Course on Stereochemistry
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Lecture 04: Chirotopicity Stereogenicity

Okay now, the last time what we said about was that the optical rotation which is a very important physical parameter for optically active compounds okay? And this is useful not only to measure the to identify one compound with another compound and also to measure the percentage excess of one Enantiomer over the other. So we have introduced a concept of Enantiomeric excess or what is also known as the optical purity okay?

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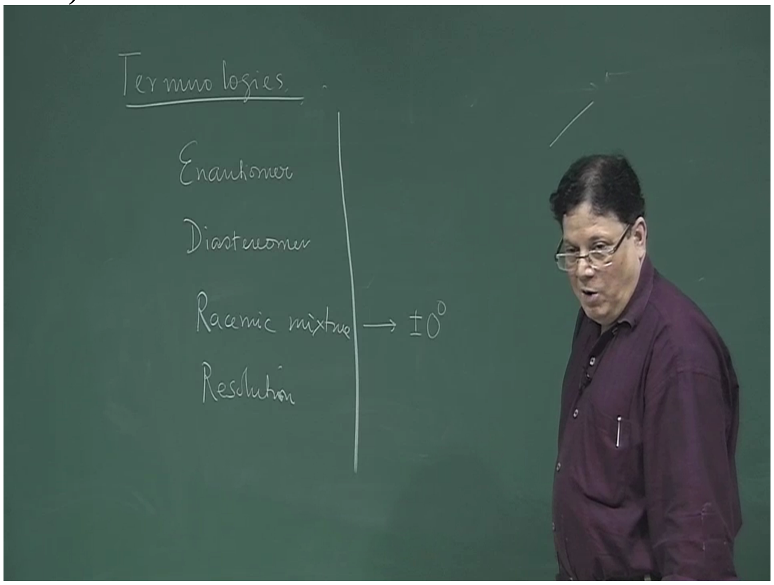

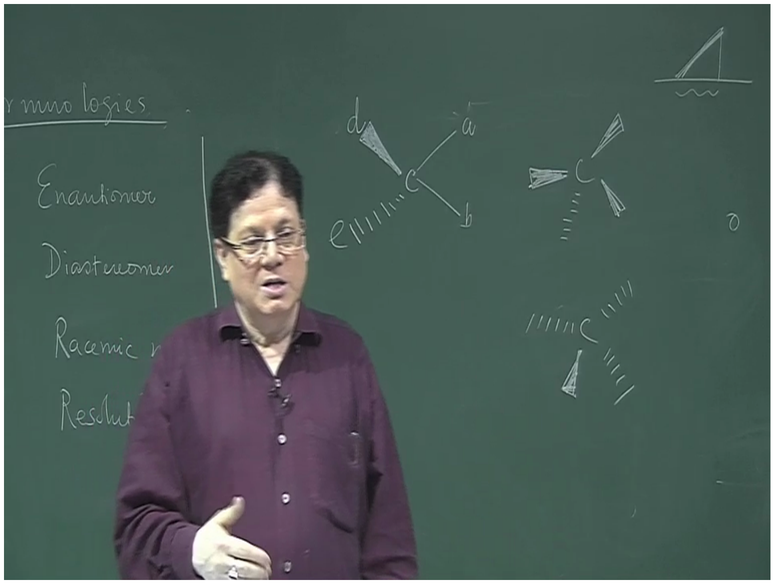

Now before I go further, let me again clarify some of the terminologies that are used in stereochemistry. We have been exposed to at least 2 or 3 of these but again just repeat these. Enantiomers, what are Enantiomers? They are not superimposable stereoisomers which are non-non-superimposable mirror images of each other. They are chiral in nature. Diastereomers, they are stereoisomers but they are not mirror images of each other.

Now what about the chirality of Diastereomers? They may be chiral or they may be achiral, both, okay? Racemic mixture, it is a 50-50 mixture of the 2 Enantiomers okay? 50-50 mixture or one is to one mixture of of the Enantiomers, of the pair of Enantiomers. So the rotation of Racemic mixture will be 0, + or - 0 because the + compound is present in equal amount, so it will try to rotate the plane of polarised light to X degree, + X degree.

The - compound will upset it by turning it back to - X degree. So the total rotation is, ultimately becomes 0. That is Racemic mixture, that is one is to one combination of pair of Enantiomers. And resolution is that if you can separate the Racemic mixture into the individual Enantiomers. So resolution is separation of a Racemic mixture into the individual Enantiomers okay?

Now the next thing is very important in stereochemistry and that is as I said that was the time of Vant Hoff and Lebel Cobra proposed that the carbon is a tetrahedral carbon. And this tetrahedral carbon, because of this tetrahedral nature of carbon, that gives the possibility of generating another molecule if the ligands, that means the substituents attached to it are different. If the full ligands are different which are attached to it okay?

So I want to make a carbon where there are 4 different league. So one is red, one is this pink, suppose this is a ligand, that means substituent. There is a fight ligand . So I have another. Suppose I put a carbon here, so if you look at this carbon, this carbon is attached to a methyl, this is one ligand. This is another group represented by white or an atom.

This is an atom or a group represented by the red. And this is another substituent represented by pink, okay? Now this is a three-dimensional molecule because this is a tetrahedral, you cannot draw a tetrahedral by putting all the bonds in the same plane because that never happens in a tetrahedral. If you inspect the tetrahedral, then it has got a it has got some special features. The features is that 1st of all, you cannot place more than 2 bonds in one plane.

So you have this tetrahedron and these 2 bonds can be in one plane. These 2 bonds can be in one plane but you cannot place 3 bonds into one plane. If these 2 bonds in a plane, then what happens to the other 2 bonds? One bond is above this plane, the other bond is below the plane. Okay? So so that is the 1st concept that maximum 2 bonds can be placed in a plane. Then the other 3, other 2 bonds, one becomes above the plane and the other 4th bond becomes below the plane.

You can actually place the carbon in the plane and then what you can have, the 3 bonds are above the plane of the reference plane on which the carbon is placed and the 4th ligand, 4th substituent is below the plane of this what I am holding. The reverse situation can also happen, the 3 bonds can be below the plane and one bond can be above the plane. So these are the different possibilities.

So 1st of all, you cannot place more than 2 bonds in the plane and 2nd one that 3 bonds can be above the plane in which the carbon is residing only. And then the 4th bond will be below that plane. Vice versa, if there is the 3 bonds are below the plane then the other bond will be above the plane okay? Now the question is, how to draw this three-dimensional structure into the blackboard which is a two-dimensional plane? So so there were some notations that were used that when we draw a bond, usually we draw a bond by a line.

Now in stereochemistry a line means a bond, no doubt but this line is in the plane of the bond is is lies in the bond lies in the plane of this board, this line. If I say a single, simple line. See if I drawn other line, that means this line also is in the plane of the board. What happens to the other 2 bonds in a tetrahedral? As I said, if 2 bonds are forced in a plane, to lie in a plane, the other 2 bonds cannot lie in that plane.

One bond will be above the plane and the other bond will be below the plane. And this is supposed the carbon which is attached to the 4 different groups. Suppose this is a group A, this is a group B and then you have a group D and then group E. So one will be now above the plane. Now how to show that to the to the students or to people who is observing this molecule that how to make them aware of the fact that one bond goes above?

And the way to do it is, you make it a dark bond but you see the way it is drawn. It was 1st narrow and slowly the dimension becomes more, the wdith becomes more. That means as you go away from the carbon, the substituent is also moving above the plane, more and more above the plane. Okay? So this is, this means the bond is above the plane of this board. And the other bond which is now below the plane of this board so that will now be looking like this.

So this is the 3rd substituent and this is the 4th substituent. So this is the way you can represent a tetrahedral. This is one way that 2 bonds in one plane, the other is that 3 bonds above the plane. So now you know this that when I draw this dark bonds, darken the bonds and show it, that means these 3 bonds are above the plane. And what did I say? That if 3 bonds are above the plane, then the 4th bond will lie below the plane okay?

So this is another way of representing the tetrahedral in the two-dimensional plane. And there is a 3rd one option I have is that 3 bonds are below the plane and the 4th bond will now be the should be above the plane. So these are the 3 situations and the both all the 3 situations can be shown in this perspective formula okay? This is what is called the OH formula, the OH representation of three-dimensional molecules.

That where, remember if you have only the single normal line, that means these bonds are in the lying in the plane of the board. If you are drawing it in the paper then that they line the plane of the paper. This is above the plane of the board, this is below the plane of the board. So these are flying OHs. However they are they are little bit hard to visualise because you have you have this alpha, beta concept here.

Now there are other kinds of perspective formula which are more useful in stereochemistry, in stereochemical representation of molecules and they are called projection formula okay? Projection formula. What is projection formula? That is projection means you know that projection means that if you have a line on a above a plane above a certain reference plane and what is the projection of this line that you draw a perpendicular from the and point to the plane and then that means you draw a perpendicular from here to there to the plane and then you draw the line.

So that is what is called the projection. The simple mathematical concept that if you have a bent line and if I see what is the say what is the projection of this line on this plane, the projection is draw the perpendicular and these becomes the projection of this line which is drawn here, okay? So based on this principle, you have different projection formula. That means what you do?

You take the three-dimensional molecule and then you you draw the projects and of the molecule on the plane and then see how does it look? What are the projections? Because what we draw is the projection that is obtained by drawing all those perpendicular to the reference plane okay? So there are 3 kinds of projection formula. The most common is the Fisher projection formula and and the the most common is the Fisher projection formula. And the others are Newman collection formula and sawhorse, okay? So let us 1^{st} come to the Fisher projection formula. What is that?

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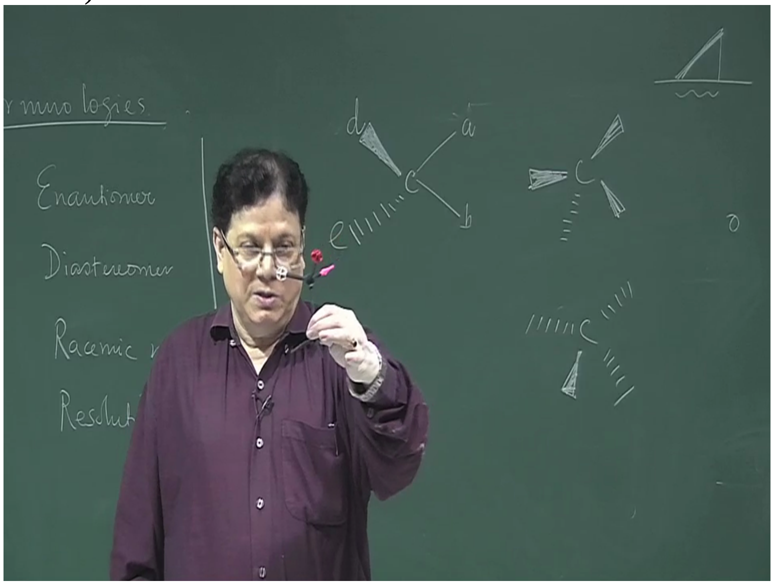

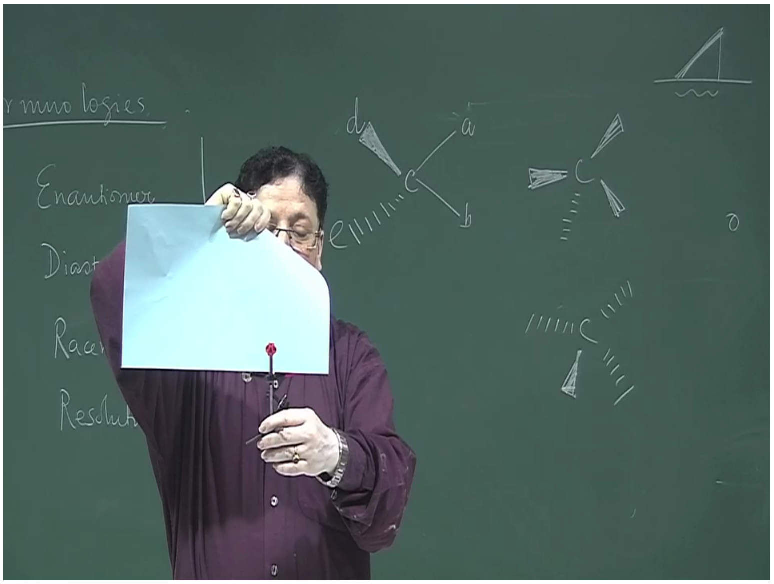

That in Fisher projection formula, you hold the molecule in such a way that suppose I am the Observer, you hold the molecule. That means the carbon containing the 4 different groups in such a way that the bonds that none of the bonds, I have a reference plane here, I consider a plane like this. So none of the bonds are in the plane. Only the carbon is in the plane of this paper. So what happens now? 2 bonds if I am the I am looking from this side and this is my reference plane, so what happens?

2 bonds will be towards the Observer if the observer is from this side and 2 bonds will be behind the Observer. That is 1st thing. So when you draw a Fisher projection formula, you view the molecule in such a way that 2 bonds are facing towards you and 2 bonds are going away from you. But not only that, there is another one, restriction and that is in put in Fisher projection is that the bonds which are towards the Observer, they should be in the horizontal direction. And bonds which are away from the Observer, they should be in the vertical position.

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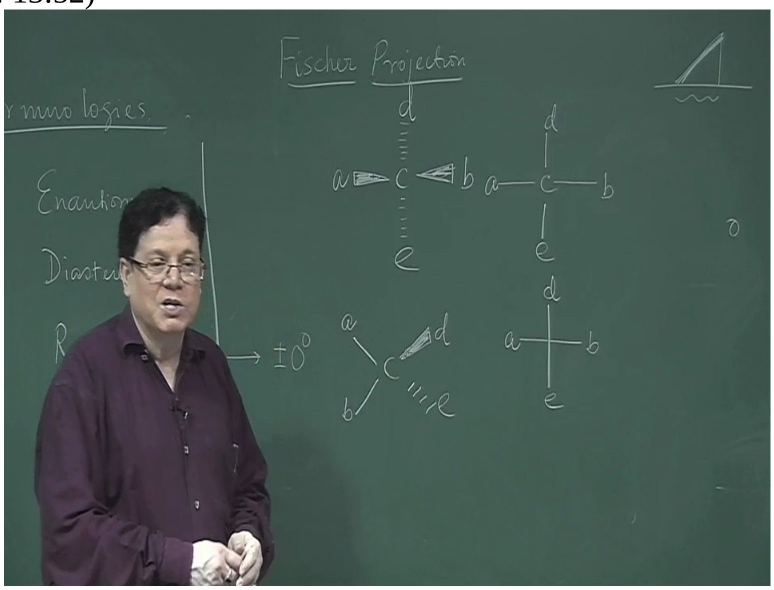

So basically what I am saying that you hold the molecule in such a way that it looks like in the OH formula, it should look like this. So the these 2 bonds are towards the Observer because they are now above the plane of this board and the other 2 bonds and the other 2 bonds are will be away from the Observer but they are in the vertical line. So if I am the Observer, so that means what I see that these 2 bonds are facing towards me, that means if I extend my hand, one is pointing to my right hand, another is pointing to my left hand.

And this D group is away from me but it is pointing towards my hand and E group, it is also going away from me but it is pointing towards my leg okay? Now what I do? I draw projection of these bonds, of these of these bonds onto the plane of the board. So when I draw the projection, that means this will go down and I get a line, simple line like this and for the moment we keep the carbon but in Fisher projection, carbon is is not shown.

So this is the protection of B, of the bond connected to this carbon. This is the projection of A and this is the projection of D. Now this projection has to be coming from the backside and this also, the projection has to come from the backside. So these are the projections that you will have of all the bonds in the plane of the board okay. Now you remove the carbon and it will look like a cross.

So this will be D, this will be B, this will be A and this will be E. So I hope this is clear. That means if while drawing the Fisher projection formula, I should write this is the Fisher projection formula. In the Fisher projection formula, what the molecule is 1^{st} holding is held in such a way that the horizontal bonds are towards the Observer and the vertical bonds are going away from the Observer. And then you take a protection on the plane, the reference plane in the in this case, the board and then you will see that you are forming a cross and then you put the atoms again.

So this is the Fisher projection of this molecule okay? Now the problem is, always the molecule will not be drawn in this fashion. The molecule can be drawn as I said, in various fashions in the OH, in the OH perspective formula. So if a molecule is drawn like this suppose, say this is beta, this is alpha and these 2 bonds are in the plane of the in the plane of the board, and I ask you to draw the Fisher projection formula of this.

Now this molecule if I, if I stand here in front of this molecule, then this is not projected according to the Fisher projection because in Fisher projection, 2 bonds has to be beta and they have to be also towards the 2 hands in the horizontal direction. And the other 2 bonds should be towards away should be away from the Observer and also should be towards the vertical axis. But this is not drawn in such a way.

So how to know convert this into the Fisher projection? Now there are several ways you can do it. It all depends on the visualisation that visualisation concept that we have, three-dimensional visualisation. But I can give you some some simpler way to solve this type of problems. So the problem is, draw the Fisher projection formula of this molecule. So what I suggest that now one option is you rotate the molecule.

You rotate it in such a way so that the 2 bonds so that it looks like what is just before drawing the Fisher projection. So you have to turn the molecule. Now while turning the molecule, you can make a mistake. That is a problem. That you have to turn this. D is already up. So you have to turn this D. So you have to turn, bring the E up also. Then you have to make out where are the As, where are the Bs. The other option is that do not turn this molecule, keep it as whatever it is. The Observer is flexible. Observer is the student or the teacher or whoever is seeing this molecule.

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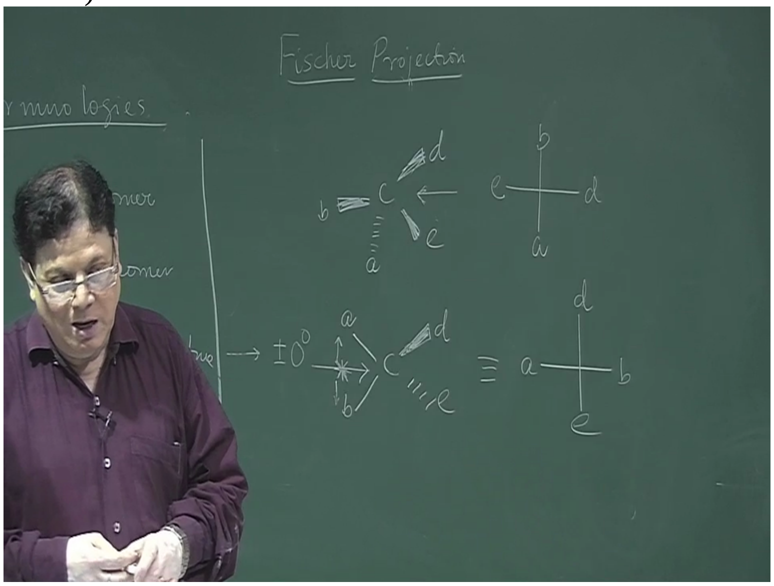

So if the Observer thinks that he is standing here in a vertical manner, he is standing here with his head up and leg down. So he is standing at this position. Head is up and leg is down and he now sees the molecule from in from this direction. So what will happen? If he extends his hand on the 2 sides, so these 2 bonds A and B are now projected towards him because he is standing here and he is standing again I repeat, he is not standing like this.

He is standing in a in a perpendicular to this pain of the board. He is standing like this, his head is here, his leg is below the plane of this ring and his left hand will be here and his right hand will be on this direction. But if he stands here, the interesting point is, he is not satisfying the condition of the Fisher projection. That means, the molecule now this A and B are towards his 2 hands and they are also going towards him and what happens?

This D is going away from him, E is also going away from him. But D since it is above the plane of the board, so this is pointing towards his head and this is pointing towards his leg. But they are going away from him. So if you are not draw the Fisher projection, that means I am seeing from this direction, my head is here, I am seeing in a, I am sitting in an orthogonal position, standing in an orthogonal position to the plane of the board and then I can draw the Fisher projection very easily.

So what will happen here? I see from here, so you draw the cross again and the left hand now you have to decide where is your left hand, where is your right hand. The left hand is on this side and the right-hand is on this side. And that is your head? D is pointing towards your head but it is going away from it and that is be the case in case of Fisher projection. So that is D and that is E. So this is the way to draw the Fisher projection.

Situation maybe little bit more complicated that if I draw it in say I have 3 bonds like this above the plane of the board and the other bond must be as I said, these 3 bonds are above the plane, then the 4^{th} bond has to below the plane. If that is the case, then how to draw the Fisher projection from this? Now the simple way to do it as I said, do not turn the molecule. The best is that you position, the Observer should position himself or herself in such a way that the molecule just looks exactly what is before drawing the Fisher projection.

That means the horizontal bond should be above the plane and the vertical bond should be below the plane. So where the Observer should place himself or herself. So if the Observer is now observing from this side and extends his hands towards this and towards on the other side then you can see that these 2 bonds will be towards him, D will be towards his right hand, E will be towards his left hand, this B will be towards his, this B and E are going away from him and they will be occupying the vertical axis and B will be at the top because it is now the it is in the headward direction and this is in the direction of the leg.

So you see from there and then you draw the Fisher projection very easily. So this will be the right-hand so that will be D. This will move into the left hand, that will be E and that will be B and that will be A. So this is the simplest way of drawing the Fisher projection even if it is given in different perspective ways, OH formula. You can easily convert.

As I said, there is no harm in rotating the molecule but rotation can draw you into trouble. That when you rotate the molecule, you have to see where it is, after rotation how does it look? The better approach is that the Observer makes room that he stands in such a way, such a corner that it looks like a Fisher projection formula and then draw the Fisher projection. Only thing you have to remember, where is the right-hand, where is the left-hand? Where is your head where is your leg? Then you can draw the criss-cross okay. Now this Fisher projection formula has certain restrictions. Restrictions means you cannot just rotate the formula at your will.

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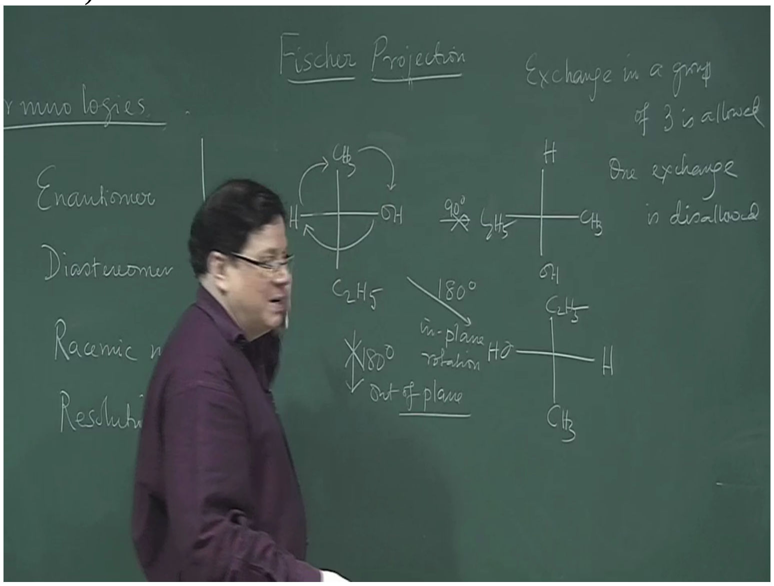

Means if you have a Fisher projection formula that there is suppose methyl, there is OH, there is a hydrogen and there is a suppose there is a ethyl group okay. Now this Fisher projection formula if you say that I will rotate this by 90, the rotate this whole thing by 90. So what will happen? methyl will come here. So rotated by 90 and then this OH will be here, H will be there and sorry C2H5 will be there and this will be H.

Now if you do a rotation by 90, you actually change the molecule. This is not the same molecule as this because when you convert remember this that when you convert a 3-D molecule into a 2-D plane, when you write that, there are some restrictions that are imposed now. You cannot rotate it at will. But if it is in the three-dimensional perspective formula, you can rotate it. There is no restriction of rotation. Here there is some rules that needs to be followed.

What is the 1st rule? That you cannot rotate the future projection formula by 90 degrees in plane. So in plane, this is in plane rotation formula. You are keeping this whole thing in plane and rotating by 90 degrees. That is not possible. So what actually is interestingly you can try that this actually is becoming the mirror image of this one if you do this 90 degree rotation.

What is allowed is 180 degree in plane rotation , in 180 degree in plane rotation. That means this methyl is here, C2H5 is there and then OH is here, H is here. So 180 degree in plane rotation is allowed, 90 degree in plane rotation is not allowed. What what other things are allowed or disallowed? Disallowed is 180 degree out of plane rotation, 180 degree out of plane. See there are 2 ways of doing 180 degree rotation.

Either you can take this and make it, you rotate it in the plane. That is one way of rotation or you can rotate it 180 degree out of plane. That means you take the molecule house of the plane and then again put it in the plane. So these other 2 ways. So 180 degree out of plane rotation is not allowed. Then what is what are the other rules? The other rules is that you have, you can exchange, if you exchange the position of these ligands.

Suppose I exchange OH with methyl, I put OH here and methyl here. Whether that is allowed or not? The rules says that exchange in a group of 3 is allowed. Exchange in a group of 3 is allowed and one exchange is disallowed okay? Now what does it mean? One exchange means this exchanging methyl with OH. So if you put the OH here and the methyl here, that is not allowed okay? That changes the molecule.

What does not change the molecule is exchange in a group of 3. That means you bring the methyl here, OH here and the H there. That is what is called exchange in a group of 3. So that is what is allowed. One exchange is disallowed. So that is I think all about the Fisher projection formula. We can come back to this issue later on when we talk about the absolute configuration of molecule. This will be extremely helpful in drawing various stereochemical molecules with various types of stereochemistry involved okay?