Symmetry, Stereochemistry and Applications
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Module No # 3
Lecture No # 13
Chair and Boat Conformation of Cyclohexane

Welcome back to the course on symmetry, stereochemistry and applications. In the previous lecture we were discussing about the conformation of cyclohexane in the chair form and then we were trying to understand how we can draw the molecule using the Neumann projection.

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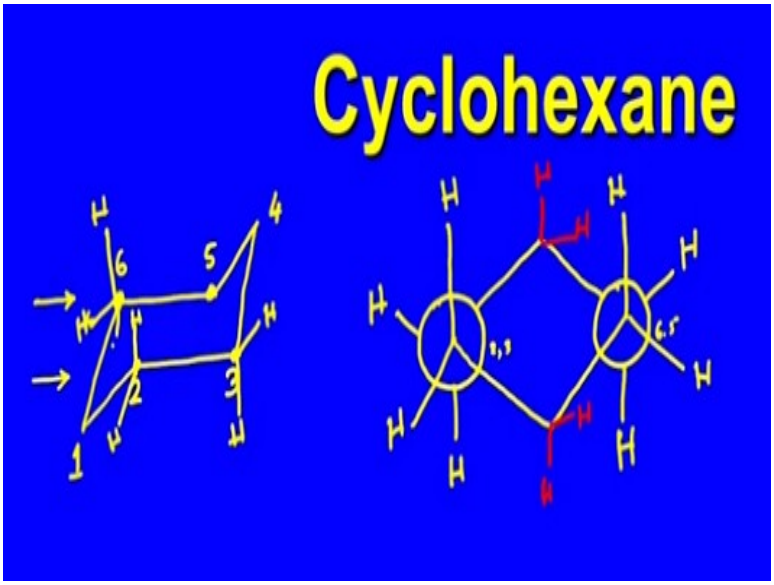

So in this case as you have seen that these 2 hydrogen atoms which are on the central carbon atoms is like that and this is how you should draw the chair form of the cyclohexane molecule.

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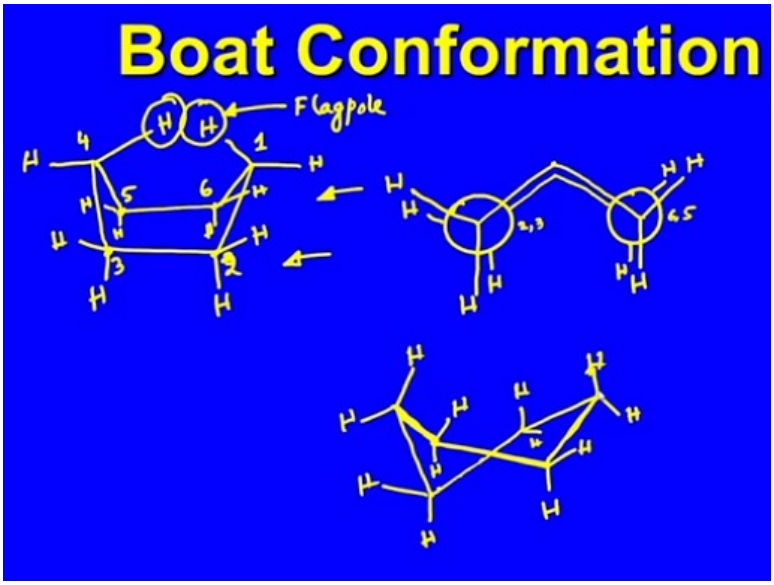

So the next important conformation for cyclohexane is the boat conformation. So the way we draw the boat conformation is the following. So here what we have are the hydrogen atoms on these 2 carbon atoms are very close. And the other 2 hydrogen are in opposite direction and in these carbons the hydrogens are down and up. So now if we try to draw this molecule in this, boat conformation in the Newman projection how should it look like.

So we should see from the side of these 2 parallel bonds and then try to draw the Newman projection. So what we draw here are the 2 carbon atoms through which we are looking at, so if we try to number them as 1, 2, 3, 4, 5 and 6 this carbon that we have here is the carbon number 2 the back carbon is 3 here the back carbon is 5 and front carbon is 6. If you look at this carbon atom 2 you have the CH 2 group at the top which connects to carbon number 6.

So this is the connection between 2 and 6 which is your carbon number 1. On the other hand if you look at 5 and 3 they are also connected in the same manner. So now the other hydrogen that we should draw for 2 are these 2 hydrogens and for 6 these are the 2 other hydrogen for 2 and 6 then on 3 you should have 2 hydrogen placed like that and on 5 you should have 2 hydrogens placed like this.

So this will be the corresponding Newman projection of boat conformation and these hydrogens which are close in the boat we call those 2 hydrogens as flagpole. Because of those flagpole hydrogens being very close this conformant is unstable compare to the chair conformation and it

always tries to go to the chair conformation from this boat conformation. So when the transformation tries to happen then the molecule goes through a different conformer called the twist boat which I am trying to draw here.

So in this particular conformation this bond is above the plane of the projection and that bond is below the plane of the projection and it is a twist boat conformation.

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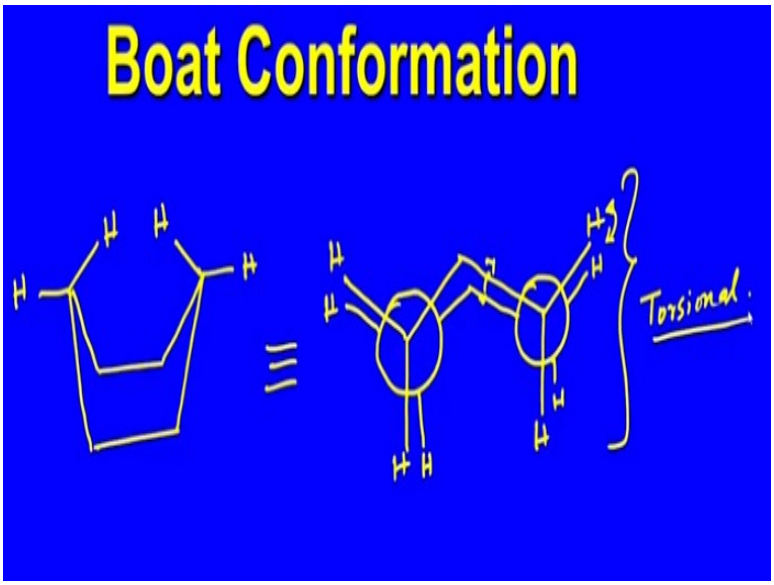

So as we have seen in the boat confirmation that the hydrogen atoms are on the flagpole and they interact very close and you have a significant amount of steric strain and also a torsional strain in the molecule. Because if, you see the molecule in the Newman projection it looks like that there are 2 eclipsed butane groups present one next to the other. So this molecule has eclipsed methyl groups, eclipsed hydrogen atoms, eclipsed methyl groups which, is equivalent to n-butane that you had in the eclipse or fully eclipsed conformation.

So it has significant amount of torsional strain compared to the chair conformation of cyclohexane which does not have this torsional strain.

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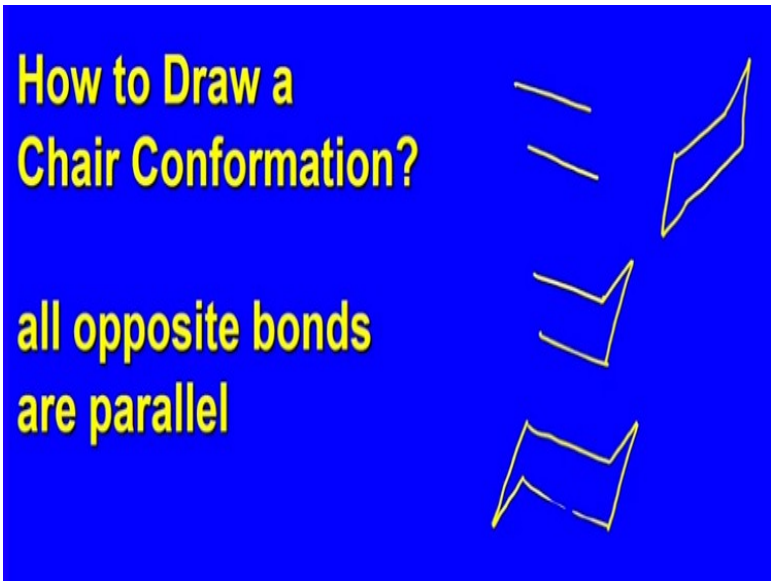

So, by now you must have practiced yourself how to draw different cyclohexane chair conformations. So, it is easy if you try to draw the chair conformer, you should draw 2 parallel lines. Then you join those 2 parallel lines with this and further those 2 parallel lines join this and you can join the other 2. Similarly, if you draw it in the other direction that you draw it like this you draw this and draw that. So, both of them are the chair conformations of cyclohexane.

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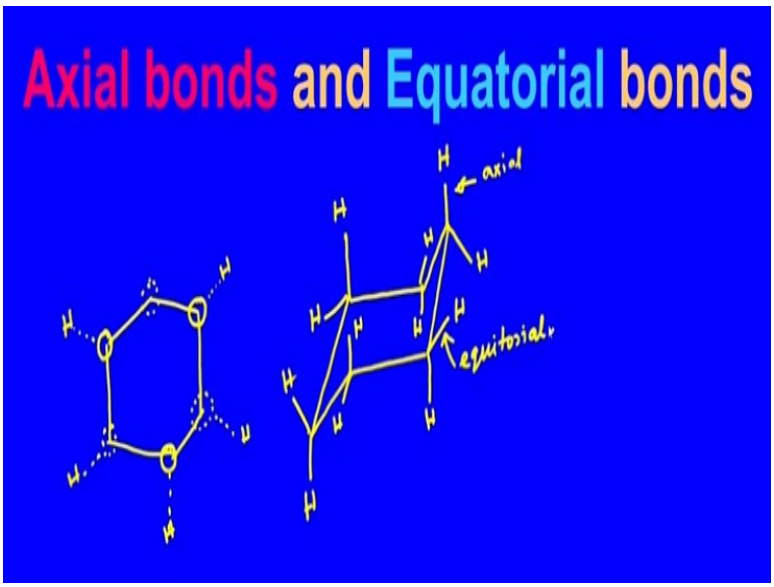

So now when we try to look at the cyclohexane molecule there are 2 different types of bonds present in this molecule. The hydrogen atom positions are identified as axial bonds and the equatorial bonds. So, when you look at the molecule from the top. It would actually look like a

planar molecule and what we will have is in case of 3 alternate carbons the hydrogens will look upwards.

And the other 3 carbons 1, hydrogen will always be downwards and the other hydrogen will be in the plane of the molecule or will look like in the plane of the molecule and it will look like that. But actually when you try to see the conformation in 3 dimension when we try to draw the molecule in chair form. I'm trying to draw it in the chair form as good as possible, the bonds which are up are the axial bonds which are like that are axial bonds; the down ones.

And the other bonds which are like this that are called the equatorial bonds. This becomes very important when we try to understand some of the chemical reaction and we try to understand the stereo chemistry of substituted this cyclo hexane is we will see in a few minute.

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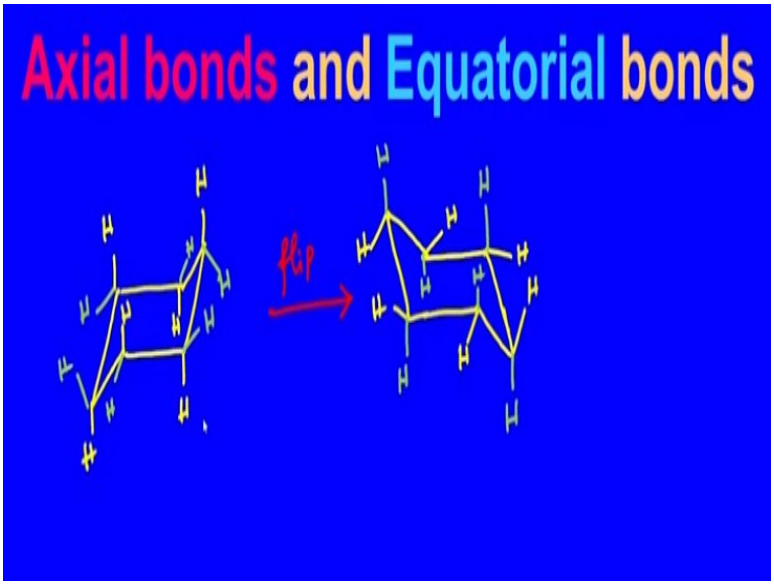

So when you have a cyclohexane drawn like this, these are the axial bonds that I am drawing and I am drawing the equatorial bonds in a different color. Now if you try to flip this cyclohexane molecule which means we are trying to convert the molecule to a different chair form where the atoms which were above are going to be down. And the one's which were down should be up. So in this particular confirmation which is a flipped conformation the hydrogen atoms which were the axial bonds are now going to be the equatorial bonds.

And the bonds which were the equatorial bonds, drawn in green they are the corresponding axial. So on flipping the axial bond becomes equatorial and the equatorial bond become axial. And this ring flip happens always at room temperature because both the conformations are of same energy therefore we do not distinguish between these 2 different conformations.

So what we wanted to indicate here that the ring flip makes an axial bond to be equatorial and equatorial bond becomes axial.

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So when you flip a chair conformation or axial bonds become equatorial, all equatorial bond become axial which essentially means all up bonds stay up. And all down bonds stay down so let us see what does it mean?

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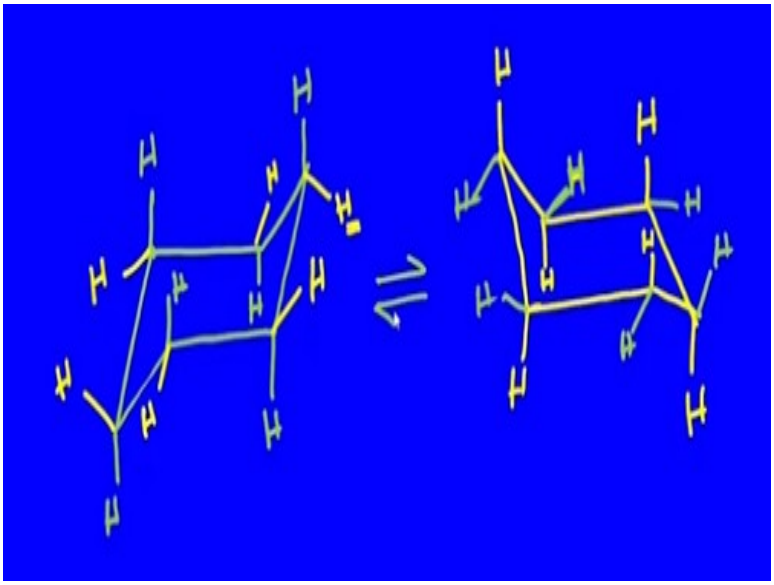

Suppose we had the molecule like this. This is the up hydrogen, this is the down hydrogen, this is up hydrogen, this is up hydrogen, this is down hydrogen, this is down hydrogen. But all of them are axial, this hydrogen is up equatorial, this hydrogen is up equatorial and this hydrogen is up in equatorial position, this hydrogen is down equatorial, this hydrogen is down equitorial and this hydrogen is down equatorial. So now if I convert this to the flip conformation which is like this, the hydrogen which is down here that was my equatorial hydrogen it should become axial hydrogen and remains down here.

And the hydrogen which is up here in the equatorial position becomes the axial hydrogen up there. Similarly this hydrogen is axial up and this hydrogen is axial up and here there should be one equatorial down, there should be 1 axial down hydrogen. So you have already drawn 6 hydrogens which were initially equatorial or now they have become axial. And the axial hydrogens are now the corresponding equatorial hydrogen.

I think that hydrogen should be down here and the other one should be the axial hydrogen which has now become equatorial. So this is how one should try to draw the flipped rings and try to understand how these bonds change their orientation depending on which way the cyclohexane ring is flipped.

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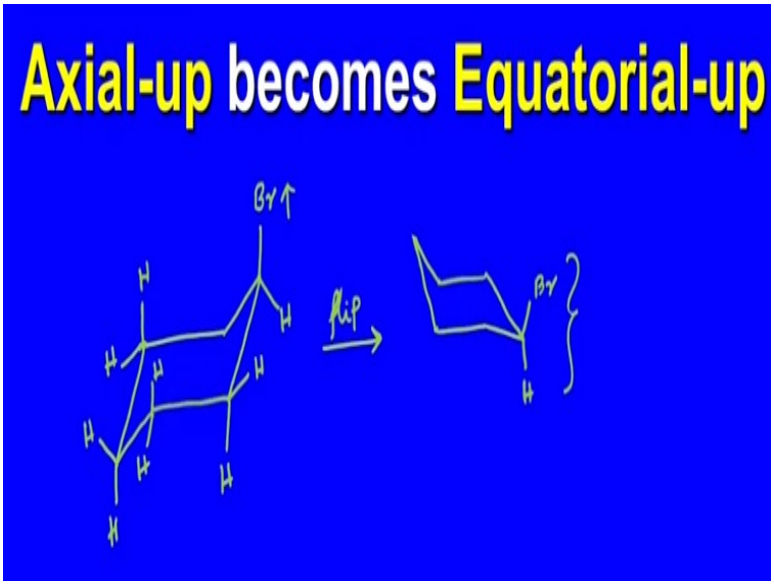

So if we try to do these using a substituted cyclohexane, suppose we have bromocyclohexane. If we flip then what should happen is we should have this and that side and this bromine which was axial up will now be equatorial up and hydrogen along with that which was equatorial down will remain axial down. This is what is meant by axial up becomes equatorial up. So, this bond which was upwards not it is still in equatorial position but it is in the upwards direction.

So this is how we should try to understand what happens when you flip the cyclohexane in chair form. Because this; is very important in understanding some the conformations and stability of various cyclohexane derivatives specially the 1, 2, 1, 3 and 1, 4 di-substituted cyclohexane derivatives. So what happens is that when you have the substitution in the cyclohexane ring.

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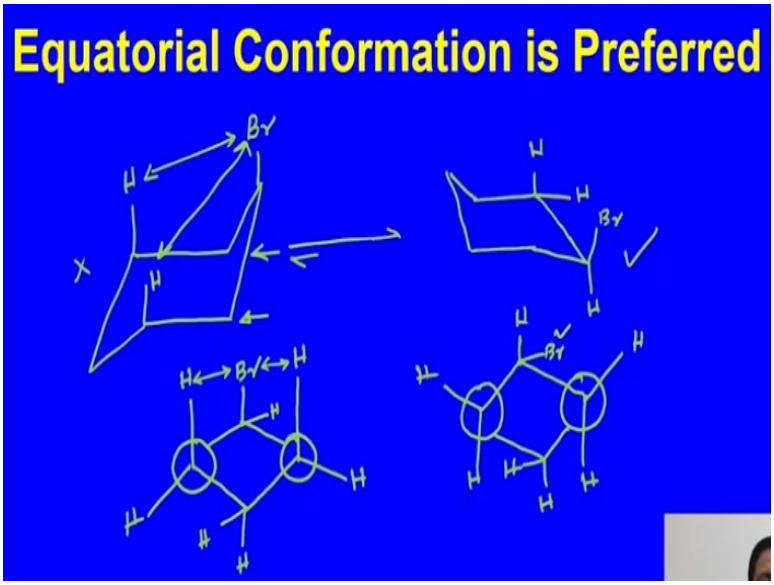

Suppose we have a Bromine atom or a methyl group in the axial position like that. There is a possibility of a steric interaction between the large bulky groups with the corresponding axial hydrogen atoms. And it then produces some destabilization in the molecule. So as soon this kind of situation arises because of large bromine atom or large methyl group present on the carbon atom. Then the ring flips spontaneously towards the other chair conformation where the bromine goes to the equatorial position and the steric strain is released.

So if we try to draw these 2 conformations using Newman projection through this bond, what should I look? So in this particular conformation, it is easily seen that this bromine is in between the 2 hydrogen atoms and that causes a steric repulsion in that. So if we draw the fifth version of the molecule in Newman projection it would look like this. So now this bond is in the equatorial position and is no longer in the interaction between the 2 hydrogen atoms which were causing destabilization in case of the axial orientation.

So, on the room temperature this particular conformation is more stable compare to the axial conformer. So we will continue this lecture from here in the next class.