Symmetry and Group Theory

Prof. Dr. Jeetender Chugh
Department of Chemistry and Biology
Indian Institute of Science Education and Research - Pune

Lecture - 4
Symmetry Elements and Operations – Part 2

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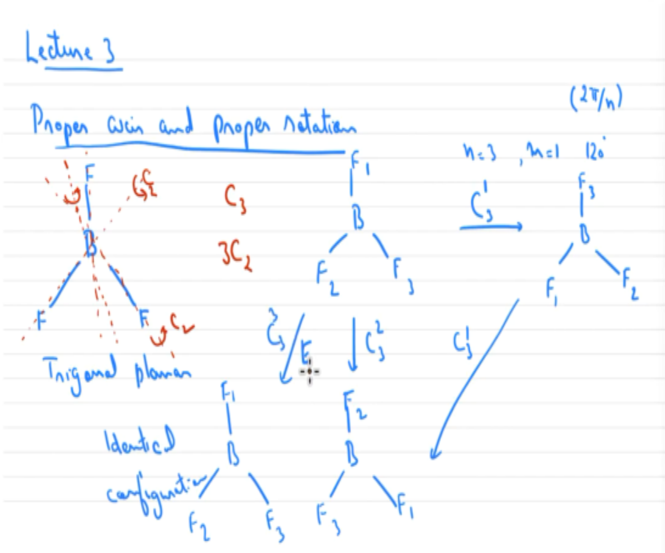

Welcome back everyone let us start with lecture 3. So, we were discussing symmetry elements and symmetry operations and in that let us continue our discussion on proper axis and proper rotation. We have seen an example of water molecule and coordinate system how C2 axis or C2 rotation affects water and Cartesian system. So, let us continue with that and let us take few more examples so that this is very clear.

So, let us take an example of a molecule called BF3. Yes, the configuration is trigonal planar molecule. Trigonal planar. Let us try to list down what all symmetry axes are present in this. So, let us first try to identify the first symmetry element or the proper axis. So, this will be perpendicular to the plane of the board passing through B. So, this is called a C3 proper axis.

And then we will see what all operations it will give. Another axis will be the one which is actually in the plane of the board and is passing through B and F atoms. So, this will be called as C2 axis. And how many such C2 axis will be present? There will be 3 such C2 axis present. So, we have 3 such B F atoms, so, we will have this C2 and another one passing through this so, 3 such C2 axes.

Now, let us see what is the effect of C3 and C2 operations on to this molecule? So, let us say if we draw this again quickly, B, F, F, F, we have 1, 2, 3. Now, we can do C3 operation, m times Cn operation m times so, n = 3 over here, and m = 1. So, if we do that, we will do a 120 degree anticlockwise rotation, because this is 2pi / n. So, what do we get over here, B, F, F, F. Now, this 1 comes here, 2 goes there, 3 goes there. So, we have so 1, 2 and 3.

Now, let us say similarly, if we do C3 operation twice, what do we get? So, instead of 120 degrees rotation, we have to do now a 240 degrees rotation because 120 is C3 ^1, so, C3 ^2 will be 240 degrees rotation, so, what do we get? B, F, F, F so, again this is rotation will be anti clockwise, but now, 1 actually moves all the way here, 3 moves all the way here, and 2 moves all the way there.

So, we have 240 degrees rotation. So, 1 comes over here, 3 over here, 2 over here, this is C3 done twice. Now, you can see that if you do C3 ^1 over here, this is also related by C3 ^1. So, if you do C3 ^1, C3 ^1, it actually gives rise to C3 ^2. So, you can see that result by yourself. So, C3 ^1, C3 ^1 gives rise to C3 ^2. So that is all C3 if you do C3 thrice, what do you get? So, let us say you also do C3, 3 times.

So, 3 times means 360 degrees rotation. So, 360 degrees rotation is 0 rotation. So, you get your molecule in identical configuration, instead of equivalent. So, these 2 are equivalent configurations so, this is equivalent, this is equivalent. Now, what you are going to get here is if you do C3 ^3 rotation and equivalent identical configuration. So, this let me write down is called as identical configuration because the atoms are actually not moving from their place. And for this reason, this is also called as identity operation, because you have not actually done any movement. So, C3 ^3 is actually equivalent to identity operation.

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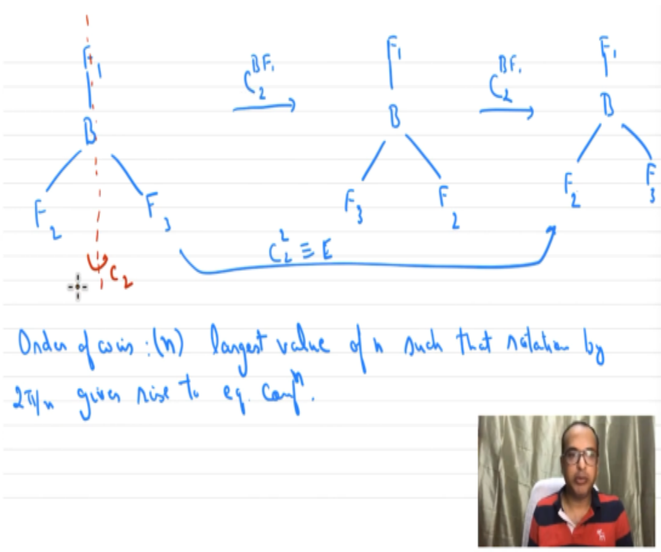

So, let us look at further let us try to do a C2 operation now, on this molecule. So, our first C2 will be in the plane of the board passing through these atoms. So, if we have 1, 2, 3 now remember anything which is lying on the symmetry element does not move so, C2 which is passing through BF1. This is just to identify which C2 we are using. Now, if B and F1 are not moving, the only atoms that will move are F2 and F3.

So, this will be 3, this will be 2, because now 2 has actually moved this side and 3 has moved this side. So, F3 is replaced by F2. Now, similarly, we can keep on doing other operations if we continue with C2 ^BF1 again we will see that we will get so, I am not moving BF1. So, what should we write here, so, this will be 2 now, and this will be 3 over here. Because again F3 will go to F2, F2 will go to F3.

Now, if you see this, if you want to go from directly from here to here, so, C2 done twice will be actually identity operation. So, identity or you can say C2 done twice. So, C2 done twice we will give you identity operation. So now, let us also see what is order of the axis? n, it is defined by n. So, it is the largest rotation so, we can say largest value of n such that rotation by 2pi / n gives rise to equivalent configuration. So, this is called as order of the axis. So, for example, this is a proper axis with an order 2. The previous one which we saw was proper axis with order 3.

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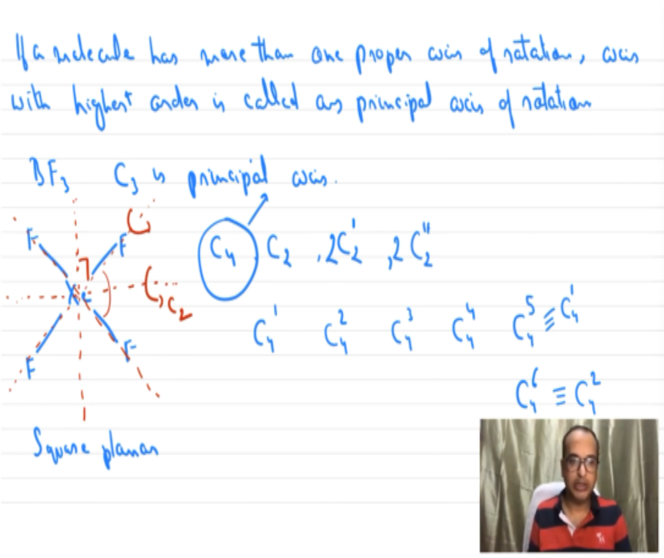

Now, if a molecule has more than 1 proper axis of rotation, axis with highest order is called as principal axis of rotation. So, in case of BF3, C3 is principal axis. So, let us see more examples so, let us go to square planar XeF4. So, what all axes it will have. So, it will have let us say 1 axis which is perpendicular to the plane of the board. So, this is perpendicular to the plane. Also, this is a square planar. So, which is perpendicular to the plane of the board this will be a C4 axis, collinear to C4 there would also be a C2 axis.

So, we will try to work it out. Now, in addition to that, if you see there would be 1 C2 axis which is actually passing through F-Xe-F bond. This will be C2' and there will be 2 such axis because there are 2 such stretches. So, there will be one more like this. So, we can write down over here 2 C2'. Then there would be another C2 which is actually bisecting the Xe-F-Xe angle instead of passing through the bonds now, it is bisecting this angle.

So, Xe F this is also a C2 so, this will be called a C2". It is just to identify or distinguish between different C2s and there will be 2 such C2". So, these are all the proper rotation axis which are present in this molecule and C4 will be called as principal axis because this is the axis with highest order. Now how many rotations each axis will give rise to, so let us try to work it out that as well.

So, C4 can give rise to C4 ^1, C4 done twice, C4 done thrice, C4 then 4 times. So, if you do C4 done 5 times this will be equivalent to C4 done once. If you go to C4 done 6 times, this will be equivalent to C4 done twice. So, it keeps on getting repeated. Now, let us actually try to work out all these operations and see for yourself.

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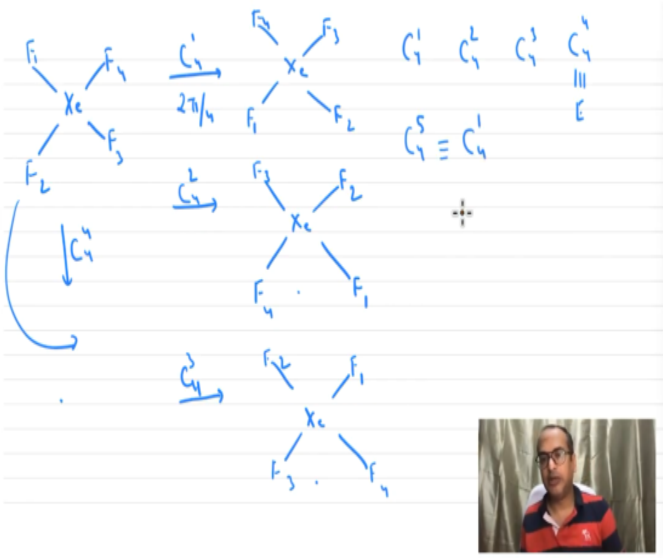

So Xe, F, F, F, F, 1, 2, 3, 4, let us quickly do C4 ^1 what do we get? X e, F, F, F, F. So, this is a rotation by 90 degrees C4 ^1 2pi / 4. So, this is 2pi / 4 rotation which is 90 degrees. So, 90 degrees anti clockwise 1 we will come over here 2, 3, 4. Now, let us do C4 ^2. So, C4 twice will be 90 degrees plus 90 degrees, so that will be 180 degrees rotation. So, 180 means that now 1 will go to its diagonally opposite position 1, 2 will go there 2, 3, 4. So again, that is 2 C4 ^3 operation. So now 3 operation means the angle will be 90 into 3, that is, this is 270 degree.

So, now 1 moves all the way to this position, 2 moves all the way to this position, 3 and 4. And now similarly, if we do C4 ^4, the rotation is 4 times so 90 degree into 4 that is 360 degree that means no rotation. So, you get the original molecule back over here. So, these are called as equivalent configurations this one would be identical configurations. So, that is why so, C4 ^1, 4 operations it will give rise to, C4 ^3 and C4 ^4, which will be going into identity.

Now, if you keep on going further C4 ^5 again you will go back to C4 ^1. So, C4 ^5 will be 90 degrees into 5 that is 360 + 90 so, 360 is cancelled out so, this will be equal to C4 ^1 operation. So, that is very straightforward to see.

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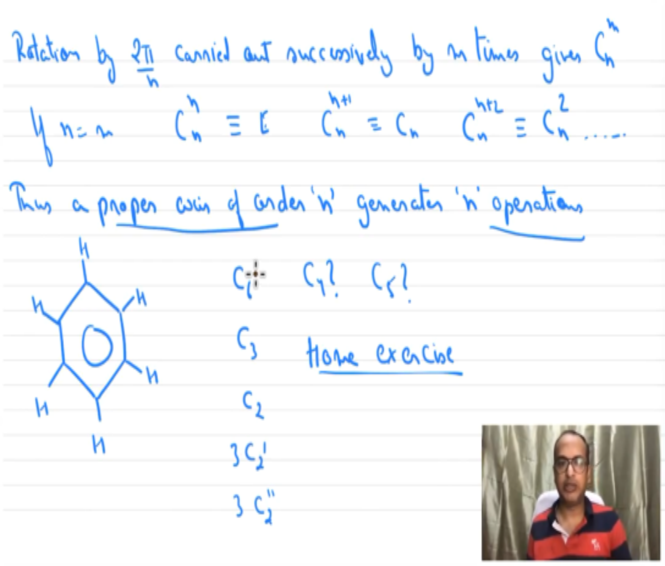

So, therefore, we can now say that rotation by 2pi / n carried out successively by m times gives Cn ^m and if n = m we get Cn ^n which is equivalent to identity and in this way if we keep on going, if we have n + 1 this is equal to Cn, if it is n + 2 it is equivalent to Cn ^2 and so on. So, thus we can say a proper axis of order n generates n operations. So, we will see later that why number of operations are important.

So, it is in the definition of mathematical groups that we are going to learn later. So, we need to understand that what are the proper axis of rotations present in a molecule and how many operations it will generate? So, this is a symmetry element and this is a symmetry operation. So, we need to know both we need to first list down all the symmetry elements, or all the proper axis of rotation for now, and what are the symmetry operations or how many operations it will generate?

So, let us take one more example to list down the symmetry or the proper axis of rotation. It is a simple benzene molecule. H, H, H, H So, I am giving you an answer try to verify the list of proper axis of rotation. So, there will be 1 C6 and also try to work out what all operations it will generate. Then you will have C3 you will have C2. These 3 are collinear to each other. Then you will have C2’, 3 such C2’s and 3C2”.

So, try to identify where these are and let us also find out if there is any C4 present, if there is any C5 present in this. And then what are the corresponding operations it will generate? So, for example, now, this should generate 6 operations, this one should generate 3 operations, 2 operations each. So, take it as a home exercise and complete this. Try to locate these axes onto the molecule and try to generate all the operations corresponding operations.

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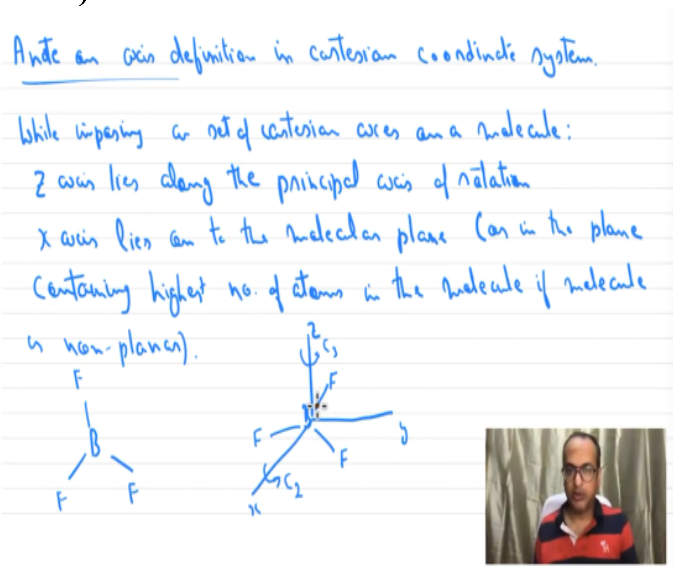

So, another important point is if you want to draw the molecule onto the Cartesian system. So, a note on axis definition in Cartesian coordinate system. So, you can say that while imposing so, sometimes it is required in this course while imposing a set of Cartesian axes on a molecule Z axis lies along the principal axis of rotation. So, you can say that if you do not know where the principal axis is, you basically you will put the molecule incorrectly in the Cartesian coordinate system.

Because, if you are not putting Z axis along the principal axis, you might not get correct results for the problems. Then X axis lies on to the molecular plane, of course, it has to be perpendicular to Z axis or the principal axis. So, we can also say or in the plane containing highest number of atoms in the molecule if molecule is non-planar. So, let us say if we want to put our BF3 into Cartesian system, how do we do that?

So, this is the right-handed coordinate system X, Y and Z. So, of course, if you have defined Z and X axis positions, the Y-axis is determined automatically by right-handed coordinate system. So, if we are keeping our molecule or the B so, we have to put it such that the C3 axis which is the principal axis lies along the Z axis. So, we will put B, F, F, F. So, this BF3 molecular plane is now in XY plane, X axis is along one of the BF bonds and Z axis is along the C3 axis. So, this Z-axis becomes our C3 axis.

X axis is now one of the C2 axes, and then these 2 F's are these 2 fluorine atoms would lie on to the XY plane. So, that is how you try to orient the molecule on to the Cartesian coordinate system.

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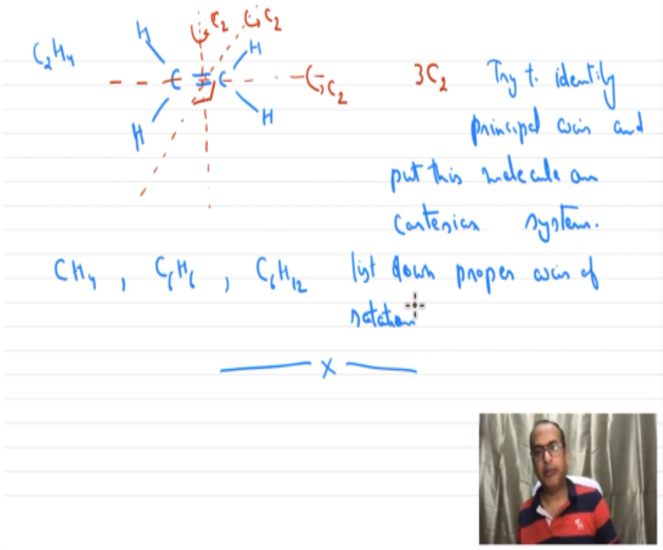

Let us take one more example before we stop, so, let us try to work out C2 H4. Where all the axes will be present in this. So C2H4 will be if you draw out the structure, it will be like this so planar molecule again. So, let us try to draw what all proper axis of rotations will be present in this. So one of them is very clear. It is passing through the C-C bond. C2 another is bisecting in the C-C double bond and the third one is actually perpendicular to the plane of the boat and through this bond.

So, it will be like, I am drawing it like this, which is actually perpendicular to the surface. So, this is third sequences so, there will be 3 C2s, all 3 will be perpendicular to each other. Now your exercise is - try to identify principal axis and put this molecule on Cartesian system, so try to do this at home. Also, let me give you a few examples to work at home. So, let us try to do CH4, then C2H4 you are going to do, then I have also given you C6H6 benzene.

Let us also try to do C6H12, both forms boat and chair. So, cyclohexane both the forms and try to see what all list down proper axis of rotations, and then find the principal axis and put the molecule on the Cartesian system, see if you can do it. So, I think that is all for today. So, let us continue our discussion on symmetry elements and operations. And we will start with the symmetry planes, that is all for today.