Symmetry and Group Theory

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Module No # 02
Lecture No # 08
Improper Axis and Improper Rotation

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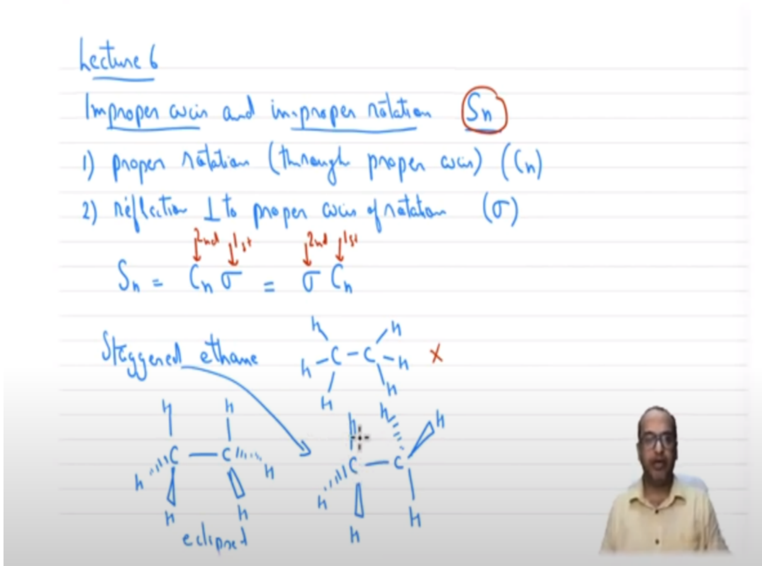

Welcome everyone, welcome to lecture 6. So, let us continue our discussion of symmetry elements and symmetry operation. In this set, we have last symmetry elements and symmetry operation, which is called as improper axis and corresponding operation is called as improper rotation. So, this particular symmetry element and symmetry operation is a combination of 2 symmetry elements and operations corresponding this thing.

So, first is proper rotation through proper axis, we have already seen what proper axis is. And the second part is reflection perpendicular to proper axis. So, reflection via plane which is perpendicular to proper axis of rotation, this also we know that this is called as Cn, this is called as sigma and improper axis or improper rotation is denoted by Sn, ok. So, we have Sn now this Sn is the combination as I said it is a combination of Cn and sigma.

And it does not really matter in which order you apply individual operations here. So, you can apply Cn first. So, in this case this will be the first operation and this will be the second operation or you can apply sigma as first operation and Cn as second operation, ok. So, let us see with an example how this particular improper axis can be understood. So, let us look at an example of staggered ethane.

How do you draw this molecule? So, we have C C H H H right. you must have seen this drawing earlier. But in symmetry class you will never draw a molecule like this because it does not tell you where the orientation of each hydrogen is. So, what is the next best thing which you can do is to draw it in which also does not give you very great details but it is still better. So, this one would be actually the eclipsed ethane.

So, if you want to draw the staggered one you can draw like this H H H, and then right. So, this will be the staggered ethane. But to carry out any sort of symmetry operation in this will be really difficult. So, the easiest way is you must have learnt this Newman projections.

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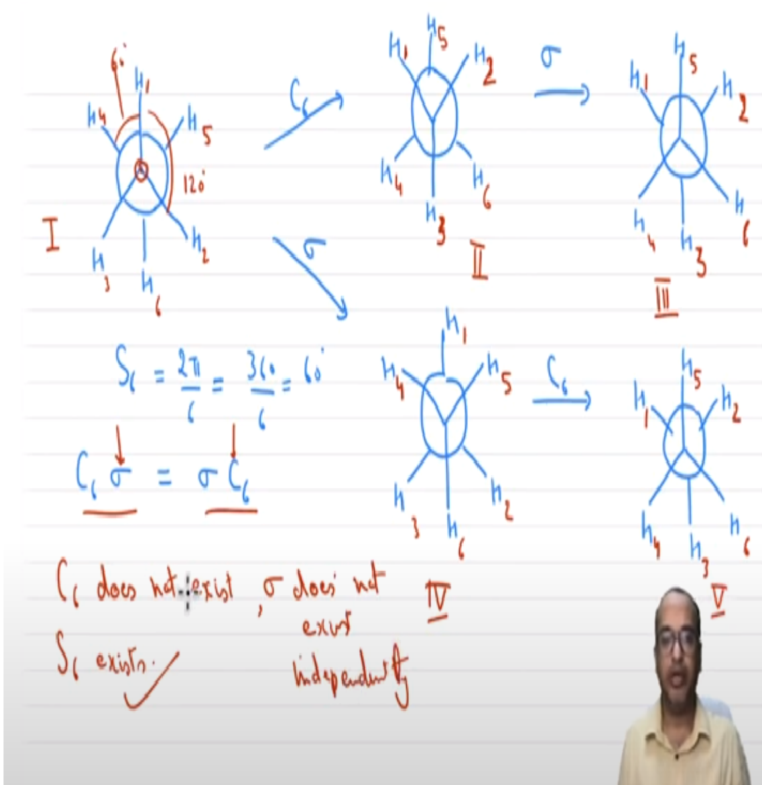

So how do you draw so this is one set of protons this is other set of protons right. So, you have H now let me also write down the numbers 1 2 3 and 4 5 6, ok. So now let see how we do this operation. So, as I said we can do C6 first, so ok so what kind of Sn we are looking for here ok.

So, we are looking for S6 in this case. Why S6? Because this will be 2Pi / 6 operation what is 2Pi / 6 what will be the angle?

So, this will be 360 by 6 which will be 60 degree of rotation. So where is the 60 degrees angle over here? So, let see this particular angle this whole angle is 120 degree between 2 hydrogen on 1 carbon but if you; look at this dihedral angle over here. This dihedral angle is 60 degree. So, we will be doing this rotation 60 degrees rotation. So, we can also see if these is any S3 axis present or not.

But let us go ahead with S6 and see this example ok alright. So, let us do so S 6 should be materialized by either doing C 6 first or sigma first or vice versa because both these operators commute with each other. We know what the meaning of commutation is right. We have seen this in first class. So, these two operators commute. We can test it out but let us first do it ok let us first do the C6 one.

So, we are doing this one first. So, C6 that is this one first right. Ok let us do both actually, it will easier. So, in this case this is the first one so we have to do in both ways ok. So now if we have to do C6 operation first this C6 operation means that H1 will move to this part. H3 will move to this part, H2 will move by 60 degree right every proton will move by 60 degrees. So how does it look. So that means, instead of inverted Y we have a upright Y right. And then instead of upright Y at the back we have inverted Y at the back.

So now let us also write on the numbers. So, this 60-degree anticlockwise rotation means H1 comes here, this will be 2, this will be 3. Now H4 comes this side, so this will be 4, then 5 goes there so we have 5 over here. So, we have to be very careful when we are writing these numbers because otherwise it will mess up everything, 6 right. So, this looks like right. Now you can see that if we denote this as molecule number 1 and this one has molecular number 2.

So, 1 and 2 are not in equivalent configurations right. You can see that the configuration of this is not equivalent to this. So, we can say that C6 does not exist in this one. So, C6 does not exist. So, we can do the operation but it may or may not result in equivalent configuration. If it results in equivalent configuration, we say that it does exist the corresponding symmetry element does exist.

But in this particular case C6 does not exist, right. Now let us do sigma, ok. So where is this so sigma has to be now perpendicular to this C6 axis. So where is our C6 axis? C6 axis is actually passing through the 2 carbons ok. So, I am drawing it perpendicular to the plane of the board. So I am drawing it as a circle with a dot inside. So, this is nice C6 axis. So, the plane this particular plane now has to be perpendicular to the C6 axis which means that the sigma is the plane of the board.

So that means whatever is in the forward will go in the backward and whatever is the backward will come forward right. So that means this H1 H2 H3 will go to the back upon this reflection and H4 H5 H6 will come forward. So that would mean that you have to draw a line like this. So, this will become your, ok let us write the hydrogen first and then we will write the numbers in red. So H1 H2 H3 and then this is H5 H4 H6, right.

So now you can see let say if this is our third, so, first and third are equivalent because you can see that this is inverted Y over here and then this is the upright Y at the back. So, you can clearly see the first and third orientation or configurations are equivalent. So, we can safely say that S6 exist right. So, S6 which is a multiple of product of 2 symmetry operations the first is C6 and the second is sigma. So, we have seen that it does exist.

So now let us also look at the commutation part, whether does it really matter with if you are going C6 first followed by sigma or we can do sigma first followed by C6. Ok let us do sigma first now. So, if we do sigma first now again this inverted Y goes back. So, the front carbon goes to the back and the back carbon comes to the front. So that means it will be something like this and the this is the back carbon which is now in the front, hydrogen write down all of this hydrogen explicitly.

The numberings remain 1 2 3, did I mess up the numbering? This should be 2 actually, right and this should be 3. So accordingly, this should be 2, this should be 3, ok. And then the 4 5 6, 4 5 6 yeah this is correct, ok. So, 1 2 3 so that is why is said the numbering has to be right and this this is my 4 5 and 6, ok. So now again you can see that let say this is our fourth configuration. So, first and fourth are not equivalent. So, we can say that sigma does not exist ok.

So now if we do C6 on this, C6 means again it is a rotation by 60 degrees anticlockwise, ok. So that would mean, now what will be the numbering, so 1 comes over here, and then 2 comes over here, 3 comes over here, and this will be 4, this will be 5, this will be 6, and we call it as fifth. You can easily see that the first third and fifth are equivalent. So, because first and fifth are equivalent, we can say that S6 exist.

So, this is verified again and because third and fifth are equivalent we can say that C6-sigma or sigma-C6 both are equivalent. So that means the 2 operators are commuting right. So ok so we have now verified S6 is present in this particular molecule. But we have seen that C6 or sigma may not, it does not exist independently in this case, ok. There is no independent sigma independently or C6, right.

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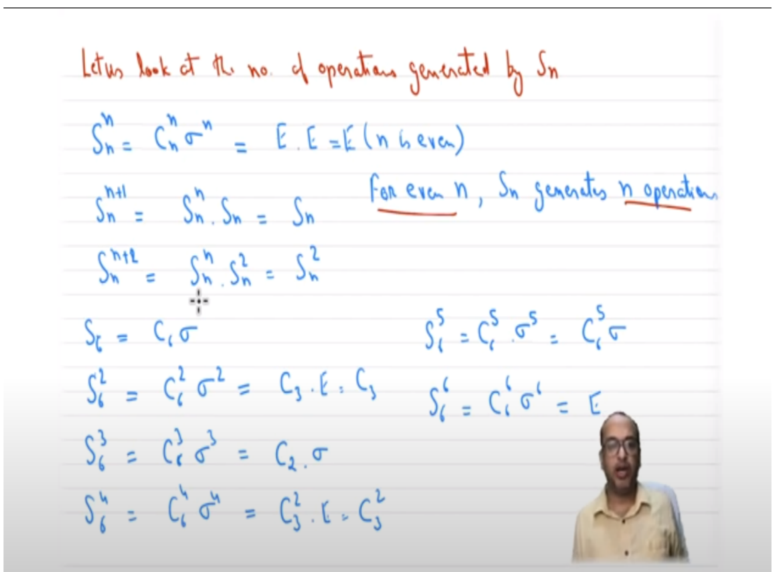

Ok so now let us look at how many operations, the number of operations generated by Sn. So, in general, so let us take the general example before we actually look at the operations. So, if we do Sn, so Sn will be Cn sigma right. If we do Sn to the power n it will be Cn to the power of n, sigma to the power of n which is nothing but Cn ^n we have seen that Cn ^n is E and sigma to the power n is E only in the case of n is even right.

So, let us first consider the case of n even n. So, this will be equal to E, right. This is easier to follow if it is not even then it will lead to sigma right. Cn to the n will remain E irrespective of even or odd. But sigma n will give rise to sigma if n is odd. So now let say Sn to the power n + 1 what happens there. So that would be Sn to the power n x Sn that means. Since this was E so this was E, so we can say this is Sn.

Similarly, if we have Sn to the power n + 2, power means how many times a particular action is done. This can be written as Sn x Sn ^2. So you can say so now there is a trend right you can see that if you are increasing this power 1 by 1 so you are getting the same operations back. So that means after Sn to the power n, it starts to repeat. So that means that it does not generate more than n operations. So, for we can safely say then for even n, Sn generates n operations. We will see for odd case also.

Let us this is for even n ok n operations ok. So now let us see the case of S6. So, we had S6 = C6 into sigma right. So, this is S6 to the power 1. So, this is the independent operation. Now let us say S6 to the power 2, this can be written as C6 to the power 2, sigma to the power 2 right. So, this can be written as C3, C6 done twice is nothing but C3. Sigma done twice is nothing but E. So, you have C3 right. So, this operation is different from this operation.

Now S6 to the power 3, this will be equal to C6 to the power 3, sigma to the power 3 that means now this is C6 done 3 times this is nothing but C2, and sigma done thrice will be sigma. So, this is again an independent operation. S6 to the power 4 will be C6 to the power 4, sigma to the power 4, which is C3 square, E. So, this is C3 square. So, C 3 done twice and S6 done 4 times, ok. S6 to the power 5 will be equal to C6 to the power 5, sigma to the power 5, which will be C6 to the power 5 sigma right.

So again, this is not come so for. So, it is non-redundant operation. S6 to the power 6 is nothing but C6 to the power of 6, sigma to the power 6 and both are equal to E. So again, this also a non-redundant operation ok so this is the case for even n when n is even how many operations it will generate.

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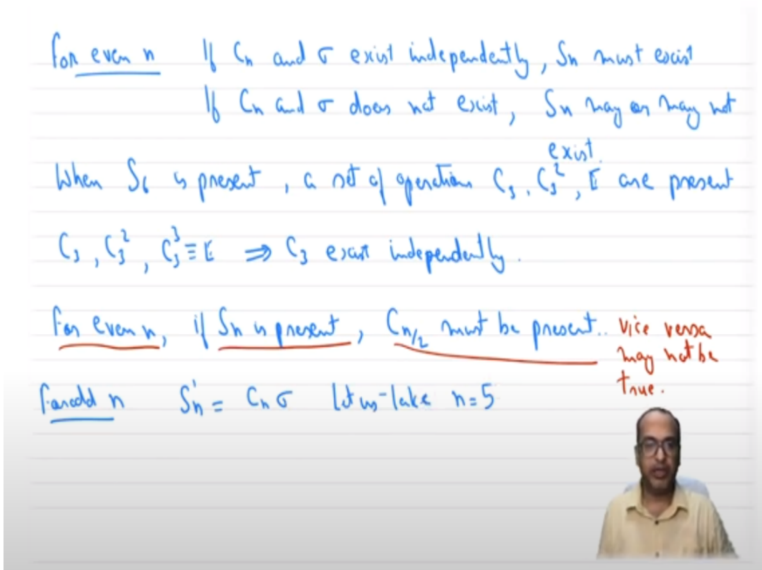

So now we have seen that for even n, we can also say that if Cn and sigma exist independently, Sn must exist right. This we have seen from this one over here. So, if you have C6 and sigma present independently the S6 will be present because it is the product of the two. If Cn and sigma does not exist, Sn may or may not exist. So, we have to actually do it and test, there is no rule which says that it must exist or it must not exist.

If Cn and sigma does not exist, we have seen this example in this particular case C6 or sigma either of those 2 were present, but still S6 was present right. So, we can safely say that if they do not exist Sn may or may not exist. So, you actually have to test it out whether it is present or not but actually doing the operations. But if they exist independently, we can safely say that it must Sn must exist ok. So, one more interesting thing if you notice over here that when S6 was present three operations were present.

So, if you notice over here there is C3, there is C3 square, there is E right. So, when S6 is present a set of operations C3, C3 square, E are present. Why am I interested in this? Because C3, C3 square, and E can also be written as C3 cube, right, so this is equivalent to E. So, these three operations indicate that implies that C3 exists independently right. So, when S6 was present C3 was present independently, irrespective of C6 and sigma.

So that means we can generalize this, for even n, if Sn is present Cn/2 must be present ok. So, we will see these kinds of corollaries a lot. So, this is an important one so you should know if Sn is present Cn/2 must be present vice versa may not be present. So, if C3 is present it is not necessary that S6 will always be present. But vice versa may not be true ok. Now let us look at the case for odd n so for odd n what happens?

So, let us do the same exercise that we did for Sn, but in this case now we have Sn even. So, if you have Sn, what do we have Cn sigma right Sn ^1. Now it is easier actually if we take an example so let us take let us take n = 5 we can also take 3 let us take 5 just to make it clearer. So, let us move to next page and see.

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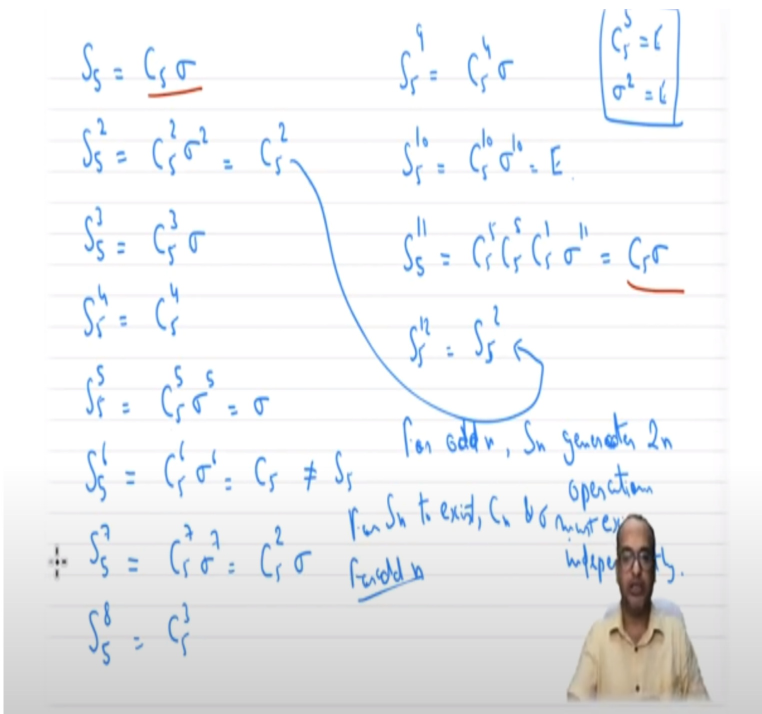

So S5 is equal to C5 sigma. S5 done twice is equal to C5 done twice, sigma done twice, which is nothing but C5 done twice because sigma square is E. Now S5 done thrice is equal to C5 thrice and now I am short cutting to sigma. Sigma done thrice is equal to sigma. S5 done 4 times is equal to C5 done 4 times, now sigma to the power of 4 is equal to E so I am not counting that right. S5 to the power of 5 is C5 to the power 5 and sigma to the power 5 which is this will be E and this will remain as sigma, right.

So, we are generating all of these operations are non-redundant operations so far. So, we have reached S5 to the power of 5. So that means now we if should see whether we start to get this operation back or we are getting some different operation. So, what I mean is in case of Sn+1 when we tested here so we were getting Sn back, right, Sn+1. So, in case of n + 2 we were getting Sn2 back so we will see what are we getting here. So S5 to the power 6 do we get Sn back or not.

So, this will be C 5 to the power 6 sigma to the power of 6 which is C5 done once and sigma and to this is not equal to S5. So that means we need to keep going because we are still getting non redundant operations. So, let us keep on going unless we actually get the same operation back so when the redundancy starts, we need to stop. Unless we get non redundant operation so we need to keep on going. Now C5 to the power 7, sigma to the power of 7 so, this means C5 done twice and sigma right.

So again, this is non-redundant operation because this earlier was C 5 square now it is C 5 square and sigma. S5 done 8 times is C5 done 3 times and that is all right. So now again this is a non-redundant operation. Now let us do continue S5 to the power 9, so we have C5 ^4 and sigma. So, I am short cutting this you can explicitly do it and see. So, what you have to make sure is that whenever you are hitting this is equal to E whenever you are hitting sigma square or even powers this is equal to E.

So, I am using this ok to simplify this ok. Now S5 to the power 10, we are getting C5 to the power 10 that means sigma to the power 10 that means again E, right. So again, we have got a non-redundant operation. So, let us see what happens next 11, C5 ^5 C5 ^5 C5 ^1 sigma ^11 right. So, this is E, E so we have C5 and sigma. Now if you notice that this is a redundant operation right C5 sigma C5 sigma. So now if you go with S5 ^12 you will notice that this will be equal to S5 ^2. So, you can do this yourself.

So, you will get this thing back over here right ok. So that means for odd n, Sn generates 2n operations right. Instead of n operation so we are getting 2n non-redundant operations. 2n+1 was same as or S1, 2n+2 is same as n = 2 and so on, ok alright. So, this is simple and one more point here is the Sn, for Sn to exist, Cn and sigma must exist independently. So, this is for odd n, ok. So, for odd n, S n to exist, Cn and sigma must exist independently, ok.

So that finishes the discussion on symmetry elements and symmetry operations and we will take one more class to actually see how to locate all the symmetry operations and symmetry elements. And then find out corresponding symmetry operations, and then we will move to next topic which is product of symmetry operations. So that is all for today. Next class we will look at how to implement this symmetry elements in different molecules and find out non-redundant operations, ok.