Symmetry and Group Theory
Prof. Anindya Datta
Department of Chemistry
Indian Institute of Technology-Bombay

Lecture No.2
Symmetry point group: Examples Part I

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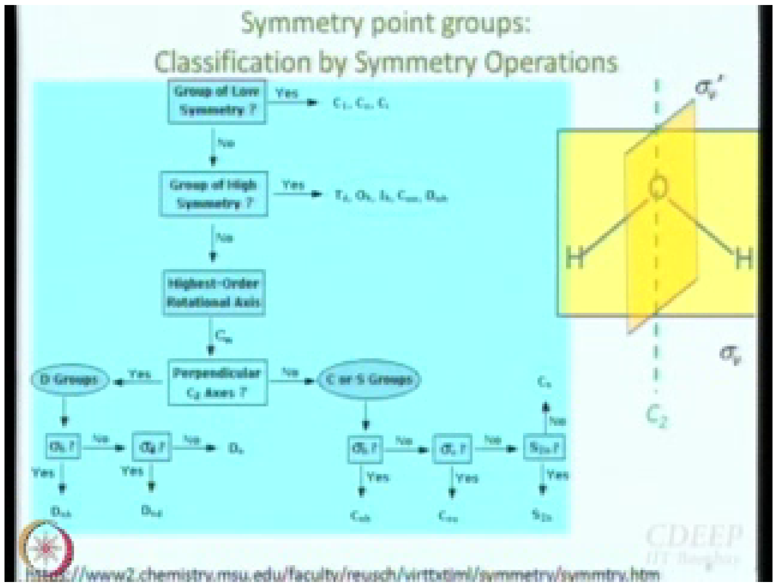

So, now let us work out some example start with water what where do I have let me hear from the gentleman in the far away benches yeah tell me do you have a point of inversion, no; do I have a axis of symmetry simple axis, yes what degree, where is it? Here and it is C2 axis ok any other axis, no, now let us look for planes I think you are going to think that I am a stupid, if I and ask you if there is a vertical plane of symmetry or vertical pain of symmetry obviously there is in. So, I would not ask that question.

Do you have a vertical plane of symmetry? Yes, where are they, this is one the molecular plane and this is one, perpendicular to the molecular plane Sigma V's go back this is easy to understand. And now think over plane that is perpendicular to the molecular plane so you are drawn it I do not know whether it is easy to see or difficult to see, the plane that is perpendicular to the Plane of the paper or the position where it is.

So, I call the first one Sigma V and call the second one Sigma V dash. And here for this very simple molecule I want to make point. The point is that these two Sigma V's that I have drawn they are not equivalent to each other will you agree with me or not. So, I will call them Sigma V and Sigma V dash and I do not call both of them Sigma V's. They are not equivalent to each other why do I say they are not equivalent to each other there is two ways in approaching this question.

First of all what happens when I apply Sigma V? When I apply Sigma V what is that happens to the molecule if I make a in this indistinguishable configuration will you agree but think of the atoms. Let us call this atom A and let us call this atom B, if you apply a Sigma V sorry reflection with respect to Sigma V, HA and H B will remain in the place right only the upper layer of HA goes without the plane and lower layer of the plane goes below the plane same is true for B, are you ok with that.

This the plane wherever I teach symmetry I always use more fingers on each of my hand I need 2 3 hands more but unfortunately I do not have so I will have to depend upon your imagination (Foreign Language: 03:38) I hope it will be better switch to principle axis of symmetry rather than horizontal plane like lying down, ok this is water molecule and this is the plane, the plane looking at you right what happens to this atom does it change place with reflection? No.

Whatever this atom? No whatever this atom? No, now if I think of a other plane Sigma V dash then what happened then if I reflect then this atom will go there, there atom will come here they interchange the atom right. So, even though both the Planes in the molecule in indistinguishable configuration their actions are not one and the same Sigma V does not cause at change in the position of any atom. Sigma V dash causes and interchange of hydrogen atoms ok.

The effects are different as you see whether the atoms move or not it is going to become very important in the latter discussion may be you would not be discussed in that in this course unless talk migration but we will see about that ok. So, you will agree with me now Sigma V Sigma V dash; do not exactly do the same thing to the molecule so they are not equivalent planes.
Another way of checking it is this, what is the axis that we have in the molecule C2? If I apply C2, does Sigma V get converted into Sigma V dash. If I apply C2, forget about the molecule only think of this line the axis and the two planes. If I apply C2, C2 is not connected in the rotation this is the plane this is C2 right, if I rotate then what will happen the plane will remain the same plane, it is just that my hand while still not allow my hand to go that much. But it will remain in the same plane right.

And the perpendicular plane will also remind perpendicular these two planes will never interchange. You see where the axis, the axis is at the intersection of the two planes is it not right. The axis is at the intersection of the two planes, the two planes do not get transformed to each other by application of the only other symmetry operation that is there in the molecule C2 ok. We have seen an example non equivalent plane of symmetry.

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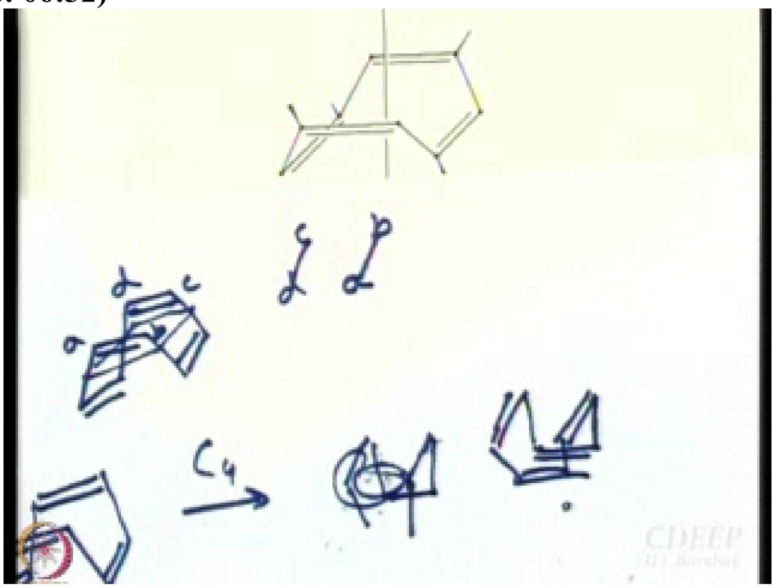

Now let us see an example of equivalent plane of symmetry ok. We will do this and come back digest a little bit actually you are wanted to give the name to water molecule and anyway let us finish this discussion and then we will come back. This is the structure of ammonia and I hope you can see it in the three dimensions. One plane in the one bond in the plane of the paper, one bond and pointing towards you singly and third bond is scared of you it is running away behind the plane right.

Now see you told me that there is a principle axis of symmetry there. There is a axis of symmetry what is it, C3 what is the axis? This is the axis, what are the other element of symmetry were, Sigma V, Where is Sigma V? Yes plane containing NH bond and the vertical axis of course. So, I can write like this; this is one plane, this is another plane I hope you get the orientation it is allow that the point that pointing at you and this is the third plane right.

Like three blades of a fan right now see what does each plain do. Let us take this Sigma V let us call this Sigma V you agree that it is a vertical plane of symmetry right, it is contains the similar axis of symmetry, the only axis of symmetry. So, now let us call Sigma V let us work with that what does that Sigma V do to the atoms. Upon operation of sigma V let us name them also, I will call them Ha Hb Hc upon application of this Sigma V first of all the nitrogen does not change place right.

What about Ha does change place? No what about Hb and Hc they change places right that is the action of Ha, Sigma V. Now this one tentatively I call it as Sigma V only, what does that plane do, will you agree with me that it leaves nitrogen and Hb in their positions and cause a interchange of Ha and Hc right on the third plane nitrogen and Hc will remain in the places Ha and Hb interchange places right. So, see the three planes has similar kind of actions nitrogen and hydrogen contained in the plane would not move.

The other two hydrogen atoms will interchange places that is the name of the game right. So, this all the three planes then are identical will you agree with me, I am sorry they are equal and they are not identical they are equivalent planes you do not have the completion of writing of Sigma V and Sigma V dash any more that they behave similarly. So, I can call them Sigma V ok so that was the first definition. Let us check the second definition.

This here is the C3 axis, you tell me. Now if you perform C3 axis will you agree with me that 3 planes interchange places remember what happened in the water we applied C2 and the 2 planes did not interchange their places Sigma V remain Sigma V, Sigma V dash remain Sigma V dash. Here however 3 Sigma V's get interchanged among each other upon application of C3. So, there is another element outside the set which causes an interchange of the members of the set that is a second Definition of equivalence right.

Right Maheth sure ok, so, I do not want to call them Sigma V Sigma V dash Sigma V double dash ABC nothing. Sigma V is good enough they are indistinguishable ok this is very important difference between equivalent and non equivalent symmetry of elements right. Now you see let us; I can see but you cannot see the flowchart now, is it not. Even if you are looking at the flowchart and I think it is very easy for you to tell me the symmetry point of group of ammonia.

So, C3 principle axis and the only other thing that is there is principle plane of symmetry so it has to be C3v right. What about water, there is C2 and Sigma V and Sigma V dash are different by the way it is look somewhat foolish call it C2 vv dash there is no provision for that in your flow chart. So, you are contained calling it C2v alright ok. Now instead of me drawing that diagrams since I have this projection facility I will make sense to you to show you the book right away ok, then next molecule you want to talk about is hydrogen peroxide can you see this clearly Is this big enough, can you see this alright.

You know the structure of H2O right it is not planar what are the axis of symmetry all elements of symmetry that are there unfortunately the answer is given that is one problem of showing on the book right only thing is you have C2 axis one bond is like this and one bond is like this ok. So, you take something in the middle perpendicular you turn then the two bond will interchange ok what will be the point group C, C6, C2 here it is C6 here fine.

Now I will cover some of the these, whatever is this, this molecule how do I not cover that and cover this there you so you see XY axis you turn by 90 degree what will happen this will come there just turn by 90 degrees what will be the molecule look like with respect to the axis this axis here you turn by 90 degree then what kind of the structure it will be. These are the molecule right let me name them abcd the bond is between a and b and c and d ok you turn by 90 degrees with respect to the axis what will happen.

In case of b you will have a right in case of c you will have b, in case of d you will have c in case of a you will have b and you forget the bond is between a and b and c and d. So, now we have turned by 90 degrees and what you have his a not indistinguishable configuration right. The b has to be the bond as well then what you see is if you now after turning by 90 degree if you reflect with respect to this plane joining the midpoints then you will get back the same kind of molecule.

There is S4 for you let me see what we can write start from here turn by 90 degree so C4, C4 operation what do you get so that is for it is, now if you deflect then what happened, if you reflect along the plane that will perpendicular to the axis then again this will come up this will come up, earlier you had a bond in this orientation again you have a bond in the same orientation are you sure you got the model it is very easy to see the model ok this is a S4 axis alright.

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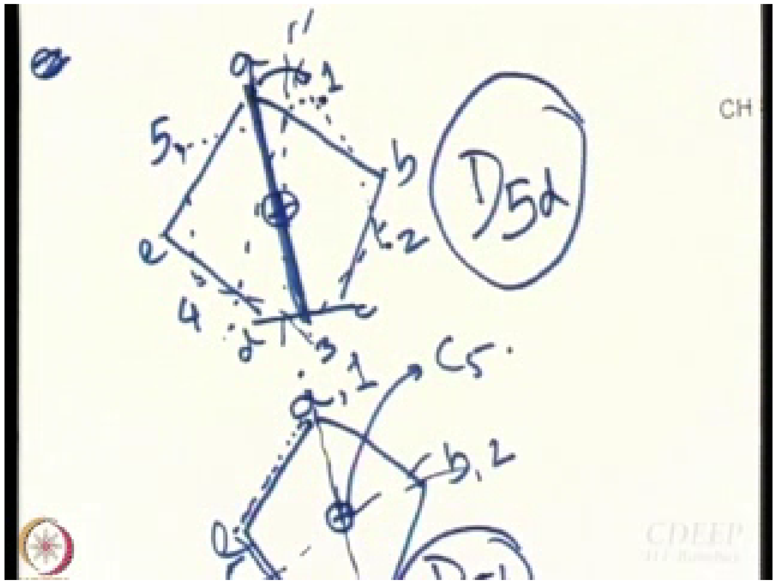

Let move to a interesting example and let me draw it actually ok. So, what is the structure of ferrocene, what does a ferrocene look like look down from the top you see a five member ring not very good here and you see another five member ring like this and their eclipsed now it is very it is to figure out do you see the C5 axis of symmetry, C5 is not very difficult to see. This is the C5 axis of symmetry right when the rings are five members you turn by to 2 Pi by 5 you get back and indistinguishable configuration have you all ok are we in the same pace.

Any other axis of symmetry Sn S10 yeah C5 axis of symmetry is also S10 axis of symmetry right because then this carbon atom will come here and then get reflected upon this ok other than that this is a simple axis of symmetry right. First of all C2 has to pass through the ion right we have done that ferrocene what is that if Fe2 or Fe0 2+ ferrocene so any C2 Axis must pass through the ferrous ion ok. Any axis passes through the ferrous ion what will it do, it is going to inter convert the 2 links it is very simple to understand.

This is ferrocene right anything we can do this is going to be C2 axis is it not. This is ferrocene this is the axis through this which will give you something like that. Now draw the structure and figure it out, it is little better than whatever I did earlier. This is C2 these are the two rings right iron is exactly in the middle, if you want that 2 to inter convert then it must be something like this right. I like to get the planes and right at the centre and this must be through iron. The question is at which angle, of course perpendicular to C5 I said that earlier but perpendicular to C5 you get infinite number of lines right so now if I do this orientation which lines ok I will take that let me not draw it will you agree with that that is C2.

I wish I have pen of another colour let us look at it point by point then only we can understand ok yeah this is one way of making small diagram look big fortunately. Let us name them a b c d e f g h i j hope you can read that. Now see when I turn that with respect to this axis do not forget what the axis is. Axis is equiv distance from the two strings it goes right through the ferrous ion and it is perpendicular to the C5 axis. Now if I rotate by 180 degrees what I am saying is a and g should interchange position right here.

You cannot see where ever I write it I over enthusiastic with this zoom in a and g would change places will you agree with me a and g will change places. The angular distribution is exactly between I take the centre and if I take projections in the middle the angular distribution is exactly in between the two lines right. So, a and g will interchange places b and f would interchange places c and I cannot even read it say c and h will interchange places this c and g, I am sorry a b c d and e and h should interchange places it is clear and you can work out correlation for every atom.

Let us take the simpler case of the ruthenocene it is very simple this is the ruthenocene where you have eclipse five member rings I just draw this two sides you just figure out right. They are on top of each other, now see what you have C5 right do you have any other axis C2, in this case C2 is very easy to understand C2 would be like this but still do not forget this C2 is not on any of those planes. Even this C2 goes to the ferrous ion and it is perpendicular to the C5 axis have you all ok with that your answer right ok.

This C2 passes through the ferrous ion it is not on any of the any of this rings as perpendicular to the C5 how many such C2 are there 5, here you need to figure out this drawing I will have another one you understand that there are 5 ok. What else is there, which plane, first which plane do you look for horizontal do you have horizontal plane of symmetry yes you do not have to look any further. For the nomenclature at least we have done.

So, what it will be C5h, Crd it will be d because you said there are 5 perpendicular C2 axis, 5 C2 axis perpendicular to principle axis right little more than C it is D. So, this is D5h that was easy now what you are I am doing is this are the planes where I am turning down just a little ok. There is a case in ferrocene this one right that is a case in ferrocene now what are the three elements that is survive? What are the symmetry elements that will be destroyed think like that.

C5 I see if I still survive right because C5, C5 is for individual rings because the 2 rings do not talk they go get mixed by C5 they do not care right C5 is still be there. Horizontal plane goes do you agree with that. Horizontal cannot be there anymore, we turned a little bit right so Sigma is what that was there are no longer survive agree with that or not. What is there in top of each other right sigma H is gone. Now what about C2 now let us ask the question is C2 there or not there. Now let us think like this earlier in ruthenocene in a b c d e and bottom of a you have I will call them 1 2 3 4 5 right that the carbon atoms top five or a to e and bottom 5 are 1 to 5.

When you apply C2 what happens? Where does a go and what about ruthenocene bottom one easier one D5h we apply C2 where does a go ok, good question this is C2 a remains where it is, no, a and 1 interchange do not forget where the C2 axis is, C2 axis is not on any of the planes, C2 axis goes through the ferrous ion that is there, equidistance from both the plane perpendicular to parallel to them. So, a and 1 will inter change is that right. Then b and b and 5 not right b and 5, e and 2 right then c and 4, d and 3 nothing else is left do you all agree.

Now what I have done is I have turn just the little this is your a b c d e and let us say this is 1 2 3 4 5 so how much I will turn with one think with respect to the other 36 right. I am going from ruthenocene e to ferrocene what is the angular twist I have given keeping the one fixed and how much I read the other one 360 by 10 right. if it is 360 by 5 once again you will have ruthenocene kind of structure ok. We have rotated by 36 degree ok. Now let us say turn this simple axis by 18 degrees half of 36 ok where it will go like this is it not.

I am sorry it is going through the centre that is a bad drawing four atoms in one side let us see 11 22 33 between the 3 now it is perfect right now you see same a1 kind of correspondence is there ok C2 survive even if you give a twist is just unless the two pentagons are really credible very difficult to draw that line ok. When you see it using a model you will look but it is also important to try to develop the vision without the model.

So, 5 C2 survive ok C2v survive Sigma h is gone what about the planes are the planes are there or they gone vertical planes. Vertical plane is something like is it not; it is there or not there? It is still there. You just that you would not call that the vertical plane anymore, is perpendicular C2 are there and the vertical plane plain would bisect the angle between them. So, you call them dihedral planes right. So, what do you have here principle axis of symmetry C5, you have 5 C2's are perpendicular to C5. So, that makes the name D5 you do not have horizontal plane so you will look for dihedral plane so this D5d alright fine.