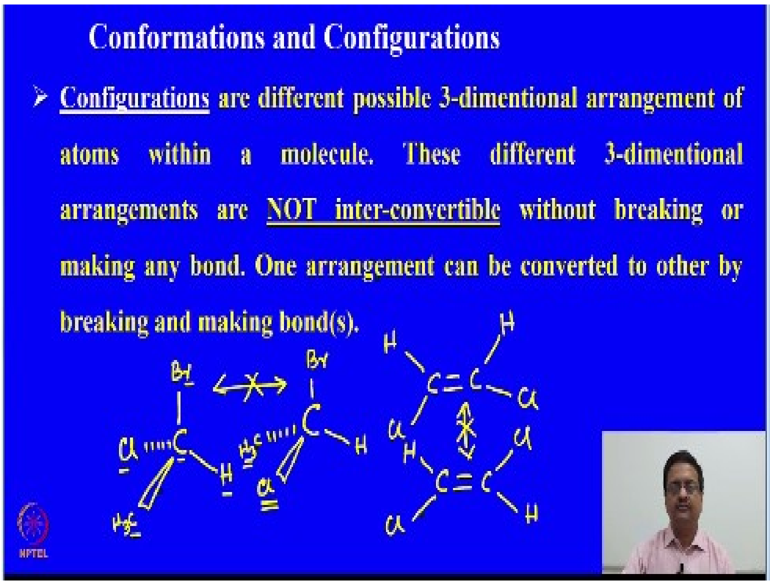

Conformations and Configurations

- Configurations are different possible 3-dimentional arrangement of atoms within a molecule. These different 3-dimentional arrangements are NOT inter-convertible without breaking or making any bond. One arrangement can be converted to other by breaking and making bond(s).

What are configurations? Configurations are different possible 3 dimensional arrangements of atoms within a molecule. These different three dimensional arrangements are not inter-convertible without breaking or making any bond and one arrangement can be converted to other by breaking and making bonds. So, let us take one example. A very simple example is a compound like this which I am drawing here. It is a derivative of ethane, 1 bromo, 1 chloro ethane.

So, the way I have drawn here is that this bromine, the carbon atom and the hydrogen are on the plane of this board and the methyl group and the chlorine are respectively above and below the plane of this board. A different configuration of this molecule is being drawn here where I have in-plane atoms as it is.

But, the groups which are above and below the plane are drawn separate in a different way and what we see is the chlorine, which was below the plane has come above the plane and the methyl, which was above the plane has gone below the plane and these two cannot be inter-converted without breaking or making any bond. So, these 2 different orientations or arrangements of this molecule are called the configurations of one particular organic molecule.

The other type of example of configuration can be seen in geometrical isomers where we have the cis and trans isomers. So, the trans compound would look like this where the 2 chlorine atoms are in the opposite side of the double bond and the 2 hydrogens are also opposite. So, these 2 geometries, these 2 different orientations are 2 different configurations of the same molecule but they are not inter-convertible without breaking or making a bond.

So, these are the configurations which are not inter-convertible without breaking or making a bond whereas the conformations are inter-convertible without making or breaking a bond.

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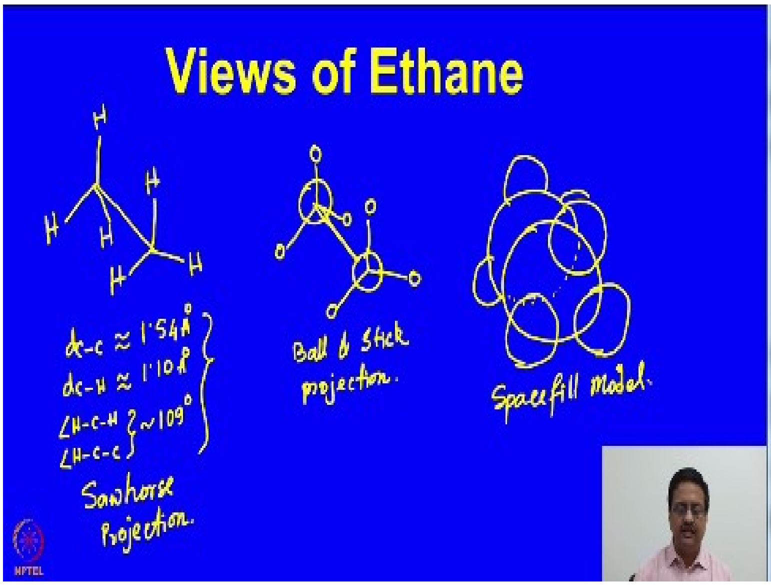

Views of Ethane

So, now, what we would like to draw are different views of ethane. So, here, what I have is a model of ethane, which you can see and this model of ethane has 2 carbon atoms and then 6 hydrogen atoms connected on either side. So, the way I am trying to draw, I am trying to see the molecule like this and trying to draw it on the plane of the board. So, in this particular molecule, what we need to know are the distance of the carbon-carbon bond, distance of the carbon hydrogen bond and the angle H C H and also the angle H C C.

So, the ideal bond length is about 1.54 angstrom for C C single bond. Ideal bond length for C H single bond is 1.10 angstrom. These angles are tetrahedral angles. So, they are close to 109 degree and if we know these parameters, then one can identify or draw the molecule in 3 dimension. So, the way I have drawn this molecule is called this Sawhorse projection. This molecule as I have shown here, it is like a ball and stick model.

And in this ball and stick model, the way the molecule is drawn on the board I am doing it here. The bigger atoms are my carbon atoms and the smaller atoms are the hydrogen atoms that are present in either carbon atoms. So, this is called the ball and stick representation or projection. The third way of drawing the molecule is to draw hard sphere object. So, the carbon in the front is drawn as a big sphere.

Carbon at the back is partially drawn like that as if it is behind the molecule, behind the first carbon. Then you have 3 hydrogens, which are smaller in size but occupies a certain volume is drawn like that. These hydrogens are on the front carbon. So, that is why we see them as full atom and the ones which are connected to the backside atoms are only seen a part of it and we only draw that like this. So, this is called the spacefill model.

So, in your text book, you will see this type of different models or projections of the same molecule for different purposes.

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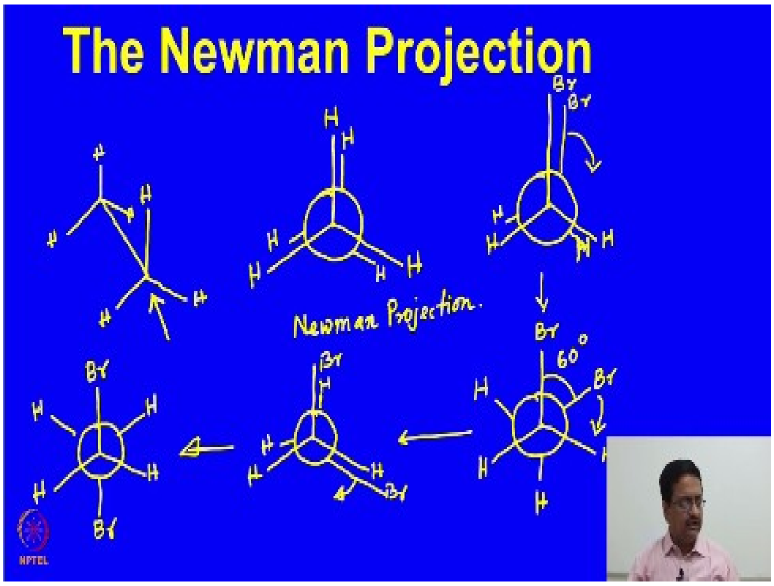

The Newman Projection

So, now, we would like to draw your attention to a method which is called the Newman projection. How Newman projection can be drawn for different molecules? So, we will start with the molecule ethane. What we have shown in the previous slide, our previous drawing is, we had drawn ethane using Sawhorse projection, which is like this, I have the hydrogens.

So, in this projection, if we try to now look at the molecule from this side so, what we are trying to do is trying to see the molecule from that side. So, when you are trying to see the molecule from the side of one carbon, what you see the front atoms are projected towards you and the hydrogen on the back carbon is projected towards me. So, this projection when we try to draw on a 2 dimensional surface or on the plane of the board.

What we draw is as a big sphere or a big circle represents the front carbon. The 3 hydrogens that are present on the front carbon are drawn at 120 degree angle with respect to each other and the hydrogens which are at the back carbon is behind. So, we draw it with smaller size bonds, following the same trend. So, this way of representing a molecule is called the Newman projection.

So, now, suppose if you have different atoms present in this molecule instead of just 2 hydrogens, suppose I replace the hydrogens by 2 bromine atoms which are shown here in red, then the molecule would look like this. I have 2 bromine atoms and 2 hydrogens on each carbon and the molecule is like this. So, if I try to draw this molecule in Newman projection, how should it look like?

In the front carbon, I have a bromine and as you know the carbon bromine bond length is much larger than the carbon hydrogen bond length. So, that should be represented and the back side also has bromine like that, this hydrogen and here is another hydrogen. So, now, if I try to rotate the back carbon like that, So, I reach a different conformation. So, how do I represent that different conformation is shown here.

I write the front carbon as usual. The bromine atom in the front carbon is at the top. The hydrogens are on 2 sides as it is but the bromine on the back carbon is now at an angle 60 degree with respect to the initial condition and the hydrogens are also dispersed like that. So, now, if I try to again rotate this further by another 60 degree, which means I am doing it like that.

So, now what happens is behind this bromine I have hydrogen, behind that hydrogen I have a bromine and these 2 hydrogens are one behind the other. So, if I try to draw the Newman projection of this particular compound keeping the front carbon unaltered, it would look like this. And then further if I rotate this bond by 60 degree, what should I get? The back carbon is further rotated by 60 degree to make it look like that.

So, one bromine is up and the other bromine is down and the hydrogens are in between. So, if I try to draw that on this projection, I would get something like this. So, what we have learnt now is to draw different conformations of a molecule using Newman projection and when you rotate the atom about a bond you get different conformations.

So, these are different conformations of 1,2-dibromoethane and that 1,2-dibromoethane conformations are inter-convertible without breaking or making any bond. Just by rotating the C C bond, you are able to draw different; you are able to make different arrangements of those atoms just by rotation. So, these are conformations, not configurations and these are very important in various organic reactions, which we will see at a later part of this course.

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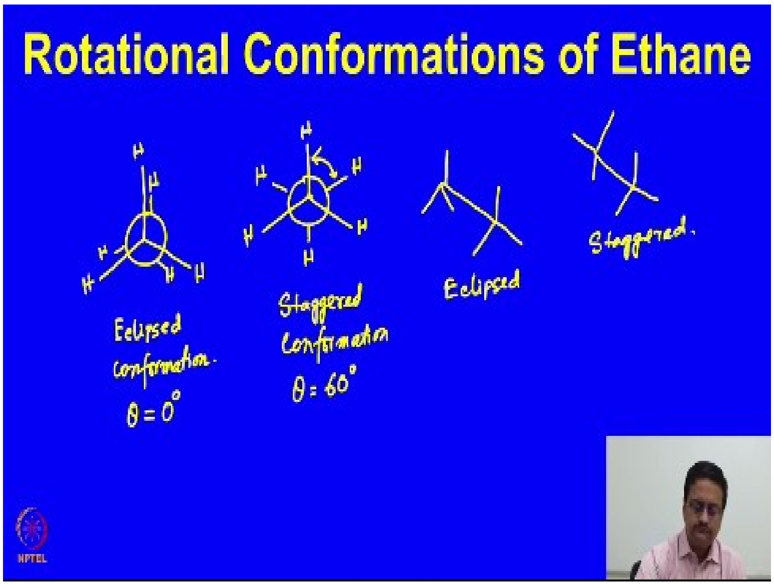

Rotational Conformations of Ethane

So, what we have learnt by now is that using Newman projection, one can identify different conformations and we have names for different, those different conformations. So, when the molecule is like that when the hydrogens are one behind the other or in case of dibromo, when the bromine is behind bromine; hydrogen is behind hydrogen that confirmation is called the eclipsed conformation.

And the second one in case of ethane, when the hydrogens are not one behind the other rather they are at an angle 60 degree to each other is called the staggered conformation. Here, the dihedral angle that is theta between the hydrogen carbon carbon hydrogen group is 0 degree and here the dihedral angle is 60 degree. So, the 2 different Newman projections of eclipsed and staggered conformation are shown here.

If we draw those as a Sawhorse projection, we should be drawing them like this. This first one that I am drawing is the eclipsed conformation and the second one that I am drawing here is the staggered conformation.

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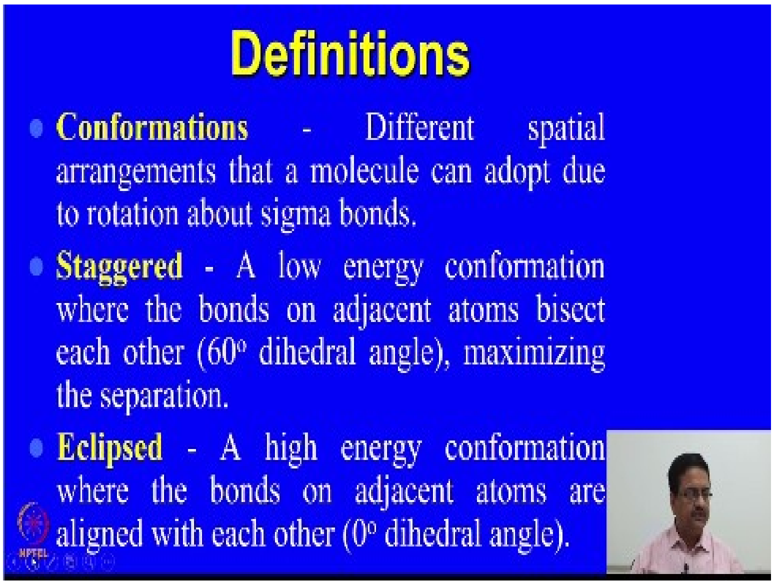

Definitions

- **Conformations** - Different spatial arrangements that a molecule can adopt due to rotation about sigma bonds.
- **Staggered** - A low energy conformation where the bonds on adjacent atoms bisect each other (60° dihedral angle), maximizing the separation.
- **Eclipsed** - A high energy conformation where the bonds on adjacent atoms are aligned with each other (0° dihedral angle).

So, what we have learnt by now is, there are conformations which are different special arrangements that a molecule can adopt due to rotation about a sigma bond. A staggered conformation is a low energy conformation where the bonds on the adjacent atoms bisect each other that is the dihedral angle is 60 degree and it maximizes the separation between the atoms in the adjacent atom.

And eclipsed conformation is a high energy conformation where the bonds on the adjacent atoms are aligned with each other. So, for example here in this case of dibromoethane, this concept of high energy and low energy can be understood easily when the molecule is drawn like that where 2 bromines are one behind the other. These 2 large atoms have Steric hindrance.

As a result, this molecular conformation is unstable. It is of high energy. When you rotate the back carbon by 60 degree, the distance between the 2 bromine atoms increases. As a result, the Steric hinderance between the 2 bromine atom is reduced. So, this particular staggered conformation is having a lower energy compared to the original fully eclipsed conformation.

But then when we rotate this molecule by another 60 degree, we reach another eclipsed conformation where there is bromine and bromine and hydrogen one behind the other in 2 occasions and this is called partially eclipsed and this also is one of the higher energy conformers of dibromoethane.

And if we rotate this back carbon by another 60 degree, we reach a conformation where 2 bromines are exactly opposite and this conformation is the most stable conformation where the Steric hindrance and the torsional strain is the minimum. So, we call it as anti-conformation. So, in the next part of this lecture, we will continue from here and discuss about various conformations of ethane and substituted ethanes.