Symmetry and Group Theory
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Module No # 02
Lecture No # 10
Product of Symmetry Operations

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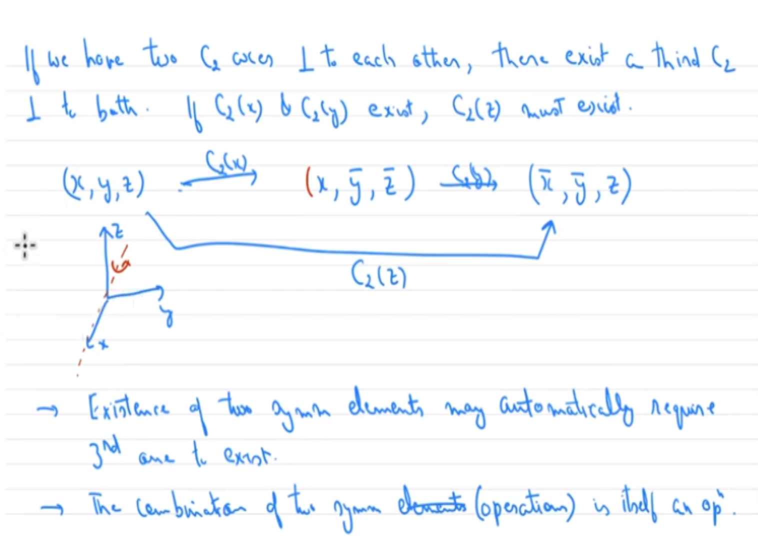

Welcome everyone, so today we will be discussing lecture 8. So, we will be discussing product of symmetry operations. So, we can also call the product as combination of symmetry operations because this is really not a product but a combination because we are applying one symmetry operation after the other. So, let us say if we are applying one symmetry operation first, followed by second symmetry operation, where X is one symmetry operation and Y is the other one.

So, let us say if this is applied first, and this is applied second, and the result of overall transformation of applying first and second symmetry operation can be directly achieved by a third symmetry operation. Let us say call it as Z, then we call it as that Z is the combination of so Z is a combination of Y and X, okay. And the order of symmetry operations does matter here because not all symmetry operations commute with each other. We have that earlier what is the computation of symmetry operations.

So, what I mean is YX is not necessarily equal to (it may or may not equal to) XY right where this is your first and this is your second operand. And in this case, X is your first and Y is your second operand. So, let us see let us say if we have x1, y1, z1 is the coordinate of a given point in a coordinate system and by operating with X we take it to x2, y2, z2. And again, by operating with Y we take it to x3, y3, z3.

Then if you find a symmetry operation which can directly take you from x1, y1, z1 to x3, y3, z3 by using Z, then Z is called as combination of Y and X in this particular order, right okay. So, for example let us say if you have, we can say that if we have, this is one such example, 2 C2 axes perpendicular to each other, there exists a third C2 perpendicular to both. So, we can say that let us say if C2x and C2y exist (because now they are perpendicular each other), C2z must exist, okay.

So, let us say if we have let us operate this C2x on x y z. So operating C2x operating on x y z. So, in this case let us see what happens. If we have right-handed coordinate system, we have x y z and now if my C2 is running along x-axis this is my C2 okay anticlockwise direction. So, what happens so y will go to –y, z will move to –z, x will remain as same because x is not moving, x is lying along the x-axis right.

So, what happens, my coordinates will change like x will remain as such, y will go to –y (I am representing –y as y bar), z will go to –z, right. Now similarly if I am applying C2y what happens now? So, x goes to –x now, –y remains as –y, and –z goes to +z, so I hope this is very very clear. So, what I have done here is now I have used C2y axis, so y remains where it was and x and z change their sign, okay.

So now you can easily see that if we have to go from here-to-here x is changing its sign, y is changing its sign, whereas z is remaining as such, which can be obtained by C2z operation, right. So thus, we have shown that if there are 2 perpendicular C2 axes, there must exists a C2 axis which is perpendicular to both. So now C2z is perpendicular to both x as well as y, right, so this is called as product or combination of symmetry operations.

So that means we can say that existence of 2 symmetry elements may automatically require third one to exist. So, for example here we have seen that C2x and C2y were existing and because their presence is there, so C2z must exist. So that means its the existence of C2x and C2y is directing the existence of C2z, right. In other words, we can say the combination of two symmetry elements (we can say operations actually) is itself an operation, right.

So, let us take an example to see and the order does matter. We will see in certain cases it may commute in certain cases it may not commute.

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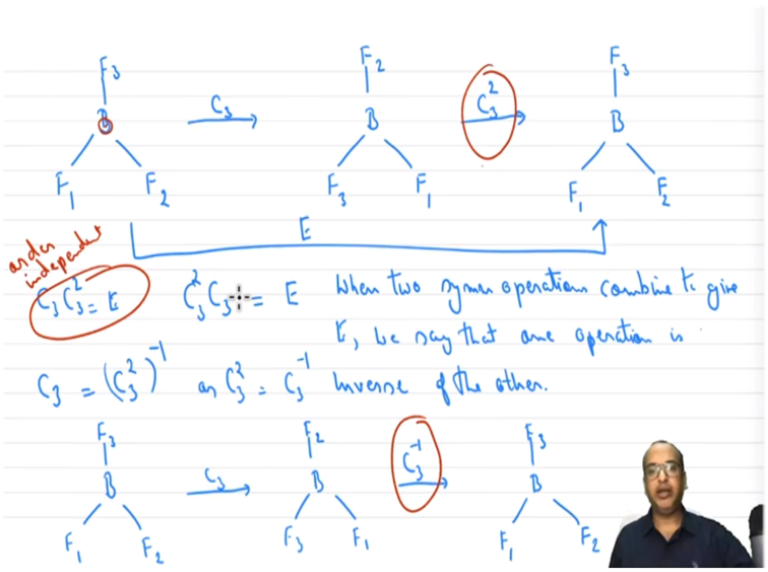

So, let us take an example so BF3. Let us say 1, 2, 3 okay, now let us do an operation. We know that there is a C3 axis here, right. C3 axis as line passing through B and lying perpendicular to the plane of this board. So, if you do a C3 operation anticlockwise what happens? It will change the, B remains at its own position, and then one moves here, two moves there, 120 degrees rotation, 3 moves here, right.

Now let us say if we do C3-square operation, okay. So C3 done twice on to this. So, what will happen? Now my 3 goes 2 times, 3 will move 1, 2 because C3 is done twice. So, in one C3 it will go from here-to-here, but we are doing C3 twice so it should move like this. So, it will be a 240 degrees rotation okay. So, F3 goes here, F2 comes here, F1 goes here, okay. Let us see we have 3 here, 2 here, 1 here so this should be very clear.

Now if you see if we have to go from here-to-here, what will be that operations? Now look at the atom position? So, it does not change F1, F2 does not change, F3 does not change that means this operation is nothing but an identity operation. So, we can say that C3 and C3-square (so remember the order we have used here is C3 is operated first and C3-square is operated second) (although in this case it does not matter, we will see why) is equal to E, right.

So whenever two symmetry operations combine to give so we can say that when two symmetry operations combine to give E, we say that one operation is, inverse of the other we will see what it means? So, we can say that C3 is equal to C3-squared-inverse, or C3-square is equal to C3-inverse. So, what do I mean by inverse? So inverse is doing the same thing in the opposite direction. For example, if I am doing C3 anticlockwise and C3-square clockwise so it would be in the same thing.

So, it is like doing the same thing but in opposite direction. So, if I am doing C3-square then it will be equal to C3-inverse right. So okay let us see that again so B F 1, 2, 3. So, if I am going C3 then what do I get? F2, F3 F1. And now if I am doing C3 inverse, then that will be doing the same operation but in the other side right. So, what do I get? So, I get the same thing back, so 3 goes back, 2 goes back, and 1 goes back.

Now you see that we have done C3 C3-inverse and I am getting the same as we got after doing the identity or C3, C3-square. So that means now C3-square becomes equal to C3-inverse, right. So, these operations because now the first set of operations are same C3, C3. And the second set of operations here was C3-square whereas here it is C3-inverse but the resultant is same. So, you can safely say that C3-inverse is equal to C3-square and you can also do the vice versa thing.

So basically, it proves that when two symmetry operations combine to give you E, we say that one operation is inverse of the other, so that should be easy. But okay now let us also see a case where the symmetry operations do not commute. So, in this particular case actually let me go back the order does not matter so we can say that C3 and C3-square if we do that then also it will be equal to E, okay.

So, order does not matter, order-independent, because they are combining to give E the order would not matter here but if they do not combine to give E the order the order will matter and it may or may not commute, okay.

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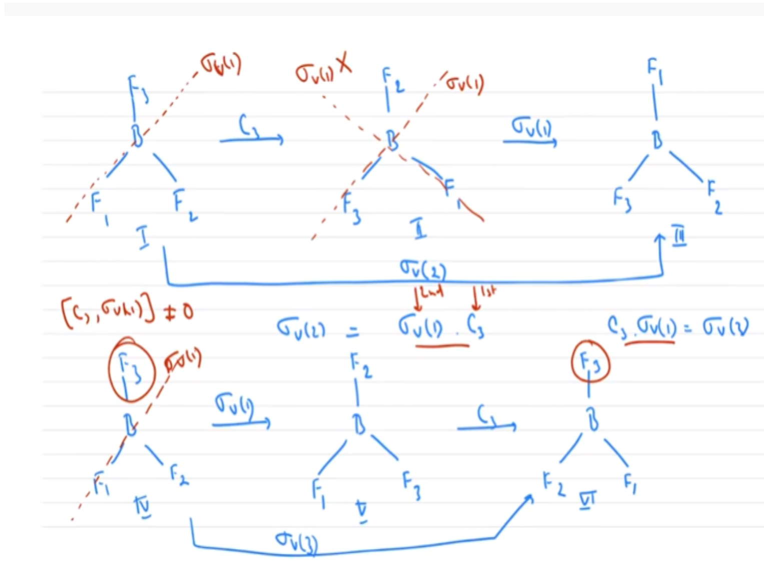

So, let us look at the same molecule again and take combination of two different symmetry operations. So, let us again do C3 first. So, we have 3, 1, 2 right 1, 2, 3. Now let us do sigma v1. So, sigma v1 will be this plane, okay. So, the plane which is passing through BF1 in the original molecule not in the transformed molecule. So, the location of this sigma v1 will be with respect to when we started with the molecule not where we ended after doing the C3 operation.

So that has to be very clear that whenever we are taking the initial configuration of molecule, we are fixing all the symmetry elements. And accordingly, we have to take the symmetry operations we cannot be moving so for example if we say that this is my location of sigma v1 that would be incorrect. So, this is not sigma v1 okay my sigma v1 will be this one okay. So, in this case my sigma v1 will be this. This should be clear. So, if I do this operation then what do I get so that means F3 does not move and the 2 F's will be reflected the other 2 F's F1 and F2.

So now if I have to go from here-to-here directly what will be my operation? So in this case if you see that F1 moves clockwise to this then F3 basically F2 does not change and F1 and F3 are reflected right. That means if I reflected by sigma v2 this will be the operation which will take it from first to so if you call it first second third. So, we can safely say that sigma v2 is equal to sigma v1 - C3. So, the order is we operated C3 first and sigma v1 second okay.

Now let us see what happens if we do it reverse so let us say the same starting point BF3 F1, F2. I am doing sigma v1 first so what do I get? So again, my sigma v1 position is this is my sigma v1 so that means the F1 does not move, F2 and F3 will get reflected. Now if I do C3 operation what do I get? So, if I do C3 operation one goes here, anticlockwise, 3 and 2. Now what is this operation? So, in this case my F3 is not moving F1 and F2 are getting reflected so I am comparing 4, 5 and 6 okay.

So, in this case if you see F3 is same, whereas F1 and F2 are getting reflected so that would be sigma v3, right. So, in this case if we change the order what do I get? C3 - sigma v1 is equal to sigma v3. So, you see how this particular product if I change the order it results into two different symmetry operations. So, we can safely say that C3 and sigma v1, commutator is not equal to 0 right. So, they do not commute is it clear okay. So C3 or we can say C3 does not commute with sigma v1 right.

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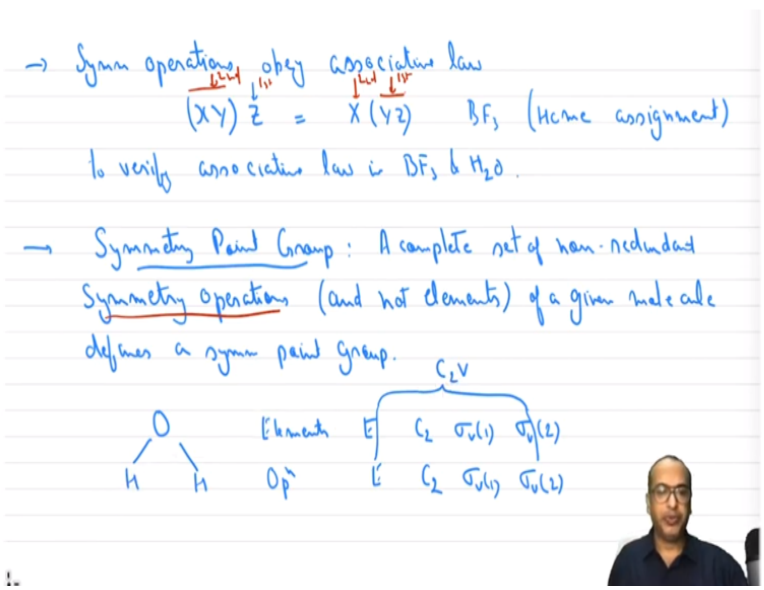

Another important property symmetry operations follow is symmetry operations obey associative law. So, what is associative law? Associative law means that if we have two operations XY and third operation Z, then our XY product of two operations into a third operation is equal to X(YZ). So, what do I mean in this case so I mean that if I doing this operation first and then the combination of this as second this will be equal to if I do combination of this as first and this as second okay.

This should be equal to always irrespective of what molecule is what the symmetry operation is and so on. So right so this should be very clear so symmetry operations obey associative law.

And we can test it out using any example like BF3. So, take it as home assignment to verify associative law in BF3 and H2O. So, let us take 2 different examples so that the operations how to do these operations will be very clear okay.

And come back to me if there is any issue with this okay. So, let us now take so we are now ready to actually go to define what is a point group? So, let us take the example of symmetry point group. So, what is the symmetry point group? So, by definition a complete set (we will see what is the complete set) a complete set of non-redundant symmetry operations so I am saying symmetry operations and not symmetry elements thus identifying the list of symmetry operations is crucial okay.

So, we have learnt how to first list down the symmetry elements and then find out what all non-redundant symmetry operations exist. So, a complete set of non-redundant symmetry operations and I will specifically write here and not elements of a given molecule defines a symmetry point group. We will see why it is called as point group and all okay. So, for example if we take example of water molecule, the symmetry elements and thus the operations so we will list down both we have seen this earlier.

So, elements are E, C2, sigma v1, and sigma v 2, right, and the corresponding operations are E, C2, C2-square will be equal to E, so we will not consider that, sigma v1 will generate 1, sigma v2 will generate 1, right. So, this forms a point group called as C2v, okay. So, we define it as C2v, this is the notation we will learn later called as Schönflies symbols of point group, let us see. So, these set of symmetry operations not the elements this set of symmetry operations will give you point group as C2v.

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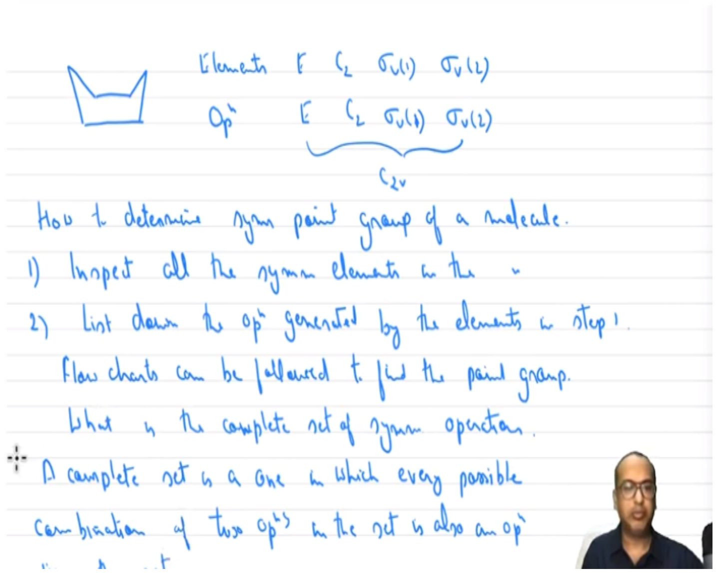

And now let us look at another molecule cyclohexane in boat form. If you have done this exercise, so here also the elements are E, C2, sigma v1, sigma v 2. So, this I give it as home exercise to identify the symmetry elements and operations. So, this is very similar as water. So although the water and cyclohexane boat form they look very different but their symmetry operation which are existing in this are same and hence both of them belong to C2v point group.

So that means any physical property which is dependent on the symmetry operations because of the classification, they will be sharing those physical properties right. So, it is interesting that how this two differently looking molecules are classified into same category, because they have same set of symmetry operations and thus their physical properties will be very similar, whatever physical properties depends on this set of symmetry operations right, okay.

So, now let us see how to determine this point group and what are different types we will see that how to determine symmetry point group of a molecule, okay. So, let us look at this. So, first thing here is to inspect all the symmetry elements in the molecule, right. Second is list down the operations generated by the elements listed in the above step, elements in step one. So up to this we have seen how to do this, right.

But this is not so easy because in certain cases where the molecule is big and highly symmetric the numbers of operations are huge. And then some times we may miss out one element or the other and unless we really practice it hard. So, you will find several books have flow charts made can be followed to find the point group, so we will see how, okay. So, but before we go there let us see what is the complete set, right. What is the complete what do I mean by complete set of symmetry operations?

So, a complete set is a one in which every possible combination of two operations in the set is also an operation in the set. So this sound this may sound confusing but let us see.

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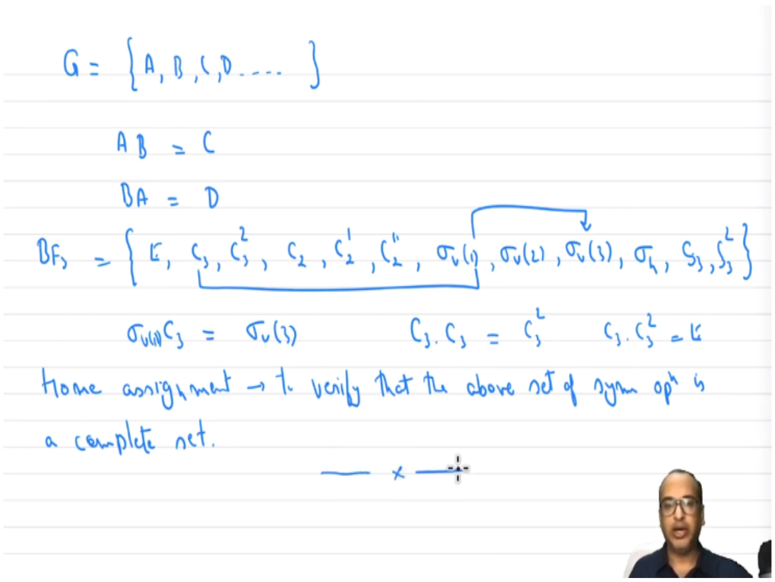

So, what I am seeing is that if we have let us say if we define a group where the set of symmetry operations are A, B, C, D and so on. Then if we combine two symmetry operations in any possible way and we get let us say C or if we are doing B A we are getting D then C and D must form the element of this group okay. So that will define the complete set. Similarly, if we do AC, we should have another product which should form a part of this set.

So, this way this is called as a complete set so again so let us take an example. So again, let us take the same BF3 case we have been discussing. So, in this case the symmetry operations let us list it down E, C3, C3-square, then we have C2, C2’, C2”. So, I am not writing as 3 C2 just so that we are listing all the symmetry operations independently. But they will be essentially equivalent so we have actually say 3C2 but let us see explicitly listing all the symmetry operations.

So, we have sigma v1, sigma v2 (or we can call it as sigma v, sigma v’, sigma v”), sigma v3 and we also have sigma h. So now if you see C3 and sigma h is there, then S3 would also exist. So, S3, S3-square, right. So now if we say that if we try to take a product so this is a complete set of symmetry operations for this particular molecule. Now if we take product of any two symmetry operations or combination of any two symmetry operations it should give rise to a symmetry operation which is already present in this set okay.

If it is not then we must include that operation also into the set okay otherwise it will never be complete. So, what I mean is that if I am combining let us say C3 and then I am doing a sigma v1 we have seen this earlier if we do this in this order what we get is sigma v3, right. So now we are combining C3 and sigma v1 and what we are getting is sigma v3, which is already present in this group.

So similarly, you should be able to test out, so take it as a home assignment number 2 for today, to verify that the above set of symmetry operations is a complete set okay. So, by complete set I mean that any combination of two symmetry operations should give rise to third symmetry operation which must be present within this set. So, you should be able to verify and the combination is not necessarily that two symmetry operations have to combine it may also be the case that C3 and C3 are combining.

For example, if we combine C3 and C3 we will get C3-square if we combine C3 and C3-square we will get E. So, I have already done at least 3 combinations for you. So, you should be able to verify how to do this okay so that is it for today and next class we will look at how exactly we find out what are the properties which are required to form a symmetry point group and how do we find out symmetry point groups okay alright that is it for today.