Chemical Applications of Symmetry and Group Theory
Prof. Manabendra Chandra
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 12

Hello, everyone welcome back. So, today is the second day of third week of this lecture series. So, we were finding the similarity between group multiplicity table which was formed of just an abstract group, and we were comparing within a particular group multiplication table which was formed for ammonia in particular which belongs to C 3 V point group. So, we figured out that when we compared both these group multiplication tables that all the elements in that multiplication table and they have one to ones correspondence so that means, elements of the group itself that is the group that had like E, A, B, C, D, E, and C 3 V point groups.

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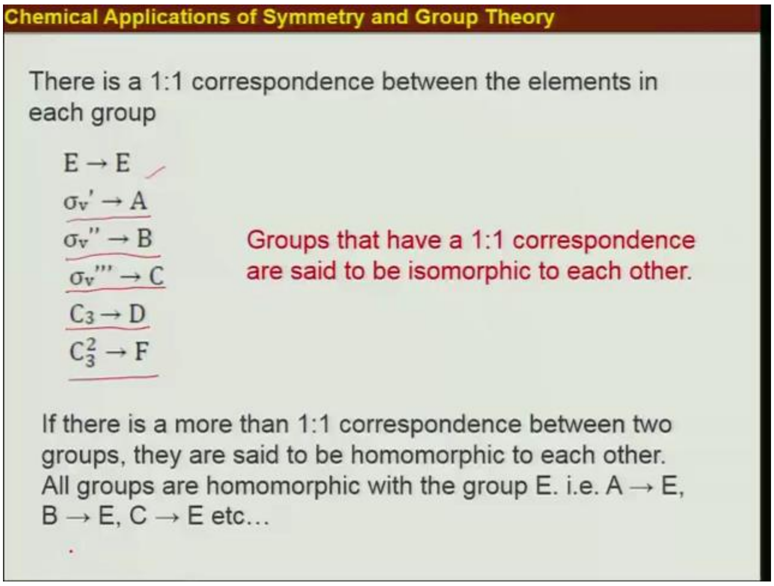

So, all the elements had one to m correspondence and we also looked at what are the actual correspondence, so which one is which. Now, the groups, which have one-to-one correspondence they are called isomorphic to each other. So, these G 6 and C 3 V point group they are isomorphous. And if there is a more than one, one to one correspondence between two groups they are said to be homomorphic to each other. And all groups are homomorphic with you know the group E; obviously, that is not a thing to be surprised off. So, where like you know A is E or B is E or C is E any element that you can think of we will have a correspondence with the identity element for that particular group.

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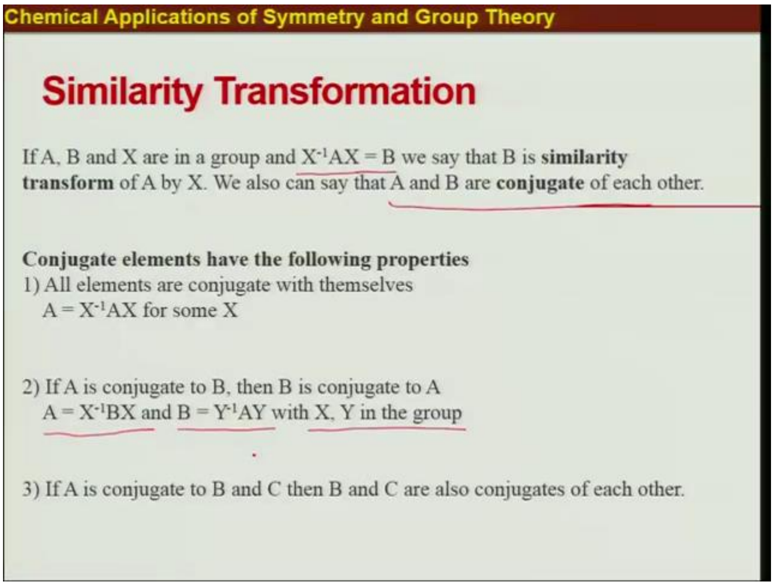

So, now let us have a look at another interesting aspect of this symmetry elements belonging to a group. We have formed a group from the symmetry operations of the molecule that is under consideration. Now, we can further classify certain operations in that that particular point group under a something called class. So, what is that class, we will know in a moment. So, before we can talk about what is a class, we should know something called similarity transformation. So, what is similarity transformation? So, if you pay little attention to the screen, you will see what is the definition of similarity transformation.

So, suppose you have A, B and X as elements of a particular group and if terms X inverse A X is equalized to B which is also another element of the group. Then we say that B is the similarity transform of A by X. So, similarly, if we have something like another element Y belonging to that group such that Y inverse B Y equals to A and again B and a are the you know similarity transform of each other. Now, when two elements belonging to a group are related through a similarity transform then we call those two elements are as conjugate of each other. So, here particularly A and B are conjugate of each other because they are related through similarity transformation. Now, there are certain properties of these conjugate elements that we will be looking at next. So, the first property that we will look is here that is all the elements are conjugate with itself.

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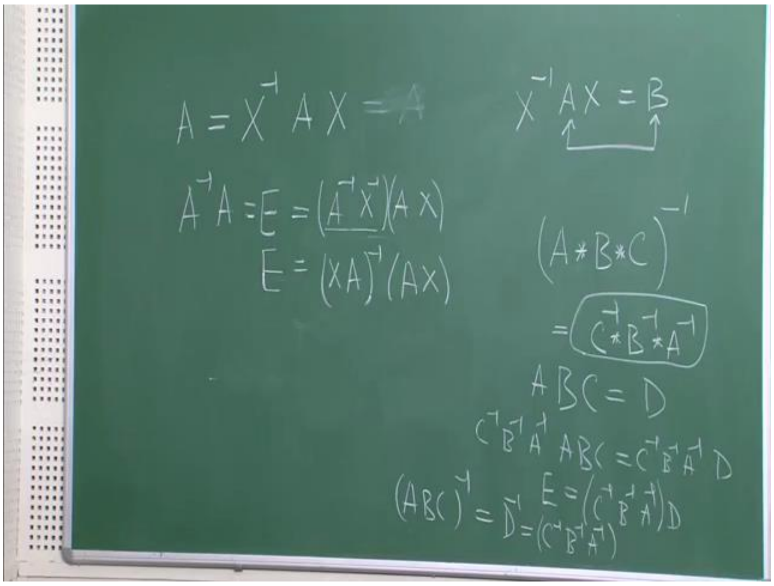

So, what does it mean? So we showed that X inverse A X can be some element B. Now, what this particular property that we are talking about says is that for any element A and X belonging to a particular group then no matter what this will always be there that is trivial case. Now that means, any element is a conjugate of itself. Because earlier what we were dealing with X inverse A X equals to B, and we said that B and A, they are conjugate of each other. And if I can have this relation that means that A is a conjugate to itself now how do we prove that that is very easily proved it can be proved very easily.

So, if I say write in this way, now if I can multiply this quantity by its own inverse that is A inverse then what we have for here A inverse A means identity, so that means, A inverse X inverse for this part A X fine. Now, what does this term mean. So, in order to find out we can utilize another property of elements of a particular group which says that reciprocal of or say if I say in this way that reciprocal of a product of two or more elements of a group is the product of the reciprocals of those particular elements.

But in reverse order, what does it mean mathematical is following that if A, B and C are member of a group then suppose I define a particular binary operation then this is equals to C inverse B inverse A inverse. So, this is a property of the elements of a group. And this also can be very easily proved like if I start with say A, B, C I am not writing this stars anymore, but this is implied and if I write A B C equals to D, and then if I multiply both the sides by this quantity. So, what we have we have C inverse B inverse A inverse followed by A B and C equals to C inverse B inverse A inverse. Now, A inverse A is identity. So, identity when it is operating on this B and C, it gives B and C. So, then next I have B inverse B C. So, B and B inverse will give again identity and we are left with C, C inverse, so that will also ultimately give identity. So, ultimately what I have is identity equals to D so that means, C inverse B inverse A inverse D.

Now what does it mean that this quantity when it is operating on D, it gives you identity; that means, D is inverse of this correct. So, in other word, I can write D is the inverse of this one. So, I can write like D inverse equals to this. So, D inverse means this A B C is D so that means, I have A B C inverse equals to C inverse B inverse D inverse that is what we started, we wanted to prove. So, the reciprocal of the products of two or more elements of the group is equals to the product of the reciprocals in a reverse order.

So, now knowing this one what can I write for this? So, this is a inverse X inverse fine, suppose if I can say for these two. So, this means X A whole inverse and then A X correct. So, this is equals to identity. Now, this is only possible when this X and A commute. So, then only I can if it commutes then only I can write it is like you know X A correct. So, in that case; obviously, I have this one. So, one element for A, I can always have like E identity, but other than identity other than this trivial solution, I can find particular element which will be commuting with this A. So, suppose that is B then B A, A B is equals to E. So, what does it mean that ultimately this comes from this expression, if this is valid then and that is valid for some X which commute with a right which is obviously, possible. And therefore, this is valid. So, in general, what we have is what we have is any element is conjugate to itself.

Now, there is another property of this conjugate elements that is if A is conjugate to B then B is conjugate to A that can also be very easily proven. So, what it says here that you know if A equals to X inverse B X and B equals to Y inverse A Y in that group then this is valid. This also can be very easily proven.

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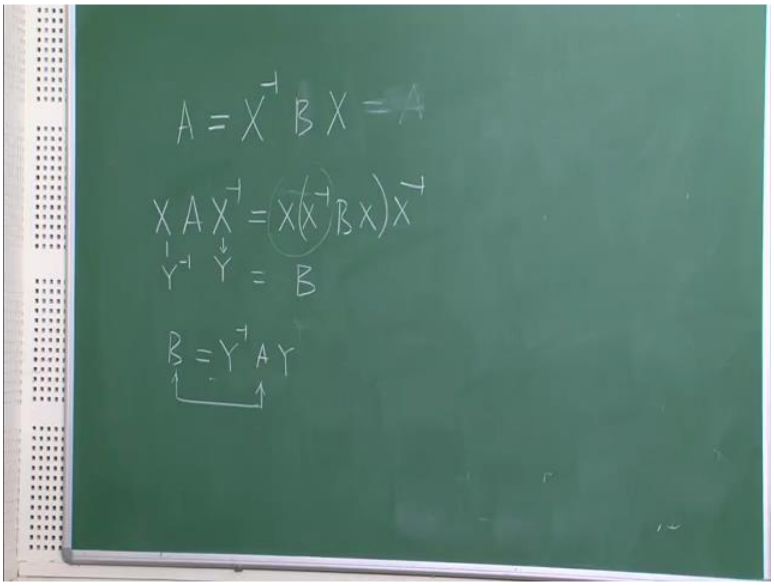

Say for example, you have this you start with equals to X inverse B X and you multiply in a way let me show you that you start with A equals to X inverse B X. So, here A and B are conjugate so that means, B and A are also conjugate. So, B is also conjugate to A. Now, how do I prove that? So, what I can do I can left multiply this A and this side also by X and right multiply with X inverse. So, let us do that. So, what do we have here, this part will give identity and this part also will give you identity. So, ultimately I have B here.

Now, in this group every element will have it is own unique inverse. So, there will be some element Y which is the inverse of X correct, and then therefore, Y inverse will be X. So, then what I can write for this part that is B equals to Y inverse A Y. So, then according to the law of similarity transformation B and A are conjugate again. So, we have seen that if A is conjugate to B then B is also conjugate to A. And thirdly if A is conjugate to B and C both together, then B and C are also conjugate, so that also can be very easily proven in the same way and I will leave it to you. So, you try it out and you prove this.

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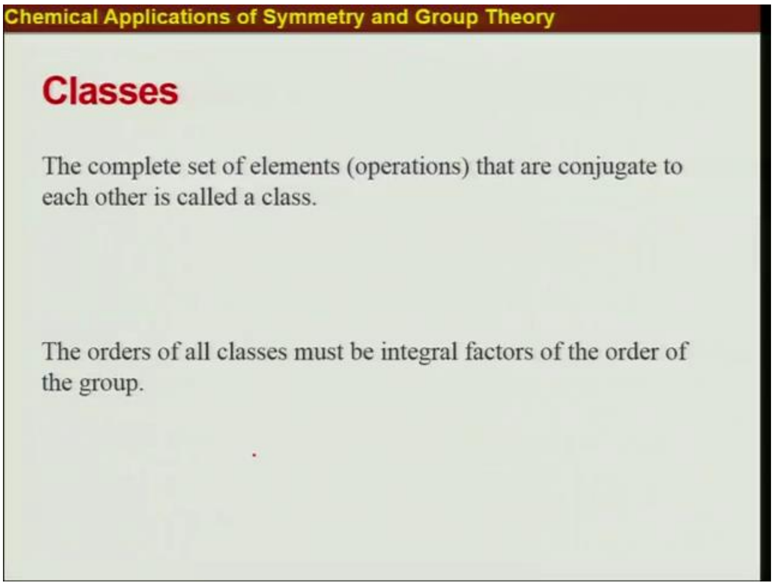

Now, if you take any particular group and then you perform similarity transformation on all the elements then if you find a set, which has to be a complete set. So, if you find the complete set of elements, which are symmetric operations here in case of point group which are conjugate to each other, then that complete set is called a class. So, this has a tremendous important in the applications that we are going to have you know few more classes later. So, you should understand what is class, how it is formed very well. So, in order to form a class, I mean one can easily verify this statement here that the orders of all classes must be integral factors of the order of the group. So, similar to the sub group, here the order of any class will be integral factor of order of the group.

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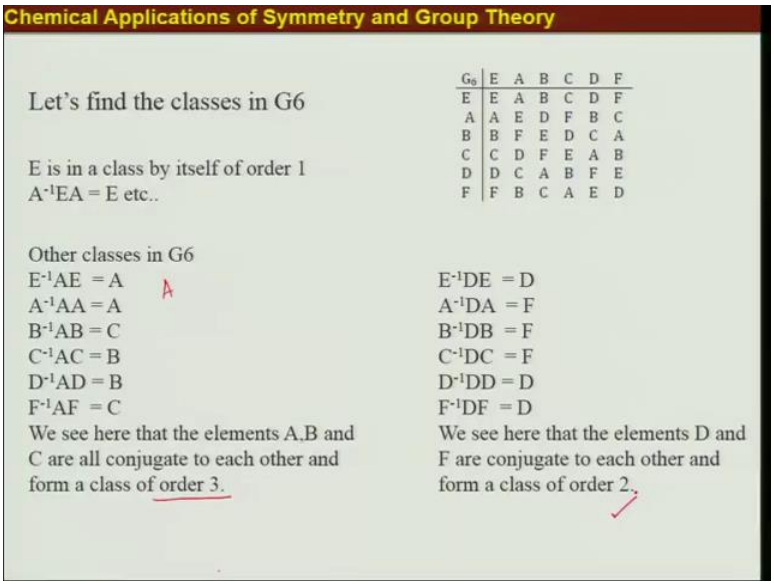

Now, with this knowledge let us try to find out the classes, which are presence in case of G 6. So, how do we find out the classes? Answer is very simple we have seen that we know the definition of class that is you know the complete set of conjugate element. Conjugate elements are you know found by with similarity transformation. So, what I am supposed to do here you have in G 6, you have 6 elements. So, choose any particular element first, and then perform the similarity transformation using all the elements present. So, for example, here you have suppose you start with the element E. So, what you do is following.

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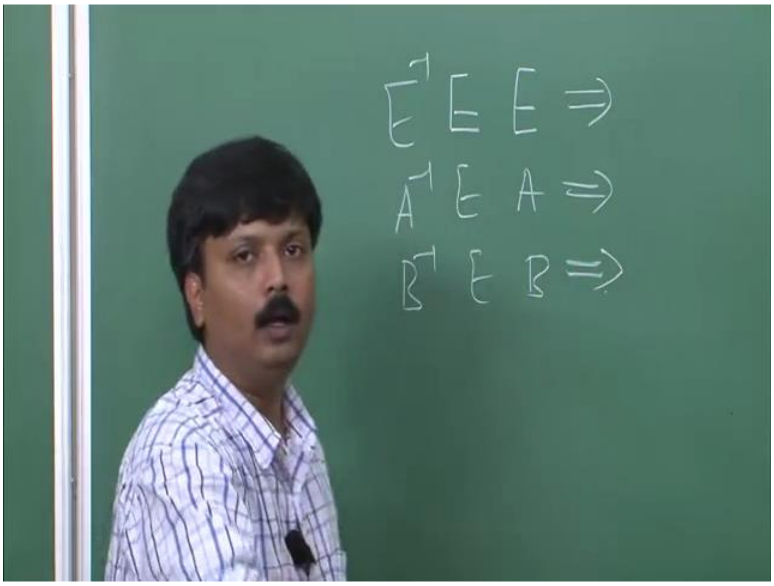

So, what you do is you take E and then keep doing the similarity transformation using all the elements that are present in this group. So, you get one answer here, then you do say A inverse E A, you get another one, then B inverse E B and you keep doing until you reach the last element of that group. And then what about the results that you get that you will 6 data right. So, 6 elements you will get out of these simulated operations because you will do another three. Now, out of these 6, you may have three different elements appearing say twice or you may have two different elements appearing thrice. So, those two or three elements that you find which are coming again and again that will form a class, and that is what exactly we are going to do.

So, first what you have to find out we will do this job for E and you get that whatever you do no matter what element that you are using to do this similarity transform on E you will get back E only. That means, that identity is it forms a class by itself that is the term that we will use. So, identity forms a class by itself. So, there are no other element in that class that identity alone forms.

Now, what are the other classes in G 6? So, you can you know you can do the similarity transformation on any other element. Say for example, you start with this element A and what you get here is written. So, on A, if you do the similarity transformation, you get A twice, B twice, C twice; that means, A, B and C they are conjugate to each other; and A, B and C form a class whose order is 3. So, we have a class of order 3.

So, here one thing I should mention that once you have started operating doing the similarity transformation on one particular element, and after this you know exhaustive similarity operations on that particular element you generate certain set of element. In the next, similarity transformation that you would like to do because you have got only three elements in this class and identity, so there are two more elements that are still left I would like to find out whether they form a class or not. So, in that case, you start with one of them.

If you do a similarity transformation on any one of them, you are going to get back A, B and C, which you have already found. So, there is no point of doing repeating the same thing. So, you do it with say D, you could choose F as well, both of them will give you same result. So, when you do the similarity transformation on D in the same manner, you find that D and F are repeated three times. So, what you have essentially that they form class, because D and F are conjugate and the order of this class is 2.

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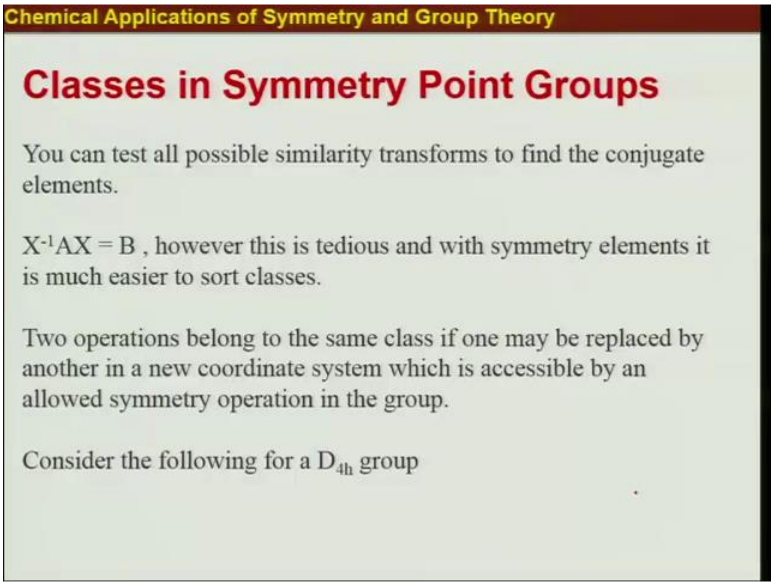

Now, this example was shown on abstract group. Now, in case of point group this is an really, really important thing. So, we need to find out the classes in case of you know symmetry point groups as well. So, you can actually test all the possible symmetry transformations like you did earlier and find out the conjugate elements. So, if you have if you have very, very large group then; obviously, this is tedious process to find out the classes, but you know once you have found out one particular class by similarity transformation then your job becomes bit more easier with you know every class that you find out.

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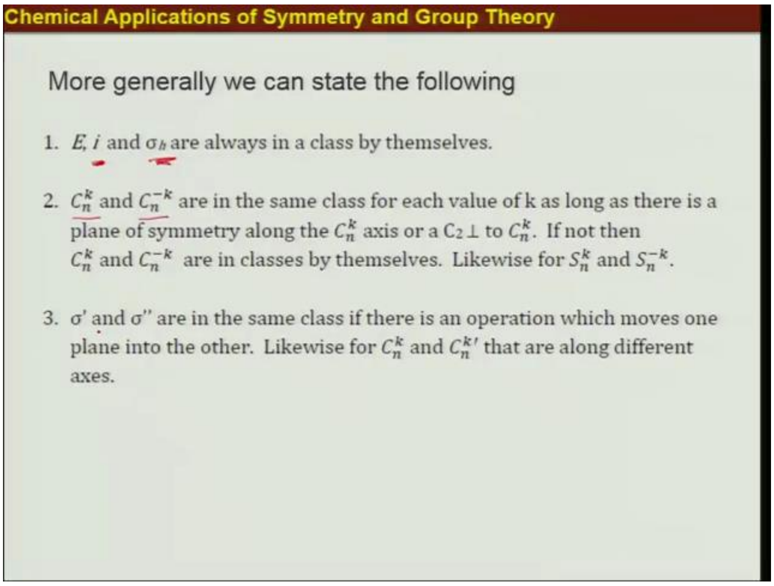

Now, let us try to find out the certain general rules regarding the classes and the relation between a particular symmetry operations and the kind of class that they will form. So, one we have already seen using the abstract group that identity forms the class by itself. There are certain other symmetry operations, which are the elements of the point group, they can also form class by themselves, one example is identity, we have already stated and inverse and sigma h string. It is not that any sigma. We will take an example later and we can see that this is valid, but whenever we have a sigma h, it always forms class by itself and so does the inverse in centre.

Again any proper axis of symmetry, and if you generate symmetry operations from that then generally this C n k and C n k inverse that is C n minus k, they are in the same class. For each value of k as long as there is a plane of symmetry along the C n k axis or a perpendicular C 2 to C n k. So, this is a generalized thing. So, if you try out for certain point groups then you will appreciate this general rule. And next time onwards, whenever you look at any particular point group, you do not have to do the similarity transformation all the time because these are certain general rules that actually have been found by extensive amount of similarity transformations on a variety of point groups. So, this is an acquired knowledge. And you can verify yourself and then you can actually you know get rid of doing all the tedious similarity transformation in order to find the class.

And similarly, we have like sigma prime and sigma double prime are in the same class when if there is an operation which moves one plane into other. Here, probably something you know that you already know; we mentioned about the equivalent symmetry operations. See, here exactly that is what you know gives you that sigma prime is a particular sigma prime suppose a sigma v.

Let us take example ammonia. So, we have three sigma Vs, you start on 1 sigma v, you apply C 3. So, this sigma v gets transformed into sigma v prime and then it transformation to another sigma v. So, these 3 sigma Vs are equivalent. So, here exactly this is being said that if you can move one of these planes into other by another symmetry operation then those sigma planes will form a class. So, knowing these it will be very easy for you to tell that 3 sigmas in C 3 v point group to which ammonia belongs they will form a class. So, sigma v, sigma v prime, sigma v double prime if I can name them in that way then these three sigmas will form a class. And you know if you look at the C 3 and C 3 square and if you perform the similarity transformation, you will easily figure out that C 3 and C 3 square they form a class by they form a class and identity obviously, it forms class by itself.

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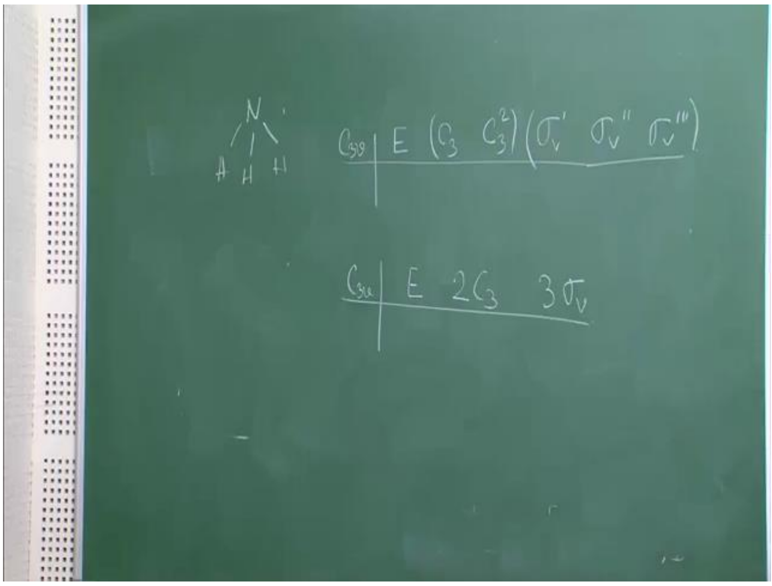

Now, one thing I will mention here that is suppose I am talking about C 3 v point group to which ammonia belongs to. So, how do I write all the symmetry operations? So, I write E, C 3, C 3 2, say sigma v prime, sigma v double prime, sigma v triple prime like this. Now, once I have found out the class, I rewrite this in a way which is C 3 v, E and I club these two because these two forms class and these three form a class. So, I write 2 C 3 and 3 sigma v. There is a specific reason for writing this way and there is a specific reason to form a class because certain properties for those symmetry operations belonging to a class are same what I mean is like any element belonging to the class will have the same property.

So, we will stop here today, and we will meet again for the following class, till then have a nice time.