Chemical Applications of Symmetry and Group Theory

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Lecture – 29

Hello and welcome to the day 4 of the 6th week of the lecture series. So, we have learnt about the SALCs, how to found the SALCs using position of it. Now, the question is like what we will do with these SALCs what information that this symmetric constrains toward the linear termination of atomic orbitals will give us.

Now in case of this chemical bonding or bond formation, so like the vales band theory that was put forward by (Refer Time: 00:56) and many others. They considered this the bond to be it is like a two center bond, so interaction between the atomic orbitals of two atoms a molecule will make where functioning localized within the bond. But, when the molecular orbital theory came into the existence then that give much more freedom, because in management theory it did not consider any kind of interaction between two bonds that are formed.

So, in molecular orbital theory we have this idea that the wave functions for in molecular orbital they extent up to the overall molecule. So, essentially you can fill the presence of the orbitals all over the molecule. So, that in one sense it is helpful for us because in that case we can actually use the use that are symmetry adopted and what that will help us in solving for various problem including the energy of the orbitals of the occupancy of the orbitals of the bond orders, all these things without going into detail our heart core computation.

So, in one way we can save a lot of time and without doing too much of work we can say about the energies of molecule how will be energies of the orbitals and all.

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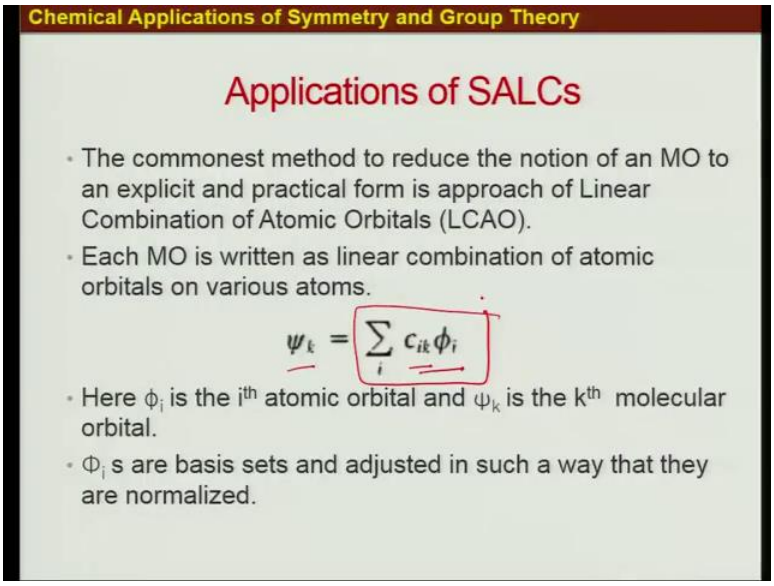

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Applications of SALCs

- The commonest method to reduce the notion of an MO to an explicit and practical form is approach of Linear Combination of Atomic Orbitals (LCAO).
- Each MO is written as linear combination of atomic orbitals on various atoms.

$$\underline{\psi_k} = \boxed{\sum_i c_{ik}\underline{\phi_i}}$$

- Here ϕ_i is the i^{th} atomic orbital and ψ_k is the k^{th} molecular orbital.
- Φ_i s are basis sets and adjusted in such a way that they are normalized.

And certain rules associated with this will help us in assigning different particles many different say different wave functions to different molecular orbitals. Now one of the the commonest approach to reduce the motion of an molecular orbital, in an express it and practical form this approach of linear combination of economic orbital in short l c a u.

So, what you approach that it is atomic orbitals they can combine in a linear fashion and they ultimately give us the molecular orbital. So, all in (Refer Time: 04:19) orbitals they are spread over all the molecules, it seems they are quite delocalized. So, this is an approximation and here we write a molecular orbital as the linear combination of four atomic orbitals, which is clear for his name and how would we do that. So, if we have the function for the atomic orbital ith orbital in a molecule as pi i and psi k is the kth molecular orbital then I can express psi k in terms of the all pi i s with a particular coefficient which is denoted as c i k, so this particular combination is nothing, but a linear combination right.

Now, this pi i s are that they represent the atomic wave function or the atomic orbitals here. So, this act as a basis function so all the atomic orbitals that is complete set of the pi i s act as the basis set and we allows (Refer Time: 05:35) would like to work with ortho normal basis functions. So, sake of ortho normal functions as my basis, so therefore this pi i s are waiting in such a way that they are normalized all right and any q atomic orbitals, so atomic wave functions they form the basis of universal presentations and automatically they will become ortho gonal, so if you make them ortho normalized also then they will become ortho normal.

So, we will get as set of ortho normal basis function, so by using this LCAO molecular orbitals approach; a particular form of the wave equation.

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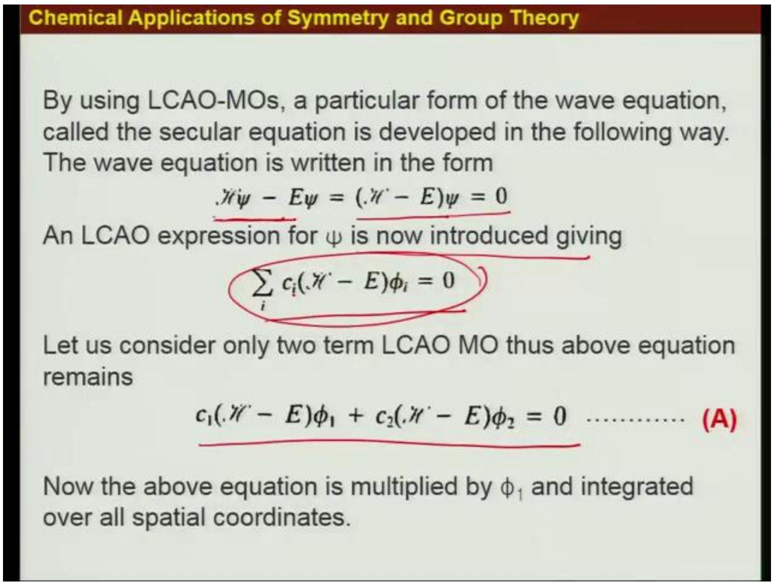

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By using LCAO-MOs, a particular form of the wave equation, called the secular equation is developed in the following way. The wave equation is written in the form

$$\mathcal{H}\psi - E\psi = (\mathcal{H} - E)\psi = 0$$

An LCAO expression for ψ is now introduced giving

$$\sum_i c_i(\mathcal{H} - E)\phi_i = 0$$

Let us consider only two term LCAO MO thus above equation remains

$$c_1(\mathcal{H} - E)\phi_1 + c_2(\mathcal{H} - E)\phi_2 = 0 \quad \ldots\ldots\ldots\ldots \quad \textbf{(A)}$$

Now the above equation is multiplied by ϕ_1 and integrated over all spatial coordinates.

Using this wave functions we form this wave function, atomic wave function; we get the wave function to be molecular orbital and then we can get and by of equation which has a particular form and which is called secular equation we will see in a while what is that and that can be developed. So, how it can be developed, so the wave equation can be written in a usual way, so by using (Refer Time: 06:51) equation, so h psi equals to e psi.

So, I can write h psi minus e psi which is nothing, but I can write in this form where both Hamiltonian and energy is used as operator and is equals to 0, this is something which we are all familiar with. Now l c o expression for the psi that is the molecular orbital is now introduced by giving this expression. Now, if I consider only two term LCAO, MO thus above equation that is here what I get is this because I am considering this i to be 1 and 2. So, I have already have two terms I could consider n terms, so for that I will have like c 1, h minus e pi 1 plus c 2 then h minus e pi 2 then c 3 and so on, what I take the simplest example were already two terms will exist.

So, as if I have two basic functions pi 1 and pi 2 and for that I can re write this equation as this fine. So, I turn this particular equation to be as a, now if I multiply this particular equation by pi 1 and integrate over all the spatial coordinates meaning by over d tau, then what do you get, so what I just say is written here.

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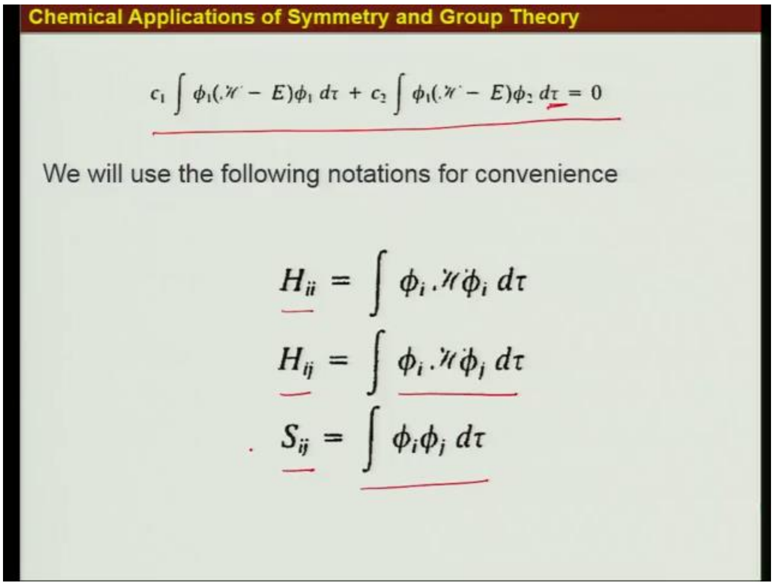

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$$c_1 \int \phi_1(\mathcal{H} - E)\phi_1 \, d\tau + c_2 \int \phi_1(\mathcal{H} - E)\phi_2 \, d\tau = 0$$

We will use the following notations for convenience

$$H_{ii} = \int \phi_i \, \mathcal{H} \phi_i \, d\tau$$

$$H_{ij} = \int \phi_i \, \mathcal{H} \phi_j \, d\tau$$

$$S_{ij} = \int \phi_i \phi_j \, d\tau$$

So, I multiplied both the sides by pi one and then I integrated over d tau, so that will remain equals to 0. Now in this expression what you can see is that there are several different integrals because you can separate these different quantities like h minus e when you expand then you can get several integrals.

So, we will use certain notations for simplicity, the notations are H 11, which stands for psi i, h pi i integrated over d tau where H ij is the integral which is given as this the two wave functions it define pi i and pi j and operated may still the same Hamiltonian and then there is a another integral which is the integration over d tau for the product of the two functions pi i and pi j and that is given by this (Refer Time: 09:57) term S ij and this S ij is known as the overlap integral.

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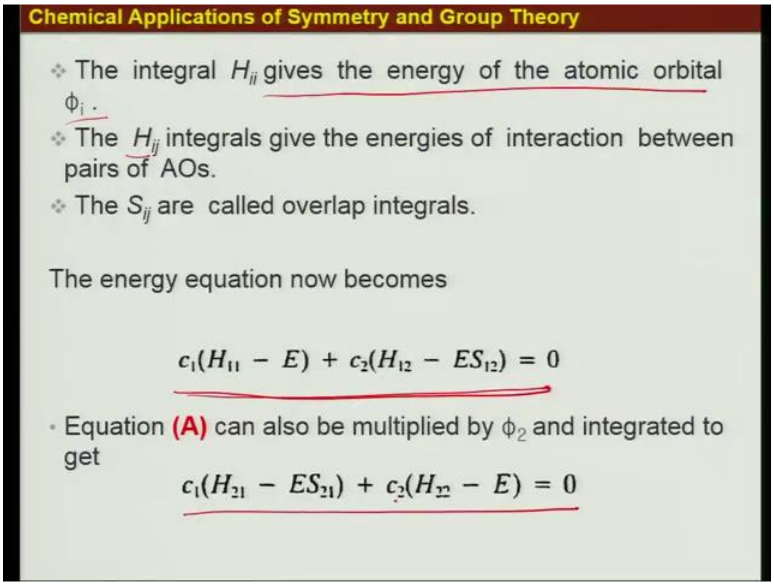

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- The integral H_{ii} gives the energy of the atomic orbital ϕ_i .
- The H_{ij} integrals give the energies of interaction between pairs of AOs.
- The S_{ij} are called overlap integrals.

The energy equation now becomes

$$c_1(H_{11} - E) + c_2(H_{12} - ES_{12}) = 0$$

- Equation **(A)** can also be multiplied by ϕ_2 and integrated to get

$$c_1(H_{21} - ES_{21}) + c_2(H_{22} - E) = 0$$

So, here we explicitly say what are which particular integral is gives what so this H ii, so it can be H 11 or H 22 then in that pi 1, h pi 1 integration over d tau or pi 2, h pi 2 integration of d tau that gives the energy of the atomic orbital pi i because here there is no interaction between two different orbital, the same atomic orbital for which I have the wave function as pi 1. So, that I am considering, so this gives me the energy of the atomic orbital whereas, H ij that gives me the energy of interaction between pairs of atomic orbitals, which is not too difficult to understand those. I have two different wave functions corresponding to two different atomic orbitals and they are interacting energetically and this integral H ij will give me the energy of this particular interaction and as I said S ij is called overlap integral, so how much two orbitals overlap will be given by this S ij integral.

So, now I have the energy equation that I can write in this fraction right using those notations. So, I got this particular energy equations considering only by multiplying that that secular equation by pi i and integrating. So, I could also do the same thing with pi 2; that means I could multiply this regulation by pi 2 and integrate over all the space and in that case what I could get, I would get something like this right, so you can see the similarity between these two equations that we got.

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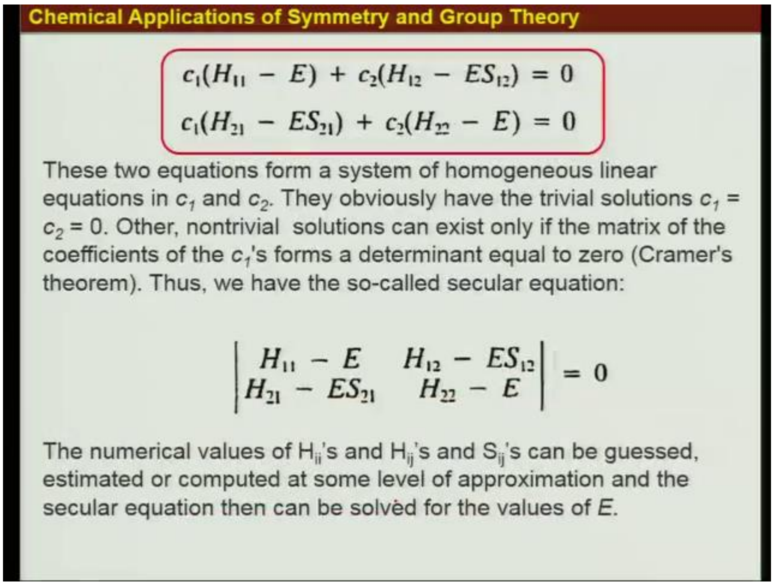

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$$c_1(H_{11} - E) + c_2(H_{12} - ES_{12}) = 0$$
$$c_1(H_{21} - ES_{21}) + c_2(H_{22} - E) = 0$$

These two equations form a system of homogeneous linear equations in c_1 and c_2. They obviously have the trivial solutions $c_1 = c_2 = 0$. Other, nontrivial solutions can exist only if the matrix of the coefficients of the c_1's forms a determinant equal to zero (Cramer's theorem). Thus, we have the so-called secular equation:

$$\begin{vmatrix} H_{11} - E & H_{12} - ES_{12} \\ H_{21} - ES_{21} & H_{22} - E \end{vmatrix} = 0$$

The numerical values of H_{ii}'s and H_{ij}'s and S_{ij}'s can be guessed, estimated or computed at some level of approximation and the secular equation then can be solved for the values of E.

Now these two equations, if I put them together; so I have got this two set of equations, now these two equations form a system of homogeneous linear equation in c 1 and c 2 which are the coefficient for linear combination. So, for these homogeneous linear equations you can always have the trivial solutions as c 1 and c 2 both are 0. Now if in order to get nontrivial solution what we need to have for by crammers rule, you should have the determinant of the matrix form by the coefficients of this c 1s and c 2s to be equals to 0.

So, then only I will have nontrivial solution and here we have this secular equation in form of this determinant. So, this is the secular determinant between terms of these integrals H 11 or H 12 and we have a term particularly this S 12. So, this ES 12 that ES 21 that we can get because if you go back and see these integrals here, so you can change inter change your position of pi 1 and e. So, this is has nothing to do because it is like a just in a scalar quantity. So, therefore, you have like e an integration of pi 1 pi 2.

So, therefore, you have ES 12 right, in that way you get this term and the other terms already we have explained. So, one can get the values of this H 11 also H ii’s or H ij’s or S ij s one can also try to estimate or compute with the help of some sort of approximation and the reason that approximation one can solve the secular equation and get the value of e, which is of at most importance. Now all the integrals that we discussed right, so like this H 11, H 12, S 12, S 21; all the individual integrals if you have to solve them be it computationally or some otherwise this is fairly time consuming. So, we need to actually do some approximation, so that our job is easier we save lot of time.

So, one of such approximation is Huckel approximation, so this Huckel approximation I will explain that shortly, this is a very interesting approximation, but this serves our purpose a pretty good way. So, for us Huckel approximation will be a pretty valid approximation and that will help us in various different ways we will see that soon. So, what is this Huckel approximation, so Huckel approximation says that all the H ij s are equal to alpha ij.

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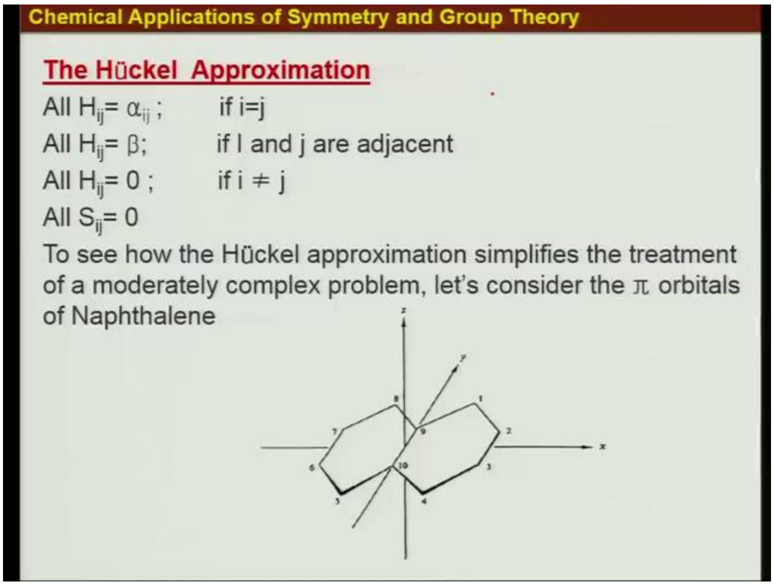

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The Hŭckel Approximation

All H_{ij}= α_{ij} ; if i=j

All H_{ij}= β; if I and j are adjacent

All H_{ij}= 0 ; if i ≠ j

All S_{ij}= 0

To see how the Hŭckel approximation simplifies the treatment of a moderately complex problem, let's consider the π orbitals of Naphthalene

For vibrate this i equals to j, so what does that mean; it means that this interaction energy is 0 until and unless this atomic orbital wave function that we are considering the pi i that is pi 1, pi 2, pi 3.

So, this interaction energy will be 0 except for the case why this i th and j th orbitals are adjacent to each other. So, I have like one orbital in the next orbital the next orbital and so on. So, this if I can see that the first one and the third one then the interaction energy is assume to be 0 under Huckel approximation, otherwise if they are adjacent they will have a value of alpha ij. So, if I consider a special case where i equal to j then I may, I have like H ii, so this H ii is alpha and this alpha is taken to be the 0 of the energy.

So, we will talk about that in detail later when we will take particular example and explain that and the overlap integral is taken to be 0 under Huckel approximation. So, with these approximations we will try to see now that how it simplifies the treatment of a little bit complex problem. So, for example, pi system of the molecule naphthalene, so what we will do; we will use all the p pi orbitals as main phases and we number this pi pi orbitals as which shown here. So, here you have a p pi orbital here you have pi pi orbital, so we have numbered them has 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 and you see the numbered are done in slightly different way, so that is because here we are considering the equi balance of the atoms here.

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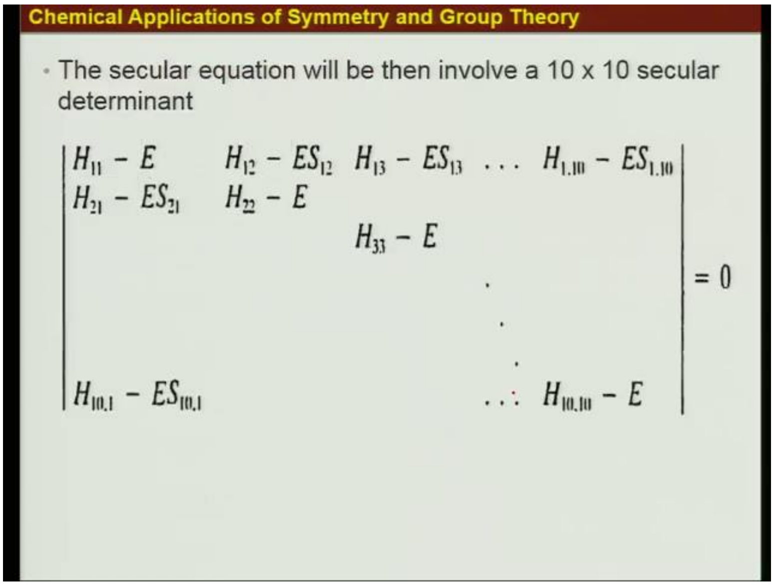

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- The secular equation will be then involve a 10 x 10 secular determinant

$$\begin{vmatrix} H_{11}-E & H_{12}-ES_{12} & H_{13}-ES_{13} & \cdots & H_{1.10}-ES_{1.10} \\ H_{21}-ES_{21} & H_{22}-E & & & \\ & & H_{33}-E & & \\ & & & \ddots & \\ H_{10.1}-ES_{10.1} & & & \cdots & H_{10.10}-E \end{vmatrix} = 0$$

So, if I take this 10 basis function involving 10 pi pi orbitals on the carbon atoms of than a prime molecule and then we do the treatment as I said in last few minutes then what we can do, we can form ultimately as secular determinants. So, in the previous examples we said that we choose only two function pi 1 and pi 2, so we had a 2 by 2 secular determinant.

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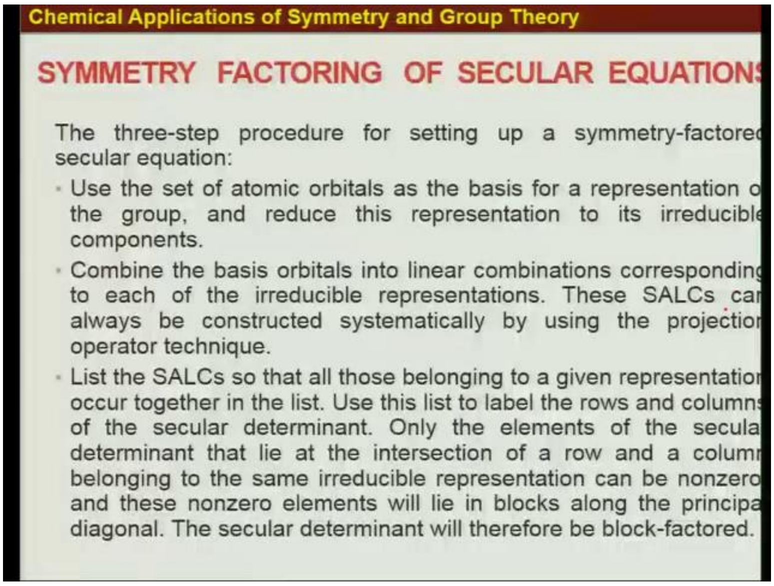

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SYMMETRY FACTORING OF SECULAR EQUATION

The three-step procedure for setting up a symmetry-factore secular equation:

- Use the set of atomic orbitals as the basis for a representation o the group, and reduce this representation to its irreducibl components.
- Combine the basis orbitals into linear combinations correspondin to each of the irreducible representations. These SALCs ca always be constructed systematically by using the projectio operator technique.
- List the SALCs so that all those belonging to a given representatio occur together in the list. Use this list to label the rows and column of the secular determinant. Only the elements of the secula determinant that lie at the intersection of a row and a colum belonging to the same irreducible representation can be nonzero and these nonzero elements will lie in blocks along the principa diagonal. The secular determinant will therefore be block-factored.

So, here we have 10 basis functions here and then ultimately I should get 10 by 10 secular determinant and then correspondingly I get the secular equation as this. Now there are there is a three step procedure for setting up symmetry factored secular equation. So, this is like we have huge 10 by 10 determinants which is really kind of scale, so can we bring symmetry restrictions here and simplify my life.

So first what we do, we use a state of atomic orbitals as sate as a basis for a representation of the group and then we reduce this representation to which we reduce the components. In the next step, we combine the basis functions here orbitals in two linear combinations. That means, this we form the SALCs by utilizing the position operated and then we list all the SALCs so that all those belonging to a given representation occur together in the list.

So, we tabulate them and we will use this list to level the rows and columns of the secular determinant, only the elements of the secular determinant that lie at the intersection of a row and column belonging to the same irreducible representation can be non 0 and these non 0 element will be in blocks along the principal diagonal. So, pretty much similar way as we did when we learnt about how to diagnose the matrix by symmetry transformation, I am saying this analogically it is similar, so the secular determinant will therefore be symmetry factor.

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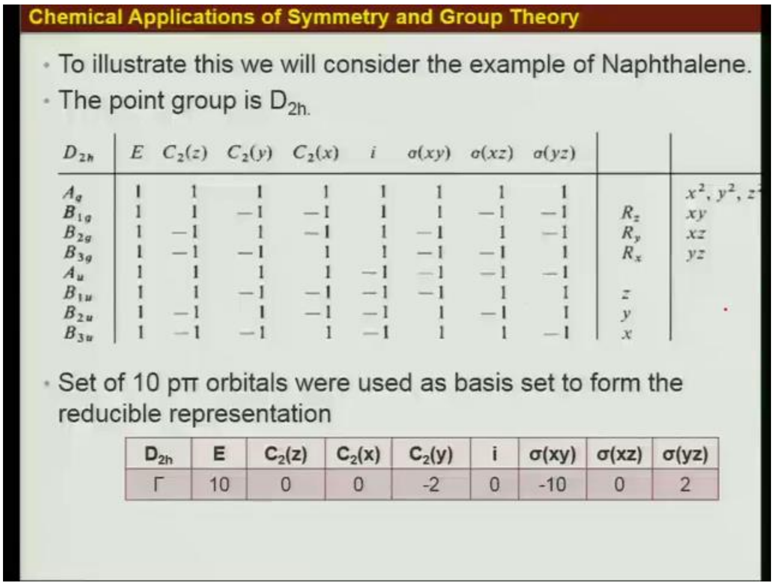

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- To illustrate this we will consider the example of Naphthalene.
- The point group is $D_{2h.}$

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	xz
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

- Set of 10 pπ orbitals were used as basis set to form the reducible representation

D_{2h}	E	$C_2(z)$	$C_2(x)$	$C_2(y)$	i	σ(xy)	σ(xz)	σ(yz)
Γ	10	0	0	-2	0	-10	0	2

So, let us take the example of this particular molecule naphthalene, so we said that we have 10 p pi orbitals as my basis. So, the point group of the naphthalene is d 2 each and here is the category for this particular point D 2h. Now using the concept of unset of atom, you should be able to form the representation. So, directly writing the characters we get the representation as gamma and this shown here, so we have the non 0 characters for identity for C 2 i for sigma xy and rest of the characters are 0.

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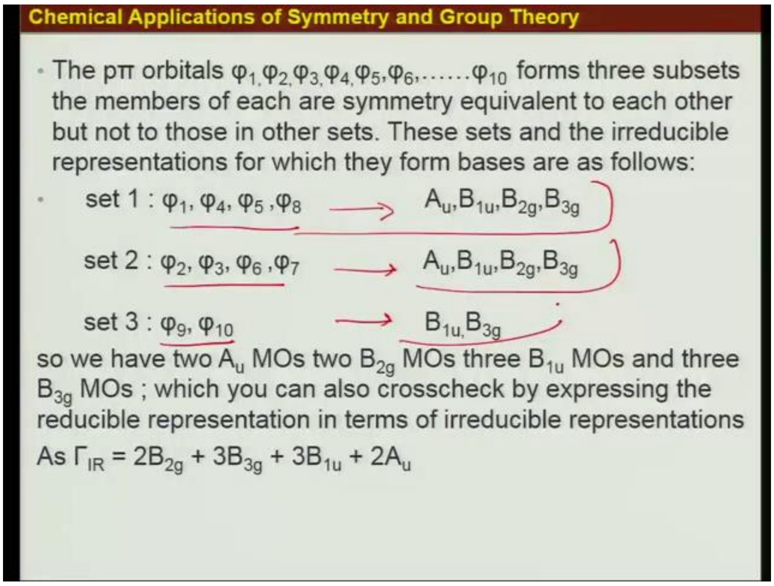

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- The pπ orbitals $\varphi_1, \varphi_2, \varphi_3, \varphi_4, \varphi_5, \varphi_6, \ldots\ldots \varphi_{10}$ forms three subsets the members of each are symmetry equivalent to each other but not to those in other sets. These sets and the irreducible representations for which they form bases are as follows:
- set 1 : $\varphi_1, \varphi_4, \varphi_5, \varphi_8 \rightarrow A_u, B_{1u}, B_{2g}, B_{3g}$

  set 2 : $\varphi_2, \varphi_3, \varphi_6, \varphi_7 \rightarrow A_u, B_{1u}, B_{2g}, B_{3g}$

  set 3 : $\varphi_9, \varphi_{10} \rightarrow B_{1u,} B_{3g}$

so we have two A_u MOs two B_{2g} MOs three B_{1u} MOs and three B_{3g} MOs ; which you can also crosscheck by expressing the reducible representation in terms of irreducible representations

As $\Gamma_{IR} = 2B_{2g} + 3B_{3g} + 3B_{1u} + 2A_u$

So, what we are supposed to do, we are supposed to reduce in the next step. So, now at the beginning we say that this p pi orbital corresponding to octane carbon atoms with naphthalene they are not all the equivalent, but they had they form some subsets which contains the equivalent the basis function c f.

So, we have essentially three different sets; in the first set we have the p pi orbital comprising function pi 1, pi 4, pi 5, pi 8 and we have another set having pi 2, pi 3, pi 6, pi 12 and the third set contains the pi 9 and pi 10. Now what you can do, you can either form the basis representation as we just said in terms of the gamma right here or what you can do, you can consider the individual sets just like the example that we gave in the previous class for p f 3.

So, if you do that if you take this basis functions as a basis set and then another set, another set then you form a representation and then reduce to get this irreducible representation. Now whatever way you do the results should be the same, so what you can do, you can form this way and all together you can find out how many irreducible represent which type of reducible representations occurring in how many times. You should get the same result if you take the reducible representation comprising the form by using the basis having a set having 10 p pi orbitals; you will get the same result.

So, what you have here; you have total 2 au orbitals, two orbitals with a symmetry three orbitals with 1u symmetry and 2 orbitals with B 2g and 3 orbitals with B 3g symmetry.

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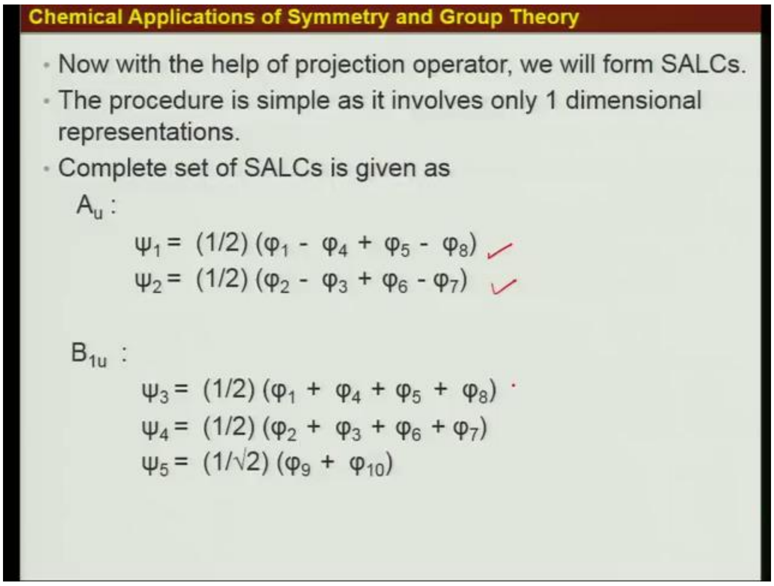

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- Now with the help of projection operator, we will form SALCs.
- The procedure is simple as it involves only 1 dimensional representations.
- Complete set of SALCs is given as

A_u :

$\psi_1 = (1/2)(\varphi_1 - \varphi_4 + \varphi_5 - \varphi_8)$ ✓

$\psi_2 = (1/2)(\varphi_2 - \varphi_3 + \varphi_6 - \varphi_7)$ ✓

B_{1u} :

$\psi_3 = (1/2)(\varphi_1 + \varphi_4 + \varphi_5 + \varphi_8)$

$\psi_4 = (1/2)(\varphi_2 + \varphi_3 + \varphi_6 + \varphi_7)$

$\psi_5 = (1/\sqrt{2})(\varphi_9 + \varphi_{10})$

So next is we have to find out the SALCs corresponding to each one of this irreducible representation. So, we have u or u 1u and B 2g and B 3g. So, we have learnt how to get those and all of these irreducible representation that we found by reducing this irreducible representations found out of those basis sets, three basis sets. Then we found the projection operators for those irreducible representations and find the SALCs that we can form and normalize them.

So, you get the SALCs using the same concepts that we have used earlier.

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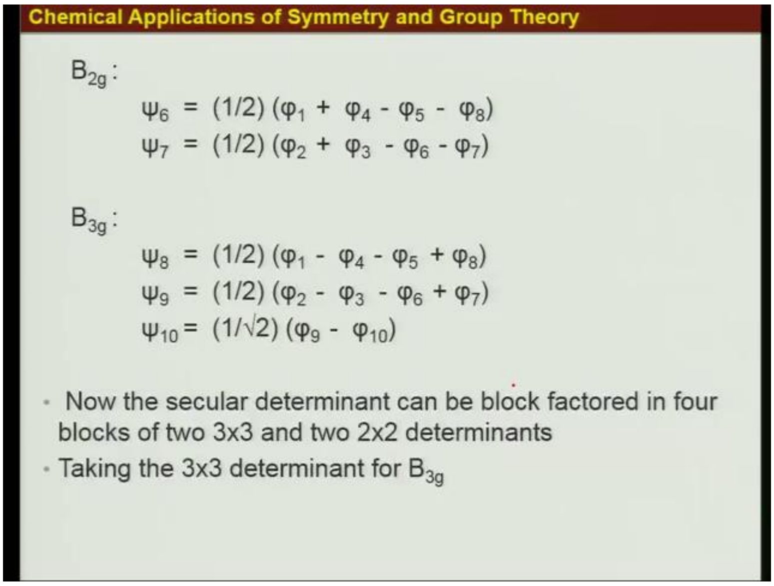

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B_{2g}:

$$\psi_6 = (1/2)(\varphi_1 + \varphi_4 - \varphi_5 - \varphi_8)$$
$$\psi_7 = (1/2)(\varphi_2 + \varphi_3 - \varphi_6 - \varphi_7)$$

B_{3g}:

$$\psi_8 = (1/2)(\varphi_1 - \varphi_4 - \varphi_5 + \varphi_8)$$
$$\psi_9 = (1/2)(\varphi_2 - \varphi_3 - \varphi_6 + \varphi_7)$$
$$\psi_{10} = (1/\sqrt{2})(\varphi_9 - \varphi_{10})$$

- Now the secular determinant can be block factored in four blocks of two 3x3 and two 2x2 determinants
- Taking the 3x3 determinant for B_{3g}

So, all together out of ten basis set, basis function you should get ten SALCs and we see that we get ten SALCs. So, SALCs that we got we are writing in terms of this psi, so psi 1 to psi 10 are our SALCs. Now we can get the secular determinant in terms of blocks and we get 2; 3 by 3 blocks and 2; 2 by 2 blocks. So, essentially we have 2; 3 by 3 determinant and 2; 2 by 2 determinant and let us start one by one.

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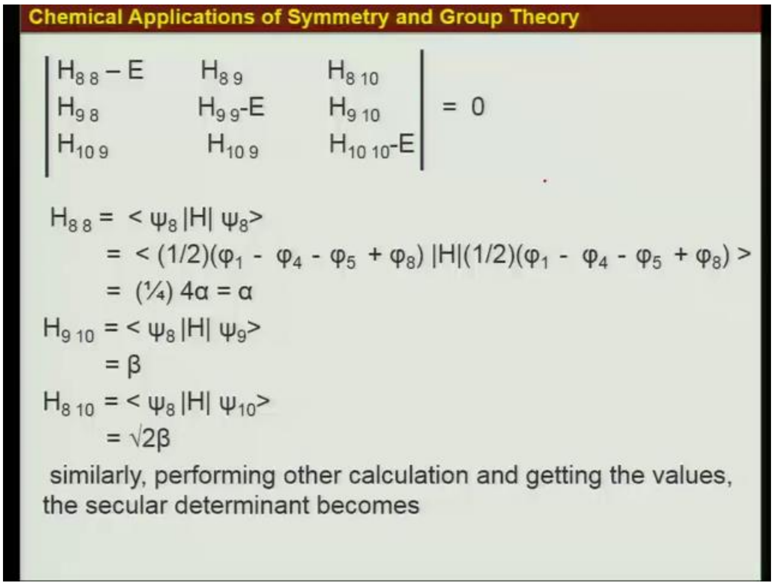

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$$\begin{vmatrix} H_{8\,8}-E & H_{8\,9} & H_{8\,10} \\ H_{9\,8} & H_{9\,9}-E & H_{9\,10} \\ H_{10\,9} & H_{10\,9} & H_{10\,10}-E \end{vmatrix} = 0$$

$$\begin{aligned} H_{8\,8} &= \langle \psi_8 | H | \psi_8 \rangle \\ &= \langle (1/2)(\varphi_1 - \varphi_4 - \varphi_5 + \varphi_8) | H | (1/2)(\varphi_1 - \varphi_4 - \varphi_5 + \varphi_8) \rangle \\ &= (1/4)\, 4\alpha = \alpha \\ H_{9\,10} &= \langle \psi_8 | H | \psi_9 \rangle \\ &= \beta \\ H_{8\,10} &= \langle \psi_8 | H | \psi_{10} \rangle \\ &= \sqrt{2}\beta \end{aligned}$$

similarly, performing other calculation and getting the values, the secular determinant becomes

So, B 3g had 3 by 3 determinant and we take that and solve the equation right, so when we write the secular determinant and then the secular equation for sebi 3; 3 and you try to solve that, you get it is all in terms of the notation that are used under Huckel approximation that is either alphas or betas. Now I mention that alpha is taking to be the energy 0, so what is the energy 0, so what is the energy 0 here, so in case of molecular orbital when we draw the molecular orbitals so as function energy. So, energy follows in a vertical relation and then we have different molecular orbitals form. So, now the energy of energy equals to 0 will lies somewhere where essentially you have the atomic orbitals having their energy. So, meaning that there is no interaction between these atomic orbitals at that particular energy at that particular energy, so two atoms are not at all forming a bond.

So, that energy level is taken as a 0, so an under Huckel approximation this alpha is taken to be at 0. So, and beta is the unit of energy, so beta will give me 1; so taking those terminologies and s 1, 2 ys 2 1 these are 0 under Huckel approximation, we get the results as 8, 8, 8 equals to alpha h 9 1 0.

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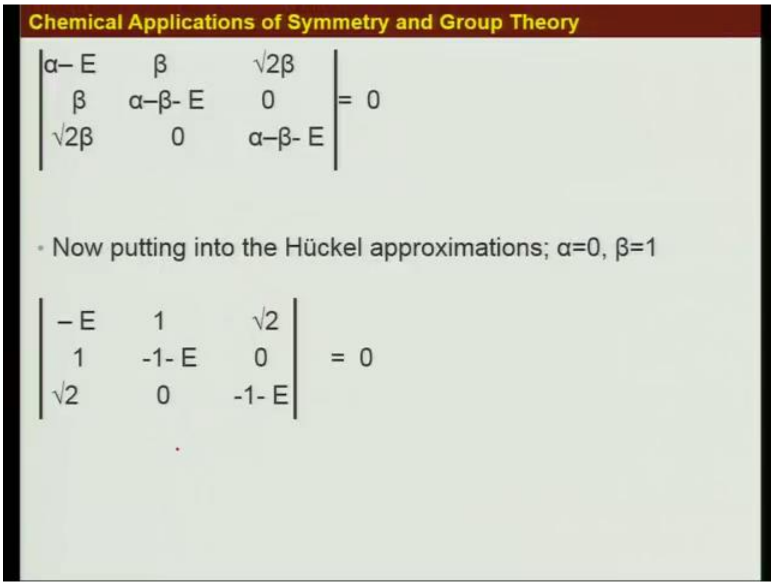

Chemical Applications of Symmetry and Group Theory

$$\begin{vmatrix} \alpha - E & \beta & \sqrt{2}\beta \\ \beta & \alpha - \beta - E & 0 \\ \sqrt{2}\beta & 0 & \alpha - \beta - E \end{vmatrix} = 0$$

- Now putting into the Hückel approximations; α=0, β=1

$$\begin{vmatrix} -E & 1 & \sqrt{2} \\ 1 & -1-E & 0 \\ \sqrt{2} & 0 & -1-E \end{vmatrix} = 0$$

So, 9, 10 is equals to beta and h 8, 10 has root to beta, so we can keep going and calculating all the other secular determinants for other irreducible representation and then put the conditions that is imposed by the Huckel approximation and you ultimately get the total energies.

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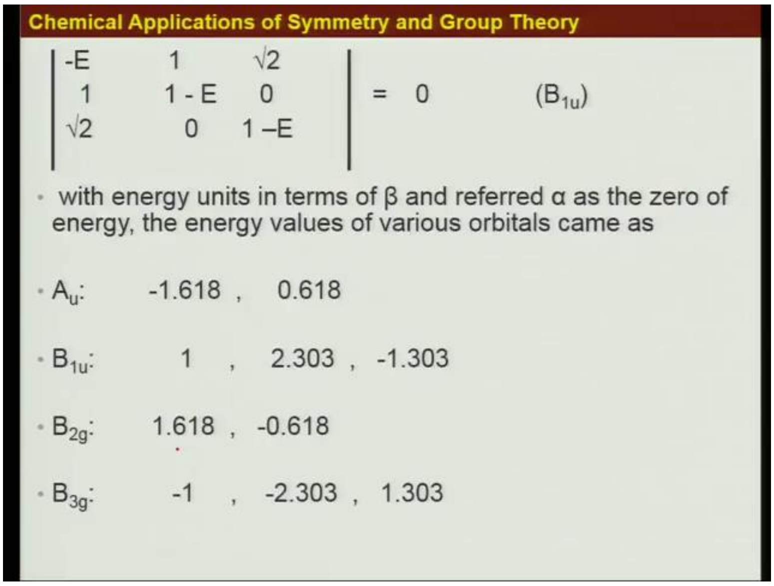

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$$\begin{vmatrix} -E & 1 & \sqrt{2} \\ 1 & 1-E & 0 \\ \sqrt{2} & 0 & 1-E \end{vmatrix} = 0 \qquad (B_{1u})$$

- with energy units in terms of β and referred α as the zero of energy, the energy values of various orbitals came as
- A_u: -1.618 , 0.618
- B_{1u}: 1 , 2.303 , -1.303
- B_{2g}: 1.618 , -0.618
- B_{3g}: -1 , -2.303 , 1.303

So, energies corresponding to which irreducible representation essentially meaning that for say a u, you have 2s ls meaning that two orbitals will be formed. So, when you solve for the determinants, if it is two dimensional you get two roots, if it three dimensional you get three. So, you get two or three different energies, so once you solve for all the determinants that you get, you get these energies and then you have to arrange these energies with energy scale.

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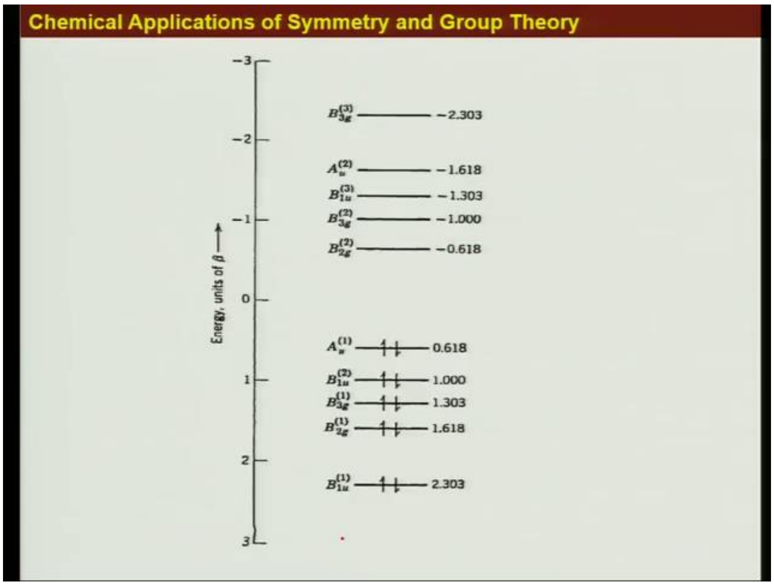

Chemical Applications of Symmetry and Group Theory

So here we have done that; that is after finding this energies corresponding to a particular orbital with a particular symmetry.

So, then we just add over this energies from lower to higher, so energy 0 is here in the unit of beta of course. So as you go higher you have this negative because beta itself is a negative where about there is interactions you get the energy has negative.

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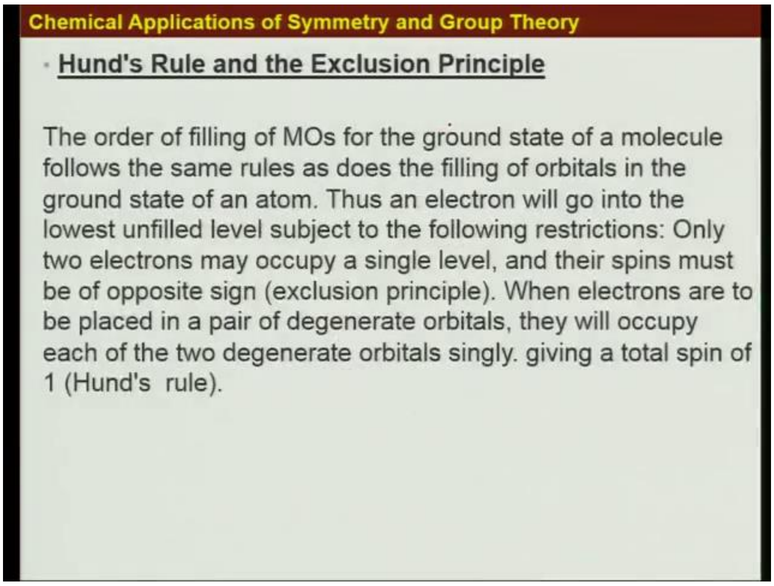

Chemical Applications of Symmetry and Group Theory

- **Hund's Rule and the Exclusion Principle**

The order of filling of MOs for the ground state of a molecule follows the same rules as does the filling of orbitals in the ground state of an atom. Thus an electron will go into the lowest unfilled level subject to the following restrictions: Only two electrons may occupy a single level, and their spins must be of opposite sign (exclusion principle). When electrons are to be placed in a pair of degenerate orbitals, they will occupy each of the two degenerate orbitals singly. giving a total spin of 1 (Hund's rule).

So, when you fill up the molecular orbital that you form, you follow the hound rule and the exclusion principle. So, when you follow the hound rule and exclusion principle, you should be able to fill up the all the electrons into the orbitals. With this we will stop today and we will come back tomorrow with some other applications of this symmetry and the group theory that we have learnt so far till then.

Thank you so much.