Symmetry and Group Theory
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Lecture - 30
Tutorial - 6

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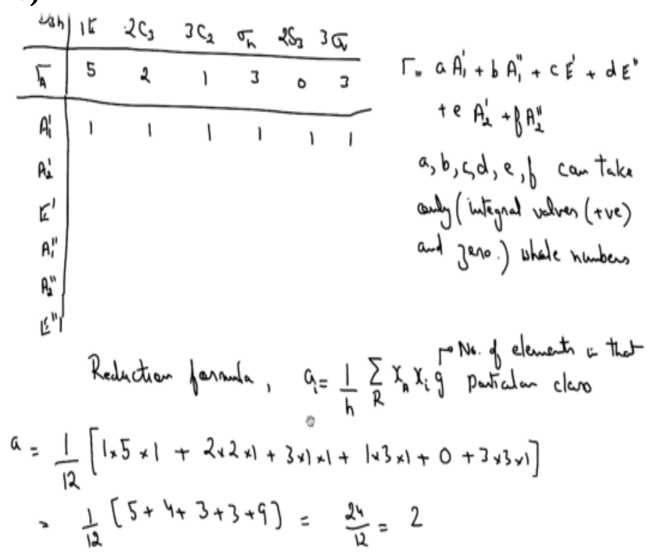

So, welcome to tutorial 6, let us see what are the problems, that we will be solving today. So, the first question is so, this is all related to character tables and reducible versus irreducible representation. So, I know we have already done this, but let us look at it more carefully again so, reduce the following representation. So, once it is saying that reduce the following representation it means that it is already a reducible representation which you have to reduce into component irreducible representations.

So, into their sometimes it will say component species sometimes it will say component irreducible representation so, either way the meaning is same that you have to reduce it into component irreducible representations. So, the given example is of the point group D3h and the reducible representation is tau and the corresponding elements this operations are 2C3, 3C 2 sigma h, S3^2 and 3 sigma v now, the characters are 5, 2, 1, 3, 0, 3 whatever is the basis that will come here.

But we do not know what the basis is to create this reducible representation, our job is to reduce this representation so, for to reduce now, what we have to do is we have to write the irreducible representation set of irreducible representations. So, let me write down the character table first. So, what we have here is A1 prime, A2 prime, I will not solve it completely, but I will just give you again how to solve it one by one point by point, A1 double prime, A2 double prime, E double prime.

So, let me see that I am writing all of this as 1, 1, 1, 1. And then there are other characters corresponding to other irreducible representations. So, now, we know that this tau can be expressed as a1 times let me write down the symbols or let me just say a times A1 prime + b times A1 double prime + c times E prime + d times E double prime + e times A2 prime + f times A2 double prime, the order does not matter.

So, idea is that this particular reducible representation is a linear combination of all the irreducible representations. Now, the coefficients we have to find out all these coefficients some of the coefficients will be 0, a, b, c, d, e, f some of the coefficients will be 0 some of the coefficients will be real numbers. So, they will always be real numbers you cannot have fractions.

So, I will say a, b, c, d, e, f can take only integral values which are positive and 0 it cannot take fraction. So, that is a test whether you are getting these coefficients as correct numbers or not. So, the test is that there will always be so basically it is a set of whole numbers starting from 0 towards positive infinity. So, integral positive so, this will be whole numbers so, anywhere in whole numbers this will take the value so, that is the test that otherwise if it takes negative value, for example, that means your calculation is not correct.

So, let me just do one calculation for A 1 prime and then the rest of the calculations will be very, very similar. So let us see so we know the reduction formula. So, we will use the reduction formula, what does the reduction formula say? So, reduction formula says any coefficient a will be equal to 1 over h, h is the order of the group, summation over all R chi A, chi A let us say this is the reducible representation and chi i let us say this is a i.

So, this is for i th irreducible representation, and this will be multiplied by a factor g, where g is the number in front of the symmetry element. So that means it is the number of class elements or number of elements in that particular class. So, this is number of elements in that particular class, this is very important, otherwise, you will mess up the whole calculation. So, this g comes here, so let us now see how it is done.

So, we will calculate a and rest of the calculation you can do as a homework. So 1 over h so, now, h is the summation of number of all the elements here, so which is the order of the group. So, it is 1, 2, 3, 4, 5, 6 and 6 more so 12. So 1 over 12 so, there are 12 elements 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, so 12 elements in the group which are categorized into 6 classes so, we have 12 here. Now summation over all R that means, we have to take all the values of R so R is changing from E to sigma v. So, we have 6 different classes here.

Now chi A is the character under reducible representation, let us say if this is A so, this is the character under reducible representation chi i is the character under irreducible representation of which the coefficient we are trying to find out and g is the corresponding class element corresponding class size. Now, this would be so, I will take 1 from here, so, this 1 into this 5 into this 1 over here then, this 2, 2, 2, 1 so, 2, 2, 1, 3, 1, 1.

So, 3 into 1 into 1 then I have 1 into 3 into 1, then this is 0, so, does not count 0, 3 into 3 into 1. So, this gives me 1 over 12, 5 + 4 + 3 + 3 + 9 which is, so, 9, 9, 18, 18 and 6, 24 so, this is 24 / 12, which is a whole number. So, this is 2 so, that means, A1 prime will appear twice in this irreducible in this reducible representation. Similarly, the rest of the coefficients can also be found out so, I will leave that to you.

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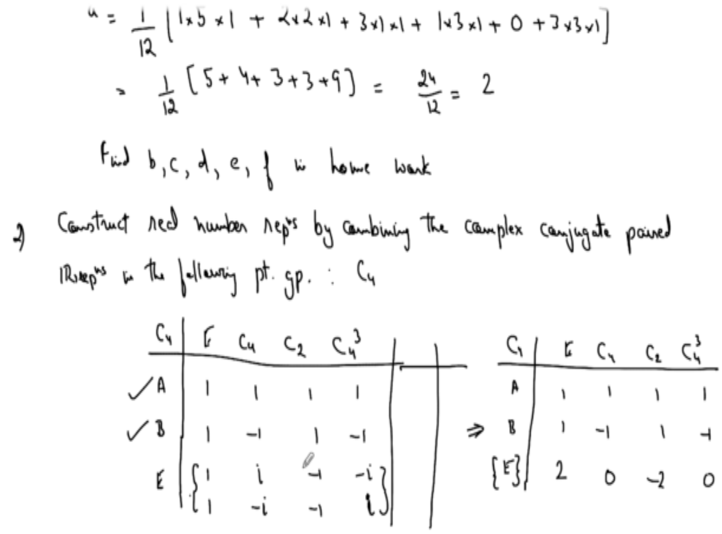

So, complete this find out b, c, d, e, f in homework. So, this course is all about calculation. So, it would be better to do the calculation yourself by your hand so, that it is very, very clear in the head and also the speed will also matter. So, with the speed at which you are doing the calculation would also matter in the exam. So, sometimes if you are not doing it optimally then it will affect your answering capacity or capability in the exam.

So, it is better to practice a simple maths problem. So, you should be able to practice now, let us look at second question. So, far we have learned about character tables, we have not looked at characters, there are some special groups called a cyclic group, which we will learn in next week. So, but I am giving you a problem which has some component of cyclic groups, so, let us say but it is related to character table.

So, construct real number representations by combining the complex conjugate paired, I will tell you the meaning of this, irreducible representations, in the following point group, point group given is C4. So, there are some cyclic groups for which the character table is not real numbers or not integers positive or negative. So, there are some complex numbers always coming into those character tables.

So, let us see how the character table for C4 looks like. So, C4 will have group elements as E, C4, C2 and C4 cube and the character table is something like this A which is all ones totally symmetric representation, B will be negative with principal axis 1, - 1 and then there is a 2 dimensional representation E. And then if you notice, you will see that there is a curly bracket written normally so far the character tables which you have developed, they do not have those curly brackets, but in cyclic groups, these curly brackets will come.

And then we will also see that how great orthogonality theorem cannot be used to actually write these character tables. And then there is a separate method to do that, we will discuss that next week. But I am just trying to give you an example of how those character tables look like. So you have 1, 1, iota, - iota, - 1, - 1, - iota, 1. And then this side also there is curly brackets.

So, this is closed in curly brackets and then the rest of the components of character table are same so, you have some unit vector basis here, binary products as a basis here written. Now, the question is asking that construct the real number representations by combining the complex conjugate paired IR representations. So, if you see that A is already a real number representation, B is already a real number representation, whereas E has complex numbers. So, now, these complex number would always come in pairs.

So, if I have a complex number here, I will have a complex conjugate here. Similarly, if I have a complex number here, I have a complex conjugate here this is i. So, how do I combine this, what I have to do is I have to just take the summation and write the character table like this. So, E, C4, C2, C4 cube, the A and B part remains same, because those are already real numbers, 1, -1, 1, -1. Now, E will be written as, so if you take the summation of this 1 + 1 will be 2, i + minus i will be 0, minus 2, and 0 again.

Now, I do not know here by just looking at this character table like this, whether it is a summation of 2 complex conjugate pairs or not. So, to indicate that what I do is, I will do a curly bracket here. So now my E is represented within the curly brackets. So that means this E is actually not an independent real number IR representation. It is a 2-dimensional representation.

But it is composed of complex numbers and complex conjugate paired IR representations. So, all you have to do is you have to just take a summation and write down the number which comes as a result let us do one more example of this so, that there is no doubt.

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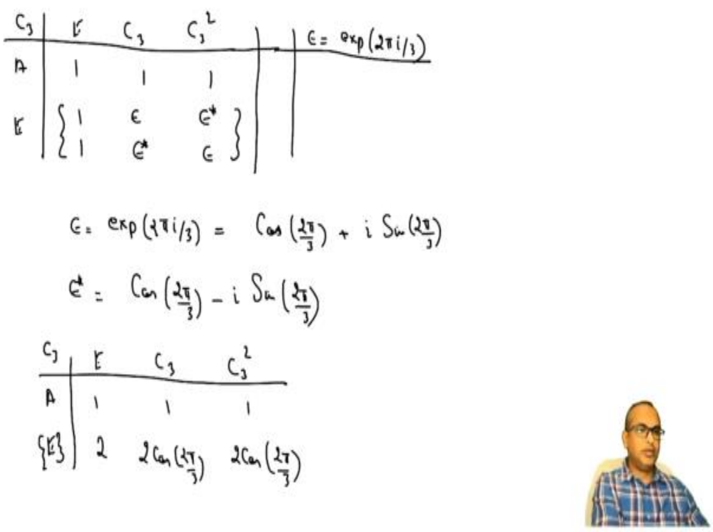

Let us look at one more character table like this. So, I will take a simple one C3. So, you have E, C3, C3 square and I have A here as 1, 1, 1 and E is written as complex conjugate pair. So, I have 1, 1 and now if you see you have written epsilon, epsilon star, so, this epsilon is a complex number and epsilon star is the complex conjugate of that and epsilon star and epsilon we will see what is the meaning of, how do we write these epsilons. So, in the character table itself epsilon will be defined and it is written as exponential 2pi i / 3.

Now, what does it mean? So, this means, if I am writing it as exponential 2pi i / 3, I can always write it as, I can expand it in terms of so, this is nothing but E i theta if 2pi / 3 is theta then E i theta so, this can be written as cos theta, which is 2pi / 3, which is the real part of this complex number and the imaginary part can be written as iota sin theta. So, epsilon means this and epsilon star will be cos 2pi / 3 minus so, it is a complex conjugate of this. So, whatever is the i coefficient that goes negative i sin 2pi / 3.

So, now, you know the value, so, now, this character table can be transformed into real numbers and what we have to do is to just take the summation of these 2 vertically so, E, C3, C3 square A, 1, 1, 1 and E will be now written in curly brackets 2 now, if you take summation of epsilon and epsilon star, your iota will get cancelled and you will get only real number. So, this will be 2cos 2pi / 3 similarly, here also it is epsilon + epsilon star so, this will be 2cos 2pi / 3.

So, this representation and this representation are same, this is the real number equivalent of the original character table. So, sometimes in calculations you need real numbers let us say if you want to calculate the irreducible components of a reducible representation, then you would need this and you cannot do the calculation with complex numbers. So, that is how basically you convert it into real numbers and then you do the calculation. So, let us see our next question which will deal with that. So, I hope this is clear, if not please shoot me an email.

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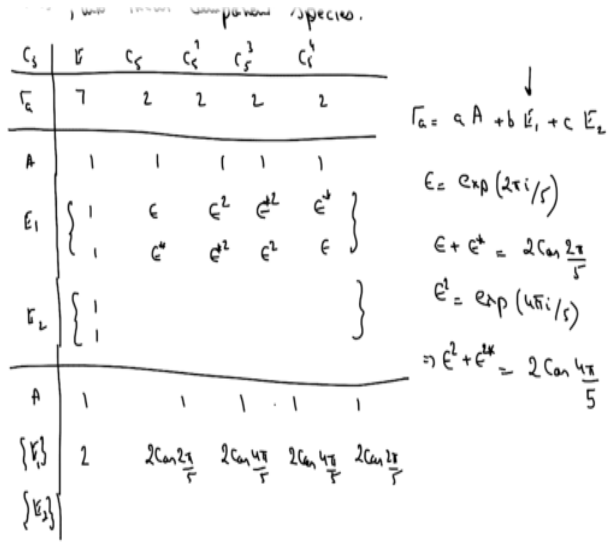

So, third question is, reduce the following so, we will be doing lot of this we will be using a lot of this these results, reducing the reducible representation into irreducible representation when it comes to application of group theory into chemistry. So, it will be better if you do this practice now itself. Because this will be used as an exercise like as a passing by comment that by using reduction formula, we get this but how to do this is taught here. So, later on in the later parts of this course, results will be used directly.

So, it will be better if you practice a lot. So, reduce the following representation from groups whose irreducible representation contain imaginary characters into their component species. Let us first write down C5 we have E, C5, C5 square C5 cube C5^4 and our tau a is 7, 2, 2, 2, 2 and if we now look at the character table the characters are like so, for C5 I have A which is all 1, and then I have E1 and E2 and these are complex conjugate pairs and what I have here is 1, 1, 1, 1 and I have epsilon, epsilon star.

Now, here I have epsilon square epsilon star square or epsilon square star whatever does not matter, epsilon star square, epsilon square, epsilon star, epsilon and here also there be some characters similar to this. So, now, let us look at the linear combination of tau a linear combination of tau a should be a times A, b times E1, c times E2. So, let us try to find out what is the component for E1 because we are interested in looking into complex numbers calculations.

So, also epsilon here will be given in the character table as will be equal to exponential 2pi i / 5, because it is C 5 groups of 2pi / 5. So, now if I take the summation, I will have to convert to be able to use a reduction formula I will have to convert this into the real numbers. So, for real numbers, I will have to take a summation of this. So, when I take summation of epsilon and epsilon star, I will get 2cos so, epsilon + epsilon star will give me 2cos 2pi / 5 which is the real number.

Now, for square of this if I take a square of epsilon that means, my theta will become 4pi / 5. So, epsilon square will become exponential of 4pi i / 5, that means, if I am taking epsilon square + epsilon square star this will give me 2 cos 4pi / 5. So, that will be the difference between summation of epsilon and epsilon star in summation of epsilon square and epsilon star. So, now, that would mean that the characters which I have as real numbers will be A, E1 and E2.

So, A will be all ones this will be 2 and this will be 2 cos 2pi / 5 this will be 2 cos 4pi / 5, 2 cos 4pi / 5, and 2 cos 2pi / 5. So, now that you have all the real numbers so, you can use the reduction formula easily. So, let us do one calculation for E1 and for A and E2 you can do the calculation at home.

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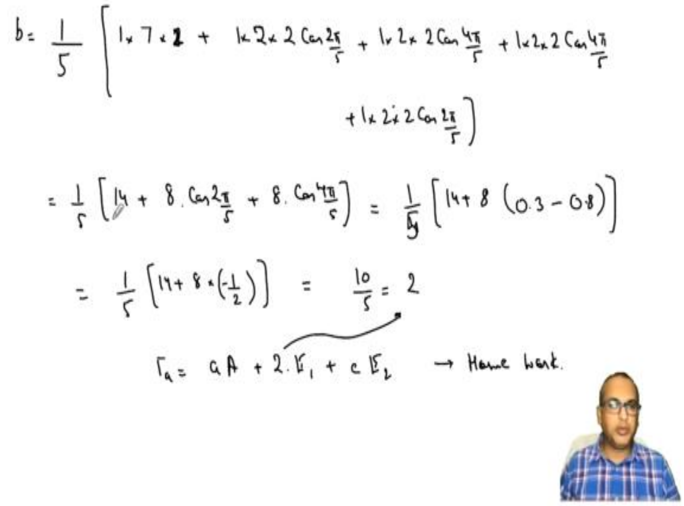

So, let us quickly do this so for b component. So, the order of the group is 5 and what I will have is now the class size is 1 and then I have 7 coming from the character under reducible representation and 2 coming from the character under E1 representation. Then similarly I have 1 into 2 into 2 cos 2pi / 5, 1 into 2 into 2 cos 4pi / 5, 1 into 2 into 2 cos 4pi / 5 + 1 into 2 into 2 cos 2pi / 5 now, you would need calculator for this because this becomes cos 72 degrees this becomes cos 144 degree the values I do not expect you to remember.

But, if we do the calculation what I have is 14 plus this will become let us combine this and this so, you will have 8 times cos 2pi / 5, and 8 times cos 4pi / 5 this simple combination and this becomes 1 / 5 14 + 8 can be taken out. So, cos 72 will be 0.3 and cos 144 will be -0.8 then you will get - 0.5 here. So, what I have is 1 / 5 14 + 8 into 1 / 2 with a negative sign now, this cancels so, you have 10 / 5 and that needs to so, that means your tau a will contain at least twice the E1 representation.

Similarly, you can calculate for coefficient of A and coefficient of E2. So, now, you should be able to do this calculation rest of the calculation please. So, tau a is a times A + 2 times E1 this 2 is coming from here which we have determined plus, c times E2. So, I have shown you how to determine this b now, try to do this same calculation for finding a and c. So, that will be your homework for this tutorial.

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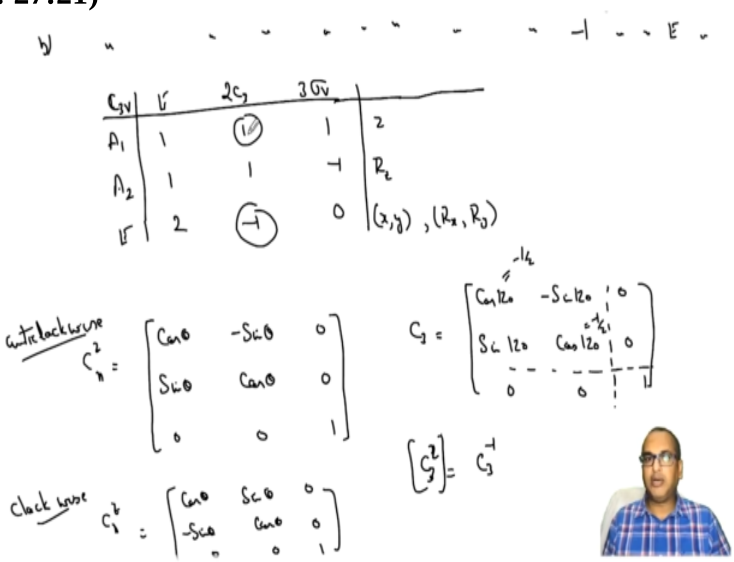

So, the question says that in C3v both C3 and C3 square belong to same class, this you already know, and that is listed as 2C3 in the C3v character table. Now, because these are members of same class, so, their characters are same under different representations. So, now, the question is saying that demonstrate so, there are 2 parts to this question demonstrate. So, first part is to demonstrate that both C3 and C3 squares which are of the class 2C3 have a character and 1 for the A1 representation.

And second part is to demonstrate that both C3 and C3 square have a character -1 for the E representation. So, to do that, let us first write down the character table of C3v. So, you have

C 3 v, E, 2C3. Now this 2C3 they are saying that C3 and C3 square both belong to this class and 3 sigma-V. So, we have A1 which will be 1, 1, 1. Now, both the characters of C3 and C3 square are 1, A 2, 1, -1, 1 and for E this is 2, -1, 0. Now we also list on the unit vectors I have z, Rz, then x, y and then Rx, Ry.

Now the meaning of this is that z transforms as A1 and x, y transforms as E, now we want to write the characters. We want to demonstrate that the characters of C3 and C3 square under A 1 is 1 for both of them and for E it is -1 to do what you have to do is you have to simply write down the transformation matrix for x y z under C3 operation and under C3 square operation so, for C3 operation. So, let us first write down any general operation for Cnz.

So, this will be we already know that cos theta, - sin theta, 0, sin theta, cos theta, 0, 0, 0, 1. So, this implies that C3 will be now, the angle will be 2pi / 3, 2pi / 3 is 60 degree. So, you have a cos 60 - sin 60 0, 2pi / 3 now, this will be 120 degrees sorry this will be sin 120 cos 120, 0, 0, 0, 1 now, this is for C3 now, if you see that this is blocked diagonalized matrix in this form into in 2 is to 1 form. So, that means, the x and y are jointly transforming as the upper part of this matrix whereas, the z is transforming like this.

So, the character for z basis will be 1 here for C3 and character for x,y that is E representation will be summation of cos 120 + cos 120 and the value of cos 120 is minus half. So, what you have here is minus half and this will also be equal to minus half. So, the character for C 3 becomes -1 if you take the summation of these 2 because the character or the trace of the matrix goes here as the character so, trace of the matrix is obtained by summation of diagonal elements.

And we will take summation only up to here because z is a separate representation which is A 1 so, this part is a separate representation corresponding to A1, this part is corresponding to x,y which is E representation. So, that means character for C3 under E will be -1 character for C3 under A1 will be 1 now, for C 3 squared, how do you get the character for C3 square, now, C3 square can be understood either by changing the angle or by changing the sense of rotation.

So, we know that C3 square can be thought of as inverse of C3 or we can write if you take inverse here or inverse here that will not matter. So, C3 inverse can be taken as C3 square.

Now, what do you mean by C3 inverse? So, you can actually calculate the inverse of this matrix or what you can do is make the rotation as clockwise so, this is the matrix or this is the matrix for anticlockwise rotation.

So, for a clockwise rotation you can write Cnz, Cnz = cos theta, sin theta, 0, -sin theta, cos theta, 0, 0, 0, 1. So, this is for clockwise and this was for anti clockwise rotation. So, what do you mean by that, so, C3 and C3 inverse are related by clockwise versus anti clockwise relation. So, if you are saying that this is my matrix for anticlockwise rotation and I want to obtain the matrix for C3 inverse so, C3 inverse can be written as C3 when done clockwise.

So, I can say that the negative sign from here will go here, which will not change the character because the character is coming from this part which is still the same. So, cos 120, cos 120 is still the same as -1 so, that means the character for C3 square and C3 will remain as same. So, I hope it is clear if it is not clear so, then you can also argue that C3 square can be considered as the angle can be changed to 240 degrees because it is twice the rotation. So if you do cos 240, - sin 240, sin 240, cos 240, you still get the same result.

So basically, the idea is that summation of these 2 will give you a character under E, this character over here we go under A1 so that is all for today. I hope these tutorials are helping you do some calculations and some practice sessions at home. So, all right, so see you next week. Thank you.