Symmetry and Group Theory
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Lecture No.9
Introduction to Group Theory

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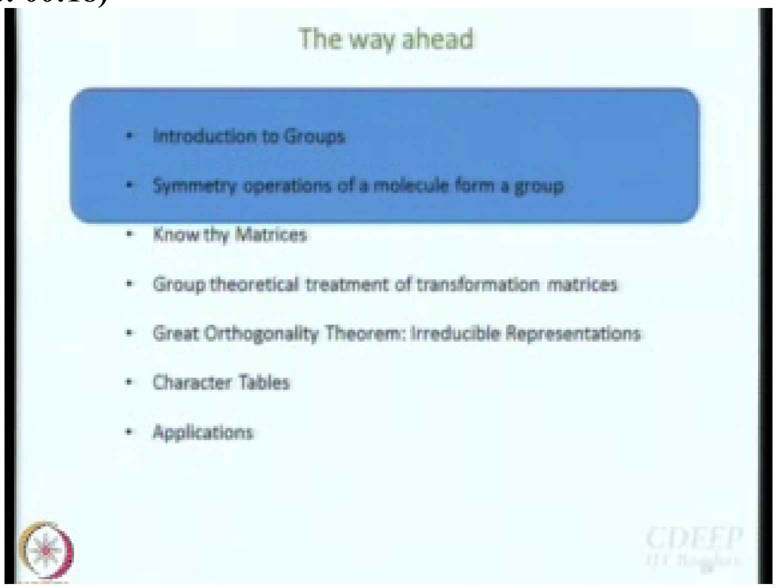

This is what we trying to do today

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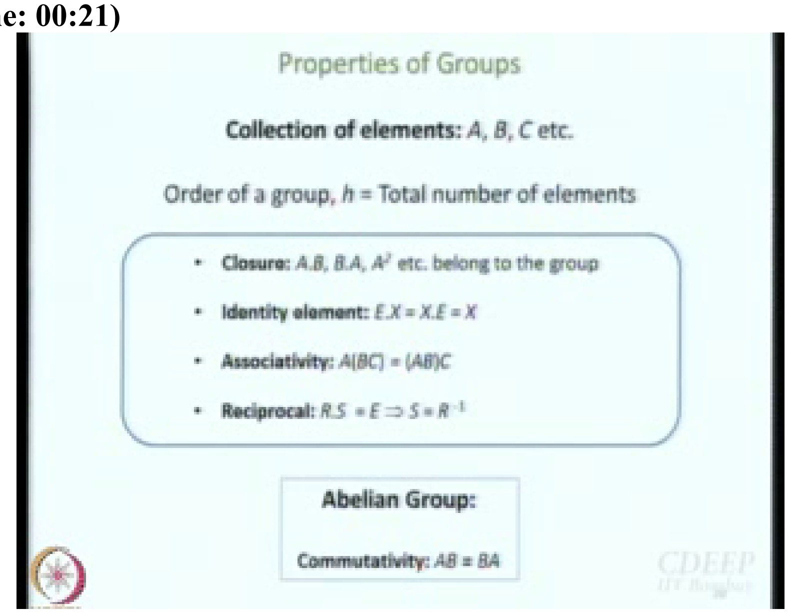

So further now let us remind ourselves what groups are what is the group? Group is the collection of elements we can call them anything right. We call them like although we have Bilal that kind of thing or you can call them a b c etcetera. For now you do not want to write too much we write abc and one thing do not forget it order of the group is total number of elements that are there ok. Now letus relate these two our problem of symmetry if you believe for a moment that the symmetry operations of a point group actually form a group.

Then what will be H for the point group What is the age what is the order for your point group you are playing a spoil Sports I am asking a simple question what is H? H is just a total number of symmetry operations but the reason why I state what seems to be obvious is that people confused between operations and elements please do not do that. H the order of the point group is the total number of symmetry operations not the total number of symmetry elements ok for example in C3v how many symmetry elements are there.

C3v ammonia I will tell you 1E, C3 then elements 3 Sigma v, 5, 2 + 3 is 5 not 4 definitely right so 5, but H is not 5 what is H? E C3 then C3 square is the different symmetry of operation do not forget that then Sigma v Sigma v Sigma v that is 6 so H going to be 6 ok please do not forget that when you talk about order in terms of context of symmetry point groups you are talking about total number of symmetry operations not elements ok, so, the collection of elements but not just any collection of element.

The collection of element that behave in a particular way and collection of element which have certain properties what are the properties of elements in a group what are the properties of group, reciprocity then associativity right identity yeah of course then closure generally I like to start with closure.

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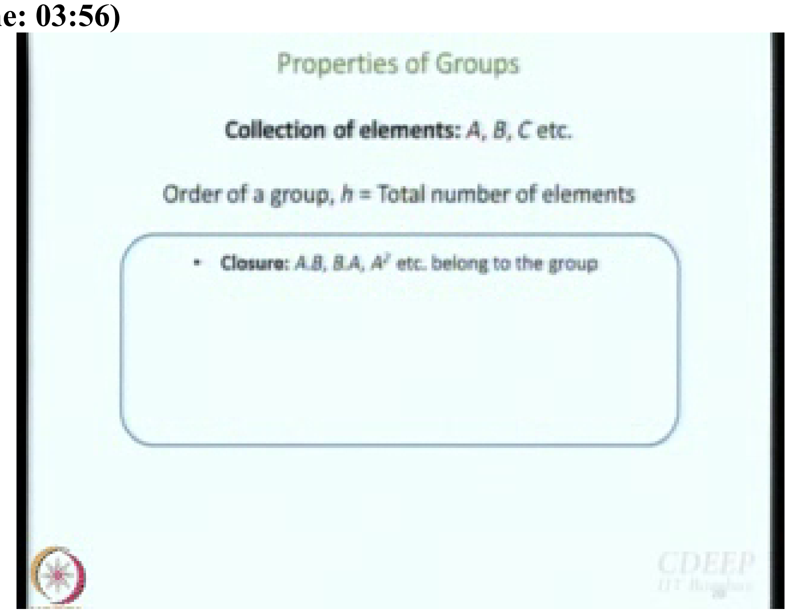

Closure means that whatever the operations are there right if you take that products product means you operate I am talking in terms of group not in symmetry operation that belong to that also. If you take the products of the elements of the group say ab or ba or a square then all this should also belong to the group that is closure ok. If I now think in terms of symmetry point group let us say C2v once again in terms of C3v what is the meaning of product what are the operation tell me C3v again Sigma v so if I write like a b if I write C3 dot Sigma v what does it mean Cv3 once again

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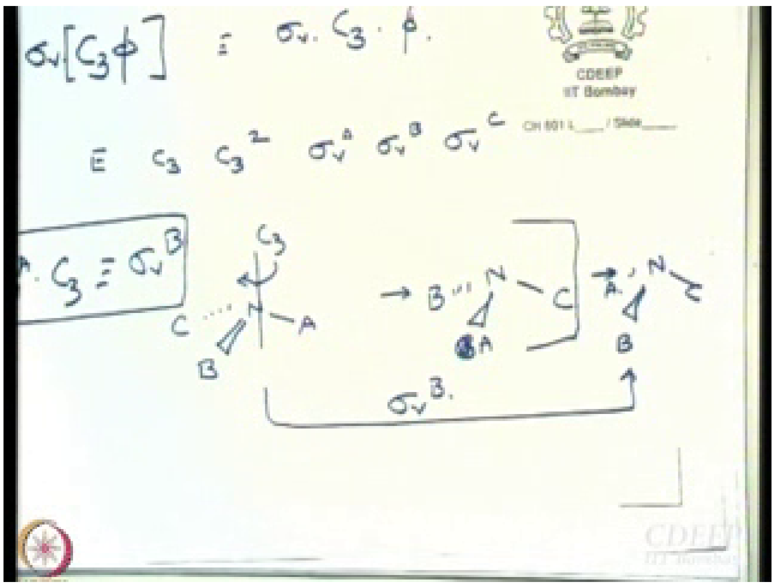

I have something Phi right, I make C3 operate on Phi and then I make Sigma v operate on whatever is the transformed coordinate this is what I write as Sigma v C3 phi ok. What I am saying is that you have E you have C3 C3 square Sigma v I call it A Sigma v B Sigma V C ok. So, if something is the function Sigma vA operates and then sorry C3 operates Sigma v operate on it then what I get should also be member of the group.

Let us see ok it is not a bad idea to like this Sigma vA Sigma vB Sigma vC can be assigned very easily is it not of course when I written A B and C, I mean HA HB HC so not get confused they are same thing just I want to write it like this. So, when C3 operates on this what do I get let us say like this where will I go B where will your B go oh sorry ABC. Now let us say you operate Sigma C rather Sigma A what was the original Sigma A the plane of the paper then what we get NCBA, what is that?

Can I go from here to here by a single symmetry operation Sigma v B right? So, what I get done is Sigma v which one they operate A C3 is equivalent to Sigma v B original molecule ok alright. So, what you can do is whenever you have a time an inclination you can work out this thing for each and every element each and every product ok. And you find that whatever you get is another symmetry operation of C3v; doubt, question, yeah we have been deceived actually.

What was the original position? No, that fellow said when we designate the plane we have to stick to the original nomenclature we have to behave as if the planes are face fixed ok Sigma C dash fine ok we can work it out you see that you will be able to draw something like this.

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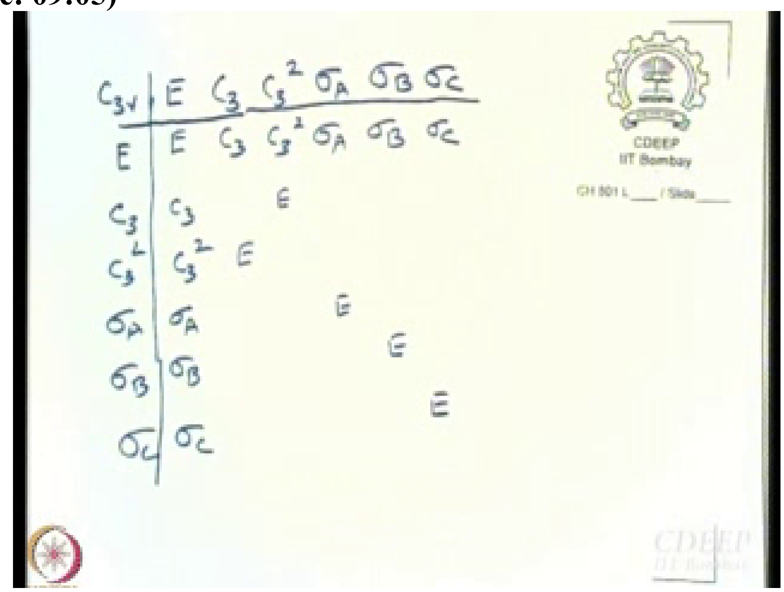

C3v E C3 C3 square in fact I write Sigma A Sigma B Sigma C ok. Now let me write it here as well E C3 C3 square Sigma A Sigma B Sigma C alright. So, how am I write this element this E which is first; this first this second this come first this come second what is E dot E, E. What is the next one actually it is E C3, C3 operation first right and E operates afterwards that is how we write it right this is C3 I think by now you will not disagree with me if I go ahead and write this ok. And similarly I think you understand how to write the first column and then what you can do is you can fill in the rest.

While doing it finds out that for each of the element you will be able to write one of these. For example what is C3 C3 square? E what is C3 square C3? E what is Sigma A Sigma A? Sure yeah Sigma B Sigma B, Sigma C Sigma C, E. I have worked out so many so you work out the rest. I worked out all the difficult ones work it out you will see that you will be able to write something one among this. I havealready demonstrated one, please try to do it yourself and convince yourselves that at least for C3v the property of closure is satisfied by the set of symmetry operations.

First property is closure ok you understood the closure and you have convinced ourselves that for C3v the set of symmetry operations satisfy the property of closure ok next one is presence of the Identity element EX = XE = X identity element is that that it multiply with any element to give back the same element not only that he commutes with any given element including itself. What is the meaning of commutes understand the meaning of commutes right they interchange so, EX = XE = X.

This is the presence of Identity identities like 1 for multiplication; multiplication is what is relevant there ok. If you are talking about addition it has to be 0 here what is relevant is multiplication. Now go back to C3V does C3 have an identity element yeah what is that? E or C1whatever you want to put, B nothing that is identity element fine, what property as you set correctly is associativity right it does not matter whether I perform C perform BC then A or whether C and then AB it does not matter you get the same result.

Now you have constructed the multiplication table of C3v personally from there try to convince yourself that associativity holds, it holds right. The last and well said correctly is his presence of a reciprocal. Reciprocal means you have for every element of R your another element S so that RS = E so you call S, R inverse ok do not forget that you are not really talking about multiplication-multiplication division-division when you write multiplication in our case the symmetry operations for example what it means is successive operation ok.

Now going back to C3v what is the inverse of C3, C3 square do you agree, C3 inverse of C3 C3 square what is the inverse of Sigma A Sigma v is Sigma B like that right. So, you see with the example of C3v what we have done is we have demonstrated convince ourselves that the symmetry operation of a given symmetry point group actually forms a group. So, we can use group theory on the symmetry operation of course it is difficult if you want keep on turning things and how will you use group theory on that is why we need matrices fine.

Before that let us remind ourselves what is a cyclic group, a cyclic group; what is a cyclic group? I have written Abelian group same cyclic that is a different issue. A cyclic group is something in which the elements are like E then X then X square so on and so forth ok, example cyclic group means take for examples C3 point group. If there is AC 3 point group what are the symmetry operations carry on there, E then C3 then C3 square ok there is nothing else. So, ABC; C is just B square ok that is what does cyclic operation is it not that is the cyclic group and in the cyclic group what happens cyclic group is also an Abelian group.

Abelian group means commentator commutativity holds AB = BA I want common conclusion that we have is that we assume that the associativity as well as commutativity holds for all groups, that is not correct, it is may or may not be commutative ok in such group however the cyclic groups are Abelian and this commutativity AB = BA holds for cyclic groups alright fine

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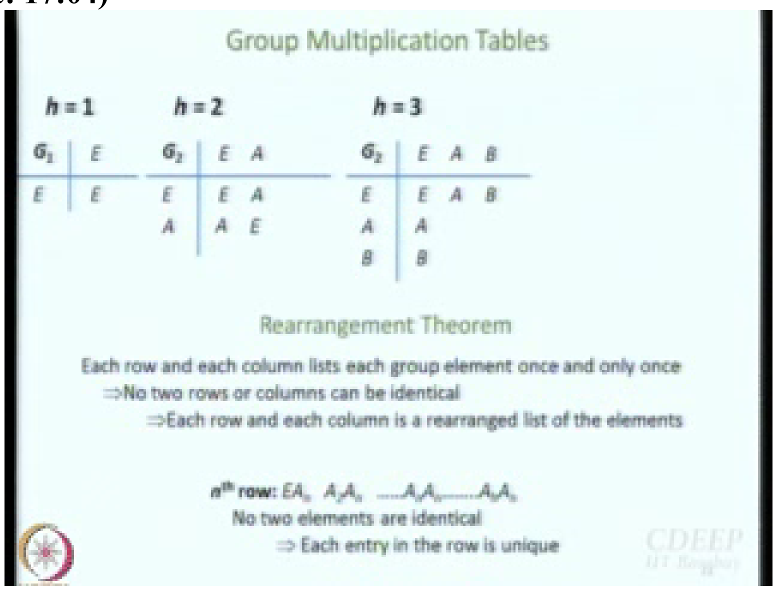

Group Multiplication Table that we already we have demonstrated what is group multiplication table using C3v but let us now do a little bit of formal introduction to the group multiplication tables ok and we are on the last right I think we have almost done it is second last. So, like C3v what we can do is we can work with abstract groups C3v is a very tangible group is it not you know exactly what is the meaning of C3 you know the meaning of Sigma v right but even before that see what we are doing now is benefit of mind set we know all the group theory holds and all that.

But then abstract group theory was formulated nobody even thought that this is going to be application in chemistry and all. So, it is completely abstract it is just people who kind of went with a flow and saw what comes out. So, let us retrace the path of those pioneers and let us see how we can work out the group multiplication table of even abstract group because knowing the value of ABC etcetera ok. So, h = 1 that is a kind of moronic group right because there is only 1 C3V in moronic group so, there is only one element what is that one element E not C.

So what would be the multiplication table look like we call it G1 you know about G8 and G10 it is not G10 it is G20 and all that group of powerful Nations and sometimes group of powerless Nation also get together and call themselves as G whatever Gn so that idea perhaps came from this group theory. Because we call them G1 G2 G3 G4 depending on what age is G1 is kind of a stupid group because there is only 1element is there that the; if you want to write the multiplication table you have to write E, E and E ok.

If it comes in the exam everybody get hundred out of hundred and goes very happy ok unfortunately life is not that going. So, let us go a little further h = 2 what is the name G2 ok for G2 let us say there we have 2 elements if it is G2 it has to have 2 elements what is the first one E and second one because it is my initial it should be EA you start writing the multiplication table now will write it you now see what will be at the cross section of E and E E E E simple. In fact you even write the first line EA right what will be E multiplied by A and what is A multiplied by E again A. Only one element is left and you know so what will be the element B my second initial B you do not write A I will write B and complete the story because if you do then you are going to violate this property of closure right.

Your closure has to be there so you better write E do not write anything else. And in fact A into A is easy not only for closure, why is it E first of all closure secondly your inverse has to be there right so A as to be the inverse of itself that is work filler for a group of order a for h G2, A has to be inverse of itself. The scope as does it have anybody else right it has to be inverse of itself alright, Mahath; agreed simple, h =3 precisely you have to give the answer EAB G3 whatever it be G2 that is genuine mistake not one made to this is a peril of copy paste.

These are the model in it this is the peril of copy paste sometimes you paste and forget to replace it is G3 of course not G2. What will be the first row simple what will be the first column now we have to work out the rest, what do I have, do I write A or do I write B, two option 50% probability A and 50% probability B what do I have there is no probability. Probability of 1 is 1 probability of the other is 0.

Because there is something called rearrangement theorem ok. Rearrangement theorem says that each row and each column lists each group element too many each's once and only once. You cannot have an element that is missing in a row you cannot have a element missing in a column you cannot have a row or column which does not have an element have you understood the meaning ok. So what did imply is that no two rows and column are identical right.

Because if that is identical that two identical rows then what will happen you go down the column you will have the same thing twice that is not done there no two rows or columns are identical ok as it remind you something? yes theta actually I am going to say that but does that remind you of something more related to physical chemistry or mathematics property of matrix what is the first question of matrix what happens when in a determinant of two rows are same or two columns are same z right fine.

So, what this implies is that each row and each column is a rearranged list of elements and hence this interesting name of rearrangement theorem ok. Each row and each column is there rearrangement list of elements do you understand that what we are doing we can actually work out the different permutation ok. First row first column is any case is defined and then we can work out the permutations in a way that no element is repeated in any row or column and we can actually construct the entire character table without even knowing what is the meaning of this elements AB ok.

If that is now how powerful abstract group theory is there ok. Now of course this is what I have got now written on stone and letters of fire? No there has to be some proof for demonstration or something right what was words of god written on stone in words of Fire, The Ten Commandments if there is no Ten Commandments right so good better be some proof and this is how we can see what we are saying make sense. What is nth row think of any group think of any general nth group?

This will be the elements there right EA and A2A and A2 means second one first one is A1 it tells that this is going to be we have written B ok. Do anyone think that this is what the nth row contain EA and N then A2 AN A3 AN and so and so forth AN AN finally Ah AN where h is the order make sense close your eyes and think what it looks like, make sense everybody convinced, I have not convinced that everybody is convinced, how do I write the elements then what do I write first one the top or one on the left?

One on the top right so what is the second element on the top A2 what is the element on the left AN so I write A2AN ok. Next one what is it A3 on the top on the left it is still AN I am going left to right in row it is A3 AN so and so forth it is finally reach end there also this going to be AN AN and then last one will be AH the last one the last element and the second one will be AN, AN is always the second one right this is what it is.

Now what will be what will you said what does the closure require that these are all elements of the group ok. Now are any two of these elements identical see everything is different right A1 A2 A3 everything to be different right. And each of that is multiplied by AN, so they are all different. So, no two elements are identical that is a proof ok, that is the proof of rearrangement theorem. Incidentally rearrangement theorem are discussed everywhere and I am following the treatment of Carton that is all.

But it is there in all the books that we are on our text fine. Now knowing that ok entering in the each row we have already said knowing this what will; can you fill in the blanks can you do this Sudoku what will this be B and what will be this then E what is this E what is A, BEEA right. So, what turns out here is that A is inverse of B and B is inverse of A ok, this is G3 and do you notice something strange there not strange but something unique here Abelian group.

Abelian group cyclic or Abelian group ok right. So, we stop here today and tomorrow we start at what 5:30, 5:30 we start at 5:30 tomorrow and we start with this we have gone up to of h = 3 next we will go to h = 4 ok and meanwhile what you could do is ok; how many are there in C3 C3v how many elements are there? 6, that is too large you think of a group which is D3 D4 what will do if we will compare the multiplication table of some point group which is either G3 or G4 and we will see that will do the same thing right so until 5:30 tomorrow.