Symmetry and Group Theory
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Module No # 03
Lecture No # 11
Tutorial-2

So, I hope you are having fun with the course so far. So, in this tutorial we will be discussing how to orient the molecules, we will look at some complex molecules. I know we have already discussed the rules and all how to orient the molecules in Cartesian coordinate system. But we will take at least 2 examples which are little bit cumbersome to orient and then we will see what all precautions we have to take. Because once you put a molecule correctly in Cartesian coordinate system, the rest of the job like applying symmetry operations and becomes easier.

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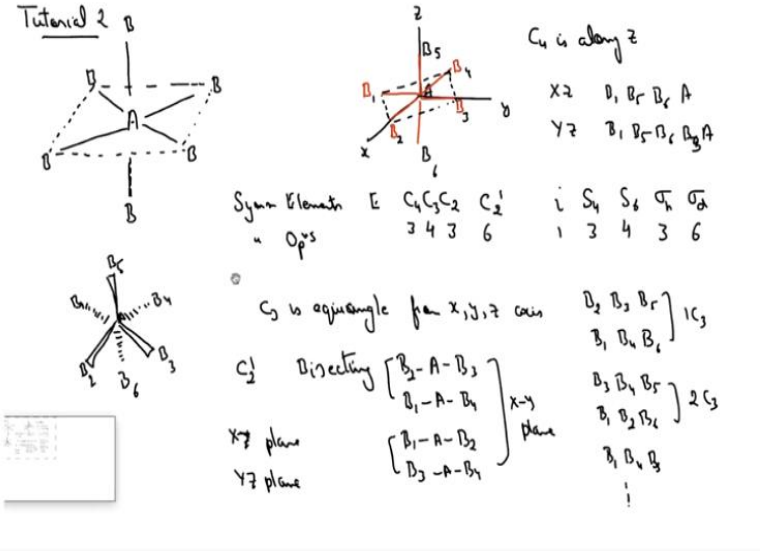

So, let us start with second tutorial. So, let us discuss, this I have already given in home assignment, but let us discuss this case. Because the next molecule will be comparison to this particular case so let us discuss octahedral case. So, to draw octahedral, I will draw it as a rectangle, something like this, where at the vertices I have 4 B atoms and these are my A B bonds. And then there is one B above the plane and one B below the plane. So now this is my X Y Z so this particular molecule is rather straight forward, it looks complex but it is straight forward in the sense that the A goes in the center.

And then you have B on the top and B at the bottom, those are, let me draw the bonds with different colors. And the other B, one of the B's will be on to this axis and other B will on to this axis, right. And all the bonds and this is the rectangle ('rectangle' incorrectly spoken as 'triangle' in the video) which we have drawn here so it is something like this. So, my principal axis is C4 axis which is oriented along z axis. So C4 is along the z axis, and then the X-Z plane as to have the highest number of atoms.

So, in this case Y-Z and X-Z plane would have equal number of atoms so this is my X-Z plane along which I have four ('four' is incorrectly spoken as 'three' in the video) B atoms, right. So, if I mark it as 1, 2, 3, 4, 5, 6 my X-Z plane contains B2, B6, B4, B5, and A (incorrectly written and spoken as B1, B5, B6, and A), right. And similarly, Y-Z plane contains Y-Z will have B1, B5, B6, B3, and A. So, X-Z and Y-Z plane, in this case, contains equal to number of atoms but if there is any confusion, X-Z plane should contain more number of atoms as compared Y Z plane, if there is discrepancy here, okay.

So, this is rather easier and while we are at this molecule let us also list down the symmetry elements and corresponding operations right. So, what are the symmetry elements present the first and foremost is E, followed by C4 (this is C4 which is along Z axis). Now, also C4 will also have there would also be a C2 along this then there would be C2 prime, C2 double prime.

So, C4 is along Z axis, now C2 is also along Z axis. C2 prime this will be perpendicular to Z axis so it will be either X or Y so there will be two C2 primes, right. Then similarly there will be how many C2 double prime so C 2 double primes which is bisecting the X-Y axis. So, there would be two C2 double primes, and there would be i. Then we have let us we will do this counting I am just counting from the top so we will do this counting again.

So, we will see will have S4, then S6 will be there and there will also be a C3 we will see where the C3 is, how many C3s are there. S6 is there, sigma-h is there, and sigma-d is there, right. Now let us try to count how many such axes are there. So, one of the C4 is along Z axis. Similarly, another C4 will also be along X axis and Y axis. So, there will three such C4 axis now about C3 where is the C3 axis.

So, if you try to draw this molecule in a way where you can so this is my A this is B, B, B and this is not all Bs in plane. So, all the three Bs are coming actually out of the plane of the board and these Bs are coming at the back going at the back so behind the plane of the board. So, this how my C3 now my C3 will be perpendicular to the plane of the board. So if you see I am looking through my X Y Z so each of this is X Y Z and I am looking through it, right.

So, if you see that my C3 is actually equi-angle, so C 3 is equi-angle from X Y Z axis, okay. It is somewhere in the middle of X, Y, and Z axis. So, I am looking at B2, B5, and B3, so this is my B2, B3, and B5. And at the back is B1, B4 and B6. So, I hope you can easily see this okay. So how many such C3s will be there now. So, you have to find such triplets so you have one such triplet then you have B3, B5, B4 another triplet and then you have B1, B5, B2.

So, you have to keep on counting all such and then you will see that there are, four such C3 axis okay. So, if you want you can list it down so you have B2, B3, B5 so you are passing through this and you are also passing through rotating B1, B4, B6 this is one C3. Now second C3 will be if you let us say if you count B3, B4, B5 so if you count this B3, B4, B5 the rest of the 3 will be B1, B2, B6, you will be rotating this. This is my second C3, okay.

Now third C3 can be now B1, B2, B6 is done. So, it can be B at this pack so B1, B4, B5, okay and so on. So, you can count that there will be 3 and then four C3 such axis. Now C2, which is along Z axis or which is co-linear with C4. So, if there are three such C4s, then there will be three such C2 axis, okay. About C2 primes, so C2 prime will be along X axis and along Y axis if we are considering the flipping of B5 and B6, okay.

So, we can say that one of the C2 prime is along B2. So, C2 prime is B2-A-B4 the second is B1-A-B3. Then there would also be another one which is along, no this is the C2 prime which we are talking about, right. So, no I think there is some mistake. This would be altogether six C2 primes. So, C2 primes, let us list them down. So not these ones, because these ones are actually this C2s, which are collinear with C4s so we are not talking about these ones.

So, you have C2 primes, which are now in-between the bonds. So, which are the six C2 primes? So, you can see that it is B2-A-B3, bisecting B2-A-B3, this angle, then at the same time this will

also be bisecting B1-A-B4, okay. And it will be flipping B5-A-B6 or B5-to-B 6, okay. So, this is one. Now let us also find another such pairs. So, you have B1-A-B2, B3-A-B4, so these are the angles which this C2 prime is bisecting.

Now this is one, this is one, similarly you will have one going in X-Z plane. So, this was in X-Y plane, both of these are in X-Y plane, right. So similarly, you will find 2 pairs in X-Z plane and 2 pairs in Y-Z plane, right. So, that gives you six such C2 primes. i is only one, S4 will be equal to the number of C4 axis if you have three C4s, you will have three S4s. S6 should be equal to number of C3 axis. So, if there are four C3 axes, so there will be four S6 axes. Sigma-h, so you have X-Y plane as the sigma-h, then Y-Z plane, and then the X-Z plane.

So that means there will be three such sigmas. And sigma-d's will be now collinear with co-planer with C2 primes. So, if there are six C2 primes, you have six sigma-d's, right. So, I hope I have not made it more confusing but I would suggest you to work out this example again by yourself so that it is very very clear.

Now, let us go to even difficult molecule then this one. It is not well the molecule is not difficult it is just that it is visualization is sometimes more cumbersome.

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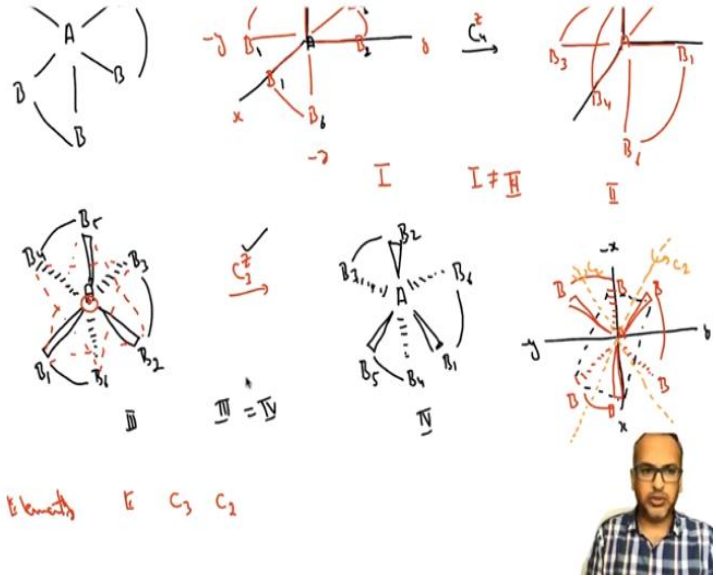

So now let us see that I have same molecule A the central metal or the central atom has the similar octahedral symmetry. But now I have these two connected with bonds, okay. So now the

case is not as simple so now if you try to draw this molecule again in the same fashion it will not work. So, if I am trying to draw it like this and then I am saying that I have connected these then it will not work, okay. This is my X, Y, Z, – Z, – X, – Y, alright.

So, let us say that this is a so now what are the symmetry elements can you identify the symmetry elements are? So, if you look at the octahedral case, we had E, so E will still be existing. C4, which was collinear with Z axis, or X axis, or Y axis cases to exist. Because if you try to do a C4 rotation, this particular B comes here so let us number these 1, 2, 3, 4, 5, and 6. So B3 goes to B1 if I do a C4 axis and B1 goes to B2 right. Now if you do that let us try to do this operation C4, okay. Let us see. So, we have A so now I have B1 here and my B3 comes here, okay, and what happens to B2?

B2 goes here and now B2 and B3 are connected, right. And what happens to B4? B4 comes here, right. And my B5 and B6 remain as such because this is C4 along Z axis. So, B4 was connected to B5 and B1 is connected to B6, okay. Now you see that these bonds, if I do C4 rotation, these bonds make these 2 configurations different. So, I can say that 1 is not equivalent to 2 right. Whereas in case of octahedral, because these bonds are not there, so 1 and 2 are equivalent so that is where C4 exist.

In this particular case C4 does not exist. So, if I cannot have C4 access which is my principle axis in octahedral case. So, in this case what is my principal axis. So the next order axis was in that case it was C3, right. So, let us see if the C3 axis exist. So, let us try to draw this molecule in the way so that we can easily draw a C3 axis. So, we have A B, so this is B5, then I have B1, we have B2, okay so I am looking from center of the X Y Z side okay.

And at the back I have B3, B4, and B6 and now what all have joint B1 B6 is joined, B4 and B5 are joined, B3 and B2 are joined. And now my C3 axis is perpendicular to this plain of the board going through these triangles okay going through this imaginary triangle equilateral triangles okay. There are 2 such triangles making a star like appearance. Now if I do a C3 axis so we want to see whether C3 axis exist or not.

So, because we are trying to find out what is the principal axis here so if I do a C3 operation what do I get? We have to also carefully see if the bonds remain at the same positions. These will remain at the same positions but if the bonds are also seen. So, this is my B1, so B1 goes here B2 comes here, it is an anti-clock wise rotation with 120 degrees and B5 comes over here. Similarly, B6 goes here, B3 comes here, and B4 comes here. Now original connection were B4 to B5, okay then B1 to B6, okay and B3 to B2, okay.

So now if you see that the bonds are also at the same position so I can say that my configuration third and fourth are equivalent right. So, then I can say that C3 is existing so that means my C3 is the principal axis. Now the rules of a assigning the molecule to a coordinate system says that you have to align your principal axis to the coordinate system right. So now how do I assign this molecule so that would mean that this is not a correct representation of the molecule along the coordinate axis, so this is not the correct way okay.

So, what is a correct way then the correct way would be if you draw this molecule that my Z axis is along C3 axis. How do I draw my Z axis along C3 axis? So, if I am looking from the top, something like this this is my X, Y, –X, –Y, and this is at the original central atom. Now X-Z plane should have more number of atoms as compared to Y-Z plane or any other random area. So, then I will draw one of the bonds which is coming out of the plane of the board as along X-Z. So, this is my 1 bond this is second B, this is third B, right.

Similarly, the opposite end will have one B, second B, so if you want to draw the same triangle or same rectangle which was drawn here. So, these are the 4 atoms which are forming the rectangle and these are the 2 opposite atoms and where are the bonds which are connecting, so these are the 4 atoms which are forming the rectangle and these are the 2 opposite atoms. And where are the bonds which are connecting so these are the bonds which are connecting (21:06).

So, if you orient the molecule like this, you should be able to find out what are the other symmetry operations. So, for example now C3 axis is along Z axis which is clear so that makes my principal axis, so what are the symmetry elements? I have E, then I have C3, then what else I have here. How many C3 axis, are there that also we can see how many C3 axis will be there?

There will be one C3 axis, okay. And then you have C2 axis and that will be all. Where is the C2 axis now?

C2 axis will be, so if I C2 axis will be in between XY. This will be my C2 axis. Similarly, there will be another C2 axis which will be like this, right. So that means I am reflecting this B with this B okay and if I am doing this one then I will be reflecting these two B's and these two B's and then these to B's. So, let us try to work it out let us draw this molecule and see how the C 2 axis works actually because otherwise it will remains as confusion.

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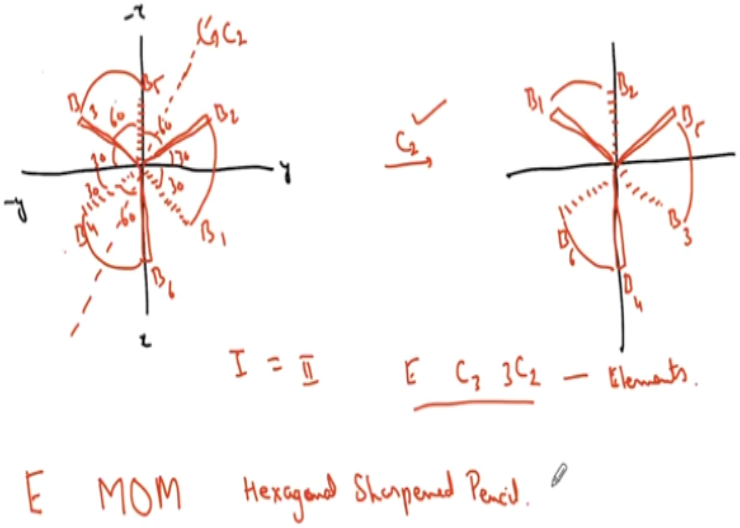

So, let me draw this molecule again this is my X, –X, Y, –Y and the molecule looks like this. You have A B so these are all 120-degree angles excuse me for the bad drawing. Then we have B now if I name them so you have 1, 2, 3, 4, 5, 6. Let me now draw a C2 axis which is bisecting B4 and B3, and B1 and B2 okay. So, if I do this will actually be a let us draw this molecule again may be, because the angles are not appearing correct.

So, let me just draw it again. So let us be more careful in drawing. X, -X, Y, -Y, so you have okay I will try to keep this angle as 30 degrees then we have and these are wedge like projections, okay. And this one would also be like 30 degrees. So, this angle is 30 degrees this angle is also 30 degrees, this is 60 degrees, 60, 30, okay. So now this is my these are my B's this looks better than what it was earlier so we have B 1, 2, 3, 4, 5, 6, okay.

Now, where is my C2 axis? So, C2 axis will be reflecting B2 and B5. So, let us also first connect the bonds. So, B3-B5, B1-B2, B4-B6, let us say these are the one's which are connected. So, if I now do a, this reflection then my B2 B5 will be replaced B1 B3 will be replaced and B4 B6 will be replaced, okay. So then if I do this, I will still have it so we have to see if the bonds are also reflected accordingly. So, this is my B now I said B2 B5 will be reflected so B2 and B5, then on doing C2, B4 and B6 will be reflected. So, B 6 goes to be 4 and B1 is replaced with B3.

Now the original connections were B1-B2, B3-B5, and B4-B6. So, my bonds are also in the same place. So, I can say my first is equivalent to configuration 2, so that is how C2 will be reflected C2 will be existing. So, the only elements in this particular case will be E, C3, and C2. And there will be one such C3, and three such C2 elements. We can of course find out what are the number of corresponding operations? But we can see that there are three such C2's. See one is between –X, Y, –Y, X.

Similarly, another will be from this side, and third will be from using the Z-axis as the plane, right. So, there will be three such C2s present, okay. So that reduces a lot of symmetry elements as compared to the octahedral molecule. Once we join these atoms with bonds, the octahedral group reduces to a very small number of symmetry elements, we will see what are the point group and all.

But let us not go into those details. So, I hope the visualization which is very important for this course is now clear to some extent. We should be also practicing lot of molecules, pick up any molecule, look out any object around you. And try to find out what are the symmetry elements and symmetry operations. I will give you some examples. For example, try to find out for letter E what are symmetry elements present try to find out for the word MOM, ok what are the symmetry elements present.

It is a 2D picture let us say. Try to see for example hexagonal sharpened a pencil, okay. Try to see what are the symmetry elements and then operation present. So, pickup any object around you and see which has some symmetry, see what are the symmetry elements present? So that this particular concept of visualization is very very clear in your heads okay otherwise it will keep on

getting accumulated and you will face a lot of issues in the later part of the course okay. So that will be all. Any questions, please shoot me an email thank you.