Symmetry and Group Theory

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Lecture – 33
Character Tables of Cyclic Groups

Or we could work out 2 more character tables. What do you want to do? Okay, let us do character tables today. I do not think time will permit. If, if time permits, we will do the second one. Okay, so see the character tables that we have talked about already, C2v, C3v so on and so forth, T1, Td, they all have real characters, right. It is not necessary that character tables will always have real characters, okay.

Imaginary characters arise especially when we deal with cyclic groups. What are cyclic groups? Example? **"Professor - student conversation starts"** EC3. EC3 C3 square, which group is that? C3 group. No. C3, C3 group, C3, right. **"Professor - student conversation ends."** So what we were saying is that we only have C3. You have nothing else. Then the operations are C3 C3 square and C3 cube which is E.

Right or wrong? Or C4 or C5 or C6, okay. What I am telling you is that the cyclic groups are groups which have this imaginary characters. Let us start with may be C4. What are the characters, how many, fine, right. For a cyclic group, Abelian group, we have said that cyclic group is Abelian group, what does that mean? **"Professor - student conversation starts"** (()) (02:28) **"Professor - student conversation ends."**

Everything is conjugated. What else did we say about cyclic groups? That cyclic group has subgroups. Every element is a group by itself. Think of, think of the C3 group. What are the operations? C3C3 square E where you cannot relate C3 and C3 square by any other symmetry element, right and we can work out the similarity transformations also. You will never be able to do the similarity transformation. So each is a class by itself. So how many rows should we have in C3, say in C4, let us say.

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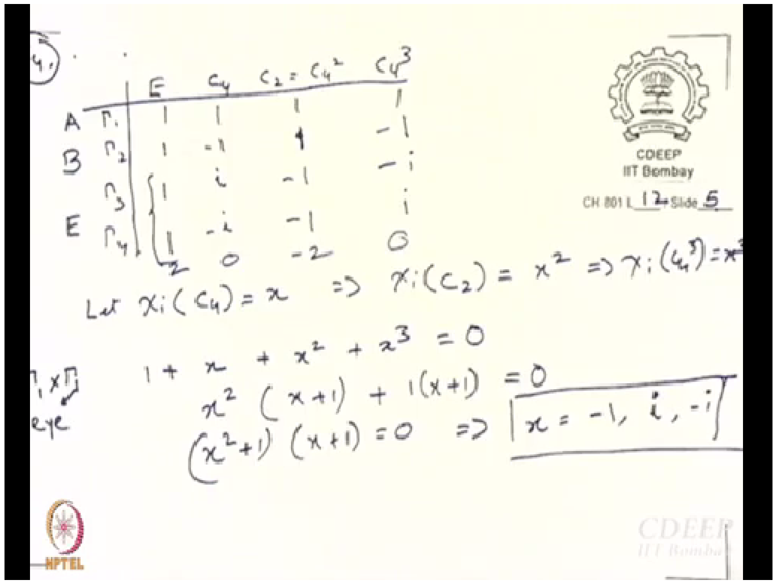

In C4, how many characters, how many rows should I have? **"Professor - student conversation starts"** 4. 4. **"Professor - student conversation ends."** I will call them gamma 1, gamma 2, gamma 3, gamma 4. We are trying to work out the character table. And what are the symmetry operations? E, C4, C4 square is also equal to C2 and C4 cube. What will be the dimensionality of each representation?

"Professor - student conversation starts" 1. 1. **"Professor - student conversation ends."** So I can write this first row and I can write the first column. Now we have to fill in the rest but as we will see, not everything will be +1 and -1. If everything was +1 and -1, what will the character table look like? **"Professor - student conversation starts"** C2v. C2v. It is not. **"Professor - student conversation ends."**

Because you have a special relationship. They are not just independent. C4, C4 square, C4 cube, okay. So let we do it like this. Let Xi of C4=x. So that would imply that Xi of C2 would be equal to how much? x square and Xi of C4 cube is x cube, okay. So I can write x, x square, x cube here. Now, now let me use Great Orthogonality Theorem. This is, gamma 1 is a reducible, irreducible representation.

Gamma i is also an irreducible representation. So what can we write? 1*1 + 1*XiC4 + 1*XiC2 + 1*XiC4 cube=1. =C4? 0, okay. Let us do that? 1+x+x square+x cube=0. How do I get it? I get it by gamma 1*gamma i. Even this looks like gamma 1. Only pronunciation, nothing else, gamma I, alright. Very difficult algebraic equation, cannot solve. Can you help me solve?

"Professor - student conversation starts" X-i=-1. **"Professor - student conversation ends."** So I can factorize like this. x squared*x+1+1*x+1=0. So x square+1*x+1=0 implies that x=-1, i, -i. So it is a little confusing maybe because here we have i and there we have i, but this i is not the same as that i, right. Not only i different from you, this i is also different from the other i. What is this i?

"Professor - student conversation starts" Iota. **"Professor - student conversation ends."** Iota. And what is Iota? **"Professor - student conversation starts"** square root.**"Professor - student conversation ends."** Square root of -1. So we can fill in these, so what will it be? 1 and what, what is x, right? So -1, i, -1. Yes, what am I saying? -1, i, -i. So I write -1, I write i and I write -i. What will this be now? C2 is C4 square.

So what will XC2 be? **"Professor - student conversation starts"** 1. 1 or i? Or -1, or -i. 1. Well let us deal with 1 first. Let us write that 1. So what is C4 cube in that gamma 2? -1. -1. As well you with me. Understood, sure, okay. Then tell me what is this, C2, iC2? i square, i square is -1. I is square root of -1. And what is XC4 cube? -i. What is this C2, XC2 here? Square of -i. Square of -i is -1 or +1? -1.

Sure. What is this? i or -i? i. Sure. Or i cube? Even this is very nice symmetry, is not it? 1i, 1-i and all that, okay. **"Professor - student conversation ends."** Now can we write the molecular nomenclature? First one is easy. I will write A. Do I need to write 1? Let us see. What is the second one? Gamma 2. Second one will be, right because character of the principle axis is -1. So anti-symmetric.

So this is B. What about gamma 3 and gamma 4? What will I write? Cannot write anything. So it is conventional to club them and name them E. So say I do not need 1, 2 at all. A and B are enough. We club them and represent them as a 2 dimensional representation E but do not forget that E is a reducible representation. In this case, if you add them, what do you get? 1+1, i-i, -1-1,

-i+i.

So this is written as E and it conforms, right. Because character of E, E here, character of the, of identity is 2. Which will make it a 2 dimensional representation and we are getting it by adding 2 to dimensional representation. Why do we like to add them up and combine them and write them together? Because that leads to elimination of the imaginary number, right. See the reducible representation is 2 0 -2 0.

No imaginary number at all. No complex quantity. It is nice. But do not forget that when we write E here, that is not the designation of the irreducible representations. Because we cannot write the designation, the Mulliken name of the irreducible representation so easily, we chose to combine 2 of them and write a combine nomenclature. A combine name but E is actually reducible, right.

If I give you 2 0 -2 0, you can easily reduce it to the constituent gamma 3 and gamma 4. Alright? Question? **"Professor - student conversation starts"** (()) (12:01) I will get the one group of equation. What, what, what? If I start solving this symmetrically by Great Orthogonality Theorem, I will get this and C2. Then how do I designate? **"Professor - student conversation ends."**

So, that is when you need to remember your group theory. What kind of a group is this? Is that too complicated. So what is the, what is the order of the group? **"Professor - student conversation starts"** 4. 4. **"Professor - student conversation ends."** So it is G4. So if you remember, we have said that G4 can give you 2 kinds of multiplication tables, right. So one kind of G4 is a cyclic group.

The other kind of G4 is not a cyclic group, okay. This is the first thing you have to remember. Secondly, you have to look at the symmetry operations. Looking at the symmetry operations, you can easily make out that this is a cyclic group, right. Right or wrong? It is nothing else. Only C4x is there. Nothing else is there and with respect to the C4x is, you can turn once to get a C4 operation, twice to get a C2 or C4 square operation, thrice to get a C4 cube operation and four times to get identity operation, okay.

That is how you know. When it is a cyclic group, that is when your antenna should go up and you should think that now I should expect imaginary numbers. No, I just worked it out. Because what is the difference between this and that, you tell me? Between this and C2E. The difference is that there is no direct correlation.

And of course, everything is correlated but then there is no direct correlation in the sense that I know that here the character of C2 has to be square of this. I know that the character of C4 cube has to be the cube of C4, right. There is no such relationship among the characters of G41, right. The symmetry operations are all different, okay. So this is where you get the marriage of group theory and symmetry.

One is not good enough. Alright? Who has read ABC's of Quantum Mechanics? It is a book, I am not saying with the figurative sense? ABC's of Quantum Mechanics. So you are too young to, that book perhaps became extinct before you were born or something. It is by like Steve Rydnik or Paul Rydnik, a small book, Russian MIR publications. So there, the name of the chapter on bonding was marriage of atoms. So this is used very frequently in chemistry, fine.

So have learnt to work out C4. Now if I ask you to work out C4, you should be able to do it. If I ask you to work out C3, then also you should be able to do it. C3 is actually easier.

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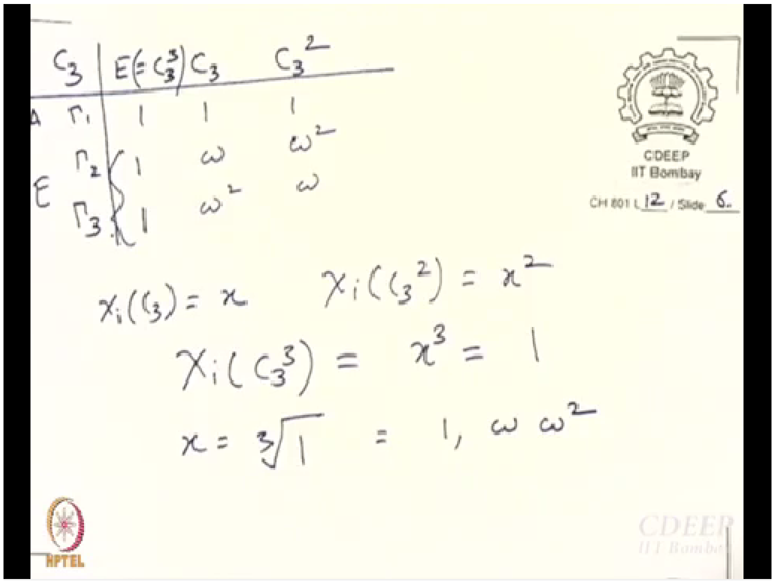

C3. What do I have? I have C3 operation. I have C3 square operation. And I have E which is equal to C3 cube operation. Once again, cyclic group. So how many representations do we expect? 3. Every operation is a class by itself. So 3, gamma 1, gamma 2, gamma 3 and L1 square+L2 square+L3 square=3 which implies that L1=L2=L3=1. So these are all 1-dimensional representations.

So I will write what I can write easily. I have only 2 places to fill. How do I fill those places? Let us say, now this is even easier, XC3=x. What will X, okay, I will write i also. XiC3 square be, very difficult algebra? **"Professor - student conversation starts"** x square. **"Professor - student conversation ends."** x square, very good. What will XiC3 cube be? Extremely difficult. Do not jump steps.

Tell me what it will be in terms of x? **"Professor - student conversation starts"** x cube. **"Professor - student conversation ends."** X cube, which is equal to your beloved 1. What is x? x=cube root of 1. How many roots should I get? What are they? 1 -1 and what? **"Professor - student conversation starts"** 1 and not -1. **"Professor - student conversation ends."** Oh, not -1, not -1, very good.

So that will be equal to 1 omega omega square. What is omega? **"Professor - student conversation starts"** Yes that is right and if I write in the exponential form. You are right, you are right. Anyway, I will show it. I need the exponential form so that I can develop the other ones. **"Professor - student conversation ends."** So now see, I can write omega, omega square here.

What will the, what will this be? **"Professor - student conversation starts"** Omega square omega. **"Professor - student conversation ends."** And what is omega*? Omega square. So I can also write 1 omega omega*. 1 omega* omega and I do not exactly know why but in character tables, it is more than often it is written as epsilon. Epsilon is actually the mode general but in this case, definitely it is omega. Alright, so this is your character table. What is this? I can say this is A and this together you call it E. Alright.

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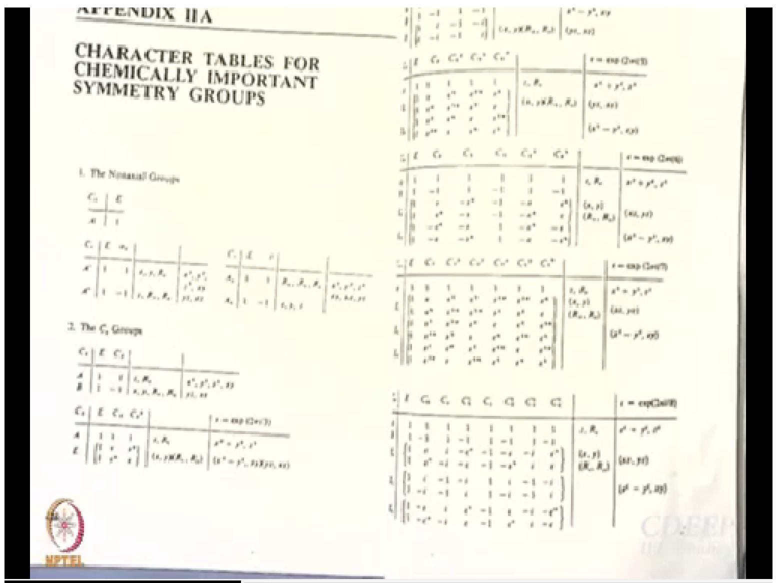

Now what I will do is, I will just show you some character tables of cyclic groups so that you get the general idea. See C3, we have discussed already. And see, now you see what is the advantage of using E. When you take x y and do this, you make this symmetry operations operate on them, then they give you a reducible representation which is actually the sum of these 2 irreducible representations, okay.

So you can say that x y jointly form a basis for this. Rx Ry jointly form a basis for this and so on and so forth, okay. So this is C4. We have discussed already, okay. Sorry. Before that. So this is the answer that we did not know. Do not know the form, E to the power 2pi i/3. E to the power

2pi i/3. Which group? C3. 3 and 3 rhyme, right. 3 times to 3.

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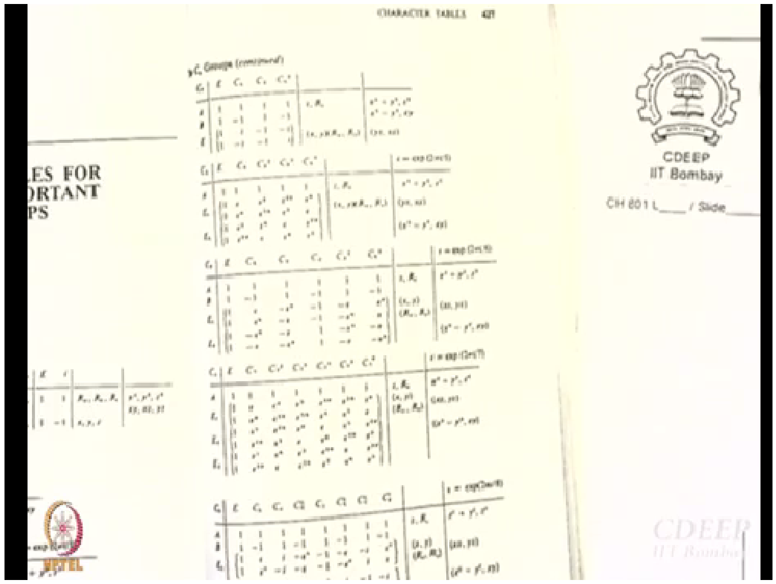

Okay, C4 we have worked out already. What about C5? Here also you get something like epsilon epsilon square and so on and so forth. What is epsilon here? Epsilon is E to the power same 2pi i but divided by 6. Oh, 5, not 6. 5, 2pi i/5 and what is the point group? C5. So again 5 and 5 rhyme. What about C6? Same thing, epsilon -epsilon* -1 -epsilon etc., etc., epsilon is exponential 2 power i/6. So that is why it is convenient to write it in the epsilon form because it will always become E to the power 2pi i/P for this CT, point group. Alright.

So this is how you can construct character tables which have imaginary quantities as well. **“Professor - student conversation starts”** Sir when we are coming to work this (()) (21:35) how will we know which group is the other. **“Professor - student conversation ends.”** In C3, it is very easy, you have only 2. Okay. Let us see, let us see about C6 or C5, C5. See we have, this is E1, right. 1 epsilon epsilon square epsilon square* epsilon cube. And this is 1 epsilon* epsilon** epsilon square epsilon. You get the message. Look at each column?

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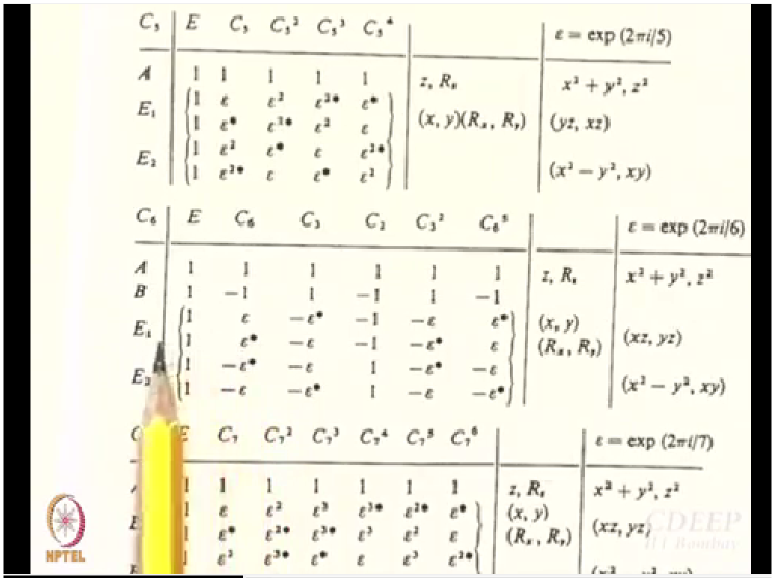

Oh, okay. Now can you see? And can you see? See epsilon epsilon*. Look at E1. Epsilon epsilon* in the same, under the same operation. -epsilon* -epsilon, -1 -1, -epsilon -epsilon*, epsilon* epsilon and here again you have -epsilon* -epsilon, -epsilon -epsilon*, 1 1, -epsilon* -epsilon, -epsilon -epsilon*. So we have basically taken complex conjugates. That is how you club, okay.

It is all symmetric, symmetry rules and that is how we get rules that govern symmetric. Okay. So I think for once we have started on time and we are finishing on time. So let us leave it here. If I start the next discussion, it will be too much. So you come back on Thursday and what I want to do is in the first, maybe 10-15, 15 minutes, I want to rush you through the normal nodes of carbonate.

I have shared the slides with you already, okay. And there the reason why I want to do is, more than anything else to show how you can decompose a complicated reducible representation into its constituents irreducible representations. We do it all the time for the rest of semester. And then we would like to go on and discuss a little bit more about the relationship of symmetry with quantum, quantum mechanics.

What is the role that symmetry plays in quantum mechanics. In fact, that is what the rest of the course is about once again. We are going to see how you can use the symmetry to factorize things like secular determinants, right. But before that, we will perform on Thursday a general discussion of the interplay between symmetry and quantum mechanics. Then we will learn something called symmetry adapted linear combination which is of utmost importance for us to develop things like molecular operators, okay.

Once we are done with that, while doing that we will also learn something about a very useful tool which is called projection operator, okay. Once we are done with that, our arsenal is complete. We know all the tools that we need to tackle actual chemical systems. So hopefully this will get done if not on Thursday, definitely on Monday. Thursday and Monday, these 2 classes we will ready with all our tools and then we attack chemical problems full-fledged from next Tuesday onwards.