Symmetry and Group Theory

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Lecture - 11
Symmetry Point Groups, Part – 1

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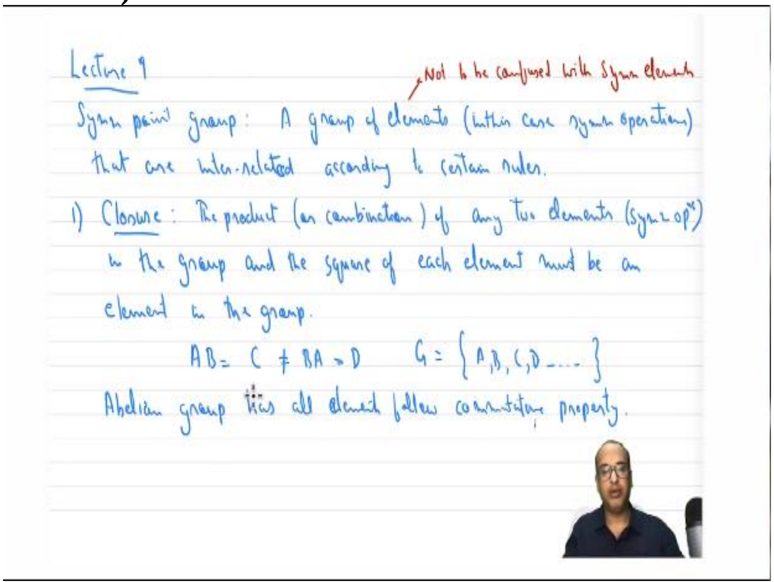

So, welcome to lecture 9. In the last class, we have seen we have learned how to carry out the product of symmetry operations or combination of symmetry operations, and we have also seen how to actually find out the complete set of symmetry operations a molecule may have. So, we have already seen that how to identify or how to find out a complete set what you mean by a complete set of symmetry operations.

So, now let us see what is a point group or symmetry point group, because our goal is to find out what is a symmetry point group, right. So, a group of elements so each member of the group is called as element, a group of elements or collection of elements in this particular case, each element is nothing but symmetry operations. So, elements are not to be confused with, so I will write it as, not to be confused with symmetry elements.

So, these are group elements which are nothing but symmetry operations, OK. So, group of elements, in this case symmetry operations and not to be confused with symmetry elements, that are interrelated according to certain rules. So, what are these rules we will see that. So, the first rule is called as, there are 4 rules which define which relate the elements and that defines a symmetry point group, the first property is or first rule is called as closure.

And it states - the product, or in some books it is also written as combination, of any 2 elements and I will again write down that these elements are symmetry operations. So, the product of any 2 elements in the group and the square of each element must be an element in the group. So, this we have already seen using the example of BF 3 that if we take a list on all the symmetry operations and we take different combinations or square of any element it must form an element in the group.

It cannot go out of that group so this is called as closure property that it is a closed group it is not infinite. I mean there can be infinite symmetry operations but again those symmetry operations within that set must be closed must follow the closure property. Also it is not necessary that AB = C and it is equal to BA that may or may or may not exist. So, this may be the case that it is actually not equivalent BA = D, in this case the group should have A, B, C, D in that set.

So, the elements C and D must be present if the commutation is not holding, so any basically any order of combination must result into an element which forms the part of the group. There is one particular group called as Abelian group has all members are all elements follow commutation law, commutative property we can say. So, in that case AB = C and that is equal to BA for all the elements of the group. So, that group is called an Abelian group that we will see later. So, now we can use any particular molecule, take any molecule list on all the symmetry operations, test for closure property you should be able to do that now.

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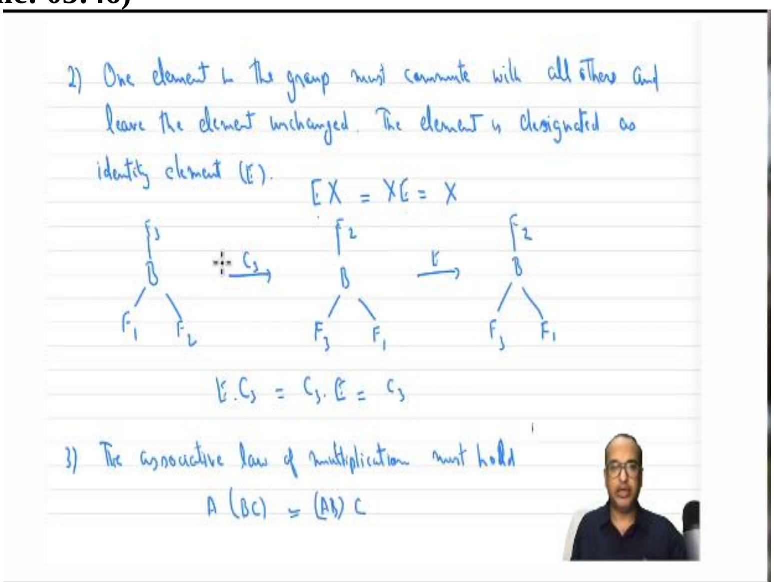

Second definition is, let me go to second page, one element in the group must commute with all others and leave the element unchanged. We will see what it means mathematically. The element is designated as identity element. So, we know that each molecule has the identity element in it, right, defined as E. So, we can say that if we take combination of EX, X is another element or XE it should give you X back.

So, one element in the group must commute with all other elements that means E is commuting with X in this case and leave the element unchanged so it will result into X. So, this is easy to show you can take any molecule do a symmetry operation perform identity operation and then do it in reverse order and see if it is equal to just the operation. So, I will just take one example over here which is I know it is very easy to follow just in case.

So, let us say if I do C3 operation, what I will get is I will not go into details but what I will do is 3, 1, 2 and now if I do E operation I will get same thing back, so F2, F3, F1. So, this is the case of C3 E. Now it is easier to see that this is equal to C3 E and it is equal to E C3. So, an element must commute with all other elements and leave element unchanged. So, again by element when I am saying element I mean symmetry operation not the symmetry element this is the group element we are talking about.

So, third property is so first property was closure another is the presence of identity which is always there. So, symmetry operations do follow the 2 properties. Now let us say the third property the third is the associative law of multiplication, which in this case is called as combination because you cannot really multiply the symmetry operations you can combine them, must hold.

So, this we have already seen that symmetry operations do follow the associative law of combination. In the last class we have seen that. So this must hold and that holds for symmetry operations.

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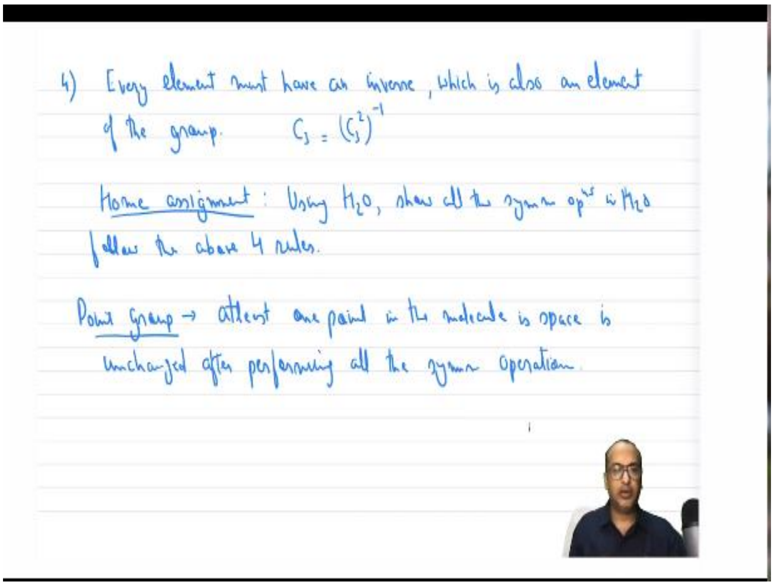

So, again this can be tested out easily and the fourth is every element must have an inverse and the inverse should also be which is also an element of the group. So, every element should have an inverse and that inverse should always be present in the group. So, for example, again going back to BF3 example, we saw that C3 is equal to C3 square inverse. So, C3 has an inverse which has C3 square and C3 square is actually present as an independent operation in the group.

So, this property should hold for all the elements, so sigmaV1, C2 any operation which is there, it should have an inverse and the inverse should also be an element of the group. So, you can take now take it as a homework assignment. Using H2O show all the symmetry operations in H2O follow the above 4 rules. So, one by one you can actually do that and see for yourself whether it is true or not.

So that once the symmetry operations, you have shown that they follow the above rules these are called as point groups and that particular set of elements is called a symmetry point group. So, why it is called as point group actually? It is because in all these symmetry operations at least one point in the molecule in space is unchanged. So, the location of that particular point remains unchanged. So that is why it is called as point group at least one point in the molecule in space is unchanged after performing all the symmetry operations.

So, you can pick up any symmetry operations of the group and by performing any symmetry operations at least one common point should be there which should not change in the molecule and that is why this particular group is called as point group. So, this is in relation to space groups where the like when we study or if you have actually gone through a course of this crystallographic where the translational operations are also there.

So, here we have seen that it is only rotation and reflection operations. So in crystallographic point groups which are called as space groups we also have something called as translational operations. So, which is out of the purview of this course, but those are called as spaced groups and these are called as point groups. So, we will not be discussing space groups in this course we will be only restricting ourselves to point groups, but there is more to symmetry basically that is which goes to explain the crystallographic space groups.

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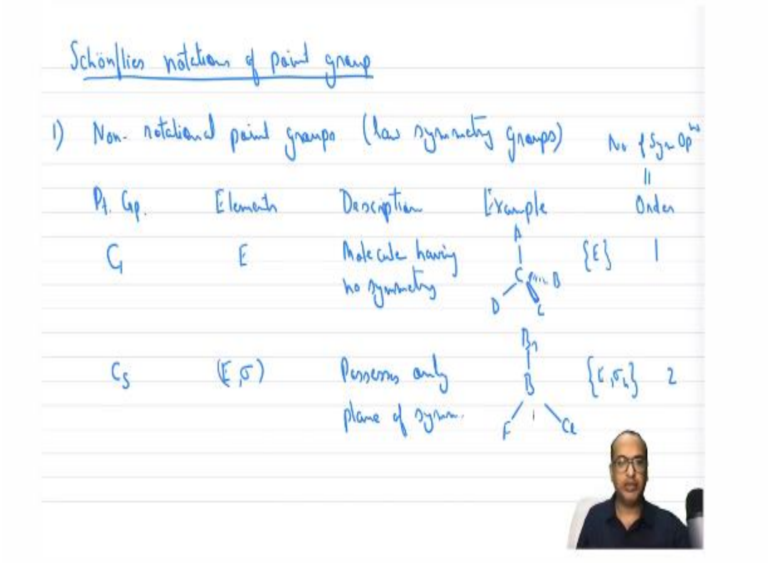

So, now let us look at next is, so now that we have learned what is the point group and how a point group is formed let us see what are different types of point groups. So, the next topic is Schönflies notations of point group, the name of the how do you actually give names to different point groups? So, let us see what are different point groups let us categorize them first and then we will see what are their names and what are the elements required to define one particular point.

So, the first in this category is called as non-rotational point groups, these are generally low symmetry groups so numbers of symmetry elements or symmetry operations are relatively lower. So, let me point group less down and then the elements of the group and I will also give you a little description and let us see example the first in this case is C1. C1 is when you have nothing but just the identity present. There is no other operation, no principal axis, no sigma, no i, no improper axis.

So, molecule having no symmetry basically, molecule having no symmetry is called as C1 point, example can be when you have let us say if you have all 4 atoms of a tetrahedral are different than say A, B, C, D. So, in this case the only the complete group is just E and we can say that the order of the group is the number of symmetry operations present in the group, order of the group in this case is 1.

So, order is equal to number of symmetry operations nonredundant symmetry operations is equal to order which is in this case is 1. So, next example so non rotational of course, because there is no rotation involved in any of this next is Cs. So, in this case you have E and sigma, the sigma can be mostly it is like a molecular plane. Molecule possesses only plane of symmetry as an element. So, an example you can take this for example here we have Br, F, Cl and this will be E and sigma-h and order will be 2. So, this is Cs point group.

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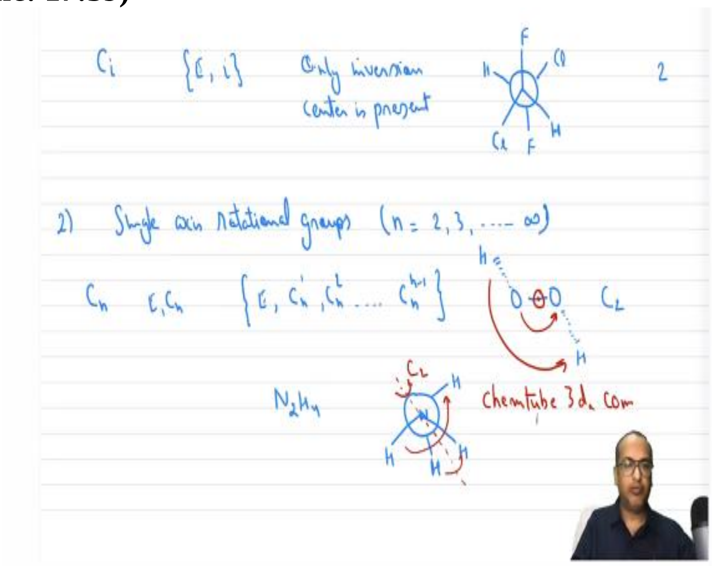

Let us go to the next non-rotational point group which is called a Ci, as it is clear from the name it should have E and i, so only inversion center. So, only inversions center present example is let us see if I can draw it correctly. So, it is a staggered fluoro-chloro Cl F goes into opposite edge. So, if you see i lies in the middle of C-C bond and that is the only symmetry element present there is no other plane nothing is present like no rotation axis. Order again is to in this case because the 2 elements of the group are E and i, so this is all for non-rotational point.

So, now let us look at the second category which is single-axis rotational groups. So, n of course cannot be one, because we have seen that if it is one it will be C_1, C_1 point group. So n can be 2, 3, up to infinity. So, we can say the point group is C_n point group the elements are C and E whereas the operations will be, so C_n will give rise to n operations.

So, C_n^1, C_n^2 and then up to C_n^{n-1} because C_n^n will be again E, so these are the set of operations an example is open book structure of H_2O_2. So, the structure looks like this. So let us say, so here my C_2 axis is actually perpendicular to the plane of the board and the rotation is, right, so O will replace O the H will be replaced with H. So, this particular group is called as C_2 point group.

So, Cn basically to the elements group, elements will be E and C2, nothing else because C2 square will be again E. So, that is single access rotational point Group Cn. Another example for C n can include hydrazine, hydrazine is N2H4 and the structure you can draw in Newmann projection let me draw as if I draw it let me see if I correctly draw it H, H and this is N and the back end atom is also drawn like this and then you have H, H.

So, here the C2 will be passing through an N-N bond so if you do this so, I would advise you to actually go to chemtube 3d dot com and look at this molecule in 3d. So that you can actually see where the cemetery operation lies, or where the position of C2 axis. So that way it will be easier to see but if you do this, there will be basically a C2 which is passing through and N-N bond and the operation will be like this so this will be your C2 axis. So, this H goes at the back this H this will be the kind of rotation we are talking about.

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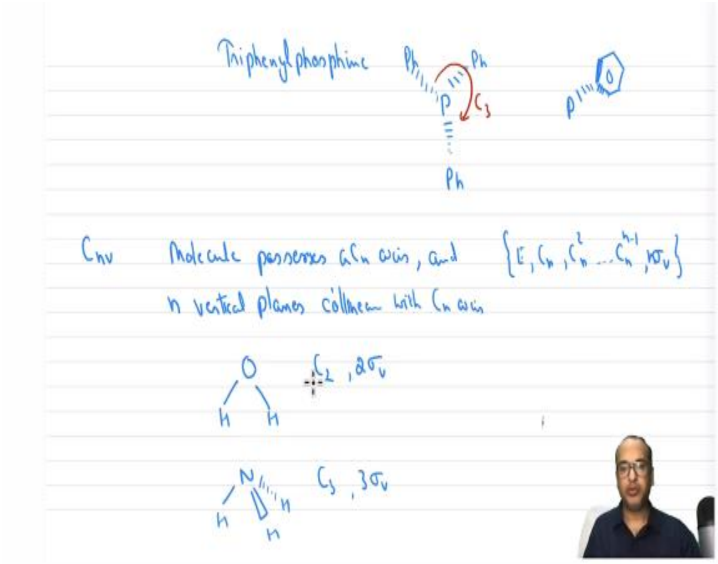

Let us take one more example for this, which is triphenylphosphine. In this case, it is phosphorus atom and then you have 3 phenyl rings which are oriented like a propeller. So, none of these phenyl ring is actually in the plane of the molecule. So, if I draw it more precisely, it is like something like this where this point is actually coming out of the plane of the boat and this bond is going to be below.

So, it is like something like propeller blade fan like a thing which is twisted phenyl ring so there is no sigma-h in this case. So, here the symmetry axis is like the C3. So all of these forms Cn point group. So, next is Cnv point group. So here molecule possesses a Cn axis, and n vertical planes that are collinear with Cn axis. So, the operations will be E, Cn, Cn^2, up to Cn^{n-1} and we should have n sigma-v, it can be sigma v1, sigma v2 and so on.

So, example we have already discussed these kind of examples so one is water, so water has C2 axis and 2 sigma-v which are collinear with Cn axis. Then similarly NH3, has a C3 axis and 3 sigma-v collinear with the C3 axis and so on so, these are Cnv point groups. So, we can also see what is the order of this particular group so, order here is 4 for example, and we can work out the order for NH3.

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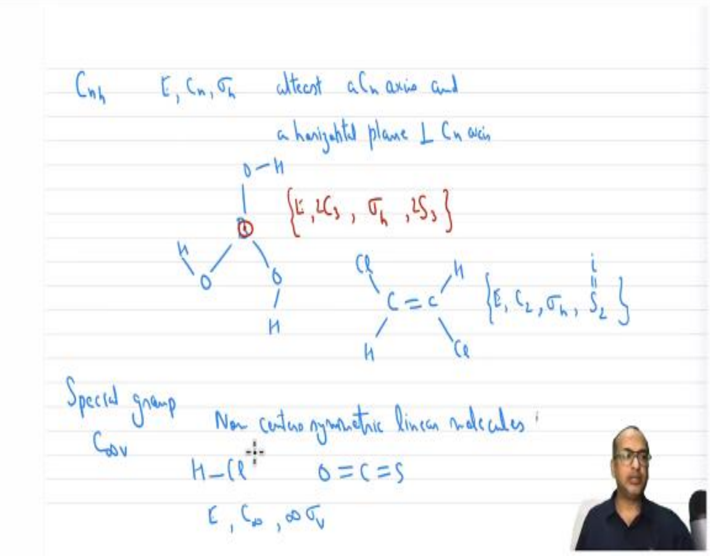

Then next single-axis rotational point group is Cnh. So, here the group elements are other symmetry elements are E, Cn, sigma-h. This is the least which is required. So, molecule should possess at least Cn axis and of course it will generate n-operations and a horizontal plane perpendicular to Cn axis. So, for example let us look at B, OH, OH everything is in plain, there is a C3 axis which is perpendicular to the plane of the board.

So, C3 and there is a molecular plane which is sigma-h. So, because C3 and sigma-h are present there would also be S3 axis and of course E would be present. So, these are the set of symmetry elements and the corresponding symmetry operations will give rise to two and two here. So, 2C3, E, 2C3, sigma-h, and 2S3 and so on another example you can look in this category is C CH Cl H Cl.

So, here the elements are E, C2, sigma-h and because C2 and sigma-h are present so, there would be S2 which is nothing but i and the operations would include E, C2, sigma-h, i because C 2 square will be equal to E only. So, these are the set of operations so, you can say E, C2, sigma-h, and i will be present and then let us also discuss one special group under single access which is called as C infinity v.

So, these are basically non-centrosymmetric, it is easier to remember like this, non centrosymmetric linear molecules. So, example is HCL, anything linear without having any center of symmetry, or let us say we have COS or CSO. So, the elements will be E, C infinity, we can see that there is a C infinity axis passing through the linear axis of the molecule and infinity sigma-v.

So, infinity sigma-v's are all sigma-v's which are containing that particular C infinity axis and we can find out the corresponding operations, there will be infinity operations are arising because of C-infinity. So, that is it for today we will next discuss dihedral and cubic point groups and then we will also see a flowchart how to discuss how to actually identify which molecule belongs to which particular point.

So that is it for today, so do practice look at different molecules, list on symmetry elements and then try to work out if the operations present in that molecule are actually following all 4 properties of the group or not. Thank you.