Crystals, Symmetry and Tensors
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Lecture 19 d
3D Point Groups VIII: Combinations of a Mirror Perpendicular to an n-Fold Axis

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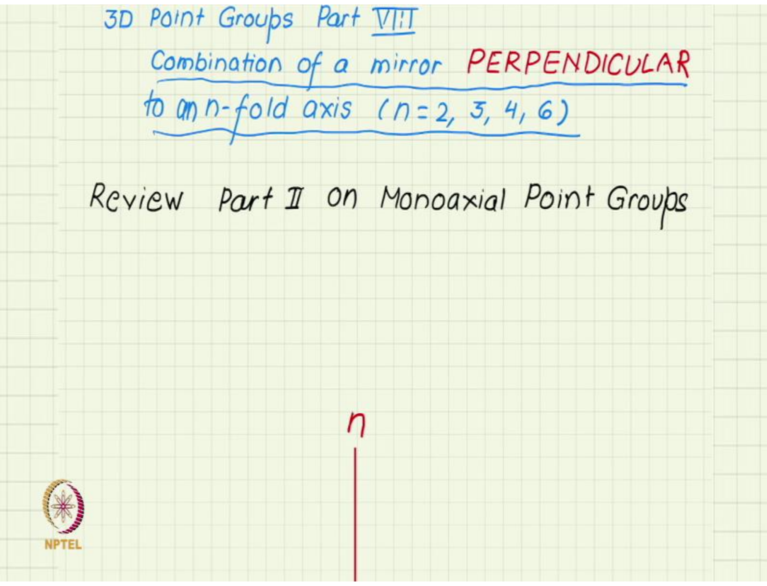

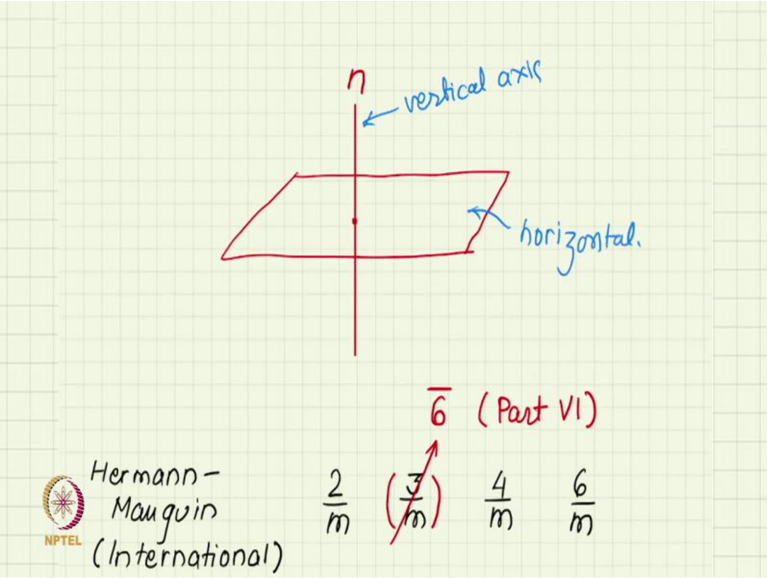

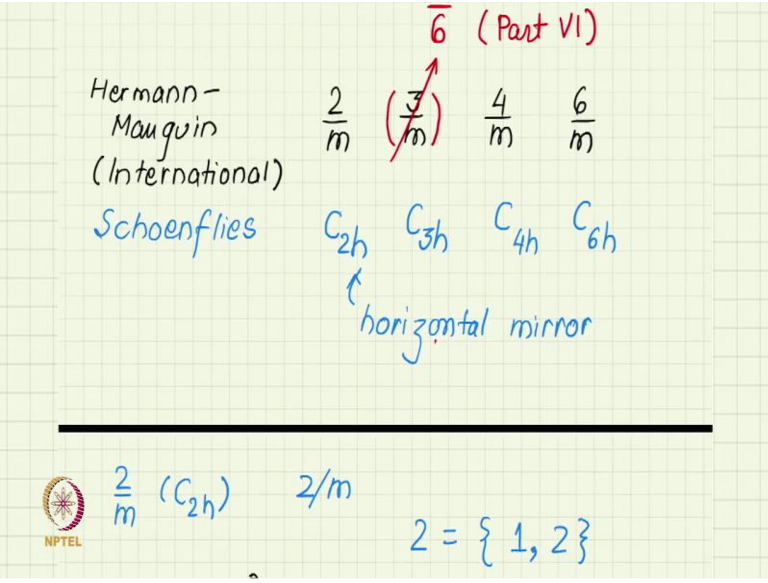

In this video, we will generate few more type 2 groups, we will generate those groups which can be represented as a combination of a mirror plane perpendicular to an n-fold axis. And we will see what happens with n is equal to 2, 3, 4, and 6. So, this is my n-fold axis, and now, what I do is to put a mirror plane not parallel as I had done it in the previous part of this series, but this time perpendicular to the n-fold axis. The Hermann–Mauguin notation for these which is also the international notation is that, if you take a 2-fold axis and put a perpendicular mirror, then it is shown as a fraction 2 by m. Similarly, we can have 3 by m, 4 by m and 6 by m.

The Schoenflies notations h, C 2h, C 3h, C 4h, and C 6h, but what we will see that 3 by m actually become same thing as 6 bar. So, there is no such notation 3 by m in Hermann–Mauguin notation, it is considered to be 6 bar, which we have already met when we were discussing the mono axial rotoinversion groups, this was discussed in part VI.

However, Schoenflies keeps the notation C 3h. So, what is considered as a 6 bar point group or a 6 bar axis is considered as a 3-fold axis with a horizontal mirror plane. So, this h, h of Schoenflies now represents horizontal mirror. So, a perpendicular mirror plane since the axis is considered to be vertical, the mirror plane becomes horizontal, in Schoenflies way of looking at it.

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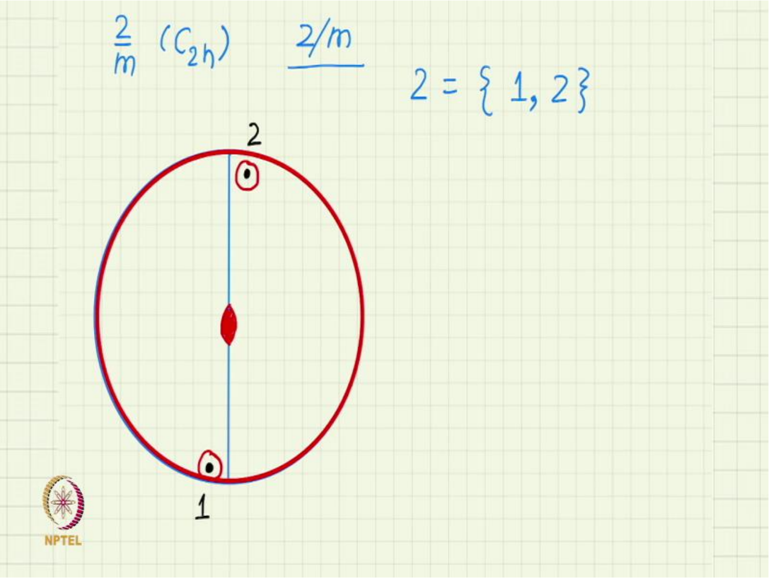

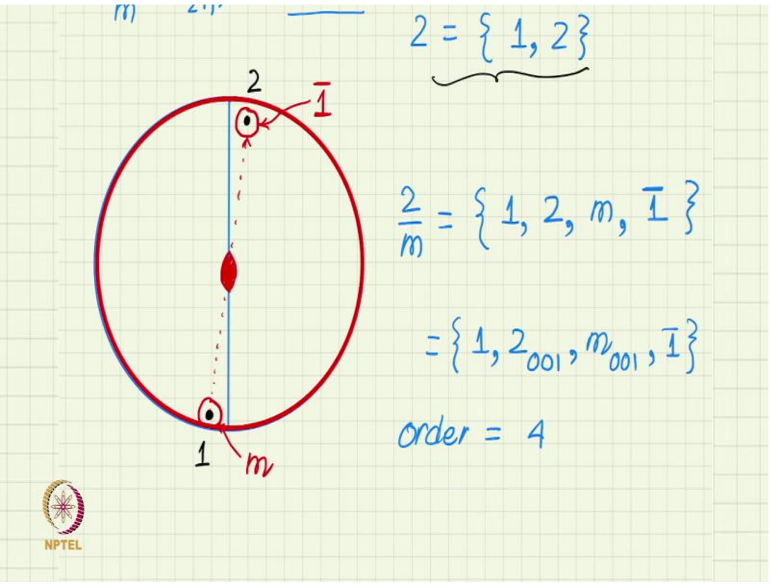

So, let us generate these groups. So, a mirror pain perpendicular to 2-fold, 2 by m or C 2h in Schoenflies notation, and these groups are also written as in a linear way as 2 by m. So, we can use 2 by m, 4 by m, 6 by m also, the international notation. So, style of writing can be different just like when writing fractions, we can write either in either way, we can in the terms of point group also we can write it in either way.

So, let us start with the point group 2, which has 2 operations, 2 general positions, but we want to add a horizontal mirror, horizontal mirrored coincides with my primitive, and it will reflect these two general positions into reflected position. So, the handedness will change. So, from black, we will now use red. And since these positions are represented as dots, are representing positions about the equatorial plane, I will now, and reflection will take them below the equatorial plane. So, now I am using open circle. So, red open circle to represent the reflected configuration.

1 and 2 black dots correspond to the operation 1 and 2 of the original point group 2. But now, we have two red open circles also. And that can be designated, this one can be designated as m, but what about this? So, you can see that that is an object of change handedness, and on the other side of this 2-fold axis. So, if I relate my original black dots to this red circle, this is related by actually an inversion centre on the 2-fold axis. So, this operation is actually inversion.

So, it is easy to write the group now, 2 by m group which has 4 operations, 1, 2, m, and 1 bar. Since there is only one mirror plane, which is perpendicular to the 2-fold, there is no need to give subscripts to define their orientation, but still if we wish to do that, we can write this as 2 oo1, that is a 2-fold along the z axis, and m oo1, that is a mirror plane perpendicular to the z axis. A group of order 4, with 2 type 1 operation and two type 2 operations.

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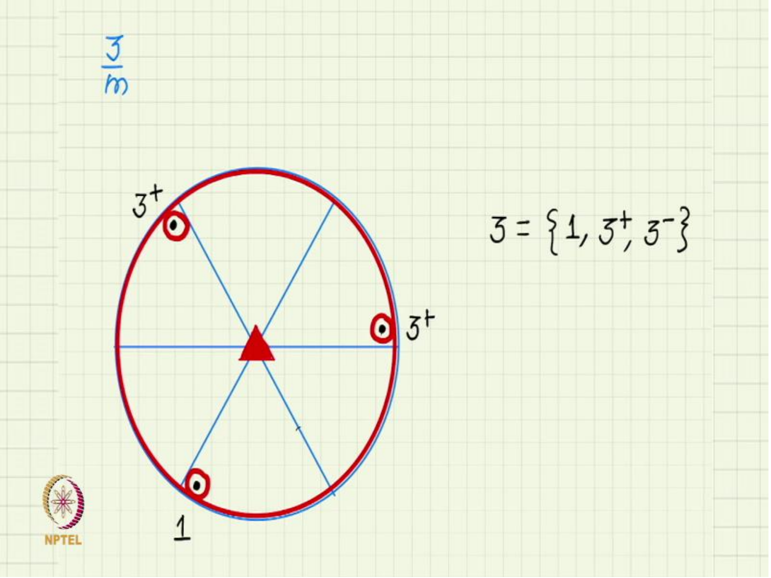

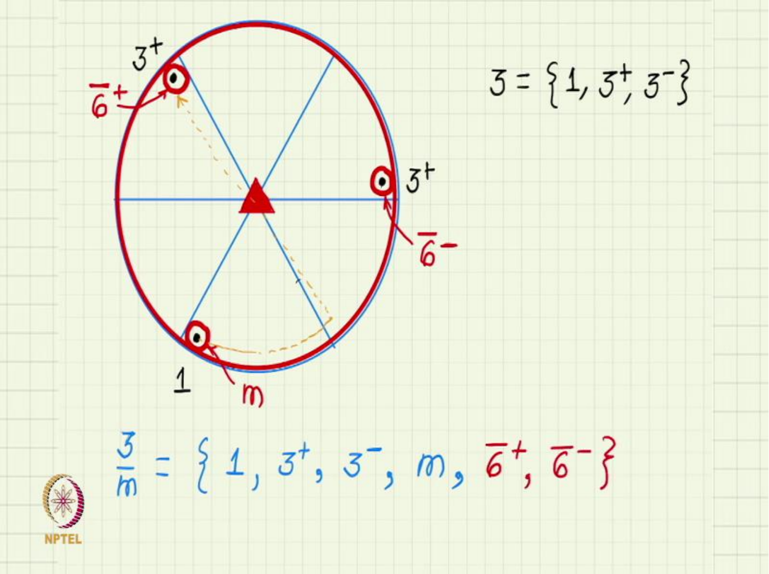

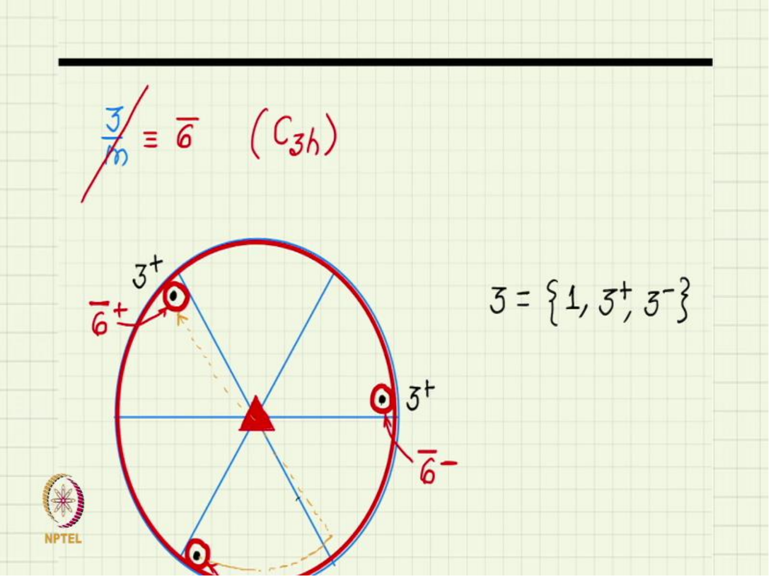

So, now let us consider the case of 3-fold, I have the point group 3, with three operations, 1, 3 plus, and 3 minus, and the corresponding three general positions. I want to develop a group by placing a mirror plane perpendicular to this 3-fold. So, I place a mirror plane along the equatorial plane. So, this horizontal plane or the equatorial plane now becomes mirror, it reflects these original objects, which were the right-handed object above the plane, into reflected counterparts, which are left-handed object below the plane. So, below represented by open circle, and the handedness changes shown by red.

So, now, I have a group of 6, I have a set of 6 general positions. So, correspondingly they will be group of 6 operations, what are the 6 operations? So, let us see, so I am trying to write 3 by m, which is 1, 3 plus, 3 minus, and I have an m, but I have two more operations. So, m was, m can be the general position is m, but what are these general positions? So, if we look at that, and if you recall what we have already said that 3 by m is going to become 6 bar. So, these 2 are actually related to the original point 1 by 6 bar. So, if I start with 1, rotate by 60 degree, that is a 6-fold rotation, and then invert. So, handedness will change from black to red, position will go from about the equatorial plane to below the equatorial plane, and I will end up there.

So, this red circle here is nothing but 6 bar plus, and this one, you can convince yourself will become 6 bar minus. So, the two additional operation in this group are nothing but 6 bar plus, and 6 bar minus. And these were exactly the operations you will recall from the group 6 bar. So, that is why in international convention, it was decided not to use 3 by m, but to use 6 bar as designation for this group, which we have already covered.

So, 3 by m becomes 6 bar. Although, Schoenflies uses this 3 by m construction for this group. And so, the Schoenflies notation is still C 3h. So, I am crossing out 3 by m. Do not use 3 by m as the designation, you can think of it as 3 by m, 3-fold axis with a perpendicular mirror plane, but you should call it 6 bar, because that is the convention.

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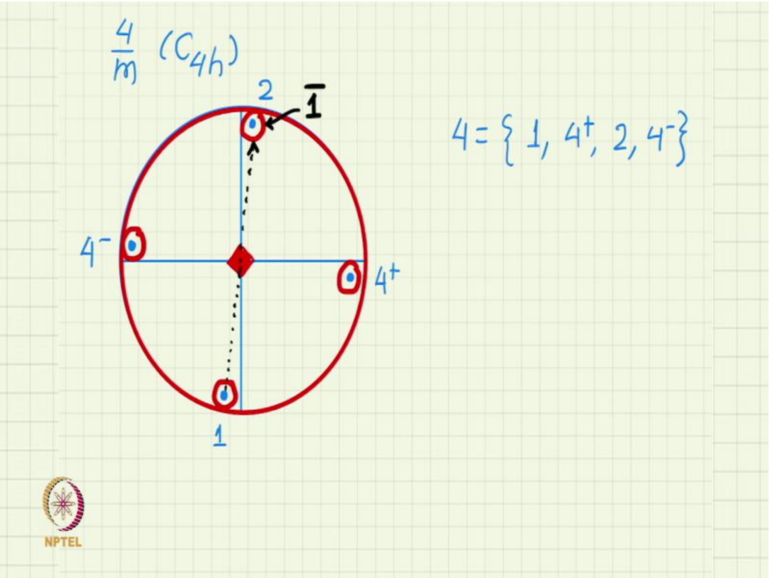

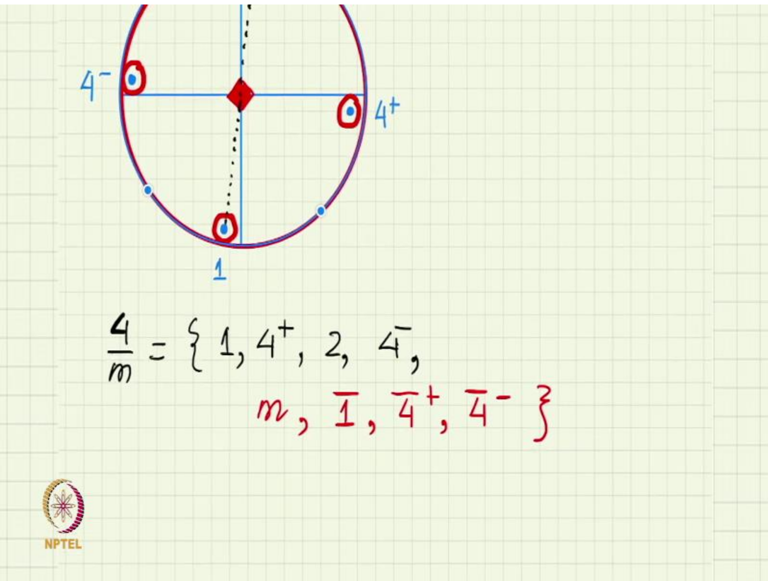

Now, we come to the 4-fold axis, we wish to place a perpendicular mirror, again the four general position of the 4-fold axis, and they will reflect into four more position of change in handedness below the plane. So, you have 8 points. And you can see here in this case, that the original blue right-handed object is converting into this red left-handed object below the plane, and that is again an operation of inversion, as we had seen in one of the previous cases. So, this is 1 bar.

So, which means, I can write the group operations using this fact. So, the group 4 by m obviously has the 4-fold axis, so, it is 4 plus, 2, and 4 minus, but now, it will also have four type 2 operations, one of them is m, one of them is also 1 bar, we have seen here. And if 1 bar is there, and 4 is there, so, the group operation requires combination of 4 plus, and 1 bar, and you know that 4 plus and 1 bar should give you 4 bar plus, and 4 minus and 1 bar should give you 4 bar minus. So, the 8 operations of this group 4 type 1, and four type 2 are these.

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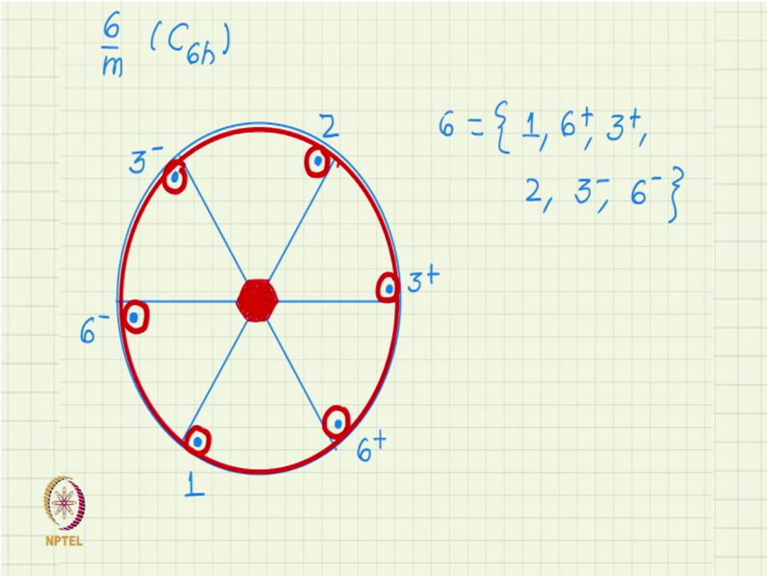

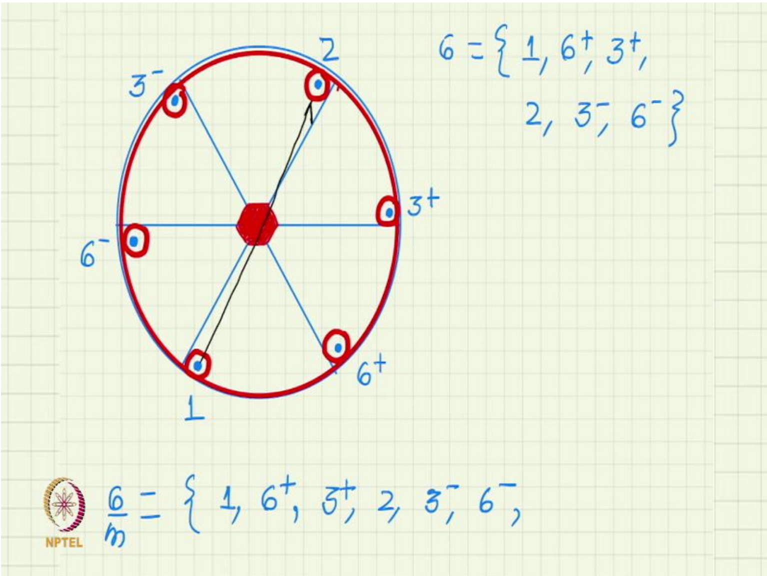

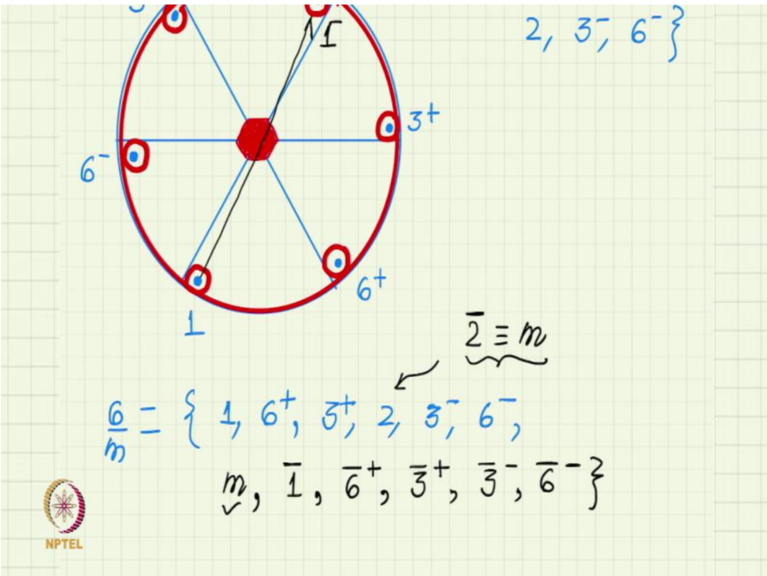

Coming out final group 6 by m. Now, you have enough practice in this kind of process. So, you can just put your horizontal mirror to a 6-fold axis, and as usual in the previous cases the number of equivalent points double up, and the number of operations will also double. So, now, you have 6 operations of type 1. So, 6 by m, 6 operations of type 1 as for the 6-fold, so, 6 plus, 3 plus, 2, 3 minus, and 6 minus. And you can see here also you generate a centre of inversion, because this point related to this circle is by inversion. And mirror anyway you had added.

So, you have a mirror who have an inversion centre, and just like I wrote for the 4 by m case, if you have 1 bar, so you should have combination of 6 plus, and 1 bar, that is nothing but 6 bar plus. Similarly, you will have 3 bar plus, 3 bar minus, 6 bar minus, so 6 operations of type 2, 6 operations of type 1.

You may notice that when combining 1 bar with these rotations, I combined 6 plus to give 6 bar plus, 3 plus to give 3 bar minus, but I did not combine it with 2, why not? Well, you can combine that will give you 2 bar, and that 2 bar is exactly as you know is m, 2 bar is a mirror plane, which I have already noted. So actually 2 is also combined with 1 bar. So, this group gives us a group of ordered 12. Thank you very much.