Symmetry and Group Theory

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Module No # 02
Lecture No # 09
Solved Examples of Symmetry Elements and Operations

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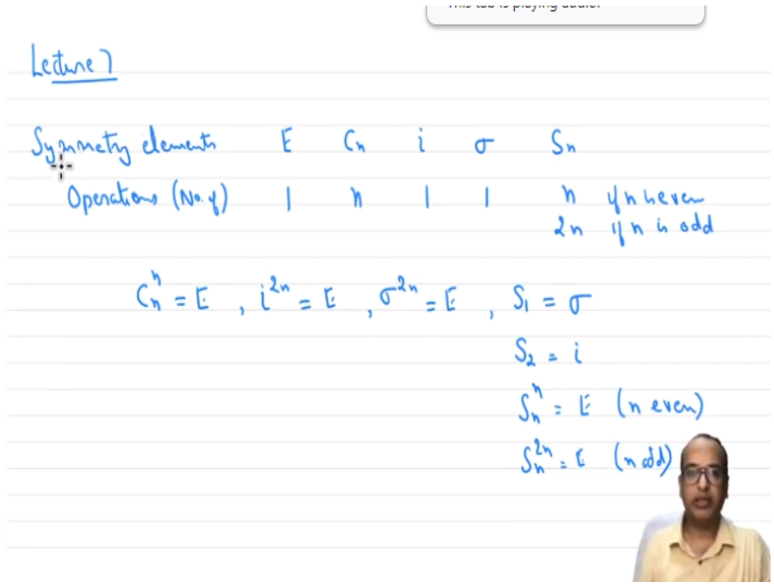

Welcome to lecture 7. So, we have been discussing symmetry elements and symmetry operation. So, let us summarize what we have learnt so far. So, let us list down all the symmetry elements we have learnt and corresponding symmetry operations, and if there are any special cases. So, let us see a symmetry element, first symmetry element is identity followed by proper axis of rotation which is symbol by Cn. Then inversion center sigma that is the plane of symmetry and improper action of axis of rotation right also called as rotation-reflection axis.

And the corresponding operations it will generate, so let us send number of operations, so E will generate only 1 operation, n-order Cn axis will generate n operations, i will generate only 1 operation, sigma will generate only 1 operation, and Sn will generate n operations if n is even, we have seen that. And it will generate 2n operations if n is odd right. Also, there was some special cases that we have seen if Cn to the power n this will be equal to E, i to the power 2n will also be equal to E.

Similarly, sigma to the power 2n would also be equal to E, for if you take only S1 it is nothing but sigma we can easily prove it. If you take S2 this is nothing but i, you need actually n = 3 or higher for S3 to exist. So, you can work this out yourself so if you take n = 1, S1 become sigma if you take n = 2, S2 become i. I have not shown it explicitly but try to work it out yourself. Now Sn to the power n = E for n even, and Sn to the power 2n = E for n odd, right okay.

So, this is the summary of what we have learnt so far so let us now look at some solved examples to help you understand how do we actually list down all the symmetry elements and corresponding operations in different molecules. So, let us start with typical molecule let us say water.

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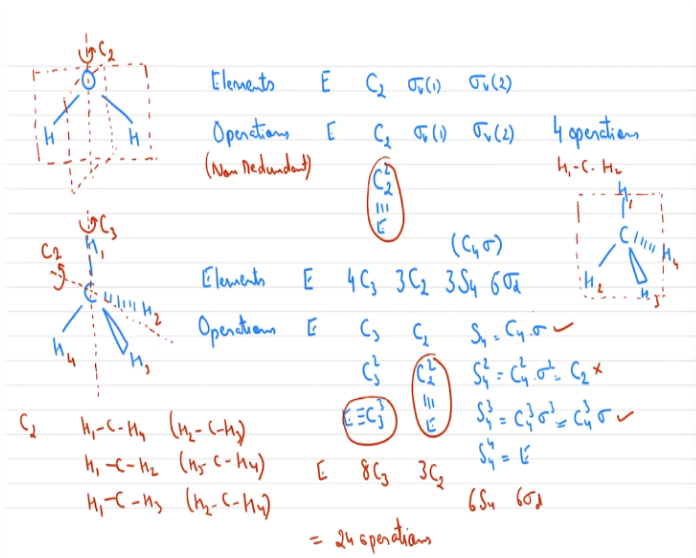

So, we have been seeing water. So, what are the symmetry elements present? So, the very first element in every molecule that we have to list is identity. It is always there irrespective of the molecule right that as we have learnt. In addition to E, so let us then look at what is the principal axis which is present? So, principal axis which is present in this case is there is only 1 axis proper axis of rotation which is C2 axis, which is lying in the plane of this board.

So, we can say C2 only one C2 so we will write only 1 here then there is one plane, which is the molecule plane, which contains C2 and another plane, which is actually perpendicular to the plane of the board and reflecting the 2 hydrogen's. So, there are 2 independent planes we can call it as sigma v1 and sigma v2, right. Now how many operations it will generate? Let us see so E will generate only 1 operation E, then C2. So, C2 should generate two operations, C2 and C2 square. But C2 square is nothing but, E so we do not need to consider this one. So, because we are considering only non-redundant operations okay so we do not need to consider C2 square although C2 will generate two operations as we will learn nth order principal axis will generate n operations. But we do not consider this because this is equivalent to E.

Now sigma v1 will generate sigma v1 one operation. Every sigma will generate one operation so we have sigma v1 and sigma v2. So total four symmetry elements and four operations. okay so this number is important. We will see later four operations that are non-redundant okay. So, this was an easy case so let us go to little higher number of operations. Let us see let us look at tetrahedral molecule methane, okay.

So, now let us see what are the elements and then corresponding operations also we will list down. So, first and foremost is always E. Now what is the principal axis of rotation here. So how many proper axes of rotation are present? So, one is C3 axis which is passing through C-H bond there are four such axes because there are four such bonds right. And another is C2 axis, so C2 axis is by setting the H-C-H angle we have seen this example before, this will be C2 right.

So, let us see we can write down so there are four C3 axis. All are equivalent so I am writing them together. If there is non-equivalent C3 axis then you will write C3, C3', C3" and so on. But in this case, all are equivalent C3 axis because all C-H bonds are equal, so that is why we are writing as 4C3. Now how many C2s are present? So, think about it how many H-C-H bonds are there that are bisected? How many of such C2 axis will be there? So, there will be 3 such C 2 axis?

So, if we list them it down by number let us say 1, 2, 3, 4, it will be easier to see that for C2 let us say H1-C-H4 then H1-C-H2 (we have to take only non-redundant ones), then H1-C-H3 right. These are the options which where the C2 will bisect, okay. The, let us say if we are taking H1-C-H4, H2-CH3 will be covered in this right. So, it is bisecting H1-C-H4 as well as H2-C-H3 angle, right. Now similarly, H1-C-H2 so this will be bisecting H3-C-H4 angle.

And H1-C-H3 will be bisecting H2-C-H4 angle, and then there are only 6 such angles in this tetrahedral molecule. So, we have 3 C2s over here, okay. So, that is how we list them. Now what else do we have, any ideas? So, we will have S4 axis. So, what is an S4 axis? S4 is combination of C4 into sigma, right, sigma which is perpendicular, okay. So, we can work it out this operation try to work it out this operation yourself otherwise we can discuss during the interactive session.

How many such S4s will be present? If there are 3C2s there will be 3S4s present okay then we also have sigmas present. In this case these will be called as sigma d's because these will be bisecting our H-C-H angles. And how many such sigma d's are present? There will be 6 such sigma d's, okay. So, let us also see where the sigmas are present, so let me draw those molecules over here again.

So, if I draw a plane which is containing let me write down 1, 2, 3, 4 so containing H1-C-H2 and reflecting H3 and H4. So, this will be once such sigma and we have seen that there are 6 such bonds so there will be 6 such sigma's right that is easier to see. Now the number of operations so E will generate only one. Now each C3 will generate C3, C3 square, and C3 cube that means 3, but now this one is equivalent to E.

So, we do not need to consider this one because E is already considered over here, so this is not required. So that means each of this C3 will generate 2 operations, so then we will have 8 such operations 8C3 operations, okay. Now C2, each C2 will generate 2 operations C2 and C2 square again C2 square will be equal to E, so we do not need to consider this one. So that means there will be total 3C2 operations. S4, we have seen that each S4 should generate n operations, right because n is even over here, S4 should generate S4, S4 square, S4 cube, and S4 ^4.

Now this will be equal to C4 into sigma, this will be equal to C4 square into sigma square which is equal to C2, okay. So, this become non redundant, this is not because C2 is already covered here. Then we have C4 cube sigma cube, which is C4 cube sigma. So again, this will be considered and this will be equal to E, right. So that means each S4 will generate 2 non-redundant operations. So that means we will write 2 S4s, and each sigma d will generate one operation so we will have 6 sigma d's.

So, these are the number of operations it is going to generate so that means total operations will be here sorry 3 into 2, 6 right. Because we have each will generate 2 so we will have total 3 S 4 axis so this will be 6. So, 12 and 12, so 24 operations, okay. So, by now we should be able to identify where the symmetry element is located and how many symmetry operations it will generate? And this thing will come out only with practice so you need to practice with a lot with a large number of molecules.

Otherwise, this will be never with clear and further down the line the course will handle this thing as if you know how to calculate this. So, you should better practice at this point itself how to identify what are the symmetry elements present locate their positions on to the molecule and generate operations and identify how many symmetry operations are there. So, let us see one more may be couple of more examples to confirm this.

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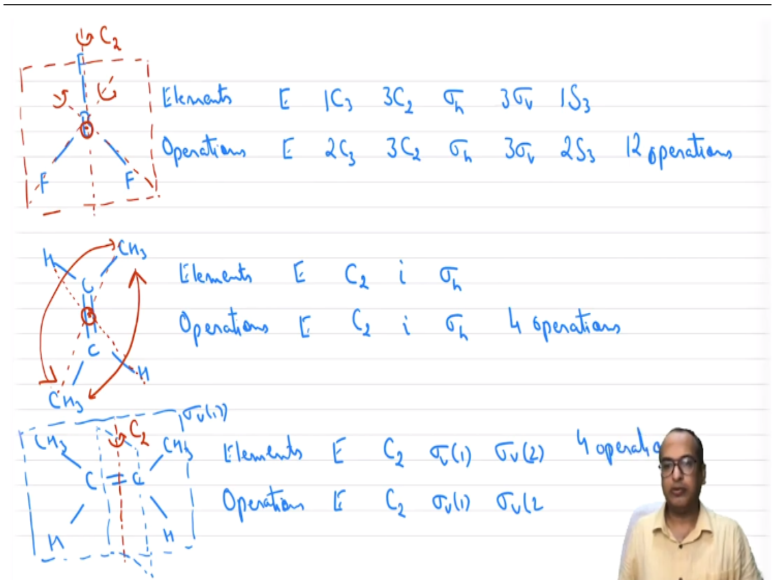

Now let us say the molecules which we have considered already, so BF3. Now again what are the elements and corresponding operations? So, elements will be E, principal axis will be C3, where is C 3? C3 will be perpendicular to the plane of the board passing through the Boron atom. Then we have how many C3s are present? Only one. Then we have C2s, where is location of C2 now? C2 is located passing in the plane of the board, and passing through B-F bond, right.

This is C2. How many such C2s are present? There are 3 such B-F bond so there are 3 such axis right. So, we have 3C2s. What else? We have a molecular plane sigma h, then, which will contain all 4 atoms, so this is my molecule plane. Then there will be 3 planes, each containing the B-F bond and perpendicular to the plane of the board. So, because it is containing the C2 axis as well as the C3 axis so this will be called as sigma v.

Now how many sigma v's will be present? There will be 3 sigma v's. Now what else is present in this case? Now you have noticed that there is a C3 present and a plane which is perpendicular to C3 is present, so that means there must be a S3 axis present, right. Now because there is only one C3 so there is only 1S3. Now let us list down the operations. So, by the way you should try each and every operation and try to do the operation and see if you are getting an equivalent configuration of the molecule or not.

So that will tell you whether the element is present or not, okay. So now the operations. E, each C3 will generate 2 operations we have seen that earlier, so 2C3 operations, each C2 will generate only one operation because the C2 square will be equal to E. So, we will have 3C2s, one sigma h each will generate 1, S3, S3 square, so each S3 will generate 2 operations, so 2S3. So now how many total operations we have? So, we have 6, 7, 12, so 12 operations.

Let us take one more example let us take sis or trans okay let us do both trans-2-butene, now elements and operations. So, elements will be E, what else will be present in this case, we will have a C2 axis. Where will be the C2 axis? C2 axis will be perpendicular to the plane of the board. And passing through C=C double bond so if you do this C2 operation this will go there and this will come here right. So that will be the kind of rotation anti-clock wise direction it will be like this C2 and only one C2 axis we have i in this case we will have i.

So, if you see here this is the center of the molecule say if you pass or line from one atom through the center of the molecule find the other atom similarly here right. So, you will have i, then we will have sigma h. So, this is easy case numbers of elements are very less in this. And the corresponding operations are E, C2, i, sigma h, so only 4 operations. Now let us also look at the case of cis-butene. Now what are the elements and what are the operations?

So, yes E this is the first one, then what else we have got, we will have a C2 axis now, where is the C2 axis, what is the location? C2 will be lying in the plane now, unlike this. So, this is the C2 rotation. So, CH3 will be moved to this CH3, H will be moved to this H, so this is my C2 axis. What else have we got? We will have 2 sigma v's, sigma v1 so this is the case like water molecule? So, 1 will become molecule plane like this is sigma v1 and other one is plane perpendicular to the plane of the board but containing C2 axis, right so it will be like this okay.

Now both the planes are perpendicular to each other and each of this will generate only one operation. So again 4 operations here, okay.

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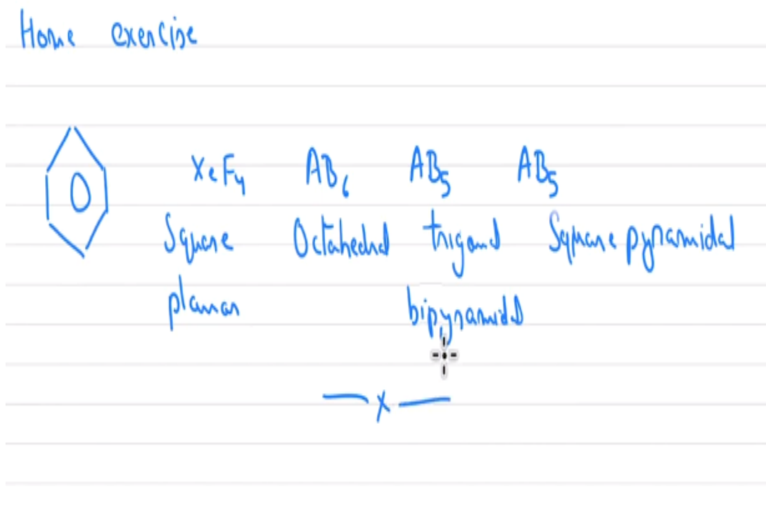

So, with this let us, I will give you some home exercise so that if you are comfortable with identifying all the symmetry elements and operations. So, let us take benzene, let us take a square planner molecule XeF_4, and let us take octahedral AB_6. Let us take a trigonal bi-pyramidal AB_5, let us take a square pyramidal AB_5, so I will write it down, so square planner, octahedral, trigonal bi-pyramidal, square pyramidal.

We have already seen tetrahedral, so this will cover a full range, so if you can identify the symmetry elements and the corresponding symmetry operations, locate the position of symmetry elements and find out the number of total symmetry operations. You will be good for the rest of the course because these are the type of molecules will be dealing with very often, okay. So, try to practice a this a lot, so that this is very clear in the heads.

So, in the next class we will be dealing with the product of symmetry and then we will take up the definitions of symmetry group and all, okay. So, let us end the class today okay thank you.