Symmetry and Group Theory
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Lecture -32
Representations of a Cyclic Group

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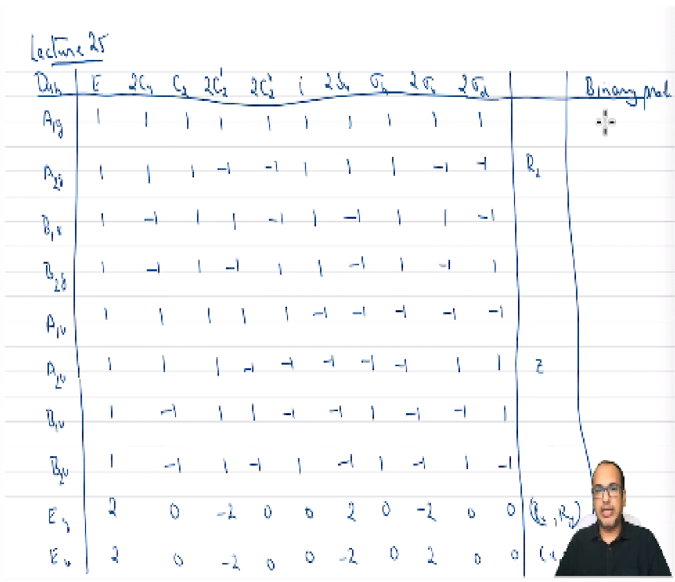

So, in the last lecture we have seen how to write character table, that is complete list of irreducible representations using great orthogonality theorem. We started with the molecule XeF4 and we found out what is the point group of the molecule. Then we wrote all the symmetry elements and operations present and then listed down the complete IR representations. We also did the nomenclature for all the IR representations using mulliken symbols.

And then we found out the basis sets for unit vector transformation, so what is the like z is forming basis for which IR representation x and y is forming basis for which IR representation and so on. So, next is in this step the last point of character table is the binary products which goes here, so which binary products form bases for which IR representation that is what we are going to see today. And why binary products are important?

Because we want to see how d orbitals transform under different symmetry operations and so certain properties, certain functions or certain binary products actually have similar properties as d orbitals.

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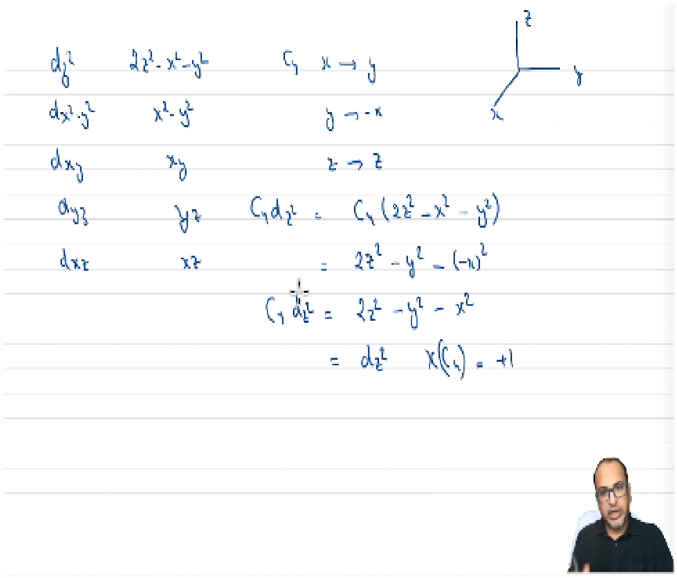

So, let us look at that. So for example dz square has the functional form of 2 z square - x square - y square. Similarly, we have d x square - y square as x square - y square and so on so forth. So, dxy will be xy, dyz will be yz and dxz or zx will be xz. So, if we want to see how the d orbitals are transforming under various symmetry operations, we must know how x, y, z are transforming. So, let us see, let us take an example of C4, so we know that C4 when we apply C4 onto x we get y.

So, let us also draw the coordinate system so that it is easier to see. So, we have x, y and z, so x goes to y upon doing C4 and then y goes to - x and z remains as z. So, now if you want to see the effect of C4 on to let us say dz square then we want to see basically what happens to this function, - x square - y square. Now this can be easily identified because we know the fate of z, so the fate of z is z so that means that does not change fate of x is y. So, that means we have y square here fate of y is - x right, so that means we have - x square here.

So, this gives rise to 2 z square - y square - x square. So, this negative becomes positive and then you have negative here. Now that means C4 dz square gives rise to dz square. That means character under C4 should be equal to plus 1. Now similarly we can find out all the characters for example, we can find out the character for under C2, C2 prime, C2 double prime using the same set of rules and find out that what is the basis for or to which IR representation dz square is forming the basis.

So, as it turns out so dz square would be lying here okay, so all the, this thing will be totally symmetric and hence we will get dz square as totally symmetric representation. So, similarly you can find out for other d orbitals as well and so let us not take this spend more time on this. So, now that it is very clear now we know all the areas of character table.

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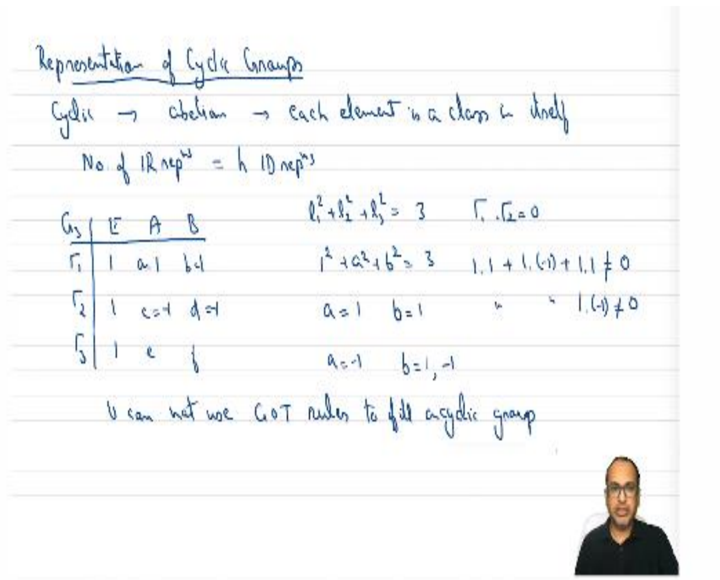

So, we can move ahead and move to the next topic which is representation of cyclic group. So, why is cyclic groups need a separate discussion? Because as you see that cyclic groups when we are trying to fill using great orthogonality theorem will not be able to fill it up and we will get stuck at some point, so let us see what are the issues. So, cyclic groups are abelian in nature, cyclic groups are abelian that means each of this will commute, each of the operation will commute with each other that results into each element is a class in itself.

So, also we will see that the number of IR representations is equal to h 1D representations, so that is the where h is the order of the group. So, that is clear, so now let us take an example that why this thing great orthogonality theorem cannot be used to fill up a cyclic group. So, let us take a cyclic group, let us take a general cyclic group G3 with elements as E, A, and B. So, because there is going to be three classes so that means we should have three IR's.

So, if there are three IR's then we should have l 1 square + l 2 square + l 3 square should be equal to 3. And the only solution for this positive values because these are dimensions is going to be 1 1 1, so I am going to write 1 1 1 under the symmetry operation E because that is the character and dimension of this representation. Now for if we say this is a and b the characters under a and b.

So, next rule says that 1 square + a square + b square is equal to 3. Now the again the solutions here can be, a can be equal to +1 or - 1, b can be equal to + 1 or -1. So, let us take this as + 1 first so that would mean that we can have it as 1 and 1. So, let us keep a equal to 1 and b equal to 1. Now let us say if this is my c, d and this is my e, f, the other two possible solutions are we can say that a is equal to -1 or b is equal to 1 or - 1.

So, if this is 1 or - 1 or a is equal to - 1, can we really put in here. So let us try to put in - 1 here and + 1 here. So, if we now try to do orthogonality condition that is tau 1 dot tau 2 equals to 0, do we get a 0? So, let us see 1 into 1, + 1 into – 1, + 1 into 1, so this is not equal to 0. If we try to keep d is equal to negative 1 we will get a negative here and that will also not be equal to 0, this will be same.

So, that means none of these solutions would work for the orthogonality condition, so that tells you that you cannot use GoT rules to fill a cyclic group. So, you have seen now an example. So how do we go about then? There are other solutions which can be non-real numbers, that is the complex numbers can also be solution of these and those complex numbers may fill it up. But it is not as straightforward as finding the real numbers real roots for this equation, but complex numbers finding complex numbers is not easy itself.

So, let us see if we can find a general complex number that will fill up the whole table. So, it is clear that the real numbers cannot be a root of this equation, so if real numbers cannot be so then the next resort is to find complex digits.

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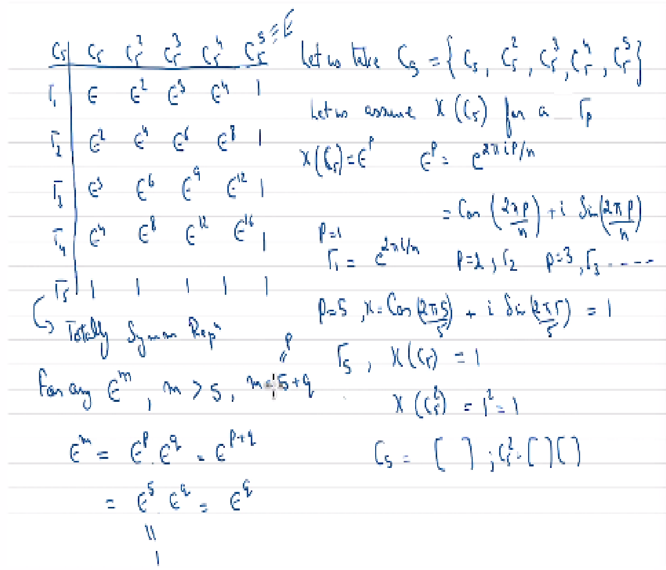

So, let us do a general group of 5, C5 so that is G 5 that is the order of the group. And now let us take C5 maybe the group instead of G5. I will just say C5 point group so I know the elements also. So, all the group elements will be here C5 and you know that in cyclic group all the group elements or symmetry operations can be generated by raising powers of one particular element. So, because this is a rotation element you can use this to generate powers to generate other symmetry operations by raising powers.

So, C5, C5 square, C5 cube, C5^4, C5^5 which will be equal to e, that will naturally come out we will see that. So, let us see that these are the five symmetry operations here C5, C5 square, C5 cube, C5^4, C5^5. So, now because there are, each element is now a class, so we should have 5 classes so that means we should have 5 IR representations tau 3, tau 4, tau 5. So, now also let us assume character under C5 for a pth tau.

I can call it as tau p or pth representation, so let us call it as tau p actually. So, we are assuming a general complex number under this as the character. So, that character let us say that it is epsilon to the power p which is now the character under C5. For any pth representation if it is tau 1 we can call it as epsilon to the power 1. If it is tau 2 we can call it as epsilon to the power 2 and so on so forth.

So, where tau p is epsilon p is nothing but epsilon p is e to the power 2 pi i p by n, that is correct, 2 pi i p by n or so we can also write it as cos of 2 pi p by n + i sin 2 pi p by n this will generate us any general complex number. So, for p equal to 1, we have tau 1 so p equal to 1 tau 1, that will give rise to cos 2 pi by p. So, that will give rise to we can say that e 2 pi i by n and similarly for p equal to 2, we have tau 2 for p equal to 3 we have tau 3 and so on.

So, that is easy, so that means now we can raise this as powers of epsilon. So, what happens at p equal to 5? We can see that this will be cos 2 pi 5 by 5 plus i sin 2 pi 5 by 5. So, that means cos 2 pi + i sin 2 pi, so that will be 1 so, this is the character. So, that means for tau 5 character under C 5 is going to be one so we can write one over here. So, also the other characters so character for C5 square, C5 cube under tau 5 can be obtained as square of this. So, for example if I want character for C5 square I can write it as 1 square, so that will be equal to 1.

Why I can take it as a square? Because so I can say that if C5 is represented by a certain matrix. Now in this case it is 1 cross 1 matrix, so C5 square will be nothing but the square of the matrix multiplication we have seen. So, if it is the matrix is 1 cross 1 it will be simply the trace of the matrix which can be multiplied. So, that means 1 square can be used so this means that I can write all the elements like this. Does that make sense?

So, also if you see that character of C5 to the power 5, so if I now write for tau 1 what will be the character for C 5 to the power 5. So, character under C5 to the power 5 would also be epsilon to the power 5. So, epsilon to the power 5 is nothing but if you take this thing again it will be cos 2 pi and sin 2 pi. So, that is going to be 1 in all these cases. So, this also conforms to the rule of great orthogonality theorem, that the sum of square of dimensions is going to be 5 and this actually turns out to be E.

And this particular tau 5 turns out to be totally symmetric representation which has to be there always, totally symmetric representation. So, we are done with at least 5 + 4, 9 elements out of this 25. So, now let us try to write down rest of them so because this is tau 1 under C5 so we can write it as epsilon. Now this will be epsilon square, epsilon cube, epsilon 4 and this will also be epsilon square, epsilon cube, epsilon 4 and this will be epsilon 4 because now we are raising the power epsilon because now P is increasing so this will be 6, 8.

Here we can write it as epsilon 6, epsilon 9, epsilon 12 and this will be written as 8, epsilon 12, epsilon 16. So, now you can easily write this because now once you have written this so all you are doing is here you are raising the power. So, epsilon goes to epsilon square because this is C5 square, epsilon square goes to epsilon 4, again squaring this so 3 goes to 6, 4 goes to 8. Again, then again if you square it, this will be, so if you cube it from here to here it will go as cube.

Now epsilon to epsilon cube, epsilon square to epsilon 6, 3 to 9, 4 to 12 and so on so forth. Now there is very important property, so if for any epsilon to the power m where m is greater than p or where m is greater than 5 in this case, let us say, we can always write m is equal to 5 plus some number q. Because let us say m is 6, m can be written as 5 + 1. If m is 7, m can be written as 5 plus 2 and so on so.

So, that would mean that if my epsilon to the power m can be expressed as epsilon to the power p and epsilon to the power q or in other words if I have it as epsilon to the power p + q, if my m is p where my 5 is p, epsilon m can be written as epsilon p + q and then that can become epsilon p into epsilon q. Now this can be if p is equal to 5, I can say that epsilon 5 epsilon q and since epsilon 5 is equal to 1 we have seen that here epsilon to the power 5 will be equal to 1.

So, we can write epsilon to the power m is equal to epsilon to the power q, because now this thing goes to 1. So, for any m which is greater than 5, we can write epsilon to the power m as epsilon to the power q, where q is represented with this relation.

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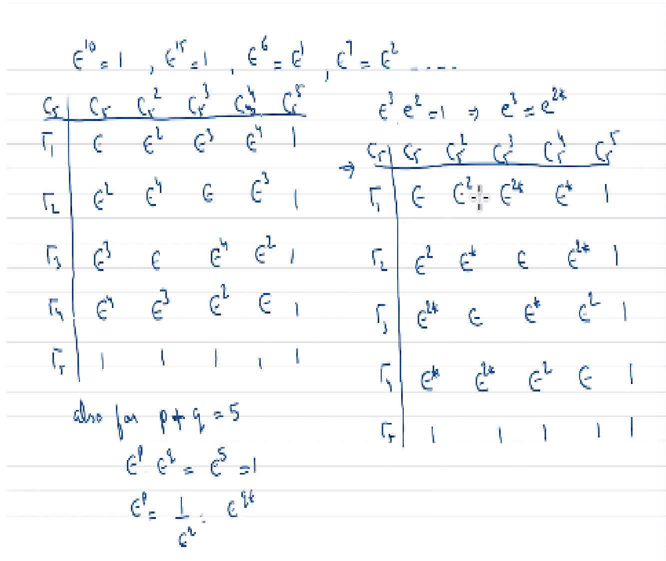

So, now that would mean that epsilon to the power 10 will also be equal to 1, epsilon to the power 15 will also be equal to 1 and epsilon let us say 6 can be written as epsilon to the power 1, epsilon to the power 7 can be written as epsilon to the power square and so on. So, this makes life little easier because we can simplify the character table now. So, let us say C5, C5 square, C5 cube, C5^4 and C5^5, so we have tau 1, tau 2, tau 3, tau 4, tau 5. So, I had 1, 1, 1, 1 here.

Now this is epsilon, epsilon square epsilon cube, epsilon 4 and if we square this, I get square, I get 4, now I get 6. Now instead of 6 what I will do is I will just write epsilon here. I will not write epsilon 6. Similarly for epsilon 8 I am going to write only epsilon 3 because epsilon 5 will be equal to 1. So, now again here epsilon this will be cube and this will be 4. Now here again if I am going to write 3 can be this will be 6, so again it will be written as 1 and this will be 2 plus 6, 8 so this will be again cube.

And this will be 3, 6, 9 so this can be written as 4, 3, 6, 9, 12 so this can be written as 2. And here 4, 8, 12. So, 12 can be written as 2 and 16; 16 can be written as 1. So, this is easy, now also for p + q this is plus equal to 5. I can say that epsilon p into epsilon q is equal to epsilon 5, where p + q is total is equal to 5 which is equal to 1. That means epsilon p is equal to 1 over epsilon q, which is nothing but epsilon q star.

Because this is a complex number so conjugate of q basically right q star. So, that means like for example if I have epsilon to the power 3 into epsilon to the power 2 this will be equal to 1. This implies that epsilon 3 can be written as epsilon 2s conjugate. So, now again I can reduce this to following. So, now if I am seeing here that this is epsilon, epsilon remains as epsilon 2 remains as epsilon 2 epsilon, cube now can be written as epsilon 2 conjugate, 2 star.

Similarly, epsilon 4 can be written as epsilon conjugate and this is 1. So, now cube is written like this and epsilon to 4 can be written like this. Now similarly here this will epsilon square this is epsilon star, epsilon, epsilon 2 star. This will be 2 star, this will be star, epsilon square 1, epsilon star, epsilon 2 star, and epsilon 2 epsilon, 1, 1, 1, 1, 1, 1. So, now very interestingly you see that there are two types of powers in this and then if we rearrange the columns and rows what we can see is that;

We can find out that there are certain sets which occur in pairs which are complex conjugate pairs. So, let us see how to do that, so what I will do is I will just rearrange this in terms of rows only.

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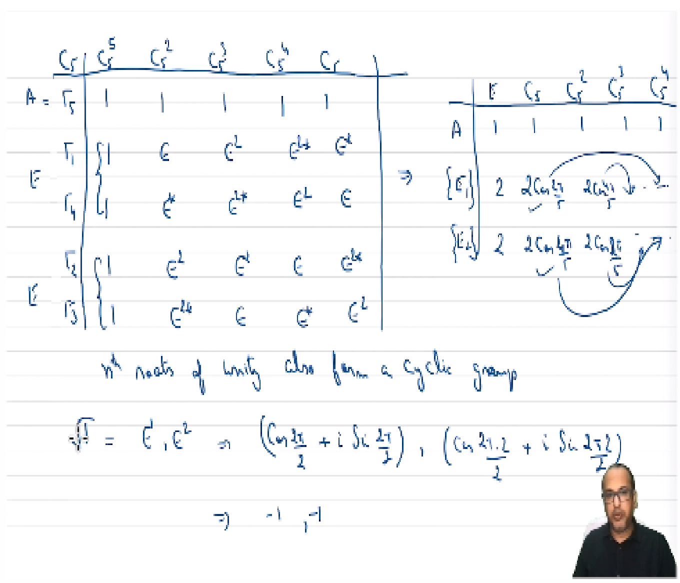

So, what I will do is let us see here and this gets really interesting after this. C5, C5 square, C5 cube, C5^4, C5^5 or actually what I will do is I will write C5^5 first, because that is the trend for writing is. So, here I have tau 5 I am going to write first followed by tau 1, followed by tau 4, and tau 2 and tau 3. I will tell you why I did this, so now if I am writing tau 5, tau 5 is all 1 which is totally symmetric representation and all the characters under C5^5 are also 1 that we have already seen.

Now if you notice the interesting thing is that epsilon star they come in complex conjugate pairs, similarly epsilon 2 epsilon 2 star come in complex conjugate pairs, all of them actually, epsilon star and epsilon and similarly here also they will come like pairs, all I have done is I have just rearranged the columns, I have just brought the C5^5 column here and then rearranged the rows here.

Just to make sure that these complex conjugate pairs come next to each other. Star, star, epsilon, star, epsilon, epsilon star over here epsilon 2 star and epsilon 2, so now if I want to give the mulliken symbol this will be A. Because this is totally symmetric one-dimensional representation, now this will be E, this is two-dimensional representation and this will also be E. And how do I write? I do not write curly brackets over here because I am considering that both of them together.

For all practical applications, we need to combine this because we cannot deal with complex numbers (wrongly spoken as real numbers) in practical sense. So, although in general it now follows the rules of great orthogonality theorem that we have arrived at 5 independent irreducible representations. But together they are combined into E because if we do a summation of these 2 tau 1 + tau 4, what we will get is real numbers. So, what we will get here is like if we combine it, so E, C5, C5 square, C5 cube, C5^4 I will get A, E, I call it as E1 and E2.

And now I am writing curly brackets here, why I am writing curly brackets here? Because this is not real E, this is a summation of two complex irreducible representations which are of one-dimension. So, either you have to represent this by curly brackets or you have to represent the mulliken symbol by curly bracket. So, if we do this this will be all once now if you do 1 + 1 this will be 2, 1 + 1 this will be 2.

And now if you do summation over epsilon and epsilon star, that means the sine term will go and the cos term will add up because now this is complex conjugate. So, I will go, so this would mean that epsilon would mean that I have 2 cos 2 pi by 5. Similarly, here we have 2 cos 2 pi by 5 and here it will be square, so basically it will be 2 cos 4 pi by 5. This will be 2 cos 2 pi by 5 and so on. So, this you can easily write now.

Because again this will be epsilon 2 and epsilon 2 let us conjugate sum so again that will be same and then this will be epsilon epsilon so this will be same as this. So, you can write this will come here and this will come here. Assume that this will come here and this will be 4 here this will come here. So, now if you notice that I have written E1 and E2 here that means I have distinguished these ones, so if you remember the mulliken symbol rules.

So, it says that the character under C5 that is the principal axis rotation has to be symmetric, so if you find out that this one will be positive so that one takes a subscript as 1. This one will be a negative number so that one takes E2 as the subscript. So, this is the representation for a cyclic group of order C 5, so I hope this one is now making sense and it is all clear. So, you can always write down this cyclic group representations either in the expanded form, where you will have 5 IR representations.

Or basically the h one-D IR representations or you can combine the IR representations into real numbers and then when you do that the corresponding mulliken symbol will get braces around it or the curly brackets around it. So, I hope that is here so let us see now a very quick application of the cyclic groups, generator so these are called as generator. The epsilon p is called as generator of the roots, so let us see we have learned that earlier, nth roots of unity also form a cyclic group.

Remember we did that for cube root of unity in initial classes. So, for example if I am talking about square root of 1, the roots of this will form cyclic group that means I can write epsilon 1 and epsilon 2 as the roots. So, this would imply that my roots are nothing but cos 2 pi by 2 and here n is equal to 2 + i sin 2 pi by 2, this is my 1 root and our second root is cos 2 pi into 2 by 2 + i sin 2 by 2 by 2 now this gives you - 1 and 1.

Which we know that the square root of 1 can be 1 and - 1. Now let us see one more example by using the same thing.

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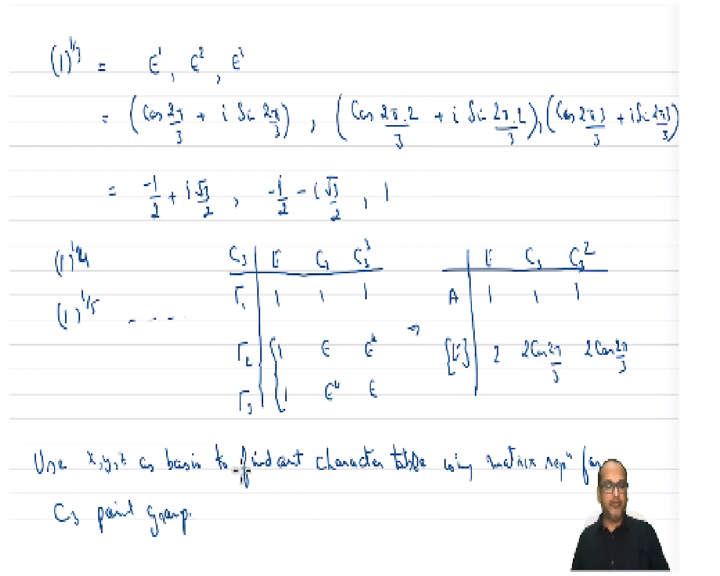

So, let us say the cube roots of unity so that is 1 to the power 1 by 3 this will have the roots as epsilon 1, epsilon 2, epsilon 3. This has nothing to do with chemistry but it is just to show you some example where cyclic groups form. So, this will again be cos 2 pi by 3 + i sin 2 pi by 3 is the first root. The second root will be 2 into this, so cos 2 pi 2 by 3 + i sin 2 pi 2 by 3. And third root will be cos 2 pi 3 by 3 + i sin 2 pi 3 by 3 and this is equal to minus half plus iota root 3 by 2, minus half minus iota root 3 by 2, and 1. So, you can keep on going and find all the roots of unity.

So, for example you can find out for 1 by 4 to the power 1 by 5 and so on, so you can keep on doing that. So that finishes the representation for cyclic group. Now we should be able to write the character table for any given cyclic group. So, let us see that what it takes to write for any cyclic group, so let us take a simple example of a C3 point group now. So, you should have tau 1, 3 of this tau 1, tau 2, tau 3. So, you can say that this will be 1, 1, 1 this will be 1, 1

And you can say that this will be epsilon, epsilon star, epsilon star and epsilon. So, now and then if we combine this you can easily write it as, so why I did that because now here I can write it as epsilon, epsilon square, epsilon cube. Now epsilon cube will be equal to 1, epsilon square will be equal to epsilon star and epsilon will remain as epsilon. So, this is now very easy so given the understanding that you have now.

So, you can write down without doing all the calculations you can simply write down the character table of any given IR representation. so E, C3, C3 square and I have 1, 1, 1 now I will call it as E and then the other one is E. If I combine it remember that I have to write the curly brackets on one side of it, if it is not combined. So, this tells me that these two representations are complex conjugate of each other.

Now if you combine this, I will get characters as 2 this will be 2 cos 2 pi by 3 and this will be 2 cos 2 pi by 3 and you can actually carry out x, y, z, take x, y, z as the bases and find out the matrix corresponding to E, C3, and C3 cube and find out what is the matrix and the corresponding phase try to block factor it and then find out whether you are able to match this character table or not, so try to do it as assignment.

So, find out use x, y, z as bases to find out character table using matrix representation for C3 point group. So, that is the end of this and next class will be starting with application of group theory and quantum mechanics.