Crystals, Symmetry and Tensors
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Lecture 19b
3D Points Groups VI: Improper Monoaxial Point Groups

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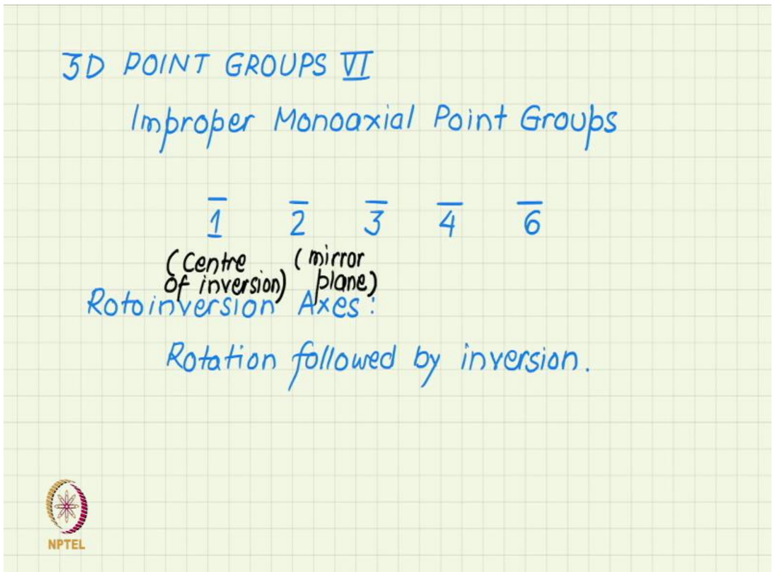

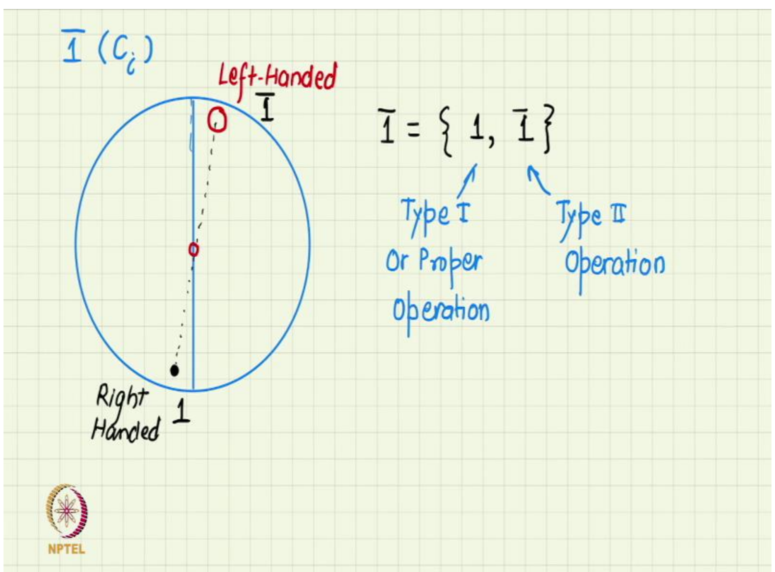

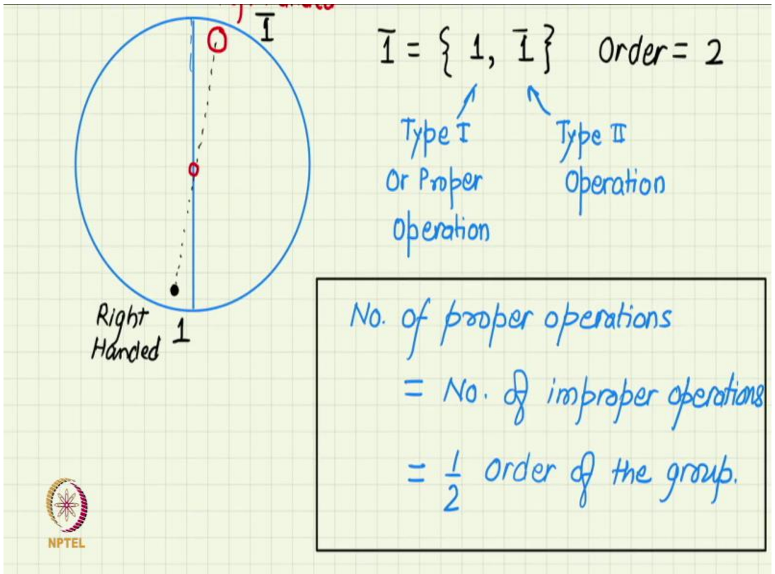

So, we now venture into developing improper point groups, there are 21 of them, and again, we will go in steps to develop all of them. We begin with the monoaxial improper point groups. So, as you know, there are 5 different corresponding to the 5 pair or proper rotation axes, there are correspondingly 5 improper rotation axes, which are the rotoinversion axes. So, we have 5 rotoinversion axes, 1-bar, 2-bar, 3-bar, 4-bar, 6-bar.

These are the operations associated with these rotation axes themselves from a group and these will be the improper monoaxial point groups. So, these are called rotoinversion, rotoinversion axes, that means, a rotation followed by inversion. So, these are rotoinversion axes, which means, they represent a rotation followed by an inversion. So, 1 by we have seen we have met this when we were introducing various kinds of symmetry operations in one of the previous videos, here, we simply know that 1-bar is also a center of inversion, it is not really an axes, it is actually a point.

Similarly, 2-bar is also not really an axes, it is a mirror plane. So, 1-bar and 2-bar will be handled separately at center of inversion and as mirror plane. So, really non trivial rotoinversion axes are 3-bar, 4-bar and 6-bar. So, as a told, the operations associated with these axes themselves form point group and those are our improper monoaxial point group. So, let us look at them one by one using our stereogram and listing of operations. So, 1-bar is a group which the Schoenflies notation, is Ci.

Now, this is an inversion center as we noticed so, the stereogram is simple, I have a circle, let me draw a reference diagonal. So, I have a point here above the equatorial plane and I have a center of inversion in the center or center of inversion really does not have any standard graphical notation, but here we are representing by a small open circle. So, that is located at the origin.

So, what the center of inversion will do to this object at general position shown by the black dot? So, we will take it through the center of inversion to an equal distance other side. So, which means, if this object was above the equatorial plane, the image will be below the equatorial plane. Also, inversion in 3 dimensions changes the handedness of the object. So, if this black object, let us say was right-handed, then the image will be left-handed and I will show left-handed image by a red circle.

So, open circle shows that it is below the equatorial plane and the red color shows that this is of a different handedness than the black point. So, if the black is right-handed, the red is left-handed and that completes the group, because if I now apply the inversion again on this red point, it will bring me back to the original black point. So, the black represents the identity operation, whereas the red circle represents the inversion operation.

So, this group 1-bar has only 2 operations 1 and 1-bar. Notice that 1 will always be there in all groups identity will always be there in all groups. So, an identity is a type 1 or proper operation. Thus, even in improper groups, you will always have some operations which will be proper. So, in this case 1 is a proper operation and 1-bar is type 2 or improper operations. In fact, an interesting theorem from the group theory tells that the number of type 1 and type 2 operations in any improper group will always be equal and equal to half the order of the group.

So, let me I am not proving it here, but let me just know that for any group number of proper operations is equal to number of improper operations. So, in this case, both of them are 1, the order of the group obviously, is 2. So, since these two are equal both are equal to half of the order of the group maybe I can extend my box to include.

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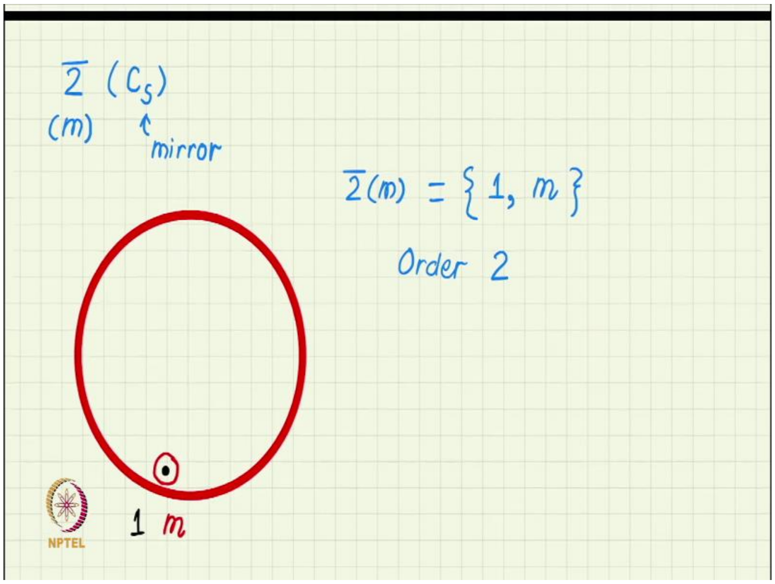

So, let us go to the next group, 2-bar which is the Hermann Mauguin notation for this is CS, S stands for the German word for mirror and sometimes in Hermann Mauguin notation also 2-bar can be represented as M, to represent that this is actually a mirror plane. So, this is also a simple point group, we can quickly develop it stereogram and the operations it represents. So, if we consider the mirror plane to be, so, let us show the point in general position and if we think of the mirror plane as horizontal, so, it will coincide with the equatorial primitive circle.

So, that becomes the mirror plane and if an object is above and it is reflected in a horizontal mirror plane, it will go below and it will change its handedness. So, a change of handedness represented by an below represented by an open circle and change of handedness shown by red. So, in black you have the identity 1 and in red you have the operation of mirror which we represent by m, we could have represented it by 2-bar also, but I am using m.

So, both these points are there, if I reflect reflection of reflection is the original object. So, if I reflect the open red circle again in this mirror plane, I will come back to the black point above. So, the group is complete and I can write my 2-bar group which also can be represented as m, as an identity operation and a mirror plane. So, order is again 2 and you can again see that the number of proper operation which is 1 in this case, and improper operation which is m, the 2 are equal both are 1 and 1.

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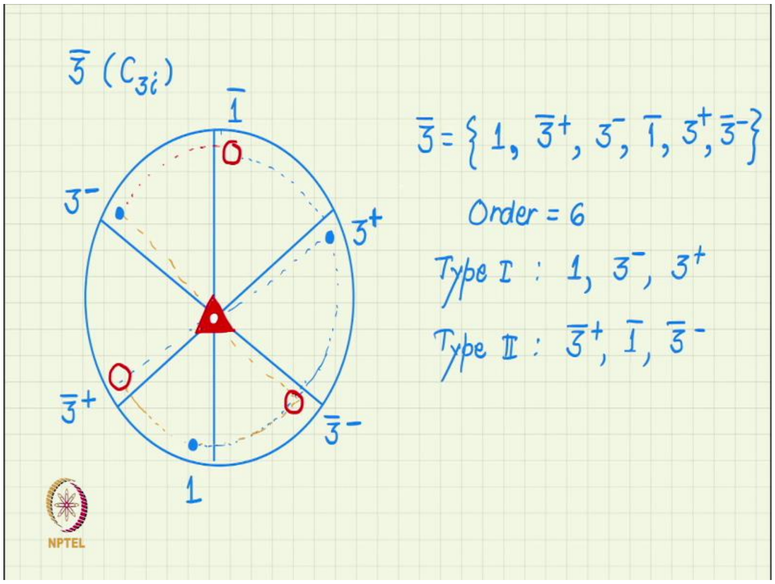

So, our third group is 3-bar. 3-bar has an interesting Schoenflies notation, C3i, notice that for 1-bar Schoenflies would have used CI and for 3-bar here is using C3i. So, somehow it is indicating that this also had center of inversion, which is not obvious in the notation of Hermann Mauguin as 3-bar, we will see that. So, let us develop the stereogram as usual for 3-fold rotation use the reference lines at 60-degree, and starting with an object in a general position I have 3-fold rotoinversion axes. For this, there is an international notation where for 3-fold axis there was a filled circle to represent the 3-fold rotoinversion axes, we use a circle with a hole in the middle.

So, that represents 3-fold rotoinversion. So, which means, now I have to rotate, I have to rotate by 120-degree, I have to rotate counterclockwise by 120-degree, I arrive here, but the operation is not complete because this is a 3-fold rotoinversion. So, after reaching there, I have to invert it in the axis to come here, the rotation part did not change the handedness, but the inversion part will change the handedness, rotation part also did not change its level it remained about the equatorial plane, but inversion took it down.

So, I have an open circle at that location. So, effectively you can see that it is rotated 60-degree clockwise and then reflected in the equatorial plane if I continue this, so, this should be representing our operation of 3-bar plus, if I again rotate by 120-degree. So, if I again rotate it by 120-degree I will come here and then if I invert I go there, but, I come above the plane with the same handedness as the starting point.

Now, from your 3-fold axis stereogram, you can see that relation between 1 and this new point is nothing but 3 minus, it is a clockwise rotation by 120-degree, so, a negative rotation by 120-degree. So, applying 3 plus 3-bar plus 2 times I get 3 minus. Now, you have what the field that how it is going to go. So, the next operation brings you here, but you can see it is related to the original 1 simply by inversion in the center.

So, we can note this to be 1-bar in the next stage in its journey, it comes here again with change handedness and you can see that this is related to the original point 1 by a positive rotation by 120-degree 3 plus and then, it comes to the final stop in its journey here. And this is nothing but 3-bar minus. So, just like we got 3-bar plus by 120-degree anti clockwise rotation and inversion. This one you will get by 120-degree clockwise rotation and inversion.

A further operation of 3-bar on this brings us back to 1. So, the group is now complete, you have 6 operations and we have already listed them. So, we just list them in the group notation. So, we have 1, 3-bar plus, 3 minus, 1-bar, 3 plus, 3-bar minus. So, order is 6 you can see that the type 1 operations or proper operations in this are 1, 3 minus and 3 plus and type 2 or improper operation are 3-bar plus, 1-bar, and 3-bar minus. So, again you can see that they are equal in number, proper and improper operations 3 each half the order of the group.

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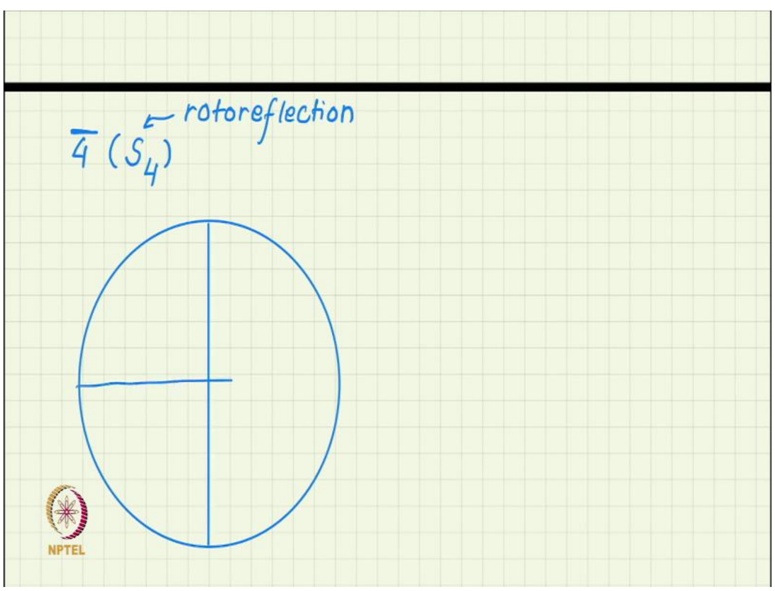

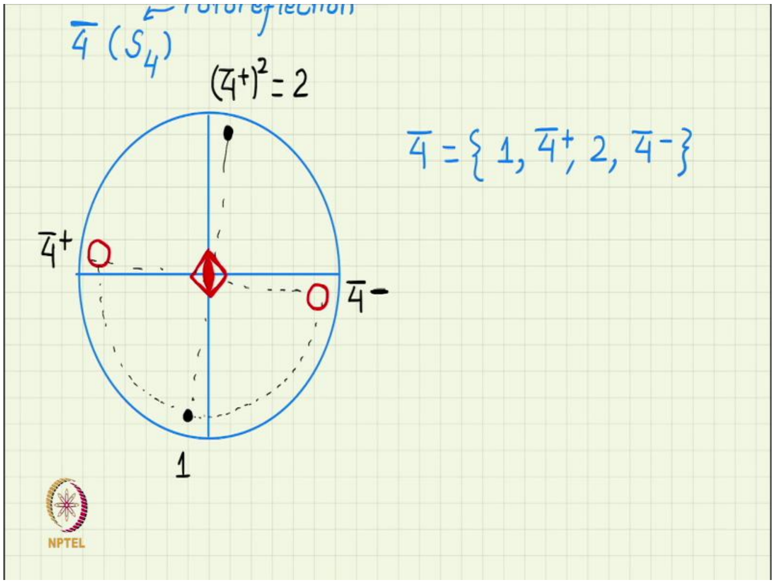

Now, we come to the group 4-bar. This is the Schoenflies notation S. Schoenflies is interpreting the rotoinversion axes as rotor reflection. So, S as we saw in CS, we are just standing for mirror in German. So, S stands for roto reflection in Schoenflies, just like bar represents roto inverse in in Hermann Mauguin, S represents roto reflection. So, Hermann Mauguin will call it a 4-fold rotoinversion axis, Schoenflies we like to call it 4-fold roto reflection axis and in this case, they happen to be equivalent. Since 4-fold rotation is involved, we take reference axes at 90-degree, reference lines start with a general position 90, so, 4-fold rotoinversion symbol very, very interesting.

So, let us make that, a field a square was representing a pure 4-fold rotation proper for 4-fold rotation axis. For 4-bar axis, the international symbol is an open square, but with a filled lens inside you will see why this symbol has been chosen. So, now, you rotate by 90-degree counterclockwise and invert. So, you come there and you come there with changed handedness. So, you get that point. So, if this was 1, this is 4-bar plus 1 more step of 90-degree rotation, 90-degree anti clockwise rotation and inversion brings it up and change its handedness. So, it is back to the same handedness as the original object.

And you can see that although we have applied 4-bar plus 2 times, so, we could have written it as 4-bar plus square. But, actually it becomes nothing but a 180-degree rotation. So, we will use the notation 2 and it is final stop of journey, 1 more 4-bar plus operation, we will bring it here. We will bring it here. So, which will be equivalent you can convince yourself to 4-bar operation in the opposite direction. So, that is 4-bar minus, if we apply once more to this, 4-bar minus I come back to 1. So, the group is complete and I can write 4-bar group as well 1 4-bar plus 2 4-bar minus, 2 operations are the first kind 2 operations of the second kind.

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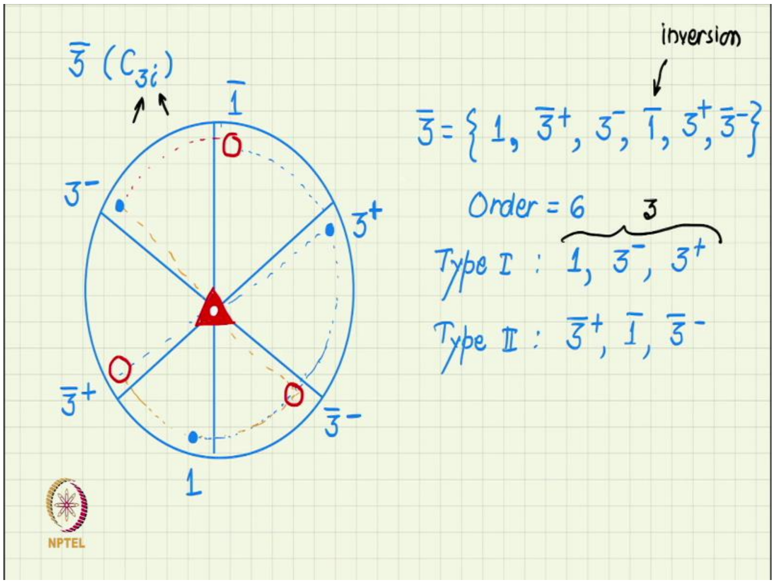

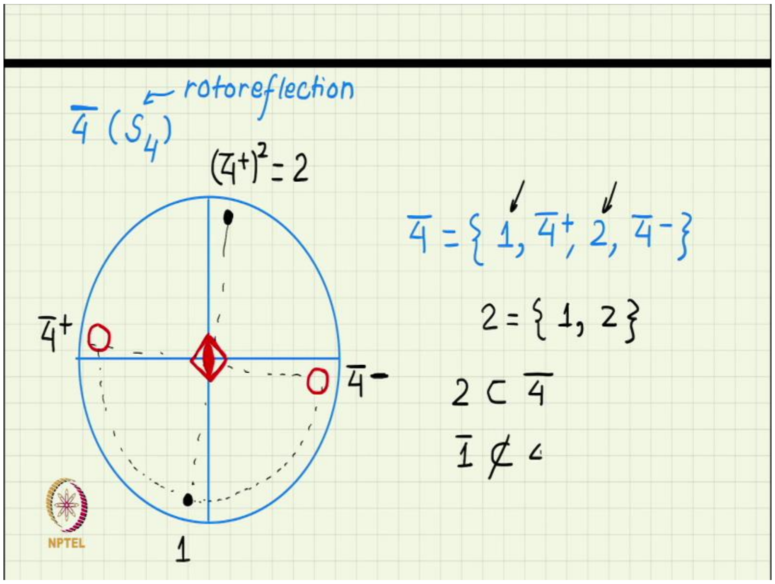

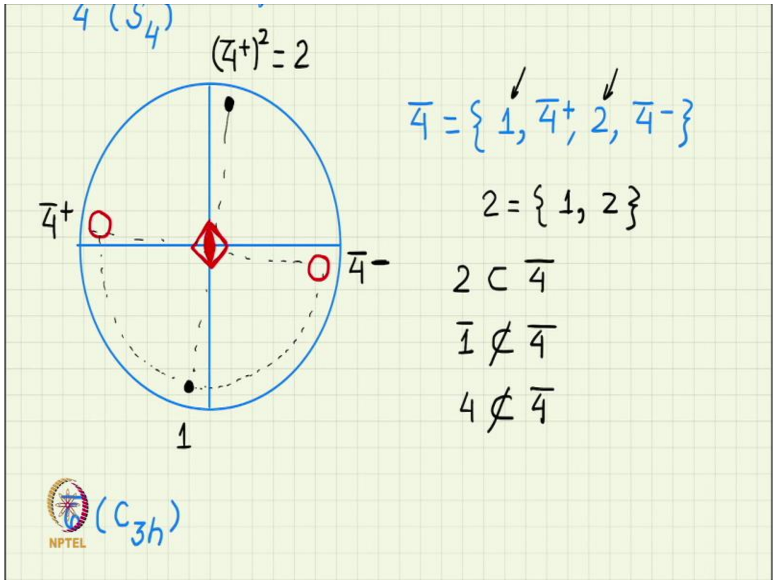

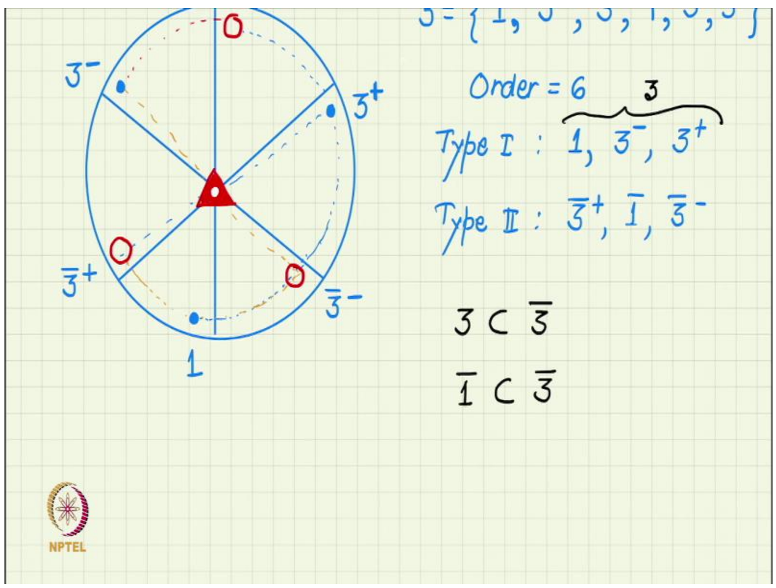

And the final group to be developed is the 6th bar which is interestingly called C3h. I forgot to mention here, I said that, we will talk about this i. So, you can see that each point here is also related to another point by inverse in center. So, 3-bar automatically has 3-fold as well as the inverse in center, you can see from the listing of the operations also, that 1-bar is part of the group. So, that is the inverse in center, inverse in and you can see that it contains 1 it contains 1 3 plus and 3 minus, which is nothing but the point group 3 or 3-fold rotation.

So, 3-bar contains both 3-fold rotation, 3-fold rotation and the inversion center. That is what was Schoenflies symbol C3i and the graphical international symbol also is representing this by having this hole in the circle. So, you have a filled circle, almost filled circle, which is representing the 3-fold and the hole in the middle is showing the inversion center. If you compare this with 4-bar, you will see the points are not related by an inversion center. So, 4-bar does not have an inversion center.

However, each point can be related to another point by 180-degree rotation. So, 2-fold is part of the group, you can see that 2-fold group 2 is 1 2 and both 1 and 2 are there in 4-bar. So, 2 is a subgroup we can write this like this 2 is a subgroup of 4-bar, but inversion center is not there, there is no 1-bar operation and in the stereogram also, you cannot invert the point. So, 1-bar is not a subgroup of 4-bar. Whereas, here if we write the same in the same notation, so, we can say 3 is a subgroup of 3-bar and 1-bar is also a subgroup of 3-bar.

So, 3-fold rotoinversion includes both 3-fold rotation and inversion. 4-fold rotoinversion does not contain the does not contain the inversion. It also does not contain the 4-fold axis. So, 4 is also not a subgroup of 4-bar, because you do not have a point equivalent point at 90-degree rotation. Because at 90-degree rotation, you will have a point which is above the equatorial plane, but here you have below the equatorial plane and with change handedness. So, this difference between 3-fold and 4-fold should be seen.

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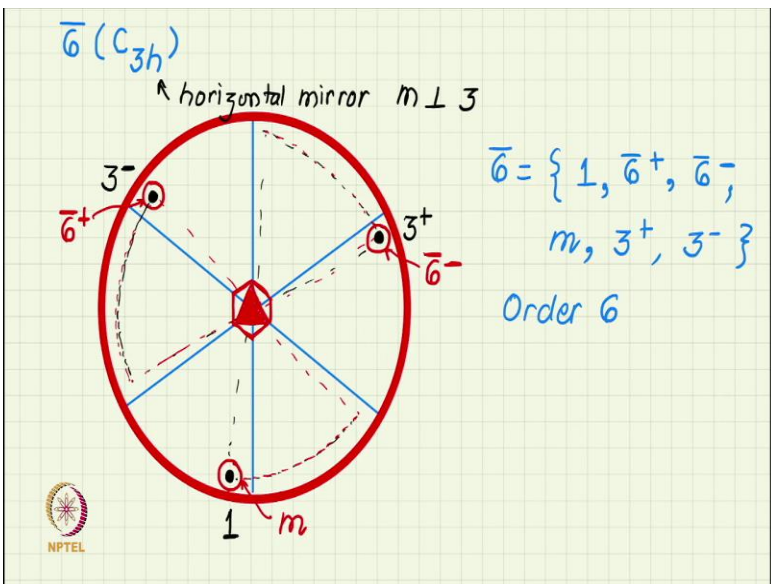

Now, here again we will discuss the Schoenflies notation after we have developed the 6-bar, axis 6-bar group. So, let us develop this 6-bar gives us a hint that we should take the reference lines at 60-degree we start with an object of right-handed object about the equatorial plane, then 60-

degree rotation counterclockwise rotation, followed by inversion. So, that takes us there, change the handedness and change the level.

So, it goes below, 60-degree counterclockwise rotation and inversion brings it again above and with changed handedness, so, from red, it again becomes black. Further 60-degree rotation and inversion seems to be bringing it to the original position but not really because it was above the equatorial plane from where we are starting. So, inversion takes it below the equatorial plane and also change its handedness, so in the same location now, we have an red open circle 60-degree to the red open circle and inversion, you get a black dot where red open circle was existing.

Now, continuing our journey 60-degree rotation followed by inversion. So now I get an red open circle, where a black dot was existing. And now from this red open circle, if I repeat the operation of rotation and inversion, I come back to the original black dot. So, the group is now complete and no new points will be generated. So, I have 6 equivalent positions 3 above and 3 below. So, it is a group of order 6 and let us note the operation.

So, we can see that I have 1 and these other black dots can be related to 3 plus and 3 minus because they are of the same handedness and they are 120-degree away. And the 3 red dots, if you see red circles if you see, so, just 1 below the equatorial plane below 1 is of changed handedness and is exactly below 1. Similarly, below 3 plus also you have changed handedness and exactly below the equatorial plane. And same thing is repeated for 3 minus.

So, what you know is really, the equatorial plane has become a mirror plane. Although you did not start it by making it a mirror plane, but the equatorial plane turns out to be a mirror plane. That is interesting, and I have not yet given the then geometrical notation for the 6-fold axis, the geometrical notation for the 6 6 bar axis, 6-bar axis is a hexagon with a triangle in between which is filled.

So, you can see 1 3 plus and 3 minus. So, every point is related to other points by a 3-fold rotation. So, 3-fold rotation is part of the group, this is what the filled triangle in the geometric representation is showing. But the 6-fold the hexagon is not filled, because you do not have a 6-fold here because at 60-degree you are not finding equivalent position. So, that is why an open hexagon with a filled triangle is the geometric symbol for the 6-bar axis.

But look at the Schoenflies way of looking at it, what Schoenflies is seeing that every point is related to other point by a 3-fold rotation as well as the h represents a horizontal mirror that is perpendicular to 3-fold because 3-fold is assumed to be vertical in Schoenflies notation. So, there is a mirror perpendicular to 3-fold, this is important to keep in mind. So, you can think of 6-bar as a mirror perpendicular to 3-fold and that is exactly what is shown in the Schoenflies notation.

But Hermann Mauguin represents it as 6-bar. So, for the other group operations we can write here now. So, this one is just represented as a reflection of 1 we can call it m. Now, here the red one, how to relate this with 1. So, we have seen that this 1 was simply, if I rotate 60-degree and then invert, I got to this circle. So, this is actually a 6-bar it is representing 6-bar plus operation. Similarly, this 1 will be representing 6-bar minus operation. So, this gives us now, the idea of how to write the group operations.

So, 6-bar group, a group with 1 then, you have 6-bar plus, then you also have 6-bar minus, also have m, 3 plus, and 3 minus. So, group of ordered 6. So, that completes the development of monoaxial groups, all of these have their improper axes, but there is only 1 of them, which we have placed vertical in these stereograms. In the coming videos we will now just like we did for the proper groups we will try to combine more than 1 improper groups, improper operations or improper axis, more than one improper axis in the same group. Thank you very much.