Chemical Applications of Symmetry and Group Theory
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Lecture - 13

Hello and welcome to the day 3 of week 3, this lecture series. I hope you tried practising finding out conjugate elements for was different point groups if you have not, please try it some more. Today we will start there, where we left the other day.

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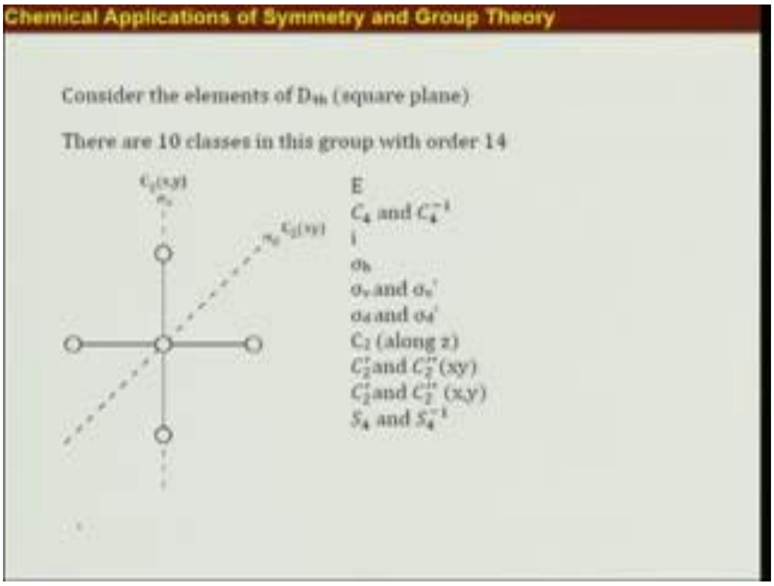

We are talking about how to write this you know classes for 1 particular point group. We showed that for C 3 v, we write E 2 C 3 and C sigma B because all the sigma v is, they belong the same class and all the proportionate symmetry operations, and they belong to another class and E that is identity from class by itself.

The reason we club them together and that the reason is that their properties, their characters are same likes the characters of C 3 and C 3 squares. They are same, the characters of sigma v prime sigma v double prime sigma v triple prime. They are all same for C 3 point group, but the characters for you know this C 3 class and character for sigma v class, they may not be same when I say about character that has a deep meaning. We will come to that, the following 2 or 3 classes and so. Let us come back to the, you know classification of symmetry operations. On your screen you can see that there is D 4 h point group and the classes that are possible for this particular point group are written here.

You have 10 different classes. You have class by identity inverse and the sigma H they form class by itself. You are already told that here you can see that and then you know 2 different sigma vs, they form you know class 2 sigma d is they form a class then C 2, there is a C 2 which is along the Z axis in case of D 4 h, D 4 h is Z axis means is the you know same axis through which you proper axis of symmetry C 4 runs. C 2 forms class by itself and then perpendicular C 2s they formed you know class by themselves and there are you know improper axis of symmetry. This S 4 and S 4 inverse, they form also class by they form a class. You have to try a lot of point groups and you find out the, you know symmetry operations and then you perform the simulative transformation on them and you try to find out classes.

Suppose I give you this you know D 4 h or some other say that D 4 d then there are certain you know travels in front of you. What are they like? Just like that, if I give you D 4 d, how will you know what point group or what that is symmetry operations that this point group has? Because if I give you the molecule may be you can try to look at and find out you know what the symmetry operations are. All you have to, you know think about a molecule which may have a point group D 4 d, but this is little bit problematic. I have easy option will be to just go and find out the book of book of group theory and at the end of this book, you will always find a set of tables which are known as character table and this character table gives you all the symmetry operations, but they will give you in terms of you know this classes, but that will you give you wait hint, but otherwise how will you find out about the symmetry operations that will a point group has? Like we are going in a reverse relation now earlier we figured out all the symmetry operations for a particular molecule and then figured out which point group this molecule belongs to.

Now, what we will do that in general if someone gives me a particular point group can I find out what are the symmetry operations that you know point group will have and that is what we will look at now.

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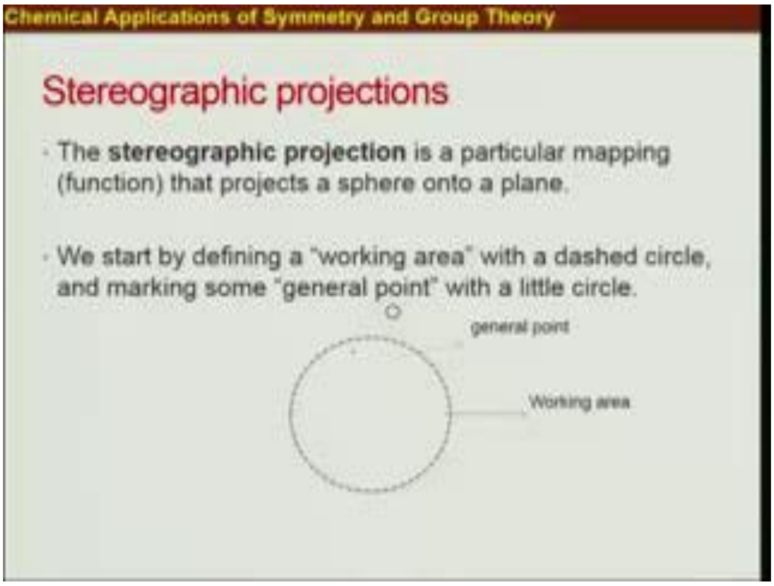

How will you do that? We will do that using something calls stereographic positions. Let me be clear, this point that we will not go into the deep, you know details of the stereographic positions or deviation of the stereographic positions, we will tell you the basic things of the stereographic positions and we will show you how to use this stereographic positions to find out the symmetry operations that are possible and also we will try to show you that by using stereographic positions and you can find out the products of symmetry operations that is an added advantage of this stereographic positions.

What is this stereographic position? Any molecule will be dispose in a space. It is a 3 dimension of space. So, anything you know if you take it like 3 dimension sphere and you know you project everything on to this, you know plane at the middle of the sphere you can take it like you know mapping plane. The stereographic position is a particular mapping that projects a sphere on to a plane. What we do here? We defines our working space or working area and we perform this you know positions of any point and utilises symmetry operations to generate several you know points that are also positions of any point the 3 dimensional space. We generate different points and thereby we figure out what are the symmetry operations other than which are very clearly defines by the point group rotation that represent.

Let us get it started so that it becomes bit more clearly. There are some issue in this particular try here. This circle actually is meant to be here. What I will do I just draw circle here that will solve the problem, alright. This circle big circle here shown by a dash line is our working space and everything that we do here will be in this working space and then what we do, we take any general point on that particular working area or working space and then we perform the symmetry operations. Now which symmetry operations that we will be performing, see when will be look at the symbols that is the (Refer Time: 07:51) rotation for any point group, certain symmetry operations which having that particular point group pretty obvious, let us say for examples if I take the case of C 2 v. What we know about that, you know C 2; that means, there is definitely there is C 2 axis and v is and v is transfer of vertical plane of symmetry that is there is a sigma v. So, this 2 at least I know and E is always implied.

I will start from first 1 that is a C 2 then after I will operate all the possible you know operations that are generate 2 C 2s. Here it is only 1 C 2 because C 2 2 or C 2 square is identity and then we will move to the next symmetry operations that is obvious from that point group rotation, that is sigma v S, you will apply sigma v. Similarly if we have say like you know D 6 8, what will you do? D stands for like C N. D 6 means a C n then there are perpendicular C 2s and H means there is a sigma H square. This 3 at least I know now, I do not know whether other than this there are you know centre of inversion whether there are other sigma v is the other sigma d is whether there are improper axis of symmetry all those things we can actually find out by using this stereographic positions.

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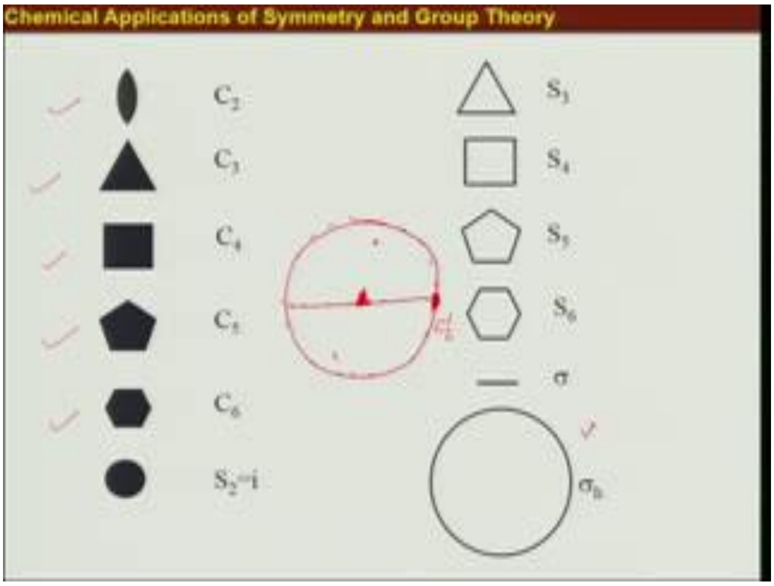

Let us get started now before we actually use if we before we start stereographic positions, we will first you know look at certain symbols that are used here.

Any proper axis of rotation is defined by some solid symbols. Like done here this is for C 2, C 3, C 4, C 5, C 6 and you can keep going. You know and triangle is for C 3 you know a square is for C 4 and pentagon is for C 5 and so on. It is not very difficult to remember also and this particular geometry have been 2 points on the 2 sides is symbol of C 2 for improper axis, what will we use is the same symbol, but not solid 1 , but the hallow now any sigma plane is given by a solid line. Let me clarify this thing little bit here. Suppose this is my working area and then I find out that there is a C 2 which is a proper axis symmetry which is here then what I do we mark it here. That it means there is a C 2. For any given object here will you know come to this point by a C 2 operation.

If there is a C 3 then I mark it here. Now there if there perpendicular C 2s that, that is very interesting thing like. This region is for peaceful axis of rotation or even improper axis of rotation that is given in centre while any perpendicular C 2s are you know drawn at the periphery suppose there is a perpendicular C 2s here. Say suppose this is C 2 perpendicular C 2 axis then, you draw that sign here. This means perpendicular C 2s or if I write C 2 prime. All the axis, you know proper axis or improper axis, they are written here or any perpendicular C 2 are written on the periphery fine now, you know this whenever I draw a line particularly, when it is dash line; that means, nothing. That has no physical significance here whenever you see the solid line; that means something. This dash lines are just for you know guidance that is all.

Now, suppose this line is by sigma plane then I will specify this 1 by a solid line across this is sigma plane if there is a sigma E, what will you do? This is sigma E means this whole plane molecular plane; you can imagine is a plane of symmetry. Then this whole thing will become solid, I will you will make it solid to signify that is sigma E that is shown here with this basic knowledge we will start looking at stereographic positions of second particular point group.

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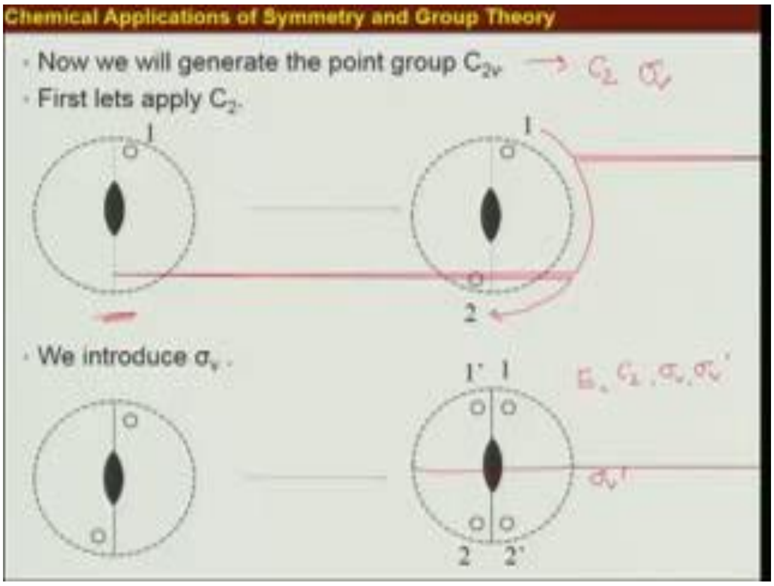

So, the easiest 1 will be look at something like C 2 v I know by it law you know what is the symmetry operations that C 2 v point group has, but it would be a good idea also to this C 2 v. It will verify immediately whether you can use stereographic positions to find out what are the symmetry operations that are possible. We will start here. You look at you know the figure here. We have the working space here as usual and what you know from C 2 v point group that we have a C 2. From C 2 v, what I know we have a C 2 definitely and then I have a sigma v, sigma v you know what is the definition of sigma v.

Now we start with C 2. We take a general point here and then perform C 2. If you perform C 2, if you do a clock wise rotation then this point will come on the way and go right here and that is what it is shown on this figure from here. You know originally it was here and now I have here this of course, from reason this writing (Refer Time:

13:40) function, but that is ok. That is what we generate by using C 2. Now we know that we have sigma v. Next I will use a sigma v prime. Where we will use sigma v, let us try sigma v right here, in this direction now will you generate something new and we can see that S, this will have a replica here and this line have a replica over here. The result of applying of sigma after applying this C 2 is this.

Now you see I am marking here also this point was 1 and this point was 2 now this 1 prime and 2 prime have been generated by reflecting the points 1 and 2 through this plane which is our sigma v now you see that you know 1 prime can be formed through reflection on a plane which is here of the point 2. 2 and 1 prime can be generated from each other if there is a plane here. I do not need to you know. I get another actually sigma v here. We call it as sigma v prime. Now, from this next part we should look at is that I have applied both the symmetry operations that I could find out from the (Refer Time: 15:22) rotation itself that is C 2 sigma v and operates both of them and generates all the point that are possible so that those are the I know actual number of points maximum that you can generate and after generating those you see if you know 1 of the points could be generated from another point through any other symmetry operations which you have already you have not looked at already and we could figure out that less there are stood exits plane here which we are calling sigma v prime by which you can generate 1 prime starting from 2 or vice versa similarly 1 to 2 prime or 2 prime to 1.

We have now figured out that they are all C 2 sigma v sigma v prime and no matter what identity. These are the 4 symmetry operations that are possible for the point group C 2 v and you already know that. You can see how useful this stereographic position can be in order to find out the symmetry operations for a given point group alright.

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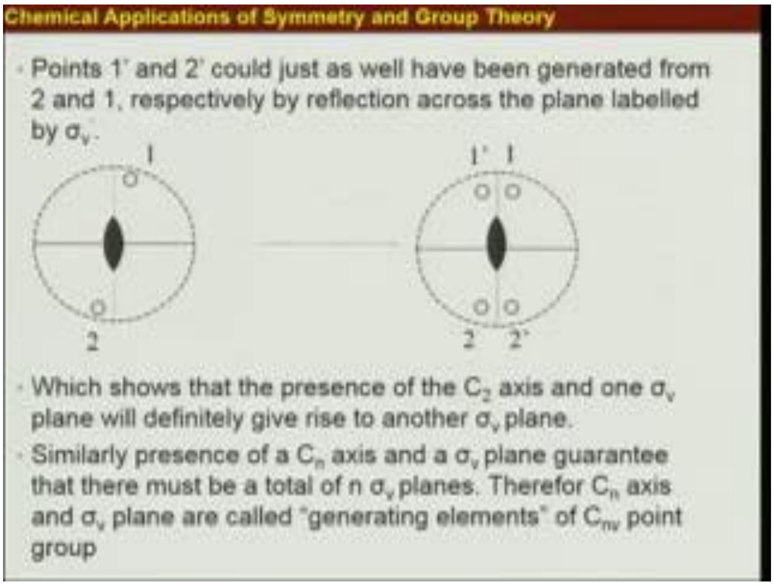

This is on your screen, this what I just now said that is you know this 1 prime and 2 prime could be generated from a reflection of the point you know 2 and 1 through a reflection plane here. From this example also you find out that the prells of C 2 axis and 1 S sigma v plane will definitely give rise to other sigma v plane here 1 sigma v prime. This is no matter, what this is true if you have 1 C 2 axis sigma v prime, there will be another sigma v plane and similarly presence of a C n axis and sigma v plane guarantee that they are there must be a total N sigma v planes, we have already you know learned that while forming the point group will had gone through the various steps. If you remember you know step 1 2 3 4 5.

In those steps, we mention that if you have C N, do you have a N C 2 primes do you have a N sigma v do you have a N sigma d is. We know that if you have you know principle axis of symmetry that C n, n, if you have 1 sigma v if you figure that out the doubt from that so implies rotation point group then you left as sure they all will be such to tell a N sigma vs. That is why this C n axis and sigma v plane they are called the generating elements of C n v point group; for example, if you would have taken C C 3 v you should be able to that very quickly. Let me help you about in doing that very quickly.

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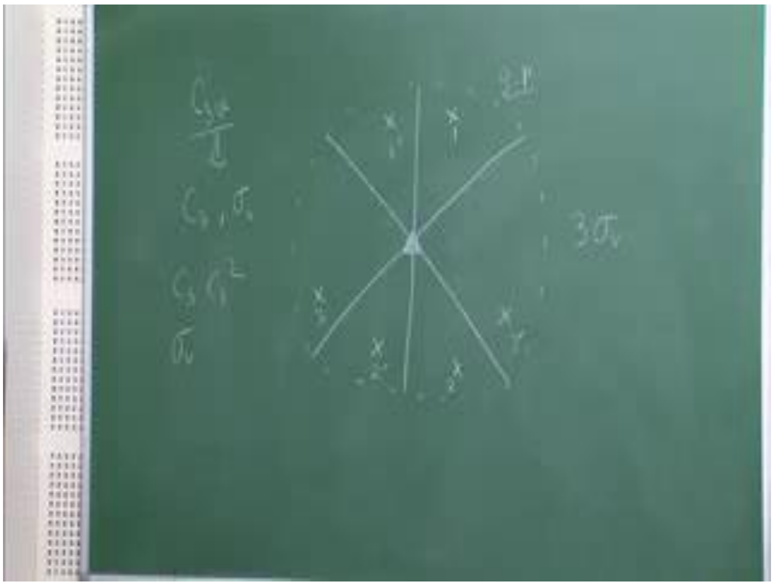

What you have for C 3 v you first find out the (Refer Time: 19:00) working space. You took trying to figure out C 3 v. C 3 its principle axis of what I know from this is that I have a C 3 axis and I have sigma v plane and already we have learned that for C 3 there must be 3 sigma v plane. I already know that now I will start from here for a C 3. Let us put the C 3 symbol here alright. This is solid triangle symbolising C 3 and then let us take any general point here. This is my general point and for my own understanding I am writing this dash line. This is us to help myself; this does not have any other meaning alright, 3 means 120 degree rotation. Let me, I have taken this generalise point. This is a generalised point any general point also (Refer Time: 20:12) and then I will operates C 3.

C 3 will take this 1 from here to somewhere here, now my job is to complete the operations that can be generated from a C 3 element. Then other operations that can be generated are C 3 square; that means, C 3 and another C 3. This element will reach somewhere here after C 3 operations, correct? C 3 square operations, sorry now I have sigma vs. Next I have to operate the sigma v. What I will do? I will say first take this 1 as my sigma v 1 of the sigma v. I will get 1 that, here now this point here will have a point 1 here. If I reflect and then this will have all similar points here.

Now I have generated all the points that I could use the information that I have from the impulse rotation. I have used the C 3 performed all the operation C 3 C 3 square and then I have applied 1 sigma v and I see the effect here now. I have got C 3 C 3 square; I have got 1 sigma v now. Let us see now, let us mark this point. Like you know say this is my point 1 2 and 3. Now this is say 3 prime and this is 2 prime and this is 1 prime now we just from here, you can see that this X 3 and X 2 prime they could be generated from a reflection through this plane. If you drive properly, it will be much clearer and then this X 2 and X 3 prime they could be generated that is X 2 X 3 prime could be generated from X 2 through a reflection on this particular plane.

What we get? We got total 3 sigma vs fine. You can try doing many other point groups.

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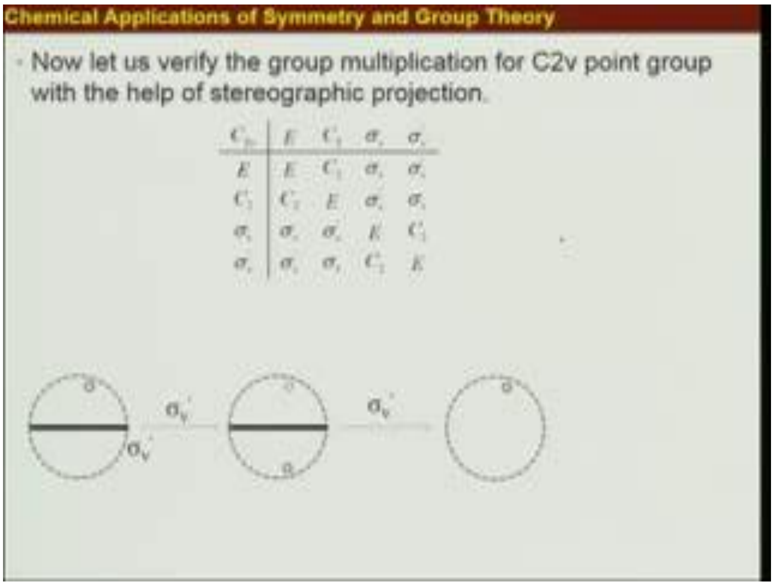

And you can you know from the point group symbols, you can find out all the symmetry operations that you can generate now. We also showed that you know with stereographic position we can find out what is the result of combining to symmetry operations that is you know successive you know successively if you operate 2 symmetric operations on any particular structure what will happen, can be figured out by a stereographic position that will you tell me that what will be the result at symmetry operations? Now while looking at the group multiplication table, we also we have figured out that like you know here in front of you, have the you know group multiplication for C 2 v prime groups and there you can see that all the binary products are written here. Now stereographic position also does the same thing. Using stereographic position you can actually find the group multiplication table.

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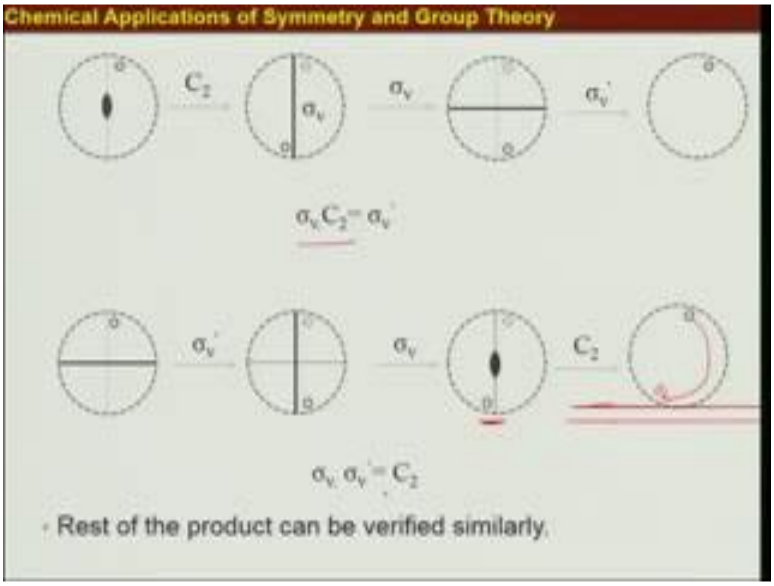

They are all interlinked, you can see that. Now you will try to verify that you know what will be the effect of you know doing this successive of operations. Now, suppose I try to find out that what happens when you operate C 2 and sigma v successfully that means, I have to get sigma v C 2 which means first you operate C 2 and then operate sigma v. First we operate C 2. This point it goes over here. This particular place is the original you know point that I took now after I got this structure then if I operate sigma v here, what we get is the reflection and in that case sigma vs in this plane. Reflection will take back to the original point. We get it we get here now. So sorry there was a mistake let me correct that.

You have you know operate C 2, it comes here and you take a sigma v which is around this plane and you generate a similar point over here, that you can see here and then you know, you if you would have taken a plane which is here perpendicular to the sigma v plane. I would call it sigma v prime then reflection through that sigma v prime plane could take the original point to this point which we got after operating C 2 and sigma v so that means, that sigma v C 2 it becomes to sigma v prime. Now let us go back to the group multiplication table and see if that is correct. If you operate C 2 and then sigma v then you get this product which is sigma v prime. This works.

Now, similarly if we try to figure out what happens? If we operates sigma v prime and then sigma v what is the result? We start from the general point and the sigma v is this plane. If you have reflection then I will go somewhere here, right here and then if I operate sigma v, which is along this then I will generate a point over here. That is what we generated here. Now if I would have taken a C 2. Here it is shown like, inform here I can go to this point by C 2, similarly from here I would come to this point, if could operate C 2 from this original point, I could reach over here which is identical to this structure.

That mean the sigma v sigma v prime is nothing, but equal to C 2 and if we just have a quick look at the a group multiplication table, then we can see that sigma v sigma v prime gives me C 2 and also from here you can see that you know it does not matter which here come that sigma v is sigma v prime or sigma v prime sigma v. It gives me C 2 which also mean set I can find out about the commutativity. So, you can verify the all the, you know other products that you can form. You can take any other point group and I will suggest to you to go steps like you go from C 2 v C 2 8 then higher orderly C 3 v and then you know D 4, D 4 h, D 4 v, D 4 d and try to generate all the you know possible stereographic positions and you know start verifying that is the group multiplication tables that you can have.

What it will do? It will you know, it will give you enough practise that you know if you have to answer the questions that what are the symmetry elements present for this particular point group you will not take much time and you can do it immediately, but the most important thing is that in the following groups, what you will do? We will start moving towards the actual applications of group theory and symmetry aspects into actual chemistry problems. Essentially for you know far we have them preparing the, you know basis for this applications. While we go for this, those parts particularly like you know find out section rules or forming a particular symmetrical after linier combination will be using something called representations. We have to actually prepare a presentation of this you know symmetric point groups and then symmetry elements. There are you need know this symmetry you know operations elements are very must and in order to you know we able to that very quick so that you can go to the actual problems you should you know practise doing this stereographic positions more number of point groups.

I will leave at that point today and we will come back in the following class with something more by will look at the matrix representations of different symmetry operations till then, Good Bye.