Chemical Applications of Symmetry and Group Theory
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Lecture – 04

Hello, I hope all of you doing well. So, I welcome you to the day four of this course. So, we stopped in the last class after finishing the mirror plane symmetry, and we just started the center of inversion. So, we will start from pair itself. So, what is the symmetry inversion or also known as center of symmetry, inversion symmetry? So, inversion symmetry is a point and this point may not contain any atom if I consider a molecule, so if I take any point or any point of molecule, and pass it through that particular point and go equal distance on the other side, I will find an equivalent point. And then this center point or origin through which I am passing is known as center of inversion.

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Let me take an example. So, I showed you this model in the previous class. This is the benzene right. Now you can look at this molecule, pickup any hydrogen atom here. So, I am picking up a hydrogen atom right here. Then I am passing through the center of this molecule, the center of this mass of this molecule and then going equal distance, what I am finding, I am finding another hydrogen. So, this is just equivalent through the previous hydrogen. And I will take anything, I take this point particularly, I take this point and pass through this central point again, I get another similar point over here. So, similarly you take point anywhere on this molecule, you pass through this point of the center and you know what the same amount same distance you will find exactly similar point on the other side. So, this point here in the center for this particular molecule will be the inversion symmetry point or the center of inversion.

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So, you can take many other molecules; let me show you another example. So, this particular model that you can see, you can see if it is zoomed little bit more then this is model for ethylene C double bond C and then 4 hydrogen here, so suppose you mark here 1, 2, 3, 4 then you take one and you start walking which this midpoint of this C-C bond and then keep going in the same direction by same amount, you will reach here. So, similar thing will happen for this hydrogen, this will reach here, and the other one sitting here will come here correct. So, if I have started with a, b, c and d, then a will go to the position of c, c will go to the position of a, and b will take the position of d, and vice versa. So, I have to start with a, b, c, d, now after having this inversion symmetry, I have c, d, a and b. So, this point of the center of C-C bond this particular molecule is the inversion symmetry or center of inversion.

So, like in the last class, toward the end, I told you that if I can select any point or a molecule which passes center of inversion, then you consider any even point not necessarily you have to consider an atom, but you can consider any point in given bond you will find the exactly same point on the other side of the molecule once you pass through that center of inversion.

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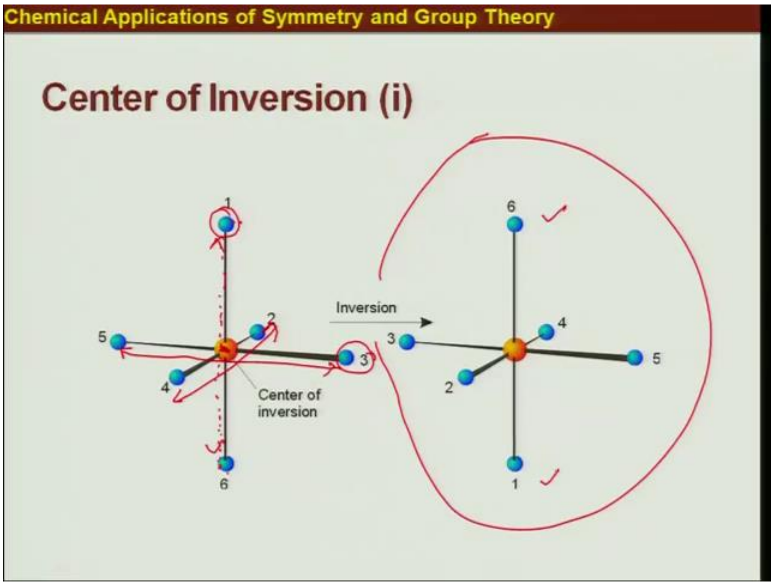

So, now if you consider the screen that is being played in front of you, I take another example of an octahedral molecule. So, you can take this molecule like here any transition metal complex like you know C O H 2 O whole 6 ignoring the metal charge. So, this will form an octahedral complex. So, all the C O bonds and if I take this O each as you know like a ball, so each of the ball is like an O or you take it like you know CO Cl 6, cobalt chloride (Refer Time: 05:19). So, each of this is you can take it a chloride, chlorine atom and center is a metal CO cobalt. Now, they will occupy an octahedral geometric. So, they will all the chlorine atoms will be disposed at you know or six vertices of an octahedral.

So, we have mutt here like 1, 2, 3, 4, 5, and 6. So, 1 and 6 they are occupied axial positions while the chlorine atoms at 2, 4, 3 and 5 they are in the equatorial plane. Now, all the CO, Cl bonds are equal. Now, having that in mind you start from chlorine 1 and we have a point right here at the center of this you know cobalt atom. Now, if we start from this chlorine 1, and keep walking through this bond and come here to this point and then keep going in the same direction an equidistance you know then we end up having you know chlorine finding this 6 chlorine atom.

So, similar thing will happen for 3, 3 will go to the place of atom 5; 2 will come to opposition of 4; and 4 will go to the opposition of 2. So, 5 will come to the position of third chlorine atom; and 6 and 1 will interchange the position of this inversion symmetry operation. So, what will be the structure, structure is shown here in this right. So, you can see I say one will go to the place of 6, and 6 will come to the opposition of 1 that is what exactly this happening right 6 and 1 they are interchanging their position.

So, whenever you have a center of inversion and you want to operate that particular operation on in given molecular structure, the rule of thumb is all the atoms or bonds which are disposed the on two different sides of this particular point in space, they will interchange their positions. So, we can see here (2, 4,), (3, 5), (1, 6), they are all interchanging their position. So, knowing this, we should be able to right the structure of any molecule after operating inversion symmetry operation, if the molecule causes a center of inversion. You cannot operate any symmetry operation on a molecule, which does not have it.

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So, for example, we talk about this CH Cl 3 chloroform. So, in case of chloroform, do you think there is a center of inversion, answer is no, because there is no such point through which I can pass and no which an equivalent point on the other side. Suppose I want to start from this hydrogen, I will not find another you know hydrogen on the other side, if I even consider any point. So, there are actually is no such point in this particular molecule which can invert the structure center of inversion the symmetry operation actually inverse the structure. So, this molecule does not have one, but the other molecule that I should used at benzene and ethylene, they have a symmetry operation known as center of inversion.

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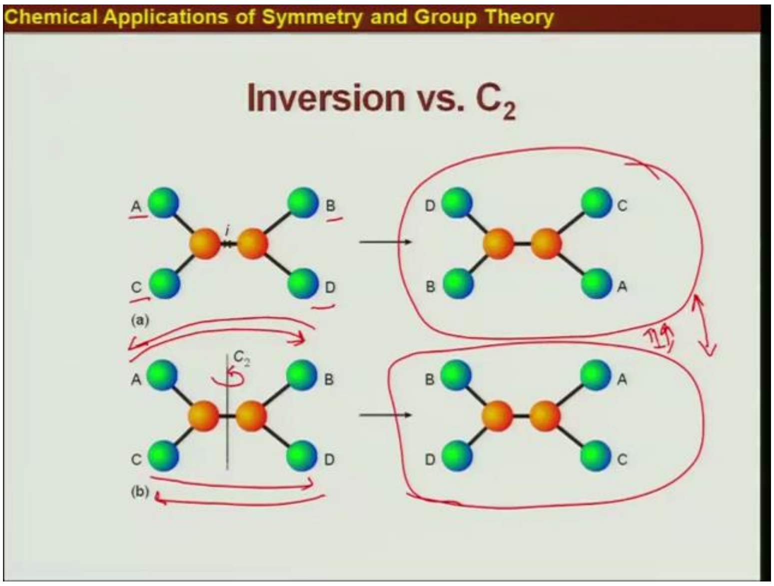

Now, here in on your screen, you can see that I have tried to compare this inversion symmetry with another similar kind of a symmetry operation that is rotational symmetry of order 2 that is by using a C 2 axis. So, I have a molecule exactly the one that I showed you earlier that is ethylene. So, I have an ethylene molecule. So, if you look at screen, you can see that all this hydrogen atoms of ethylene they are marked by A, B, and C and D. And then we can perform the symmetry operations I or C 2 on this two structures. So, here clearly I that is inversion operation will invert the structures. So, we will go to opposition of D and vice versa. So, will this D and C will interchange their positions. So, you will ultimately get this particular structure of a inversion symmetry inversion operation.

Now, C 2 on a first (Refer Time: 10:28) it gives you a feeling that it will end up doing a same thing, but will it really do that let us have a look at it. So, if you look at on screen, you can see that the C 2 axis, which is in the plane of the molecule. So, this C 2 is not perpendicular to the plane of the molecule, but it is in the plane of the molecule. So, what will happen, this C 2 will you known make a rotation of 180 degrees. So, this A will now go to this place, C will go to this place, and others will come here and here. So, I should have a structure like this. So, though apparently I and C 2, you can think that they are similar, but you can see these two structures when I marked them with A, B and C and D you can see they end up in a two different structures, but if I forget about A, B and C this marking then this two structures are equivalent. So, they are indistinguishable in that sense, so that is about the inversion symmetry. So, here also I suggest you to take some molecules particularly the molecular model and you try to look at the inversion symmetry points the center of inversion in the given molecule. So, more you practice to find out about the symmetry elements it will be more better for you.

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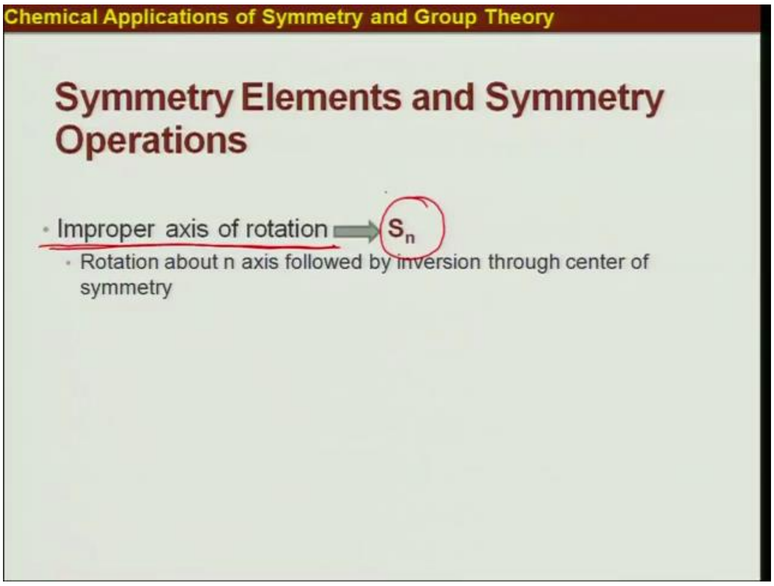

So, let us move to the next symmetry element that we need to learn. So, the next symmetry element is known as improper axis of rotation. So, this is a symmetry element which is symbol is S n, S subscript n. So, now, we have something on improper because initially we started with proper axis of rotation and I told that find the meaning of this proper this term will be clear it will be more clear when I discus something which is improper, and here we come. So, the name itself suggest that probably there is no such existence of axis in reality, let us have a look at it what does it mean. So, let us look at the definition of this improper axis of rotation. So, this improper access of rotation, so if I think about this particular operation first, so this operation is not a single operation, but this a combination of two operations - one rotation and one reflection.

So, you take a molecule, you can find an axis, which actually may not be one of these you know C n(s) that means, it may not be allow any proper axis of symmetry. Now, you suppose you find such an access about which you can have a certain degree of rotation followed by a reflection on a plane, which is perpendicular to that previous axis of rotation, and you end up getting and indistinguishable structures. Then this axis that you choose will be called an improper axis of symmetry or improper axis of rotation. And as I said it does not necessarily mean that this particular access will also coincide with a proper axis of rotation and that is why it is called improper axis of rotation.

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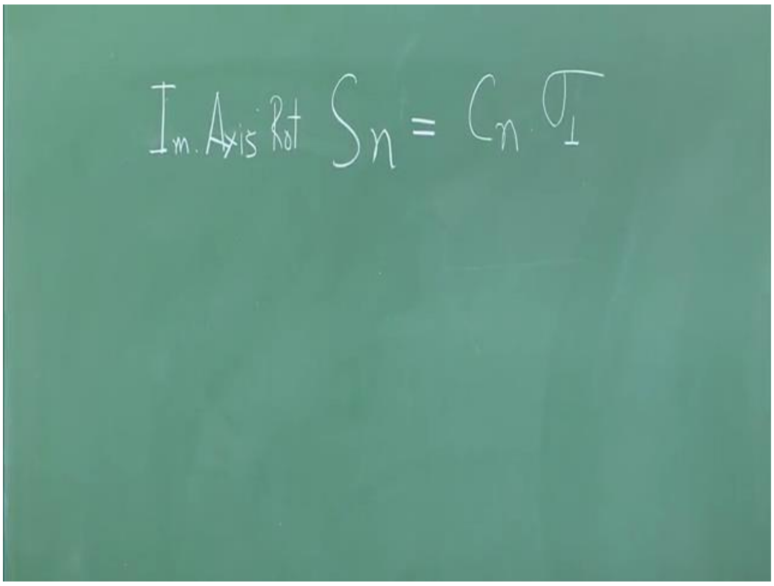

So, essentially if I can write this S n operation I should write it in this way. So, S n this is an improper axis of rotation. So, this S n is first rotation operation followed by and reflection and this reflection is such that this plane sigma plane perpendicular to this C n. So, I can write this is a perpendicular to this C n. Many occasions, you will find in many books that this is written as sigma h which may not be grammatically correct because as I say this improper axis of rotation may not be you know along the proper axis of rotation. So, sigma h is defined with respect to the proper axis of rotation the principle axis of symmetry.

Now, if I have the perpendicular plane to that axis of rotation that I am talking about for S n operation and if this C n does not lie in the same direction as that of the principle axis of rotation then this sigma cannot be called sigma h even though day it is perpendicular to this axis. So, in general, I will call it like sigma perpendicular. So, S n is an operation which is done in this way C n followed by as sigma plane and that will return you in distinguishable structure.

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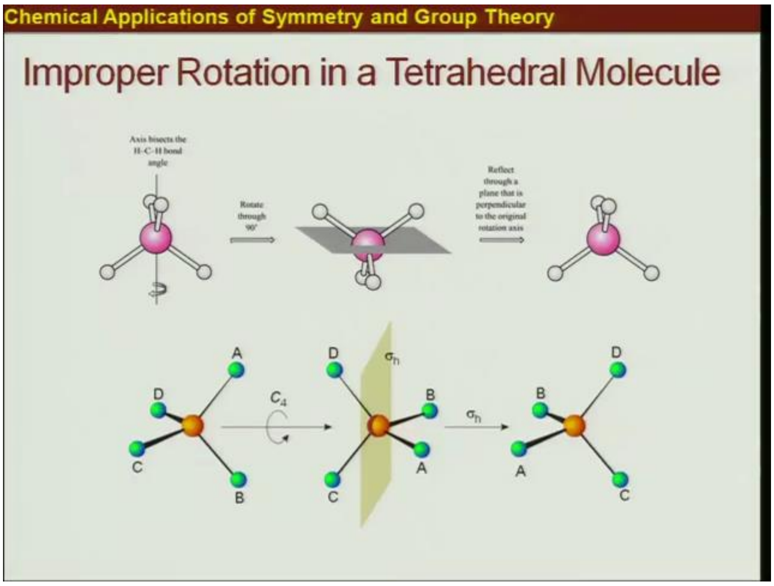

Let us take one particular example, so that it is clear to you. So, here on your screen, we have the molecule called methane. So, this is not model methane though. So, now, let is concentrate on the molecule that is on your screen right now. So, you look at this molecule methane and consider an axis, which bisects 2 H-C-H angles simultaneously.

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So, if I can show you that then it will be probably much better. So, I will show you using a model. So, this is what in shown on your screen. So, now if you look at on this particular model, which is the model for methane, so you can see all red sticks represent is C H bonds. Now, you can hold this molecule like this, where you can see this C 3 you know access principle access of rotation, but at the same time, you can find the C 2. So, C 2 will be like this, like one axis passing through the middle of this angle. So, you can see this angle. If you oriented in such a way that you can see only C bond because the other one is such blocking down other C H bond. And then this axis obviously, we cut this angle into half. So, essentially this axis is cutting this angle and this angle into half. So, there I give a rotation, it becomes like this. So, 120 degree rotation will give you in indistinguishable structure that is a C 2. Now, that is fine.

Now, can I imagine an axis to this one, which will be an improper access of rotation, answer is yes, how. So, look at this properly. So, I am using that same C 2. I took an example, which will be very easy to follow; we can go to much complex structures as we progress. And for the timing being, I should give the C 2, so that you can actually identify this SN axis here also. So, I take an axis through the same C 2 axis here, now instead of giving a C 2 rotation, I give a rotation by 90 degree. So, what I do is about this access I give a 90 degree. So, if I give a 90 degree rotation, this will go toward you. So, now imagine a plane, which is perpendicular to this axis. So, any reflection will bring this molecule here this atom here and this angle will be like this now and this bond will be coming like this. This will now go here, and this bond will now go here, because I am reflecting on a plane, which is situated here, so that will make the structure like this.

Now, if you just return to this video couple of minutes back then you will see we started with the structure. So, what does not mean, I could find an axis at a particular angle of rotation by which I can turn the molecule to structure which is very much distinguishable, but then if I give reflection perpendicular to that axis then I get an indistinguishable structure. So, this combine effect of rotation followed by a reflection perpendicular to this axis gives me an indistinguishable structure.

Now, if you go back to the original definition of a symmetry operation, we said clearly that movement of a body, which produces an indistinguishable structure. So, obviously, here this operation and rotation followed by reflection perpendicular to the rotational axis, if it gives an indistinguishable structure, this is a symmetry operation. And this all together C n sigma perpendicular as we showed here, this all together forms the symmetry operations and that is denoted by S n.

So, here I will also mention that a many times I am going back and forth between these two terms symmetry operation and symmetry element, I have discus what is what in my first or the second class. So, you should not be confused about symmetry element and symmetry operations, and both symmetry elements symmetry operations are symbolize by the same letter. So, here this S n if I can find out suppose this particular molecule I will call this axis as an S n axis. And then I can use this S n to symbolize as S n operation. And then once I use it as an operation I will change the molecular structure to another in indistinguishable, this is the molecular structure to another distinguishable one.

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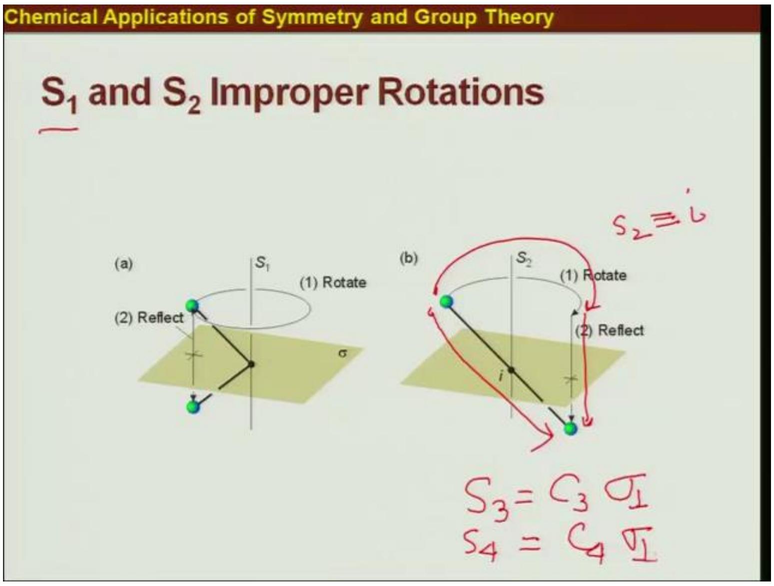

So, you have to practice a lot to find out if a molecule has a improper axis of rotation. So, now, on your screen right now, you have an example of generalized example of a some S n axis. So, this n is the order of rotation, this pretty much similar to what we had in case of proper axis of rotation. So, S n when n equals to 1, it would mean at 360 rotation right; and S 2 would mean 180 degree of rotation, S 3 would mean 120 degree and so on. And in every cases, it is implied that rotation about the particular angle followed by a reflection into perpendicular plane.

So, when we talk about S 1, so S 1 is C 1 followed by sigma perpendicular. C 1 is nothing but identity, so C 1 does not do anything. And then we are left with a sigma perpendicular. So, if there is a any reflection perpendicular to this C 1 axis, if there is a axes are imagine then essentially S 1 means nothing but reflection. So, if you see anywhere that somebody has use S 1 operation you know S 1 is nothing but operation by plane of symmetry. So, it is just a reflection on a plane.

Now, come to S 2 this is interesting; S 2 is like, you look at the screen and suppose a molecule has an S 2, so what does mean. So, I will rotate by 180 degree. So, whatever was on this side, it will now come back to this side correct, because S n 180 degree rotation. So, it is this part will come here. Now, if I give a rotation what will happen? So, now, after the C 2, it has come here, now after the reflection on a perpendicular plane, it will go here down here. So, essentially this two operations, it produces, it actually inverse the position of this object which we started with. So, it goes over here, so that means, it will have a center of inversion. So, S 2 is necessarily inversion which exactly shown here.

So, we start from this particular point give a 180 degree rotation and then we will reflect it here. Now, I cloud easily get it through an inversion symmetry here. So, S 2 is nothing but center of inversion. So, you can go to higher like a S 3 if you look at, so that will have a C 3 followed by sigma perpendicular. S 4 as you showed with this methane molecule, it will have C 4 followed by sigma perpendicular and so on. So, you can try to look at different molecular models and try to find out what are the difference symmetry elements. So, by now I have showed you pretty much all the symmetry elements and the symmetry operations that you can have in a given molecular structure. Now, you should try finding out all though symmetry elements that are possible in a molecular structure.

So, we are come to pretty end of this particular lecture. So, we have learned so far all the symmetry elements and symmetry operations, and we tried to find out some of the symmetry elements from some of the molecules. Now, in a next step, our intention is to find quantity way, so that we can talk about the nature of symmetry of a given molecule, if one is higher symmetry than other or not. And we should be able to utilize the symmetry elements present in a molecular structure in a proper way that can actually help me having application of this symmetry elements and operations. So, for that, we need an mathematical frame work which is actually a group theory.

So, in the following class, we will try to learn what group theory is basic mathematical concept of group theory. And then in the following classes, we try to see how this symmetry is being you know assimilated into the group theory and how it helps us in solving various problems in chemistry.

Thank you very much for your attention, see you in the following class.