Mathematics for Chemistry
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Lecture - 25

In the next 7 or 8 lectures I am going to talk about the topic; that is group theory and molecular symmetry.

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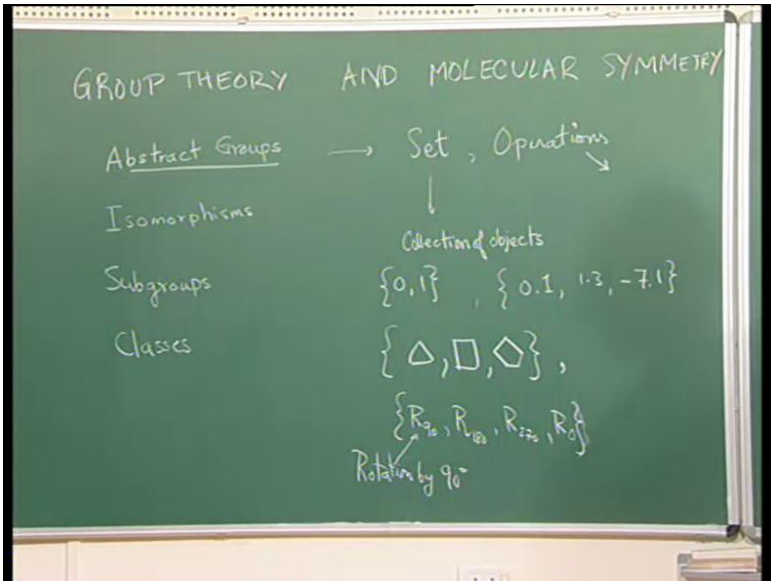

Now, this is a topic that has being introduced chemistry more recently ever since the advent of spectroscopy. So, it is very much connected to spectroscopy and this topic is also connections to quantum chemistry, so in the first part I am going to talk mainly about abstract groups, this is what we will cover today, so I will talk about abstract groups. So, what is a group? In a purely abstract sense with any reference to molecules or molecular symmetry.

And then I will talk about the concept of isomorphism's, I will tell you what are the sub groups of a group and what are the classes of a group, so this is what I will be covering today. So, let us start with abstract groups. So, what is a group? So, in order to define a group with need to have a few concepts, and I will just mention them here, so for abstract groups you need a few concepts and that is you need a set then you need operations.

So, what is a set? A set is nothing but a collection of object. And are you specifically use about object because you can take a set of numbers, you can take you can also take a set of various shapes this can be anything. So, for example, you can have the set 0 1, so this is set of 2 numbers 0 and 1 or you can take a set like 0.1, 1.3 minus 7.1. So, this is these are all examples of sets, but you could also take more abstract collection of objects for example, you could take a set of objects like this 3 could form a set.

So, it could be any such arbitrary object you could if you want, you could take so these are geometric objects. You could say that my set is composed of objects that correspond to rotation by 90 degrees, rotation by 180 degrees, rotation by 270 degrees and rotation by 0 degrees, so this is rotations by 90 degrees, so basically the set can be a collection of any kinds of object. So, each of these as a set, you do not have to have only numbers in your set, you do not have to have only figures in your set, you can have all kinds of things you can have combinations of different of all these objects. So, it is a collection of objects.

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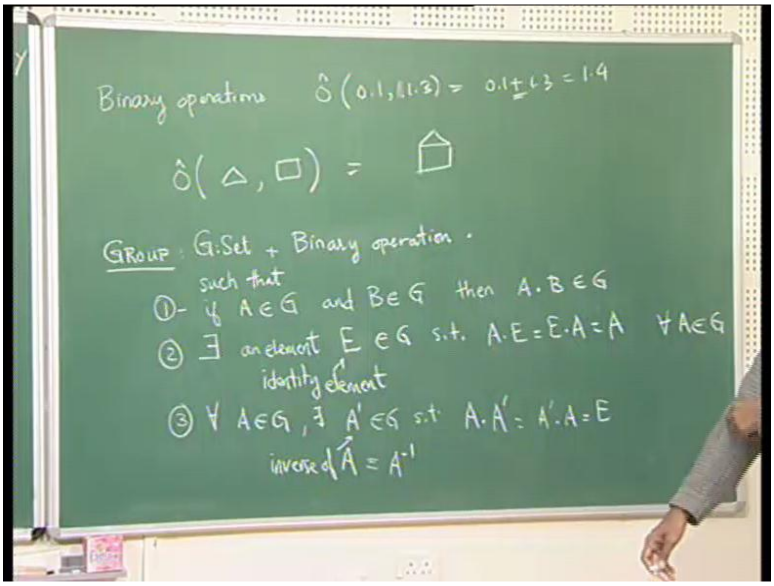

Next is the operation they act on the objects of a set, and give you new objects, so example of operations for example, binary operations, this is the binary operations, which are example suppose you have 0 and 0.1 and 1.3. So, you could have an operation that acts on 0.1 and 1.3 and it gives you 0.1 plus 1.3. So, this addition is an example of a binary operations and it is called binary because it is act on 2 object.

You could also have ternary operations, you could have unary operations, that act on one object and give you another object. So, this typically acts on an object, it gives you another object and that object may or may not be in the set. So, that object of that you get from the binary operation may or may not be in the set, for you could also define binary operation as you know suppose you do binary operations this operator operating on this triangle and this gives me triangle at top and this, so in this it could be something like that.

So, it just the important thing is it acts on 2 objects and gives you 1 object. So, the binary operation acts on 2 objects to give you 1 object. And as you can see this object may or may not lie in the set, so these are called binary operations. So, with this basic knowledge, we can define what a group? A group is composed of 2 things, one is a set plus operations. Now, so it consists of a set and then one operation sorry and an operation such that, and well I should be more specific. So, it is a set plus a binary operation.

So, it consists of a set on a binary operation such that, if let me call the set is called G and the binary operation I will denote by dot. And this group consists of the set G and this binary operation such that, if A and B are contained in G, then A dot B is contained in G. That means you multiply any 2 or you form this binary operation I will just call it multiplication but it can be any binary operation.

So, you perform this binary operation with any 2 members you will get another member of this of the group of the set G, then G is called a group. There are some more properties, so first is this is the first property, second property is there exists an element which we call E in G such that, A dot E equal to E dot A equal to A for all A containing G. So, there exists an element E is a number of G such that, A the binary operation of A with E is equal to the binary operation of E with A and that is equal to A. So, E is called the identity element and there exists an identity element.

This is identity element for this particular binary operation. And third condition is that, so for all A contained in G there exist A prime contained in G such that, A the binary operation of A and A prime is equal to the binary operation of A prime and A this is equal to identity, and then A prime is called the inverse of A. So, let us get back, so group is a set G that has a binary operation such that, if A and B are members of G then the binary operation on A and B gives an element which is also in G.

So, A dot B is also at G, so the binary operation will denote by dot. Then there exists an element E, which is called the identity element which is a member of G such that, A dot E equal to E dot A equal to A. And then for every A, for every element in G there exists an A prime which is called the inverse of A, such that A dot A prime equal to A prime dot A equal to E and inverse of A, this is denoted by A inverse. Now this is the very abstract definition because we said that the set can be anything the binary operation can be anything. But, so long as I satisfy these properties then you have a group. So, in order to look at examples of group you have to give examples of both the set and the binary operation.

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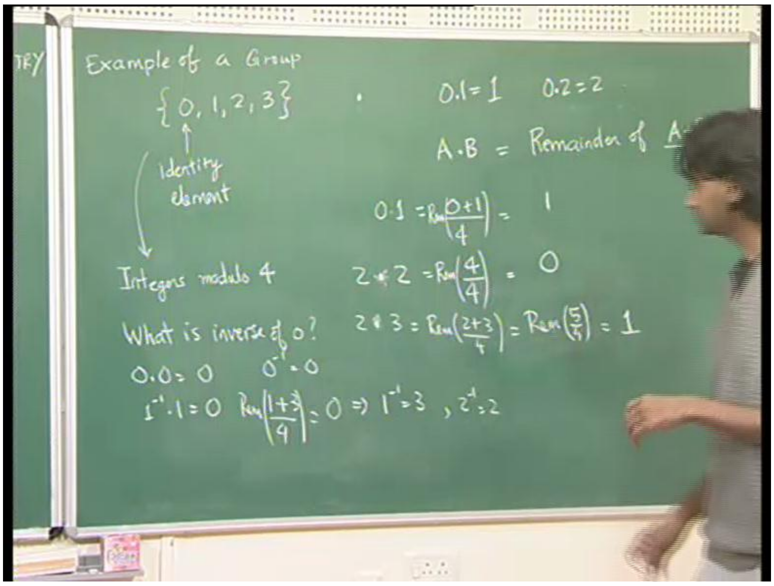

So, next we look at a few examples of groups so let us look at the set of numbers 0, 1, 2, 3 this is a set of numbers, this is example of group. Now I define my operation so this a set and you have the dot such that, so the definition we have to define what you mean by this dot. So this operation 0 dot 1 is equal to 1, so 0 dot 2 is equal to 2 and so on. And then what you want to define is, so you have 0 dot 1, 0 dot 2, 0 dot 3 they are all just the same thing, so 0 is the identity element.

Now you have to specify more about this binary operation now, I define my binary operation on any 2 integers A dot B is equal to remainder of A plus B divided by 4. So, what I mean is a following, so if I take 0 dot 1 this is equal to 0 plus 1 by 4 this is equal to 1. So, the remainder of 1 divided by 4 is, so 4 times 0 is 0, so the remainder is 1. What this let us me do is suppose I have 2 plus 2 this is equal to 4 and the remainder with 4 this is equal to 0.

So, say remainder, so 2 plus 2 is 0 then similarly, 2 plus 3 equal to remainder or 2 dot 3 equal to, remainder of 2 plus 3 by 4 equal to, remainder of 5 by 4. So, when you divide 5 by 4 you will get 4 times 1 is 4 and the remainder is 1. So, this is the set of multiplications and this will ensure that you can easily see that you take any 2 elements of the group and you do this binary operation and you get another element of the group. And you can also see that 0 is the identity element, this is sometimes called…

So, this is a set of integers module 4 so; that means, the set of integer module 4 is 0, 1, 2, 3, so even if had 75 you when you do it module 4 you will just get 3 because 75 is 18 times 4 is 72 remainder is 3. So, you can keep adding, so you can take a number and you can keep adding it and you will always get another element of this same set. So, this is called integers module 4 this forms a group you can see. So, what is inverse of 0 and the answer you can see easily that you need 0 times 0 equal to we have 0 times 0 equal to 0.

So, clearly 0 inverse is 0 equal to 0 what about 1 inverse times 1 has to be equal to 0, so clearly now you can see that 1 plus 3 module 4 remainder of that equal to 0. So, this implies 1 inverse equal to 3 and you can also see that 2 inverse equal to 2, so every element has an inverse. So, there is identity and each element has an inverse and this binary operation always gives you another number of the group.

So, this satisfies all the axioms of a group, so this is an example of a group. Now one of the things you notice is that whenever you need to check whether something is a group you have to multiply all the elements with each other. You have to do this binary operation between all elements of a group, and this is called a multiplication table.

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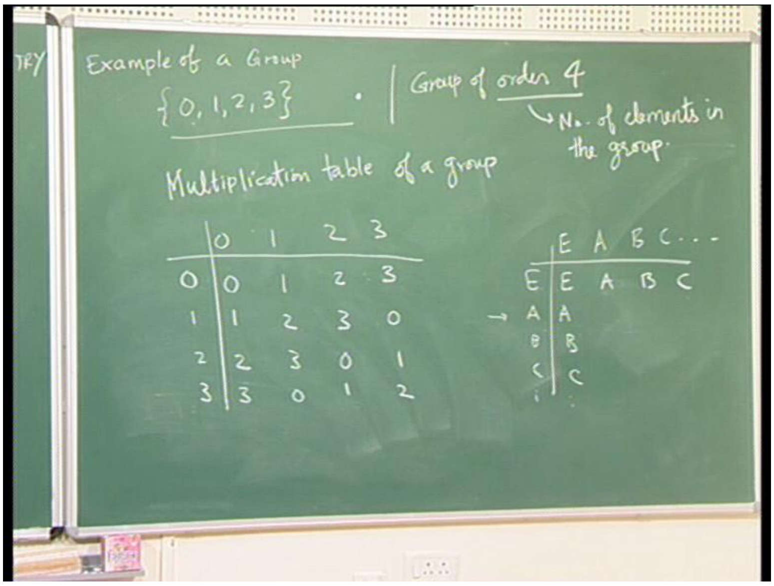

So, the multiplication table of a group, so this is over the group multiplication table this is basically the set of all products. So, this contains all the various products that you can consider and this is represented this way, so for example, in this group you have 0 1 2 3 and you have 0 1 2 3. So, I will put here is 0 dot 0, so 0 dot 0 is 0, 0 dot 1 is 1, 0 dot 2 is 2, 0 dot 3 is 3, 1 dot 0 is 1, 1 dot 1 is 2, 1 dot 2 is 3, 1 dot 3 is 0, 2 dot 0 is 2, 2 dot 1 is 3, 0 1 and 3 0 1 2. So, this is a group, so this is called a group multiplication table and if you have this table it is like a multiplication table, but this is the multiplication table for a group.

So, you have all the elements on this side all the elements on this and here you write the products. So, if you know the group multiplication table you can I mean this tells you everything you know you need to know about the group. So, if you know the group multiplication table you can easily identity what is the identity. So, the identity is clearly this element because this element the binary operation of this element with any other element gives you that element.

So, typically all groups have the following characteristics in a multiplication table. So, if I represent this identity by E and if I have various A, B, C, and so on; then here also I will have E A B C and so on. Then usually I mean all groups will have E this row will just be E times E dotted into A that has to be A because E is the identity E dotted into B has to be B, E dotted into C has to be C similarly, A dotted into E has to be A, B dotted into E has to be B, C dotted into E has to be C and so on.

So, this part of the multiplication table is common to all the groups the rest of the multiplication table it depends on the properties of the group and how you define your binary operation. So, next we will look at some more examples of group before that I just want to mention one thing this is called a group of order 3 of order 4 where order is the number of elements in the group. So, an order of a group is the number of elements in the group. So, if you want to say what is the order of this group it is 4 and you can define orders for all groups.

So, you just have to see how many elements are there in the group and that gives you the order of a groups. So, next I will consider specific examples of groups we will look at groups of different orders we will start with groups of order 1 then go to order 2 order 3 and so on.

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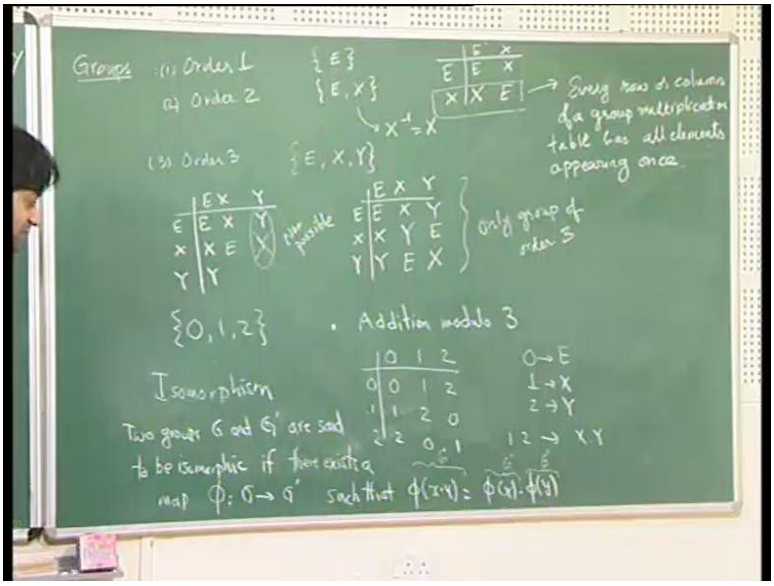

So, groups of order, so this is order 1 order 1 groups means there is only one element in the group. Now by definition that element has to be the identity and this is the only group of order 1. So, this is a very trivial group, second if you want a group of order 2 order a group of order 2 has 2 elements E and X.

I just call that element x. So, it has to have 2 elements, now the multiplication table of this group will just be E X, E X. Now this has to be E this has to be X this has to be X and so what does X into X have to be. Now it is not hard to convince your self that X into X has to be equal to E. Now there are 2 things, 2 reasons why or the most obvious reason why X into X has to be E is because X has to have an inverse and inverse of X cannot be E.

So, inverse of X has to be X, so you notice that X inverse equal to X because X inverse has to be in this group and X inverse cannot be E. So, it has to be X, so X inverse has to be X, so X into X has to be equal to E. So, this is the way you can construct the multiplication table and there is only one group there is only one choice that will work. So, whatever X you take it has to be such that X into X has to be equal to the identity, so there is no other choice for group of order 2. Now there is one more thing, you notice here this is the property of the multiplication table, so every row or column of a group multiplication table has all elements appearing once.

So, this is the property of the group multiplication table that when you look at any row or any column you have to have all the elements, so this row has both X and E this row has both X and E this column has both X and E. So, all the elements have to appear and this will be extremely useful when you construct larger groups, so when you construct larger groups then this rule is very useful. So, what we said is that there can be only one group of order 2 that has to have an identity it has to have one element such that the inverse of that element is itself.

Now let us look at order 3, so then I call it E X and I call it Y, then now the multiplication table, so E X Y it looks like this. Now X into x can either be the identity or it can be Y. So, if you look at this row you already have an X. So, you have to have a Y and an E. suppose X into X is E then X into Y has to be equal to Y if X into X has to be E this row has to have X E and Y therefore, this has to be Y but then you notice that in this row you have 2 Y's.

So, it is not possible, therefore you have to have only your only choice is E X Y, E X Y. Now X into X we said that E it cannot be E because then you have 2 Y's in the same row. So, it has to be Y and this has to be E, then this element has to be E because X Y E has to be appear in this row and this has to be X. So, this is the only group of order 3, so there is only one group of order 3 and that has to be this. Now suppose somebody tells you. how can you say that there is only one group of order 3 suppose somebody says I construct a group that contains 0 1 2 and the operation is the addition modular 3.

So, that means, at the 2 numbers I divide by 3 and I take the remainder. So, then this is also a group of order 3 we just saw that this is a group, so this should also be a group of order 3. So, why do you say but this argument said that there is only one group of order 3, so what is the connection. And to see that let us write the multiplication table of this group. So, we write the multiplication table 1 2 2 2 and 1 plus 1 has 1 times 1 has to be 2 this has to be 0 0 1

So, this is the multiplication table so this is the group of order 3 this is the group of order 3 but what you notice is that these are the same group and these are the same group because 0 if you replace 0 by E, if you replace 1 by X, if you replace 2 by Y. So, you can map 0 to E, 1 to X and 2 to Y and what you notice is that the wherever, I have 0 if I put E wherever, I have 1 I put X wherever, I have 2 I put Y then I can get the whole multiplication table.

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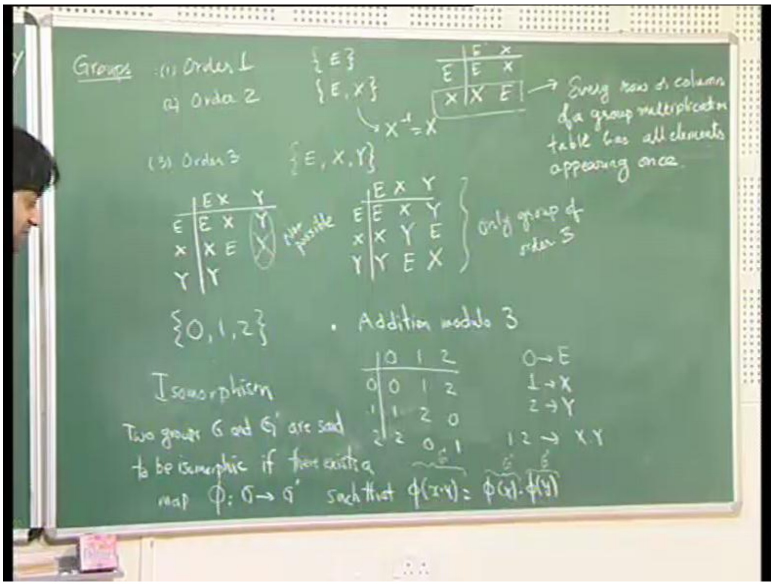

So, x times x, x times is same as 1 times 1 that is 2, X times Y X times Y is same as 1 times 2 that is 3 that is 0. So, if you map 0 1 2 to E X Y then clearly anything 1 times 2 maps to X times Y. So, in a sense the there is no difference between these 2 groups you just gave them different names instead of calling it 0 1 2 you called it E X Y here and vice versa. So, this idea that you know groups that look very different but they are actually the same is what is called an isomorphism.

And the formal definition of isomorphism is that if 2 groups or 2 groups G and G prime are said to be isomorphic if there exists a map phi and the and phi takes any element of G to an element of G prime. Such that phi of X times Y is equal to phi X times phi Y and formally this would be a objective map in the sense, if you have a map from G to G prime you should also have a map from G prime to G.

So, basically two groups are said to be isomorphism if you can map all the elements from all the elements of G to elements of G prime such that, your product of an elements is map to a product of elements in G prime. So, phi of X, so this thing is contended G prime, so you take 2 elements and each of them maps to X maps to phi of X Y maps to maps to phi of Y but the product of X times Y maps to phi of X times Y phi of the product.

So, this is the way of saying that these 2 groups are the same, so not only can I map the elements to one other but also the products or the result of these operations they also map to the same thing. So, I use the term product for this binary operation but you know that mathematically it can be any addition or something but it is just this binary operation is typically called a product and this table is called a multiplication table. So, the concept of isomorphism is very useful because that is a way of telling you when 2 groups that look very different may actually represent the same group.

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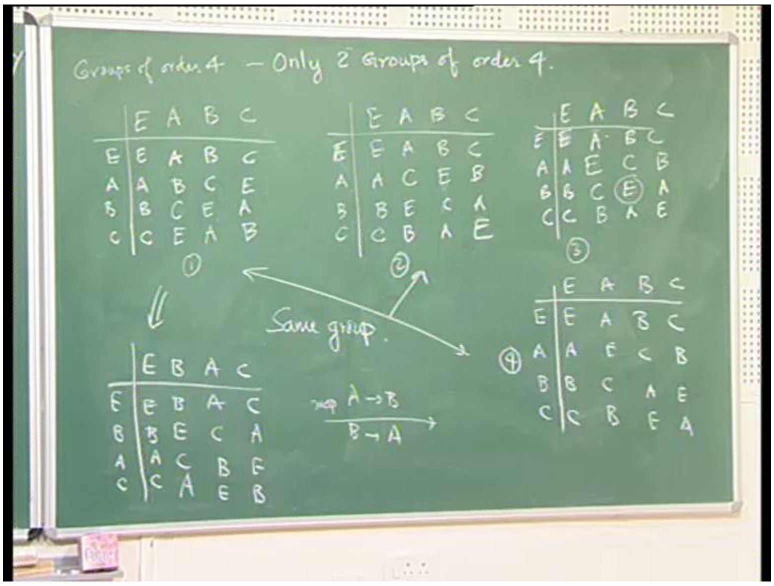

So, now next let us look at groups of order 4, so this would be for example, it would be E A B C, such that the multiplication table would look like E A B C. So, this part of the multiplication table is clear, now a times A you have 3 choices, A times A can be B C or E. So, let us start with the choice where A times A is B, now if A times A is B then A times B has to be either E or C but if it is E then A times C has to be C which is not possible.

So, A times B has to be equal to C and this has to be identity. So, once you take option I will then this has to be C and this has to be identity. So, similarly, B times A, so it has to be it can be either E or C but it cannot be E because of this row. So, it has to be like this, and then B times C B times B can be either A or it can be identity. If it is A then B times C has to be identity which is not possible. So, it has to be E A and similarly, this has to be A and this has to be B.

So, once we choose this to be B then everything else is decided, so this is 1 possibility, you could have a second possibility, now A times A instead of choosing it to be B if I choose A to be C instead of choosing this to be B I choose this to be C. Now then you can say that A times B can be either identity or B but it cannot be B. So, it has to be E B E B B times B can be either it can be C or it can be A but clearly it has to be C A A C, so this is the other possibility and the third possibility is that A times A is identity.

So, A times A we said can be B C or it can be identity A E then A time B has to be C and this has to be B B times A B times A has can be either A C or E but A and E are already there. So, it has to be C this has to be B B C this can be E or A C B this can be either E or A. So, you can have E A A E or you could have the 4 choice is C E A B C. So, you have a choice here, so C A E C B A E C B B C A E E.

So, these are the 4 choices, so on the phase of it looks like there are 4 choices but amazingly what you can show is that this and this, so these 2 groups there is there should be identity. So, it is not hard to say see if you look along the diagonal you have identity B identity B here you have identity, identity A A and here you have identity C C identity here you have all identities.

So, you can show that these 3 are the same group, they are the same group all we have done is just called A as A and so on. So, we have just permitted the rows and columns called one thing as something else but actually multiplication wise these 3 are the same groups and these 3 are isomorphic to each other. The easiest way to see this is that you look at this part of the group, this part of the multiplication table, now along the diagonal you have 1 identity.

So, in each of the cases you have 1 identity and you have 1 element and you have only 1 element appearing in the other 2 now, as such there is nothing special about this order I could always bring C here and A here, so I could always switch these 2 rows. So, if I switched these 2 rows then you can see that and I switched these 2 columns, so suppose I had written this as E B A C E B A C, now I want to find B times B B times B was identity. So, I have E here B times A is C, so I have C and A.

A times B, A times B is C A and then what I will have is B E E B, so all I did was I just switched the 2 rows B and A and notice that this looks exactly like this E E A A instead of A A I have B B, so but it looks exactly the same other than that so now I can do a map A to B and B to A. So, if I switch A and B then this map will show that is isomorphism.

So, basically what all we are saying is that these 2 groups are the same similarly, you can also show that this group is the same as this group. So, there are only 2 groups of order 4. So, what we have seen is we have constructed groups of. You know we have constructed all the small groups.

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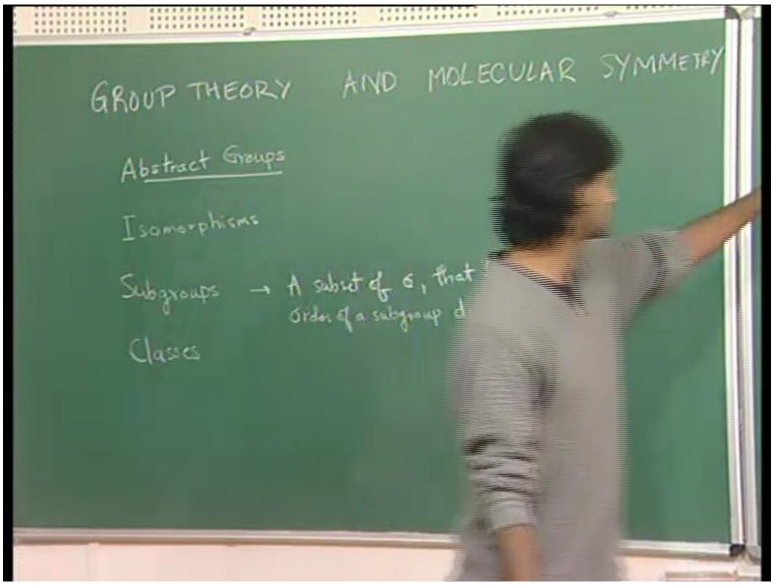

Now, there are 2 more concepts that we will discuss I will discuss the sub groups. Sub group is a sub set of G that forms a group, so the simple example is right here. So, if you take the subset E and B then E B the multiplication table will just be E B B E and. So, E and B this sub set forms A group because E times B or B times B is just identity that has all the properties of a group and so that is called a sub group. So, sub group E B is a sub group, now there is a theorem that says that order of sub group divides order of group. So, in this case the order of the group was 4 the order of the sub group is 2. So, it has to be adivisor of the order of the group.

The other thing is every group has to have the trivial sub group that is E and it has to have the sub group that is the entire group, so those are the trivial sub groups, so the identity and the full group. So, next time we will just talk briefly about classes, and then we will go to the symmetry operations and how we construct the symmetry groups.