Symmetry and Group Theory

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Lecture-06
Tutorial – 1

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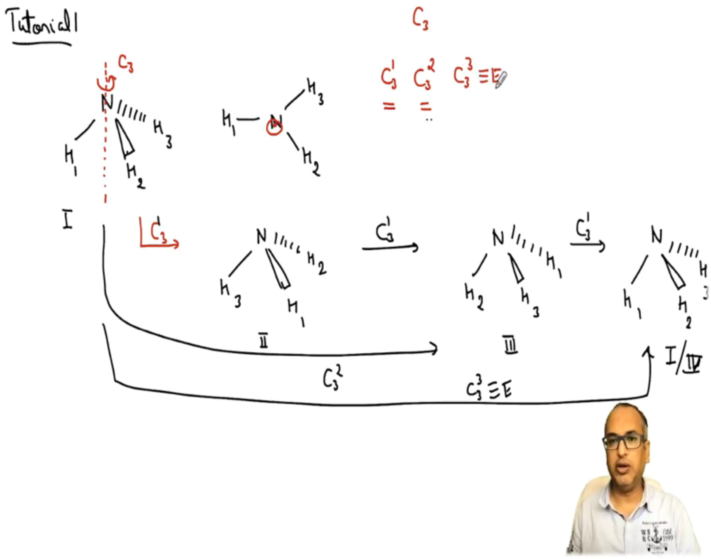

So far we have learned how to identify the proper axis of rotation and symmetry planes as the symmetry elements in different types of molecules. So, in this tutorial I will show you how to work out different or how to identify and locate different symmetry elements only including symmetry planes and proper axis of rotation. So, let us start with today's tutorial. So, let us look at this molecule which is a very simple molecule, which we have been looking at, which is ammonia.

So, you have NH3. So, this particular proton and nitrogen are in plane, this proton is coming out of the plane of board, and this proton is going behind the plane of the board. So, now, if I see what different types of proper axis of rotations are present, I can also draw this as, if I am looking from the top, it looks something like this. So, that helps me identify that there is a so, here I am looking from the top. So, now, if you see that there is a proper axis of rotation with C3 order with n equal to 3, which is actually perpendicular to let me choose a different color.

So which is perpendicular to the plane of the board, if I look from the top or otherwise, you can say that this is my C3 axis. So, this is I can write this as C3. So, in other words, either way we can we should be able to identify, and this is the only proper axis of rotation which is present in this molecule. So, the operations corresponding operations will be C3 to the power 1, C3 to the power 2, and C3 to the power 3. So, this comes out of C3.

So, now, C3 to the power 1 is an independent operation, C3 to the power 2 is an independent operation, but C3 to the power 3 is actually equivalent to E, so, why we say that? So, this is very easy to see, if we do C3 on this, let us do C3 on to this, what do we get? And all the rotations will be anti-clockwise. So, you have NH you do get equivalent configuration, but the numbers are going to be shifted now. So, 1 moves to this position, 2 moves to this position, 3 moves to this position.

So, this is C3 to the power 1. Now, I do C3 again. So, I can say that my, this operation will be C3 to the power 2. So, again I will get the H, H and now 1 moves here, 2 moves here, 3 moves here. So, this is C3 square, which is, so if I call this molecule as 1, this conformation or configuration as 2 this configuration as 3. So, 1, 2 and 3 are equivalent configuration not identical. So, if I do C3 one more time, what do I get? I get 1 here, 2 here, and 3 here.

Now, if I do this, this will be my C3 cube operation. So, this is C3 ^1, C3 ^1 on this C3 ^1 on this, 2 times C3 done so, this will be called a C3 square, 3 times C3 done so, this will be called as C3 cube. Now, if you notice this one, this one has same orientation of hydrogens as in this one. So, I would call this as identical configuration. These 2 are equivalent to 1 whereas this one is identical 2. So, then I say that because this is an identical configuration this particular or let me call it as fourth. So, fourth is an identical configuration to 1.

So, I would say that C3 cube is actually equivalent to doing nothing, that is doing identity operation. So, in this case, if we list down the operations from C3, this will be C3 and C3 square which are independent operations, and C3 cube will not be an independent operation will be equal to identity.

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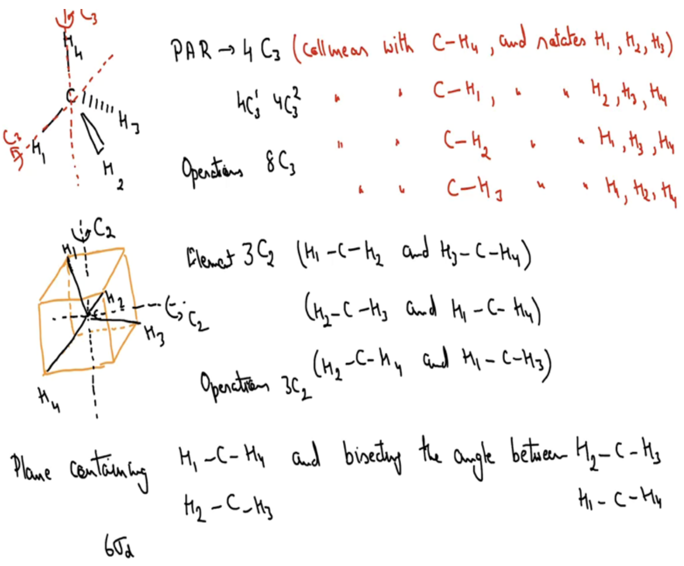

Now, let us go to a little more complex molecule where we have more, before we actually do that, let us also see what are the symmetry planes present in this. So, let us draw this molecule again the same fashion. So, 1, 2, 3. Now if you notice that there is a plane, which contains this nitrogen and hydrogen, and this will be bisecting the angle, which is H2-N-H3. So, I would draw this as plane of the board and call it as sigma V1. Now, if I am looking at the molecule from top, I can say I can draw it like this, it is very important to understand it correctly.

So, this is 1, 2, and 3. And now my plane is the one which is now I am looking from the top so my plane would appear as a line to me. This plane If I am looking from the top this view then my plane would appear as a line to me. And now this plane would contain NH 1 and we will bisect this angle H2-N-H3. So, this will be called as sigma V 1. Similarly, there will be a sigma V 2. So, sigma V1, sigma V2, sigma V3. These are the symmetry elements or symmetry planes present in ammonia.

Now, let us move to more complex molecules and look at the proper axis of rotation and planes. So, again we have discussed this case, but let us discuss in more detail so, that it is very, very clear. 1, 2, 3 4. So, now, what are the symmetry what are the proper axes of rotations present. So, proper axis of rotations there will be one C3. How many C3s will be present? So, let us try to draw it. So, if I try to see that there is a C3 axis passing through C-H4 which results into rotation of H1, H 2 and H3.

So, this is collinear with C-H4 and rotates H1, H2, H3. So, let us call this as one C3 axis. So, this is my C3 axis. Similarly, I can have a C3 which is passing through C-H1. So, I will say that there is another C3 which is collinear with now C-H1 bond and now this will rotate the rest of the 3 hydrogens which is H2, H3, and H4. So, this should be very easy to see now, this is my second C3 and this will be rotating anti clockwise and so, H2, H3, and H4 will be rotated now.

There will be another C3 which will be passing through C-H2 and rotates H1, H3, H4. Similarly the last one will be collinear with C-H3 and it will rotate H1, H2, H4. So, this is there should not be any problem in now locating the C3 axis. So, there should be 4 C3 axis independent 4 C3 axis, now, each of the C3 will give rise to C3 and C3 square operation we have seen that in case of ammonia.

So, this will lead to operations if we list on the operations due to C3, there will be 8 C3 operations because each of this there will be 4 C3 ^1 operations and 4 C3 square operations, remember that C3 cube operations will be equal to identity. So, that will not be counted. So, you will have 4 C3 elements and 8 C3 operations. So, now, let us look at is there any other proper axis of rotation in this? So, let us see what all we have.

So, there is one C2 axis, I mean not one, there are 3 C2 axis but let us see, how do we identify or how do we locate C2 axes in this one. To be able to locate see 2 axes and this one, it will be easier if we draw the molecule like inside the cube. So, let us draw this molecule inside the cube. Excuse me for the bad drawing of cube. So, now in the center of this cube, where the four diagonals will meet, this will be carbon atom, and my 4 hydrogens will be oriented along the vertices.

So from carbon to hydrogen like this, and there will be 2 hydrogens which will be meeting with each vertices. So, now, I should be able to identify the C2 axis. So, C2 axis will be present perpendicular to this top face of the cube like this, this will be going if I am going through carbon, so, let me draw it correctly. So, this will be something like this and passing through this.

So now, this is actually bisecting which angles, so if I label this as 1, 2, 3 and 4, so this C2 is bisecting H1-C-H2 angle and simultaneously it will also be bisecting H3-C-H4 angle. So, this is one C2 axis. Now, let us see if we have any other C2. So, if we carefully see that there is this particular face. So, there is one C 2 which is going through this face. So, the horizontal face. This is my C2.

Now this will be bisecting H2-C-H3 angle and on the other side this will be also bisecting H1-C-H4 angle. Now, there would be one C2 which is going from the front plane, center of the front plane to the center of the back plane passing through carbon atom. So that will be bisecting the H2-C-H4 angle and H1-C-H3 angle. Now, if you carefully notice that all 6 carbon hydrogen angles have been listed here, so that means there is no other possibility of listing another C2.

So, that would mean that there would be 3 C2 axes and each C2 gives rise to 1 C2 operations. So there would be 3 C2 operations. So, if we say that the operations it will be 3 C2 operations elements. It will be 3 C2 elements and 3 C2 operations. So, this tells you how your C2 proper axis of rotation will be oriented. Now, let us look at the planes in this particular molecule where the planes will be and how many planes will be there.

So, now if we try to list down the planes, we will see that there will be plane containing H1-C-H4 and bisecting the angle between H2-C-H3. So, there would be a plane which will contain H1-C-H4 this one and it will bisect this angle. So, now if it has to contain one particular angle and bisect the other angle and there are 6 such angles that means there can be 6 such planes, it will contain one of the angle and it will bisect opposite so for example if I am saying that it is containing H1-C-H4 this one over here.

So, if I am saying that it is containing H1-C-H4 angle over here. And it is bisecting H2-C-H3 then I can say that there would be one plane which will be actually containing this and bisecting this. So, vice versa it will be so let me mention that so this the second plane will be containing H2-C-H3 angle and bisecting H1-C-H4 angle. So, same way if we list on all 6 angles, there would be 6 sigmas present and these will be called as dihedral planes because these are bisecting the angles.

So, 6 Sigma d is will be present in this molecule. So, we are only listing down the symmetry planes and proper axis of rotation in different molecules. So, this is for tetrahedral molecule.

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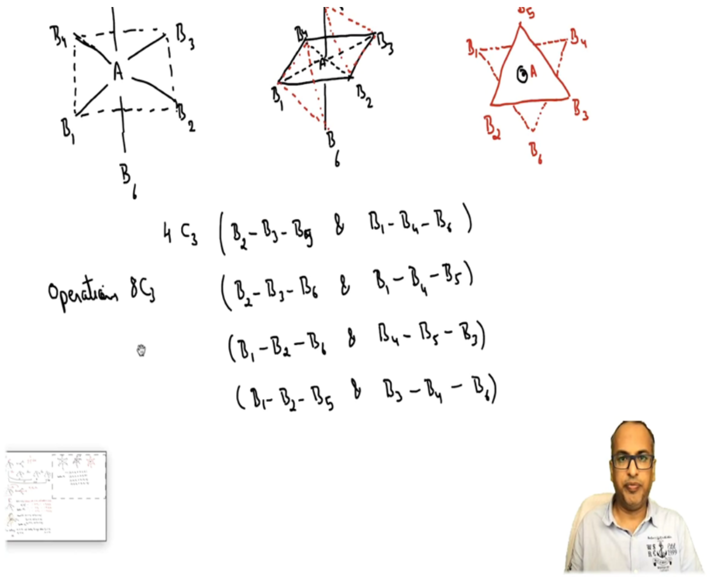

Now let us go to even complex molecule which is octahedral molecule, because there are number of elements and operations are huge in that case. So, let us list it down. Let us first draw the molecule. So, let us see, let us draw a generic molecule. Now all 6 bonds in this case are equal. Because this is an octahedral molecule and then how do we get a sense of where it is, so let us draw this draw a plane around these 4 B atoms.

So that we know that these 5 atoms are forming one plane and then this particular atom B and this B is actually coming out of the plane and this is going below the plane. So let us say if I am drawing it like this, it looks like this. So, in another words, if I try to draw it in a 3d projection, it looks something like this. So, you have at the center is A and then you have 4 B atoms, this is another way to draw. So, drawing is very, very important, because you need to understand the 3D conformation of the molecule.

Otherwise, you will not be able to draw the or write down the symmetry elements or symmetry operations present in this. So, let me also list down. Now, another way to look at this molecule is, which is very interesting. So, if I am looking from this side. So, just see that this B 5, so, if I connect B5, B3, and B2, it forms the face of an equilateral triangle. Similarly, B1, B4, B6 also forms the face of an equilateral triangle.

So, if we look via equilateral triangles keeping equilateral triangles on the front face and then how the molecule looks like. It will be interesting to see that these are the equilateral triangles that we have drawn. Now, this one is at the top because from we are looking from the side. So, you have B5, B3, and B2 and the one which is here is actually it looks like a star if you now see and the bottom is B6, B4 and the side is B1 and the center of these 2 triangles will be atom A.

So, now, it will be very, very easy to identify C3 axis of rotation. Now, if you see that there is a C3 axis which is passing through the center of these triangles these 2 triangles formed by B2, B3, B5 and B1, B4, B6. So, that way we can say that there is one C3 axis. Similarly, how many now, if we try to identify how many C3 axes are present, so, that will depend on how many equilateral triangles can we make out of this.

So, similar to B5, B3, B2 and B1, B4, B6 we can also make with B5, B2, B6, and look from the other side, this side. No sorry not B5, B2, yeah B6 we can make it as B2, B3, B6 the interesting side and this one. So, if we let us try to count how many C3 axes will be present, so, there will be 4 such C3 axes. So, let us try to list them down. So, let us try to list to the faces of the triangle that are formed by B atoms.

So, one is B2, B3, B5 and B1, B4, B6 what are the other triangles which can be formed here. So, the other triangle is B2, B3, B6 instead of top we can now go to the bottom and the second phase this will be B1, B4, B5. So, these are the 2 this side. Now similarly, we can go from the side that will be B1, B2, B6 and the corresponding at the back will be B4, B5, B3. Now, also B1, B2 will be forming another triangle with B5. So, B1, B2, B5 and B3, B4, B6.

So, these are the 4 C3 axes which will be present, can we see did we miss any other axis? I guess no, because we have covered all possible combinations. So, 4 C3 axes and thus operations will be, number of operations will be 8 operations, remember each C3 will give you 2 operations. So, 4 C3 axes will be 8 C3 operations. So, that is for C 3.

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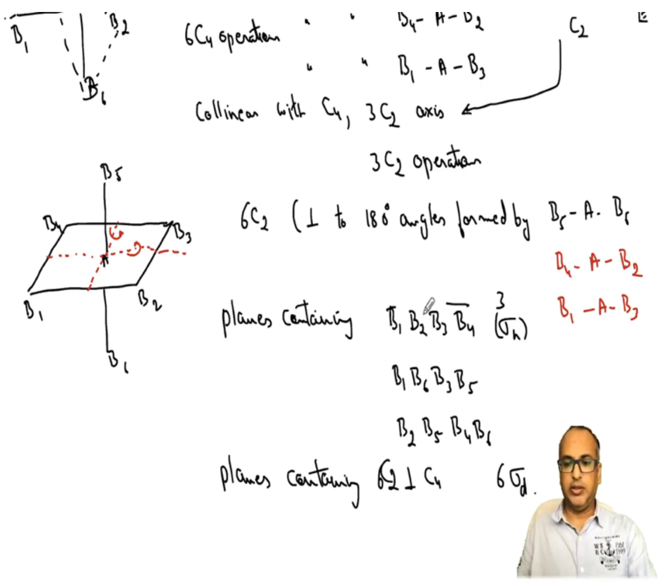

Now, let us see what else does it have that draw this molecule again? Now, there would be a C4 axis. So, C4 axis will be oriented along opposite B-A-B. So, that is the B-A-B which is making 180 degrees angle. How many such B-A-Bs are there? There are 3 such B-A-Bs. So, let us keep the same nomenclature 1,2,3,4,5,6, we have 1,2,3,4,5,6. So, this is the one which is collinear with B5-A-B6.

Then we have collinear with B4-A-B2 and there is one which is collinear with B1-A-B 3. So, there are only 3 such options, because there are only 3 such bond pairs which have 180-degree angle, others will have a lesser angle so, that will not be a C4 axis. So, now, if you do a C4 operation, it will be like this. So, this is my C4 axis, so, B1 will be replaced with B2 and so on. Similarly, if I am doing C4 operation along this axis, the rotation will be between B4, B5, B2, and B 6.

So, this will be forming as a plane and this will be my rotations C4 rotation. Now, same way collinear with C4, there will be 3 C2 axes present. Now, each C4 will give you how many operations, 2 operations. So, C4 will give you 6 C4 operations. And well this will actually give you because C4 will be one operation, C4 square will be equivalent to C 2, which is listed this one, because this is the collinear axis, then you have C4 to the power 3 as an independent operation C4 to the power 4 will be equivalent identity operation.

So, eat c 4 will give you 6 operations 6 C4 operations and collinear with C4, there will be 3 C2 axes which will give you a 3C2 operations. Now, what else any other proper axis of rotation yes, there are 6 more C2s. What are those C 2s, any ideas? So, let me draw this molecule again because otherwise it will be difficult to annotate. So, now there will be 6 C2 which are perpendicular to the 180 degrees angles formed by these C4s, so, B5-A-B6.

Now, this perpendicular can be in 2 directions. So, you have basically what you have is this axis and this axis. So, you have axis going through like this will be and will be C 2 similarly, so, each of this will have 2 perpendiculars. So, all of this will be perpendicular to these 3. So, before next will be B4-A-B2 and third will be B1-A-B3. So, perpendicular to B1-A-B3 will be passing through, if I am drawing a line like this so it will be perpendicular to this one.

So, 6 C2s will be present. So, now, let us also list down the symmetry planes, how many symmetry planes will be present in this one. So, planes are simple to see. The planes which are actually containing planes containing the 4 B atoms and the central atom for example, you have B1, B2, B3, B4 this plane will be called as sigma h similarly, you have B1, B6, B3, B5 and the third one will be B2, B5, B4, B6.

These are the planes containing 4 B atoms and, of course, the central atom will always be there and these are 3 such sigmas. So, 3 sigma h. Then planes there will be planes containing 6 C2s perpendicular to C4s. Now, these are the 6 C2s present. So, for example, this C2, so there will be a plane containing this C2 and a plane containing this C2. So, basically the planes which are dividing these planes, so, this particular plane can be divided in 2 ways.

So, one way is marked in red over here and another way is marked in red over here. Similarly, these 4 planes can be also divided by 2 possible ways and 2 possible ways. So, there will be 6 such planes, which are called as 6 sigma d. So, I hope that these 3 molecules should be sufficient or will give you enough understanding on how to locate different proper axis of rotation and planes.

So, if there are any troubles, we can again discuss during the interaction session. But the idea here is that if you list down all the atoms containing different symmetry elements, so you would not get lost and you will be able to list the exact number of symmetry elements present otherwise, if you just keep on imagining and write in air, then it would not take you anywhere.

So, it is better to list down all the atom numbers which are contained by a particular symmetry element and then try to find out how many such combinations are possible and accordingly, write down all the symmetry elements and operations, thank you very much. This is all for today.