Chemical Applications of Symmetry and Group Theory

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Lecture – 05

Hello, everyone hope you are doing great. So, in the last class we learnt about the symmetry elements and symmetry operations, we leant how to find out the symmetry elements and symmetry operations also and then towards the end we said that, after learning this whole set of symmetry elements and knowing how to find them out, we need to utilize some sort of you know mathematical frame work so that we are able to employee this symmetry elements, belonging to a particular molecule, in order to get some molecular properties out of it. So, in other word we need to learn about the applicability of this symmetry aspect of molecule. In order to have these applications, we need a quantity fame work, mathematical fame work which is known as group theory.

So, in this particular theory, which is a purely a mathematical fame work by his origin. So, long before you know chemistry stated using it, mathematician started this particular beautiful topic called Group theory. So, on this symmetry elements, can be utilized to form a particular group will come to those things in a while; now before we can form so called group something, and based on the symmetry elements of a given molecule and utilize them to find out various things like how to form a linear combination of (Refer Time: 02:08) or how to find out the probability of transition between two molecular electronic or vibration states. Before we do that we need to learn a few basic things, about this group theory, so, few criteria of something that can be called a group.

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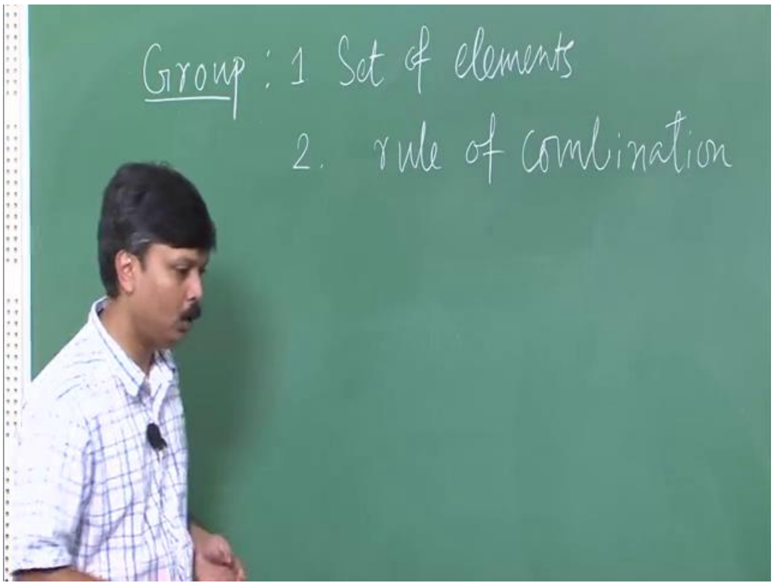

So let us start with the definition of this particular thing called Group. So, what is a Group? Group is a collection of object or set of some distinct object. So, if I can say this is the set of some elements. So, a set of element can form a group; now I hope all of you understand what is set. Set is nothing but a collection of some distinct objects; suppose I take few numbers like 1 2 and 3 together, it will form a set.

So, 1 2 3 this three numbers they are distinct objects. When I put them in a collection they form a set. So, here we are considering such a set and this set can have any type of elements, it can be some numbers, it can be different objects anything and the number of elements of any set can be anything, starting from one to infinite.

So, if I take any particular set, having certain elements in it and then if there is a particular rule of combination. So, what I need number 1 is a set of elements, number 2, well defined you know rule of combination, that can be anything; suppose I told you about a set like 1 2 3. So if I tell that as there is a big addition is a rule of combination, which can actually combine any two elements of the set.

So, I have a set of elements and I have a particular rule of combination which is well defined in this. Then I can have a group, this set will be called a group provided certain rules are satisfied. So, what I have now, I have a set of elements and a particular definition of rule or a particular rule of combination is defined in it, it will be called as Group once it follows certain rules.

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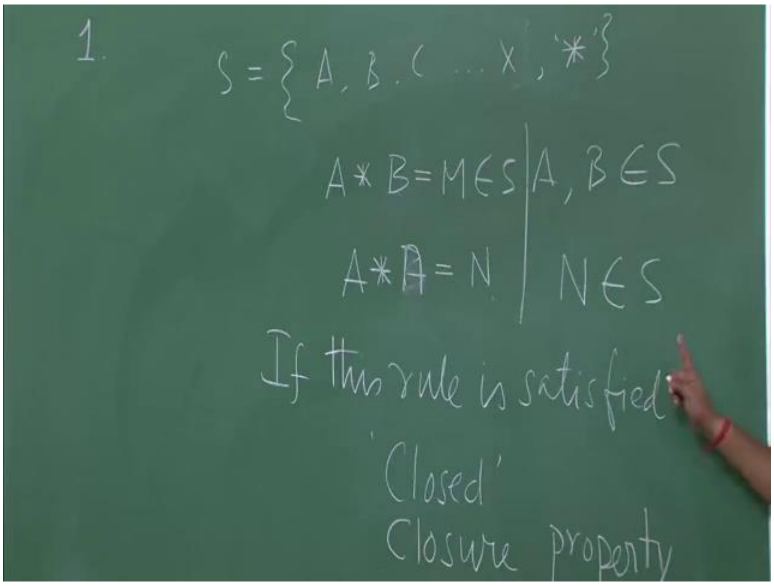

So, what are those rules? So, those rules are as follows. So, there are 4 rules or 4 laws. So, rule 1 says that, all the elements in a particular set, if I consider them and if I take any two elements from that tool of elements, then combined them with that defined combination tool, then the product or if I say that the effect of the combination this product may not necessarily mean the in the mathematical. So, called product

But if I say that you know product and combination is synonymous. So, we can take it in that way. So product of any two elements, suppose I have a set, which is formed by some element like A, B, C and so on up to x. So, there are x number of elements in that particular set and there is a particular method of combination. So, this is the method of combination set, is defined in it. Then what this rules says that, product of any two elements say A and B both belongs to this set A. So, A and B they belongs to set then the result of this combination of A and B, suppose that produces something called say M. So, then this laws says this M must be an element of set S.

Similarly, I can say that I do not have to multiply only two different elements; I can have something like this. I can have the product of A with A. So, in other word the square of any different element say if that is N, then N should also belong to S, and here M should belongs to S, then I will call this set as closed set. So, if this rule is satisfied, we will call this set as Closed and this particular property is also known as Closure Property. So, the first rule for a set that can be called a Group. So, we have to call a set or group, this first rule must be obeyed; if any s fails to satisfy this condition or this property then it will not form a Group.

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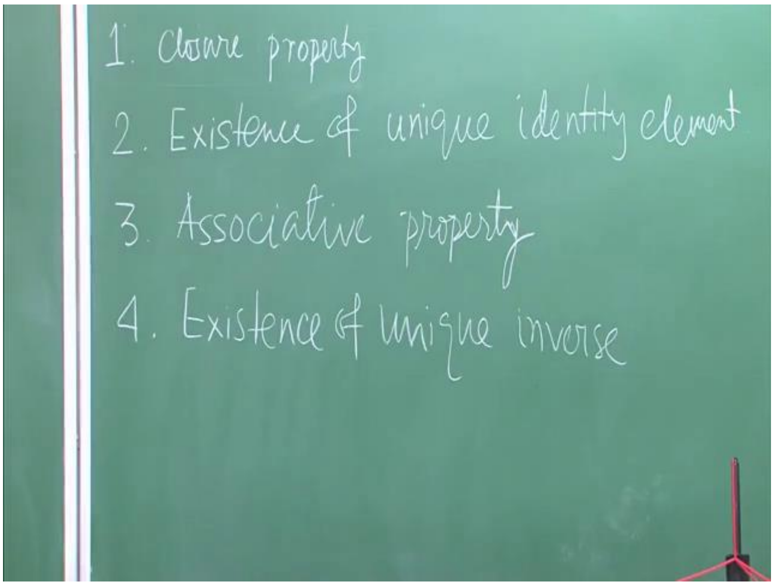

So, the first one is the closure property. So, let us write down all of them one by one over here. So, in order to form a group it must satisfy Closure Property number 1, now I said there four such condition if they are with then they will make the set, a group and we learned about first property that is the closure property.

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Now, which one is the number 2; so, number 2 says that, there must be an element within this set let us consider this set again. So, there it says the law two says that must be an element in this particular set such that it commutes with any of the elements. So, mathematically if I try to say this one it will be that there must be an element E belonging to this group S such that E commutes with any elements of this group of this set, this not yet grouped. So, E if I operate any element here, so I operate this as my defined operation; which is also binary operation because it combines two elements. So, I have E star say A now A is an elements of these group, I can take any such element then it should be same as A star E which is nothing, but equal to A.

So, it says that E commutes with A, commute means it does not matter the order of combination, whether it is E star A or A star E here only difference is the order of combination. So, the order combination does not matter and ends up giving back the element itself, this element E is known as identity element in that particular set. So, we can correlate between this identity element and the identity element that we talked about when we discussed the symmetry elements. So, you can see they are exactly the same. So, according to rule two, we have that there must be an identity element defining that group A. So, whatever you said so far, we can say single sentence that, we need an identity element to be present in the set then only I can call this as a Group.

So, this is called need an Existence of unique identity element. So, you cannot have two such elements in a set and still it is a group. So, there will be only one element of its kind, so that is why it is assuming and this element is known as identity elements. So, we are found two conditions for satisfying; that means to be satisfied in order to a form a group.

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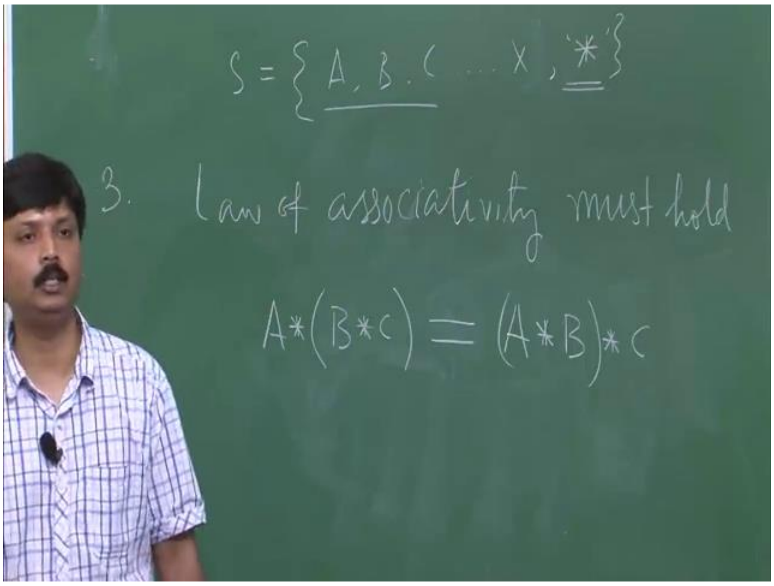

So, let us move on to law three, which says that the Law of Associativily must hold for that particular set in order to be called a Group. So, this is Law of Associativily must hold what does that mean, we know what Associativily means, associativily means the order of combination, suppose I again consider this particular set having A,B,C to X, then if I take out three elements from that, so I consider A B and C, this three elements I take and then combined them in an order like A in this way, now if I change this order of combination in such a way that, let us not put this equality, now this and this, what is the difference the difference is here this bracket is to be making on the difference, it says that first I will combine B and C and their resultant we will be combined two A, on the other side here I combined A and B first and with this results I combined with C.

Now, if the associativily holds, then this two should be equal this is Law of Associativily and in other to form a group, the set must satisfy this Law of Associativily for any element belonging to this particular set. So, we got our third condition that the set must have associative property and then we must have another rule that has to be satisfied.

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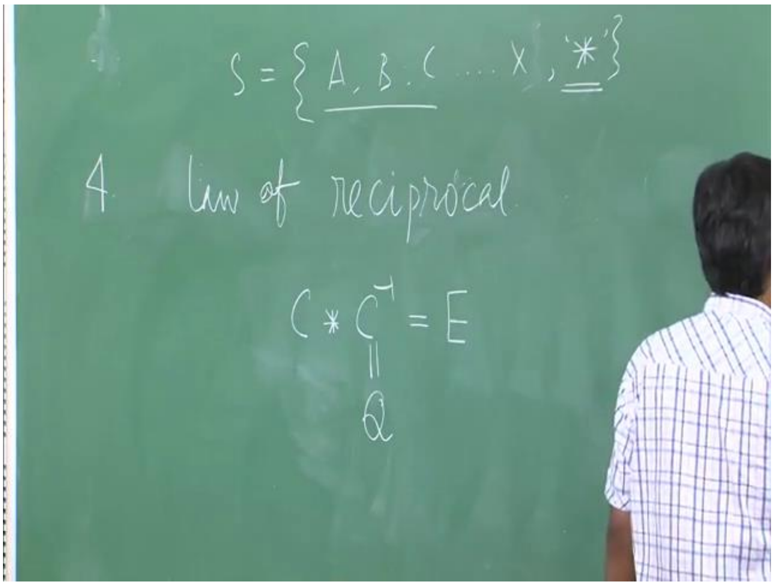

So, we come to the last rule that is the Law of the Reciprocal, Law of Reciprocal or we can say Law of reciprocation, what does it say; it says that for this particular set if I choose any element any one element if I pick up. So, arbitrarily I will pick up say C then there must be a unique reciprocal or inverse for this particular element. So, I choose say C, C belongs to S, and then there must be some element which will be reciprocal of C, which is written as C inverse, such that this combination will give E identity.

So, according to that law says that there must be some element here, say I call it like k Q. So, this C inverse and Q will be equal so; that means, for any given elements C belonging to S I will find that an elements q which will combine with C to give identity, and that is true for any elements belonging to this set S.

So, if I take a there must be some elements their R, that yields A star R equals to E. So, the forth law that we have here, is the existence of unique inverse. Now again here we have this term unique because in a set you can have only one inverse of that particular element that we are choosing, if I choose a then there must be only one element say R such that R is equal to A inverse and you will not find any other elements which will be A reciprocal of A again. So, this reciprocal or inverse of a must be one, and that must be a part of this set. So, then I will say that this set has the entire element; set has their own unique inverse.

So, once I check all these properties there will one Closure property, if it has an identity element in the set if the elements of the set follows Associative law and if there is an Unique inverse for each and every element of the set, then I can call this is set S or Group.

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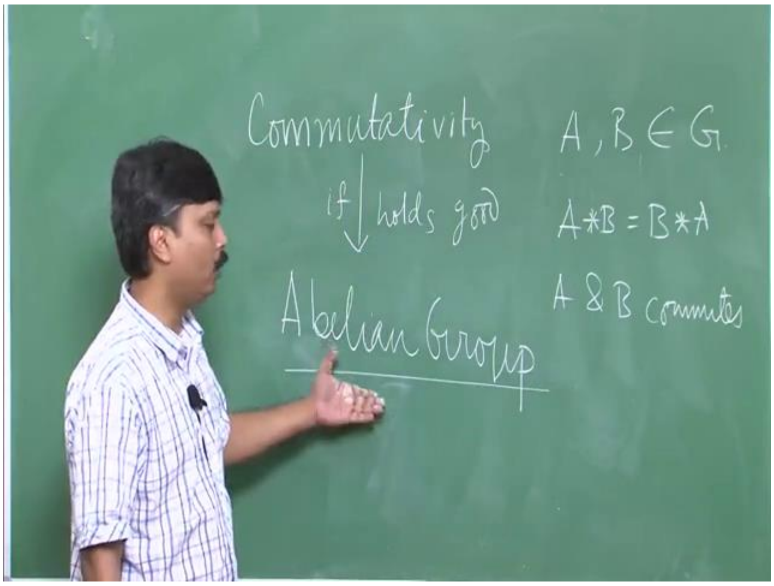

So, this S will be a called group and most of the time we give a symbol G not necessary, but you will find out that mostly we use G because group starts with G quickly use G to define a group. So, G and they you write like a set.

Now, let us revise, what do we have so far, any given set that is a collection of elements will be called a Group when a particular rule of combination is defined in it and all the elements follow certain rules one closure, second existence of identity, third law of associatively holds and fourth is the existence of unique inverse, then it will be called a Group; if the elements of a set cannot satisfy even one of this conditions, it will not form a Group. So, that has to be verified all the time when we are trying to find out if a set can form a Group if I define an define a rule of combination.

Now, if we had defined group, now at this point I will mention one an additional point about Group; a Group will definitely follow all this four rules, they will obey all these four rules, now if the elements of that set which follows all this rules and they have well defined binary operation, in that additionally if it follows a rule as, I am going to show you which is known as Commutativity. So, additionally if the elements which follows all this rules if they follow rule of Commutativity or rule of commutation, then if holds good then; obviously, that will be group because they have already satisfied all the condition for being called a Group now additionally they are you know following this particular condition of Commutativity which means for any two element A and B belonging to a particular group, if A star B equals to, B star A; that means, A and B commutes. So, once this holds good for any element A and B belonging to G, then that particular group is called an Abelian Group so this is another very important a types of group, that we will come across they have some unique properties and all.

So, we have learnt. So, far how to define a Group and also we learnt that there is a special kind of group which is known as, Abelian Group where, apart from all this four properties; an additional property of commutation also hold good they are called Abelian Group; now let us take some actual example and then try to find out if we really understand this topic.

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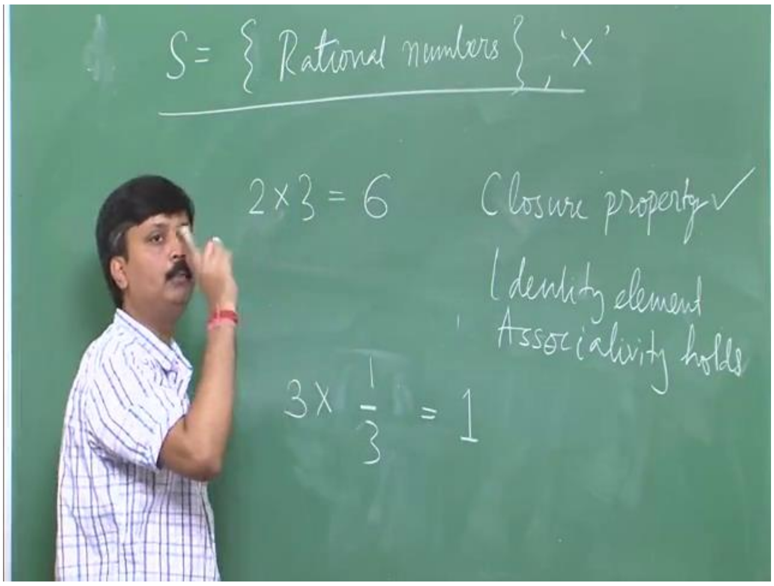

So, a let us define a set, which contains all the Rational numbers. So, which is a set by Rational numbers that is possible and algebraic multiplication as my rule of combination?

Now, is this set going to form a Group under this binary operation, which is multiplication; that is the question let us try out. So, in the set of Rational number I have everything I have infinite here, I can have one of an infinite. So, all the numbers are there. So, now, I just check, if there is a defined operation, that I already said X. So, multiplication is by operation, now first thing is that closure property. Now I take any two Rational numbers because I have all the rational numbers in my set. So, I take two and three and then see if all these properties hold.

So, two and three if I combine, it will give me 6, 6 is also rational number. So, it belongs to this one. So, I say closure property it is satisfied; now is there any identity element, it is very easy to find out; identity element will do will not change that element with which it is been combined, and it will commute with that. So, if I take any elements say I again take three; can I have something say can I have something I am putting it under a code I am not writing what it can what is it such that, I will have three into this equals to three answer is very obviously, it has to be unity.

So, now check with any given number you take it 5, 5000 anything multiplication with 1 it will return you the same number. So, I have 1 as the identity element. So, I found my identity element now does it obey associative law lets see again. So, I have 2 into 3 here. So, let us take 2 into 3 into 4. Now if I change the order 2 into 3 into 4 obvious answers is these 2 are equal. So, Associativity holds good. So, Associativity holds; now we are left with the existence of unique inverse. So, what does a unique inverse due to any elements belonging to a set that, inverse will combine with the elements to produce identity.

So, let us take 3. So, I have to combine with something which will produce my identity which I already have got as unity, and similarly if this will be commuted. So, the answer is obvious, I should have something like this. So, I have for any given element such as 3 always I have 1 upon 3 and this combination that is the multiplication of 3 and 1 upon 3 is going to give me unity, which is the identity element for this. So, this particular set of Rational number is a group under Binary Operation Multiplication. So, this I can call it as a Group under multiplication. So, I will quickly give you another example that is the set of say all integers. So, the previous one was a group under multiplication.

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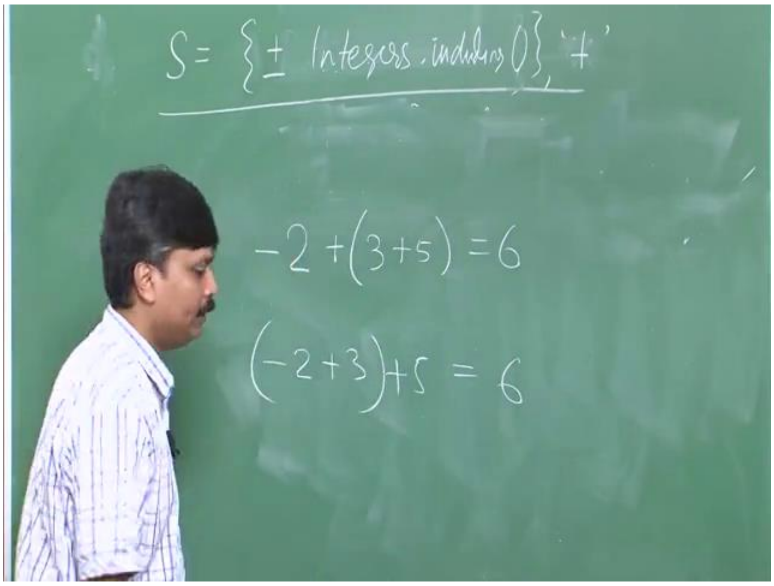

The next set I will take, say all integers both positive as well as negative integers including 0. I define an operation as addition, now quickly check if the set of all positive and negative integers including 0 will form a group, under the Binary Operation Addition; first to our closure property take any two elements, again 2 and 3, 2 plus 3 is equals to 5. 3 plus 2 is equal to 5, 5 is a positive integer, which is already a member of this, you take 5000, 1000 combine them you get 15000, what is that is an integer belongs to this particular this set. So, closure property holds for this particular set under Binary operation addition.

Now, is there any unique identity there is one, you can see I have the set which has all the integers, which includes 0 specifically. So, if you add 0 to any number it is going to return you the same number. So, it will also commute with any number under addition. So, 0 plus 5 equals to 5 plus 0 equals to 5; that means, 0 is an identity elements in this particular set when I use addition at my binary operation, let look at the third one Associativity property; it holds good because say I have something like minus 2, plus 3, plus 5, and then I can write minus 2, plus 3, plus 5 both of them are going to give me 6. So, Associativity Law holds. So, third point is also clear for this set under addition existence of unique inverse. So, inverse demands that for any given element I will have another element, with which if I combine my previous element, it will result in having the identity element.

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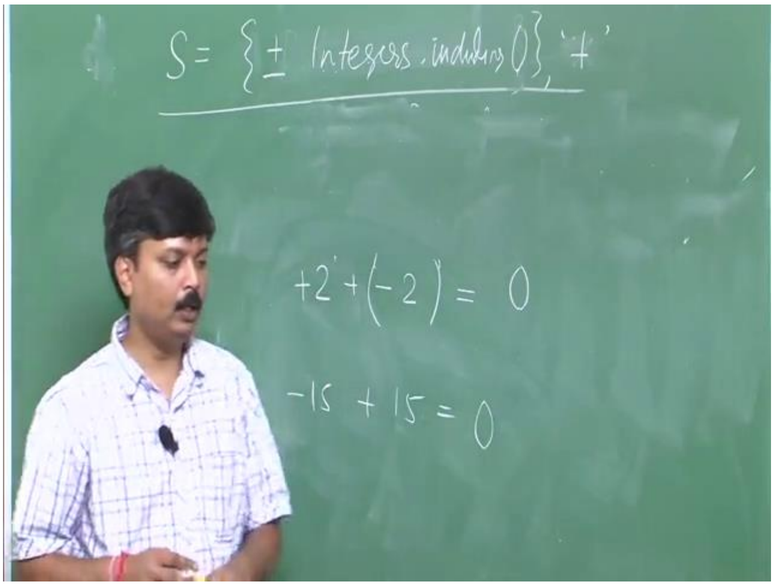

So, if I take say for example, any element says plus 2. Do I have something, with which if I add this plus 2 I will get my identity, what is my identity? I got my identity as 0, so plus 2 will be adding to something; which will give 0 and that something must be minus 2. So, if takes say another example like minus 15. So, I have to add with plus 15 in order to get my identity element.

Now, all these number are integers. So, I have unique inverse for each and every element in this particular set which has unique inverse. So, I found out that all the conditions closure property, unique and identity, Associativity as well as the Existence of unique inverse, are hold good under the Binary operation plus. So, we can call that the set of all positive negative integers including 0 forms a group under Binary operation addition. So, we should try many more such thing for example, if you remove this 0, from this set try it out, find out if it forms a group under addition; does it form a group under multiplication or the first problem that you solve today, why we define multiplication as the binary operation will it form a group under addition. So, try out many such operations and that will help you getting the basic essence of a Mathematical Group Theory.

So, with this will stop here and will come back with a little bit more about the group theory; particularly how to combine different elements of a group using something called Group Multiplication Table that will be necessary to understand the combinations of different symmetry elements which is our actual goal. So, we will learn about good multiplication table and then will move to the combination of symmetry operations. So, with that I come to the end of this class.

Thank you very much for your attention and see us next week.