Mathematics for Chemistry
Prof. Dr. M. Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 39

So, we have seen how to use the projection operators to construct symmetry adapted linear combinations, for 1 dimensional and 2 dimensional representations. For 1 dimensional representations the method of constructing is very easy because the characters are the same as the as the matrix elements. Since, it is a 1 dimensional matrix which is simply a scalar instead of using the characters of the instead of using the matrix elements, we can directly use the characters.

For 2 dimensional irreducible representations, the characters if you use the characters you have less information then using all the matrix elements. So, a character of a 2 dimensional matrix just gives it just its 1 number. Whereas, 2 by 2 matrix has 4 numbers. So, if you use the characters then what you construct or things called incomplete projection operators, but with a little bit of with a little bit of manipulation you can use the incomplete projection operators to construct, appropriate symmetry adapted linear combinations.

Now, this method of using the incomplete projection operators is more efficient because if you have the character table in front of you, you can immediately construct it. Now, let us try to see what happens when you have 3 dimensional irreducible representations, and we will try to construct a construct a symmetry adapted linear combinations for 3 dimensional irreducible representations. Now, once again I want to remind you that the irreducible representations can either be 2 dimensional or 3 dimensional.

And most of the groups have only 1 dimensional or 2 dimensional irreducible representation if you look at the character table, you will that there are very few groups that have 3 dimensional irreducible representations, and they correspond groups like tetrahedral and octahedral and various variants of those. One such group is the octahedral group that has that has an irreducible representations, which is 3 dimensional and we will see how to, how to construct suitable basis for this 3 dimensional representation. So, lets the problem the statement of the problem we will do is.

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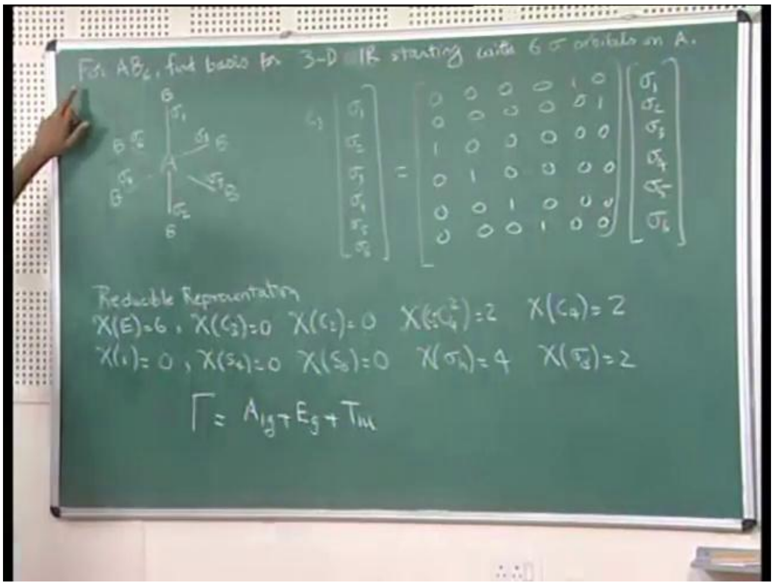

For an A B 6 and A B 6 what I mean is octahedral A B 6 molecule, find the basis for the 3 dimensional irreducible representation, starting with the six sigma orbitals on A. So, the A the A atom is bounded by 6 sigma orbitals. So, 4 are in this plane and 2 are 2 are in the plane of the board. So, you have these six sigma, sigma orbitals going from A to the B to the 6 B atoms. So, starting with these six sigma orbitals, let us let us go through the procedure and construct the symmetric adapted linear combination, and what we will is the basis for 3 dimensional irreducible representation. Now, the first we will ask is which 3 dimensional irreducible representations will you get a basis for, and to do that what we have to do is to start with the six sigma orbitals.

So, you have sigma 1, sigma 2, sigma 3, sigma 4, sigma 5, sigma 6. So, these are basis for a 6 dimensional representation, these form the basis for a 6 dimensional representation. And since, it is a 6 dimensional representation it will be reducible it will it cannot be an irreducible representation. And then so, let us go ahead and calculate the, calculate the characters of this reducible representation. So, in order to find the character any element of any class in this reducible representation, what you need to do is to operate on this vector sigma 1, sigma 2, sigma 3, sigma 4, sigma 5, sigma 6 by the various operations of the group and then find out the characters of each of them.

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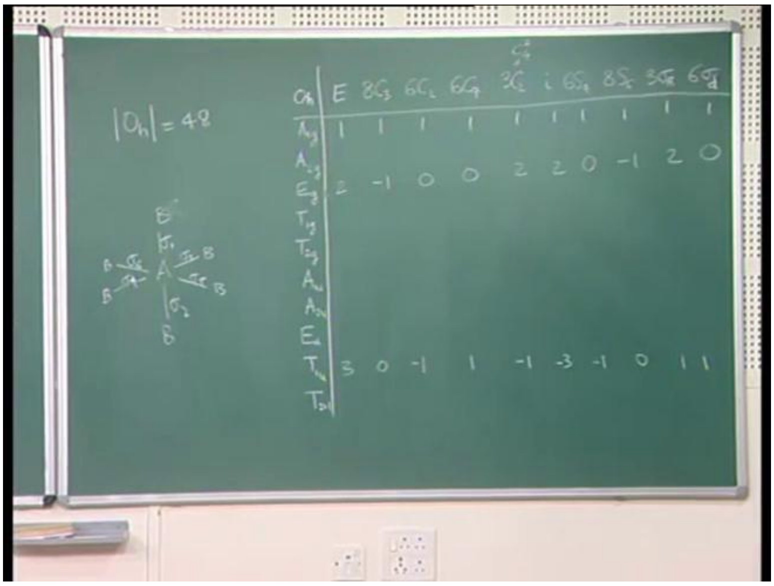

Now, the octahedral group of this molecule belongs to the octahedral group octahedral point group O h, the order of this group is 48. So, there is 1 plus 8 9 15 21 24 and then there is another 24. So, there are 48. So, the order of this group is 48. And it has 10 classes, the 10 classes are identity c 3 c 2. So, there are 8 c 3 operations and they all fall in 1 class. There are 6 c 2 operations that fall in another class there are 6 c 4 operations c 4, c 4 and c 4 cube actually which fall in a class. There are 3 c 2's which are which are basically c 4 square.

So, corresponding to the c 4 axis the c 4 axis is also acts as a c 2 access, but these 2 operations fall in different classes, there is a inversion octahedral molecule has a center of inversion the 6 c 4 axis, the 6 c 4 operations also give rise to 6 s 4 then the 8 c 3 gives raise to 8 s 6. In addition there is 3 sigma h and 3 sigma d, six sigma d. So, these are the 48 operations and these are the 10 classes and since, there are 10 classes there are 10 irreducible representations, and the dimensionality of them there are 2, 1, 2, 3, 4. So, 4, one dimensional representations 1 and 1, 2. 2 dimensional representations and 1, 2, 3, 4. 3 dimensional representations.

So, T's are the 3 dimensional representations, 3 dimensional irreducible representations. Now, I am just showing some of the characters and we will come to this in a bit, these now when we look at this the six sigma, sigma orbitals sigma 1, sigma 2, sigma 3, sigma 4, sigma 5 and sigma 6 they formed the basis for a 6 dimensional representation. And clearly a 6 dimensional representation has to be irreducible. So, we can work out the characters of various classes in this reducible representation. For example, if you operate by c 3 on this vector sigma 1, sigma 2, sigma 3, sigma 4, sigma 5, sigma 6 what you will get is sigma 1, when you operate by c 3 and you can you can you can think of c 3 as going through going diagonally in this direction.

So, then sigma 1 it takes it to sigma 4 or it takes it to sigma 5 and so on you can work out all the what happens to the remaining. So, then sigma 2 is taken to sigma 6, sigma 3 is taken to sigma 1, sigma 4 is taken to sigma 2 and so on. So, these c 3 operations they cause they can be represented there action can be represented by this matrix and so, this is a matrix corresponds corresponding to c 3, in this 6 dimensional reducible representation and once you have this you can easily work out that character of c 3.

So, the character of c 3 is 0 because every along the diagonals you have 0, character of identity will be 6 because you have 1 along the diagonals, identity will just leave all of them the same. So, you just have 1 along the diagonals and you have zeros everywhere else. So, the character of identity will be the dimensionality of the representation that is 6, character of c 3 is 0. Similarly, you can show character of c 2 is 0, character of this c 4 square.

So, there are 2 kinds of c 2's there are c 2's like this axis will be a c 2 axis and so, you have 6 such c 2 axis. In addition you will have 3 axis the c 4 axis corresponding to each of these will also be a c 2 axis, and so these have characters of 2. The character of this is 2 because if you imagine c 4, c 4 operating on a sigma 1 will leave it unchanged, will not change sigma 1, c 4 operating on, but it will not change sigma 1 and sigma 2. So, these 2 will have 1, but it will, but it will take. For example, it will take sigma 5 to sigma 4 to sigma 4, sigma 4 to sigma 6 and so on.

So, so so these 2 will have 1 along the diagonals everything else will have 0 along the diagonals. So, the character of that is 2 similarly, the character of c 4 will also be 2 and you can work out the character of the character of inversion will be 1 because sigma 1 will be taken to sigma 6 every no, no sigma orbital will be left unchanged. Similarly, s 4 is 0 s 6 is 0 sigma h, sigma h the character it will leave 4 out of 6, 4 out of 6 of the sigma's will be left unchanged. So, the character, character of sigma h is 4 and character of sigma d is 2.

So, with these are the characters corresponding to the reducible representations, and once you have characters corresponding to the reducible representations, you can decompose this into set of irreducible representations. So, you use your usual method of taking the characters of this reducible representation, and calculating how many times each, each irreducible representation appears in this representation. And if you do that you will get that this reducible representation can be written as a sum of A 1 g E g and T 1 u.

So, it is a 6 dimensional representation A 1 g is 1 dimensional, E g is 2 dimensional and T 1 u is 3 dimensional. So, it is a sum of these 3 representations, and you can you have to work it out you can easily verify this. For example, if you look at the character of c 4. So, the character of c 4 if I add the all these characters I get 2 which is a same as 2 here. So, you can verify using the character table that is indeed valid, valid decomposition of this representation.

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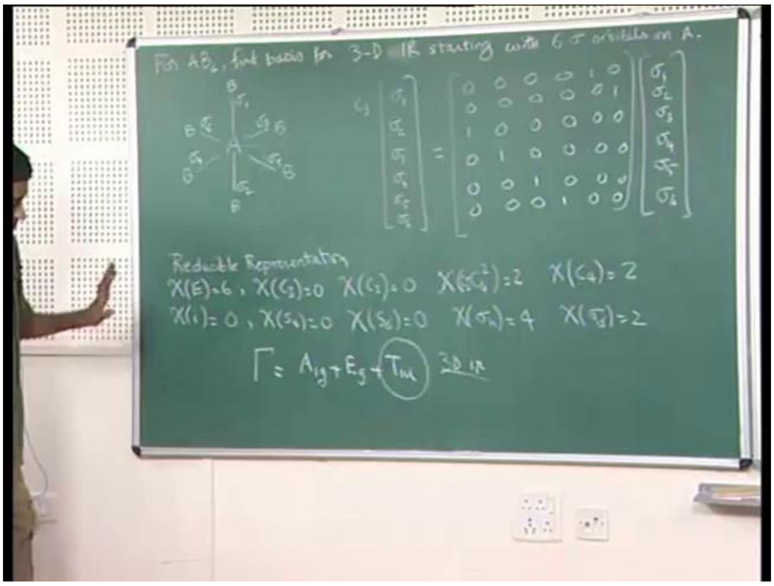

So, now you have 1 dimensional representation at 2 dimensional representation and this is the 3 dimensional representation. So, this is a 3 D irreducible representation and so, what you want to do is to, is to construct, construct appropriate linear combinations of the sigma's such that they become a basis for T 1 u. So, we want to find appropriate basis for T 1 u using sigma.

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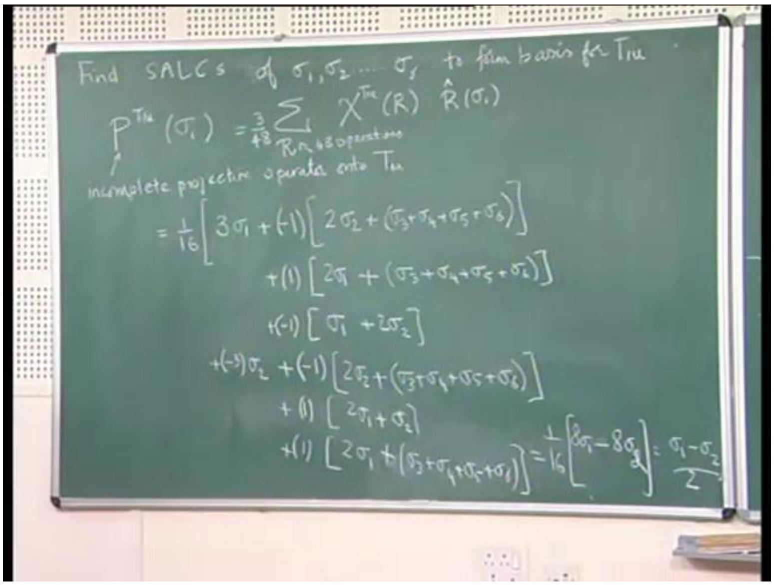

So, what we are going to do is to find the appropriate symmetry adapted linear combinations of sigma 1 to sigma 6 such that they form a basis for T 1 u. And this exercise since we, since we have the characters of all the operations. All we need to know is we can we can we can construct the projection operators and in order to construct the projection operators you need to know, how each of these operations acts on the sigma’s.

So, let us start we want we look at the projection operator of T 1 u projection on to this irreducible representation on to T 1 u of and this projection operator, projection of sigma 1 let us look at the operation on sigma 1. So, this is the incomplete projection operator incomplete projection operator onto T 1 u. So, it is a projection onto T 1 u and this acting on sigma 1 this can be written as sum over all R, and it will be chi, chi in T 1 u of R times, R acting on sigma 1.

So, the so the various operations you look at there you, you see what they give as a result of that operation, and how it operate and multiplied by the characters. So, now if you look at chi R these are the characters of the various operations. Now, this sum is overall 48 operations. So, you have to take the sum overall 48 operations. Now, that seems very tedious, but things will become a lot easier once you see that that sum of them are 0. So, you do not need to consider this here you have 8 here, and another 8 here which are 0.

So, we do not need to worry about those 16, but still you have the you have the remaining 32 that you have to consider, and let us go ahead and work it out. So, so, we need to know what happens when various operations act on sigma 1. So let us first look at the identity, identity and sorry this should be multiplied by 3 by 48, 3 is the 3 is the dimensionality of T 1 u, T 1 u is the 3 dimensional irreducible representation 48 is the order of the group.

So, this I can write as 1 by 16. 3, 3 by 48 is 1 by 16. Now, let us look at the first operation is first class is the identity, identity has character 3. So, the chi of identity is 3 and whenever a the identity operation acting on sigma 1 will just give me sigma 1 so, we will have 3 sigma 1. Next, non zero character corresponds to c 2 so that has character minus 1. Now, when now c 2 there are 6 operations corresponding to c 2, these are the c 2's as I said they thy correspond to axis that are in between in between the in between the bonds. Now, now so what they will do is they will, they will transform. Now, each c 2 will if you look at this c 2 it will transform sigma 1 to sigma 2.

On the other hand if you look at a c 2 here it will transform sigma 1 to sigma 6. If you look at a c 2 here it will transform sigma 1 to sigma 3 and so on. So, the 6 the 6 c 2 operations will so, so, so, what will happen is that 2 of them 2 of them will transform sigma 1 to sigma 2. So, the 2 that are in this plane. So, this 1 and 1 going this way will transform sigma 1 to sigma 2. So you have you have 2 sigma 2 and the remaining 4 will transform them to either sigma 3, sigma 4, sigma 5, or sigma 6.

So, you have plus sigma 3 plus sigma 4 plus sigma 5 plus sigma 6. It is not hard to see this, but importantly none of them leave it as sigma 1. So, all the c 2 operations since they correspond to axis that are between, between 2 2 axis they will never leave sigma 1 unchanged, they will always move sigma 1 to something else 2 of them will move sigma 1 to sigma 2, the remaining will move it to 1 of the other axis. So, that is as far as c 2 goes now what about c 4.

So, plus 1 the character of c 4 is 1 and you have 6 operations again. Now, the 6 operations actually corresponds to a c 4 and c 4 cube. Now, the so there are 3 3 c 4 axis 1 that is passing along each of the bonds. So, this way 1 along this so, this is a c 4 axis. Similarly, this is another c 4 axis and as is this. So, now you can see that sigma 1 the c 4 corresponding to this axis will leave sigma 1 as it is. So, 2 of them so, you have a c 4 and a c 4 cube corresponding to this axis, corresponding to this axis you have c 4 and c 4 cube both of them will leave sigma 1 as it is so you have 2 sigma 1.

Now, the remaining c 4’s remaining c 4’s will take sigma 1 to 1 of these 4, 1 of sigma sigma 3, sigma 5, sigma 4 and sigma 6. And nothing will no c 4 operation will take sigma 1 to sigma 2. So, that is that is as far as c 4 goes. Next, we can look at 3 c 2 these are c 4 square. So, the c 4 square operation, the c 4 square operation will again 2 of them. There are 3 c 4 square operations. So, 1 corresponds to along each of the axis. So, 1 of them will leave sigma 1 as it is the other 2 will take sigma 1 to sigma 2 to sigma 2 so those are the 3 c 4.

What about the what about the inversion, inversion will take it to sigma 2 so and the character of inversion is minus 3. So, you have plus minus 3 sigma 2 plus. Now, you have 6 s 4 so the 6 s 4 the character of s 4 is minus 1, and s 4 s 4 operations will be will be very much like the c 4, but then it will be c 4 followed by a reflection. And so all you will get it is c 4 followed by a reflection. So, 2 of them will take sigma 1 to sigma 2 the remaining 4 will take them to the to the other 4 plus.

So, this is the effect of s 4 and next you have, you have s 6. S 6 has character 0 so it does not matter and you have sigma h and sigma d. So, you have 3 sigma h and sigma d both have character 1 the 3 sigma h. So, they correspond to each of the planes, planes containing 4, 4 atoms so 2 of them will leave sigma 1 as they are. So, there are 3 sigma h 1 will leave sigma 1 as it is, the other will take 2 of them will leave sigma 1 as it is and the third one will take sigma 1 to sigma 2.

So, you have 2 sigma 1, sigma 2 and then you have 6 sigma d, sigma d corresponds to the planes bisecting, the bisecting the bonds. So, the planes bisecting the bonds and there are 6, 6 of them. Now 4 of them, 4 of them will contain 2 of 2 of them will contain sigma 1. So, they will leave sigma 1 as it is. So, we have we have to find the effect of sigma d’s the 6 sigma d’s. Now, the sigma d’s corresponds a dihedral planes that are in between the various bonds.

Now, 2 of them will contain sigma 1, sigma 2 and they and they will not they will not affect sigma 1. So, 2 of them will take sigma 1 to sigma 1 the remaining dihedral planes will take sigma 1 to sigma 3, sigma 4, sigma 5, and sigma 6. And this completes, this completes the effect of the projection operator, we can add it altogether and we can get the result. So, you have 1 by 16 now, let us look at the coefficient of sigma 1 you have 3 plus 2 5 minus 1 4 plus 2 6 plus 2 8. So, you have 8 sigma 1.

The coefficient of sigma 2 is minus 2, minus 2 that is minus 4 minus 7 minus 9 minus 9 plus 1 minus 8. So, it is minus 8, minus 8 sigma 1. And then sigma 3, sigma 3 to sigma 6 have minus 1 plus 1 that is 0, minus 1 plus 1 that is 0. So, minus 1 plus 1 that is 0. So, this is just this is just sigma 1 minus sigma 2 by 2. So, what we showed is that this projection operator takes sigma 1 to sigma 1 minus sigma 2 by 2.

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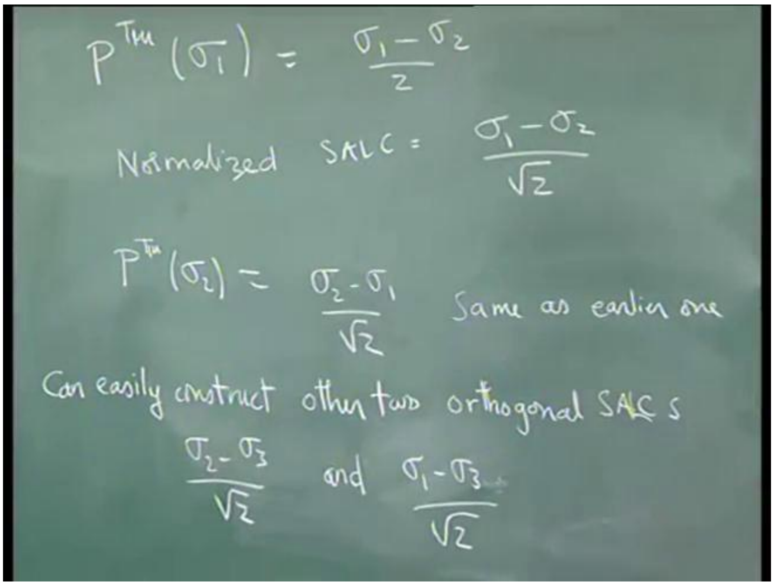

So, what we saw through this is that projection on to T 1 u the projection operator operating on sigma 1 gives me sigma 1 minus sigma 2 by 2, and if you normalize it. So, you can normalize this to get normalized S A L C sigma 1 minus sigma 2 by root 2. Now, it is not hard to show you can go through the same exercise, but it is very obvious from the symmetry that projection of T 1 u onto sigma 2 will just give me matrix elements sigma 2 minus sigma 1 by root 2 which is the same, same as earlier.

So, sigma 1 and sigma 2 they combine to give you this is the symmetry adapted linear combination of sigma 1 and sigma 2, and you can easily construct the remaining can easily construct other 2 orthogonal S A L C's and you can show that they will be sigma 2 minus sigma 3 by root 2 and sigma 1 minus sigma 3 by root 2. So, thus our 3 symmetric adapted linear combinations are sigma 1 minus sigma 2 by root 2 sigma 2 minus sigma 3 by root 2 and sigma 1 minus sigma 3 by root 2. And these 3 you can show that they form a basis for T 1 u.

So, what we have seen through this whole exercise it was it seem like a fairly tedious exercise, but it was very straight forward is that starting with, starting with a given set of set of orbitals. We started with the set that we started with throughout all these sigma orbitals act on the, a center, on the atom you had various sigma orbitals which corresponds to bonds with B. And we started with the 6 sigma orbitals and our goal was to find symmetric adapted linear combination of these sixth sigmas which would form a basis for T 1 u.

And those 6, those 6 in order to identify them first we found out how each of the operations acts on, acts on these sigmas. And using that we constructed our projection operator and once we had the projection operator acting on sigma. So, we projected we took the sigma orbital and projected it onto the T 1 u irreducible representation, and what we saw was that we got sigma 1 minus sigma 2 by 2. And so then so then we know that if we take sigma 2 we will get the same thing. So, if you take sigma 1 minus sigma 2 by 2 you will get itself. So, that means if I take sigma 1 minus sigma 2 by 2 I should get back sigma 1 minus sigma 2 by 2 and indeed that is correct.

So, this was the this was the strategy that we used and by doing this we could, we could easily construct that these 3, these 3 sigma 1 minus sigma 2 by root 2, sigma 2 minus sigma 3 by root 2 and sigma 1 minus sigma 3 by root 2 they are the symmetry adapted linear combinations. And these 3 these 3 linear combinations are the ones, are the ones that form that form a basis for T 1 u. So, far this whole exercise has shown. Now, now now you have completed the discussion of how to construct symmetric adapted linear combinations for 1 dimensional, 2 dimensional and 3 dimensional irreducible representations.

And we have seen how the projection operator can very elegantly, work to give you give you these appropriate symmetry adapted linear combinations. Now, these symmetry adapted linear combinations are used are the ones that are used to construct hybrid molecular orbitals. So, when you are doing m o theory they it is this symmetry adapted linear combinations that will that will play an important role. Also these are the ones that are used to find out how, how the how the how the various orbitals split under the influence of various fields.

So, if we if we want to take the metal lab if you imagine that the a center atom is a metal atom, and it has a and this B correspond to various legands so, then A is in what is called an octahedral field. And we want to know how the how the energy levels in this octahedral fields split, and this can be understood and what is the symmetry of the various resulting orbitals that again can be understood by these by these basis functions. Now, the next thing that we are going to do is to take this and try to do a similar exercise for a slightly different system, which is a cyclic which is a the cyclo propanyle group. And we will look at how the pi orbitals in this system play, how the pi orbitals in the system can be can be calculated.

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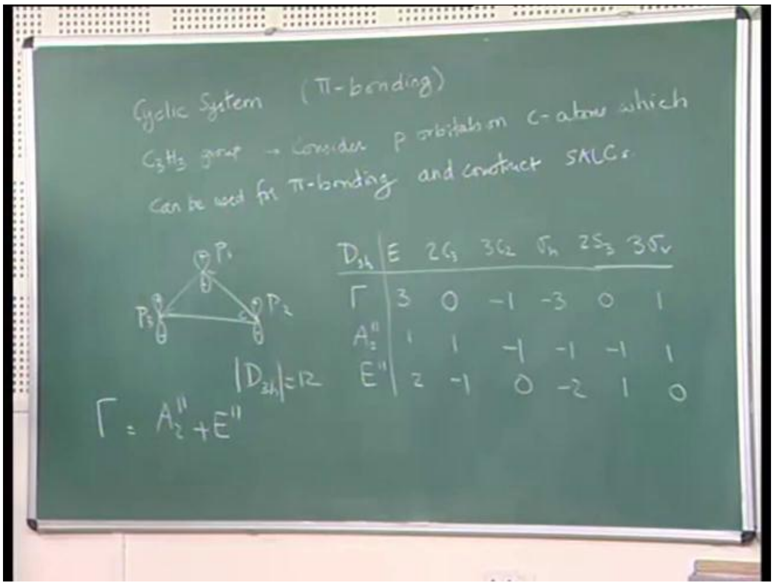

So, next we will consider a cyclic system and we will consider the we will look at pi orbitals, pi bonding this is this is what is used in pi bonding. And what we want to do is to consider a system like let us say C 3 H 3 group. So, C 3 H 3 and consider p orbitals on carbon atoms, which can be used for pi bonding and construct S A L C's. So, what we want to do is this group has it has 3 carbon atoms, and the carbon atoms has have these p orbitals. So, this is this is a planar set 3 group and the and the 3 3 orbitals, the p orbitals that are used for pi bonding are they lie perpendicular to the plane of these 3 carbon atoms. And what these are wave functions so they have a plus and minus sign. So, the sign of the wave function is opposite in the lower part.

And these 3 they can combine to form pi to show the pi bonding, and what we want to do is to construct appropriate linear combinations. So, if we call this p 1, p 2 and p 3 we want to construct appropriate S A L C's to find out what are the what are the linear combinations of these are a basis for looking at pi bonding. Now, these belongs to group the this unit has symmetry of d 3 h, d 3 h is a has the following classes, it has identity, it has 2 c 3, it has 3 c 2. Then it has sigma h 2 s 3 and 3 sigma v, the order of the group is 12 equal to 12 and it has 6 classes corresponding to 6 irreducible representations.

Now, now now now p 1, p 2, p 3, p 1, p 2, p 3 now, the sixth irreducible representations if you remember we had what, you can show that that there is they corresponds to various 1 dimensional and 2 dimensional representations. Now, so there will be 2, 2 dimensional and there will be there will be 4, 1 dimensional representations. Now, if you look at if you look at the p 1, p 2, p 3 they form a basis for a 3 dimensional representation that will be a reducible representation.

So, 3 dimensional representation which will be reducible is denoted we will denote it by gamma, and gamma is nothing but you can work out, you can work out how many times as you can work out the characters of gamma. And you can show that the character of identity will be 3 character of c 3 c 3 will be 0 because c 3 will take p 1 to p 1 p 3 p 3 to p 2 and so on. So, the character of c 3 will be 0, character of c 2 c 2 will take p 1 to minus p 1 c 2 will p 1 to minus p 1. I mean 1 of the c 2's one of the c 2's will take p 1 to minus p 1 the other 2 will take will take p 1 to minus p 2 and p 1 to minus p 3.

So, the trace of c 2 is minus 1. Similarly, the character of sigma h sigma h will change the sign of all of all p 1, p 2 and p 3. So, it will have a character of minus 3. Similarly, the character of s 3 will be 0 and sigma b will be 1. And you can you can show that this is, this is a combination of if you if you look at the character table if you look at the character table of d 3 h you can show that this, this reducible representation is a linear is a combination of A 2 double prime and E double prime. So, A 2 is a 1 dimensional representation E is a 2 dimensional representation. So, this is 1 2 and 1 minus 1 minus 1 0 minus 1 minus 2 1 1 0. So, these are the characters of so, so so so you can easily verify that gamma is the sum of these 2.

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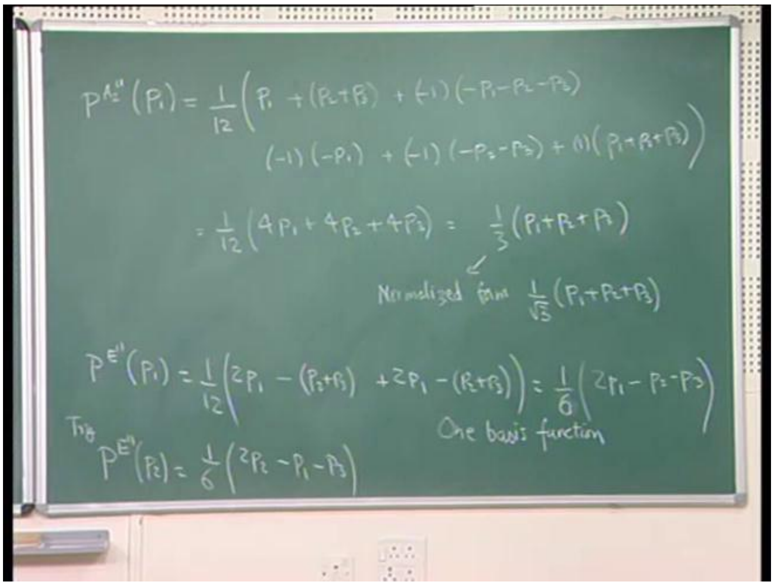

So, now let us look at the 1 dimensional representation let us find the projection onto the 1 dimensional representation, and lets this operate on p 1. So, let us, we are going to take these 3 p the 3 p orbitals, we are going to construct 1 orbital which is, which transform as the 1 dimensional representation A 2 double prime. And we are going construct 2 more orbitals which transform as E double prime which form a basis for E double prime. So, let us project p 1 onto A 2 double prime.

So, in order to do this we will so, it is 1 by 1 by 12 and if you if you work it out just like we did before, what you will get is this has p 1 this does not identity keeps p 1 as it is. Now, the c 3 we will take p 1 to either to p 2 or to p 3. Then you have the c 2's the 3 c 2's will take will take p 1 to minus p 1 minus p 2 and p minus p 3. Sigma h you have minus 1 sigma h will take p 1 to minus p 1 and then s 3, s 3 corresponds to c 3 followed by followed by sigma h.

So, we will get minus p 2 minus p 3 and then finally, the 3 sigma v's, the 3 sigma which will give you. So, sigma v's corresponds to these planes. So, they will give you p 1 plus p 2 plus p 3 and if you if you add up all these, so we will get p 1 plus p 1 plus p 1 plus p 1. So, you will get 4 p 1 then you have p 2 plus p 2 plus p 2 plus p 2. So, you have 4 p 2 and you have 4 p 3 and so this is 1 by 3. So, when you project, when you project p 1 onto A 2 double prime, when you project p 1 onto the this irreducible representation you get a linear combination of p 1 plus p 2 plus p 3, or you just get a sum of p 1 plus p 1, p 2 and p 3. And if you want you can normalize this by making it 1 by root 3.

So, the normalized 1 by root 3 p 1 plus p 2 plus p 3 and you can show that p 1 plus p 2 plus p 3 transforms exactly like A 2 double prime. So, what we have d1 is constructed, constructed a basis we have shown that the linear combination of these transforms as a 2 double prime. Now, we want to now we want to find 2 functions which together form a basis for E double prime, E double prime is a 2 dimensional representations. So, you need 2 functions so what are those 2 functions.

So in order to do that lets do p of projection onto E double prime of p 1. And this you can show if you if you again, again you can see how each of these characters operates on this on this matrix elements, but it is not hard to show this will just be you will just have 2 here minus 1 here there will be a 0 here minus 2 1 and 0. So, finally, you can show that that this will give you so it will be a 1 by 12 to p 1 corresponding to this. Then you have minus p 2 plus p 3 and you have minus 2 into minus p 1.

So, that is plus 2 p 1 and you have you have plus 1 into minus p 2 minus p 3. So, minus p 2 plus p 3 is equal to and so, I have 4 p 1 and minus 2 p 2 plus p 3. So, I will write this as 1 by 3, 2 so 4 by 12 1 by 6 2 p 1 minus p 2 minus p 3. So, this is the projection onto E double prime. So, when the projection on p 1 on to E double prime gives me this, and you can show that so, this is 1 basis function. So, this is 1 basis function. Now, we have to construct another basis function that is orthogonal to this so to construct the second basis, let us try projection of E double prime of p 2.

Now, if you do this you can show that what you will get is 1 by 6 2 p 2 minus p 1 minus p 3. So, this is what you will get if you if you if you project, if you project p 2 onto E double prime you will get this. Now, these 2 basis functions are not orthogonal. So, you can show that these two are not orthogonal so these 2 are not are not orthogonal to each other, but you can construct a second orthogonal basis function. So, what we have is.

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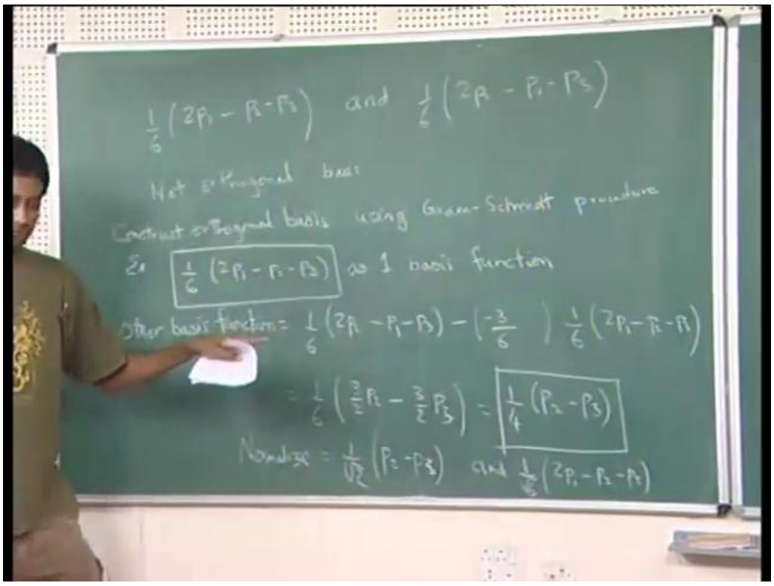

We have 1 by 6 2 p 1 minus p 2 minus p 3 and 1 by 6 2 p 2 minus p 1 minus p 3 these are not these are not orthogonal, these are not orthogonal orthogonal basis. So, if you want we can construct, construct orthogonal basis, basis using Gram-Schmidh procedure. So, I can take any one of these and I can construct the other one using Gram-Schmidt so for example. So, example you take 1 by 6 2 p 1 minus p 2 minus p 3 this as one basis function.

Now, the other basis function, function this is given by this is given by this vector this function 1 by 6 2 p 2 minus p 1 minus p 3 and from that you subtract the part you subtract the projection of this onto, onto this vector. So, if you subtract a part which is the projection of this so onto this, onto the first basis you will get an orthogonal basis function. So, what you will do is minus 1 by 6 2 p 1 minus p 2 minus p 3. So, this is the this vector and you multiply it by a constants, which corresponds to the projection of this onto this basis function, and that is not hard to work out.

So, what you will get is what you will get is here if you look at the projection, you can calculate it you take a dot product of these 2 treat this as vectors with p 1 p 2 p 3 as basis. So, if I take a dot product I will get minus 2 minus 4 and plus 1. So, I get minus 3 minus 3 divided by 6. So, I will get minus 3 by 6. And so this you can show is just equal to so, minus 3 by 6 is minus half. So, I have plus half so, if I do this plus half of that what I will get is 1 by 6. So, 2 p 2 minus p 2 3 by 2 p 2.

And then what about the p 1, so I get half p 1 and I take half of these. So, I have p 1 and I have minus p 1. So, those 2 will just cancel and what I will left with is minus 3 by 2 minus and minus half. So, minus 3 by 2 p 2 p 3. So, I can write this as 1 by 4 p 2 minus p 3. And if you normalize it you get 1 by root 2 p 2 minus p 3 and this is orthogonal to this function to this basis function. So, this right here is 1 basis function and the other basis function and you can normalize each of these if you want.

So, 1 by this will have a 1 root 2. Similarly, here what you will have is, what you will have is 1 by root 6 and root 6 2 p 1 minus p 2 minus p 3. So, these 2 are the normalized basis functions for E double prime. So, what we have shown is that is that using projection operators, we can construct symmetric adapted linear combinations for a variety of different problems. We looked at 1 dimensional representation, 2 dimensional representation, 3 dimensional representation and we also looked at problems involving cyclic permutations. So, like the p orbitals, orbitals forming the pi system.

So, in fact this symmetric adapted linear combinations is one of the most used techniques in group theory and this is this is an application, which has found, which has found its way in both in quantum mechanics and in spectroscopy. So, with this I will conclude I will conclude the group theory part of this course. And in the next class I will change gears, I will it will be the last class. So, what I will talk about is a very is the topic that is that plays an important role in all experimental methods that is error estimations. So, I will just spend one lecture on that, and then I will end the course with that.