Introductory Quantum Chemistry
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Lecture - 49
Huckel MO Theory Continued

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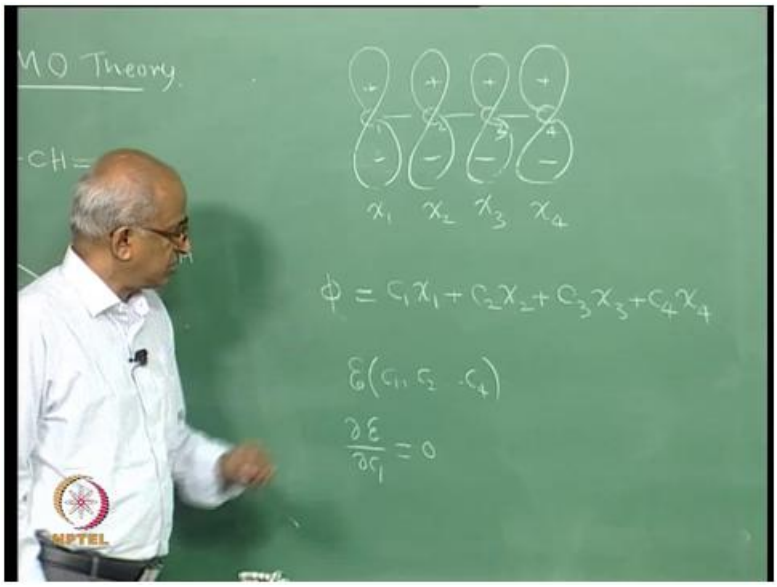

So, we were discussing the Huckel molecular of hell theory for quantitated systems. We took butadiene as an example; which is shown in this picture or in this picture. This is a better representation; each one of the carbons in the molecule has an un hybridizes p orbital standing perpendicular to the molecule. And, that is what is shown here they are called chi 1, chi 2, chi 3, chi 4. And, then we say molecular orbitals may be formed by the combination of these atomic orbitals and the molecular orbitals have this form. And, using this form it is possible to calculate the expression for script e, naturally it will depend upon c 1, c 2, c 3, etcetera.

And, then you say I will minimize energy with respect each one of them, each one of c 1, c 2, c 3, etcetera. You will get 4 equations; those 4 equations can be written or rewritten after making several approximations; they may be written in this form. And, in if you look at this matrix equation. What you find is at there is a x always along the diagonal. And, now were else x is there; what is x? x is actually alpha minus script e divided by beta. And, script e is the thing that you want to determine. And, further you also notice that the matrix is nice. For example, there is a 1 here; what does that 1 represent? It

essentially arises because your carbon atom 1 and 2 are interacting. I should not say carbon atoms. But atomic orbitals on the carbon atoms 1 and 2 are interacting.

So, because c 1 and c 2 are neighbors, you have this 1 here. So, you have a 0 there why because; carbon atoms 1 and 3 are not neighbors. So, the prescription is actually very simple; if you wanted to write the matrix which is usually referred as the Huckel matrix for any system. All that you need to do is you fill up with x along the diagonals. And, you put a 1 if atoms are nearest neighbours. If they are not nearest neighbour's right, then the matrix element is going to be 0. So, with this understanding; let me look at few simple systems and illustrate the application of the method. So, the simplest system of course, is ethane. So, in the case of ethane, what happens is you have 2 carbon atoms only.

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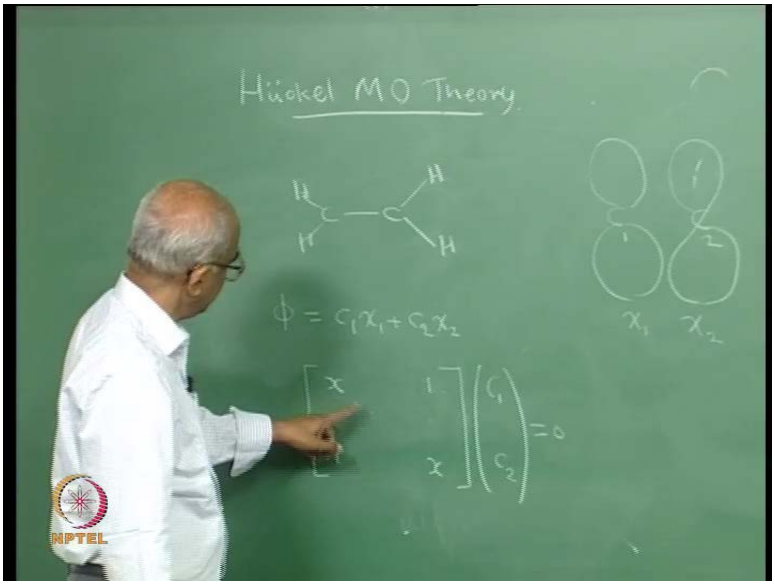

So, the structure of the molecule is actually this. This shows only this sigma bonds, the bonds found by the hybrid of orbitals. And, then the of course, there are p orbitals perpendicular to the plane of the board on both the carbon atoms. And, so I will draw a picture showing just the carbon atoms and these p orbitals. So, this is the first p orbital and this is second. Let me call this chi 1 call this chi 2. So, the trail function that we will use is Phi is equal to c 1 chi 1 plus c 2 chi 2. Now, we can just write the Huckel matrix; what will be the Huckel matrix? It is going to be 2 by 2 matrix.

You remember the prescription you have to put x along the diagonal, we will have a 2 by 2 matrix with x and x there. And, the entry here is going to be concerned with carbon atoms 1 and 2, this is 1 that is 2. So, 1 and 2 are neighbors. So, you are going to get a 1 here you are going to get a 1 here because 1 and 2; 2 and 1 are neighbours. And, this multiplying c 1 c 2 must be equal to 0. And, in out of that c 1 and c 2 should be non 0 what should happen is that the determinant of this matrix must be equal to 0. So, what is the determinant of the matrix; you can easily expand the matrix sorry, if you easily expand the determinant.

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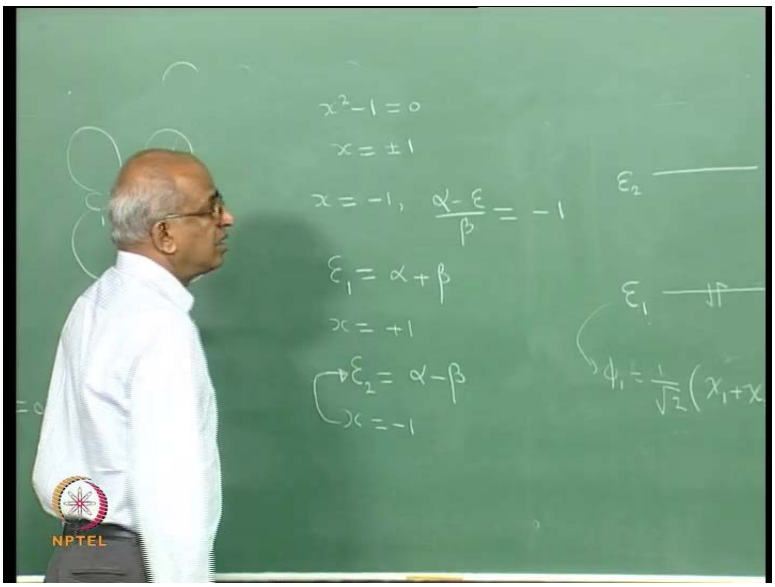

And, what are you going to get? You are going to get x square minus 1 is equal to 0. And, this means; x may be equal to plus 1 or minus 1 right, and if x is minus 1; what is that mean? It means that you see how a definition of x is here, alpha minus script e by beta. So, alpha minus script e by beta is actually minus 1. So, if you rearrange what will you get? You will get script e to be alpha plus beta right; I will call this script e 1 because; I have the other possibility where, x is equal to plus 1. In that case; you will get another value for script e which will be alpha minus beta right.

So, you have found 2 allowed energy levels; these are energies of 2 molecular orbitals. I can represent them in a picture well; the question is which one is lower? The answer is that this lower; the reason is that alpha and beta are both negative right, if we calculate alpha and beta if you can calculate it you will find that both are negative. And, therefore

alpha plus beta is the lower energy and alpha minus beta higher energy. So, this is my epsilon script e 1 and this is my script e 2. And, in the case ethylene see the each carbon actually, a carbon atom would have a 4 valiant electrons, but; these 3 of the electrons of the carbon atom are use to form 3 sigma bond so one for this bond, one for that and third for that.

That leaves one electron sitting in the p orbital. So, right each carbon has this U N hybridizes p orbitals right, which carbon has this p orbital. And, it also the carbon also contributes one electron to the phi system. So, therefore; the number of phi electrons that have to consider in the case of ethylene or ethane is actually 2. And, so what will happen if you have 2 molecular orbitals these 2 electrons will sitting this lowest, what I expect is bonding molecular orbit fine. And, then the next thing that I will do is; I will calculate the molecular orbitals, how will calculate that when x is minus 1 right, I am going to put x is equal to put minus 1 into this equation.

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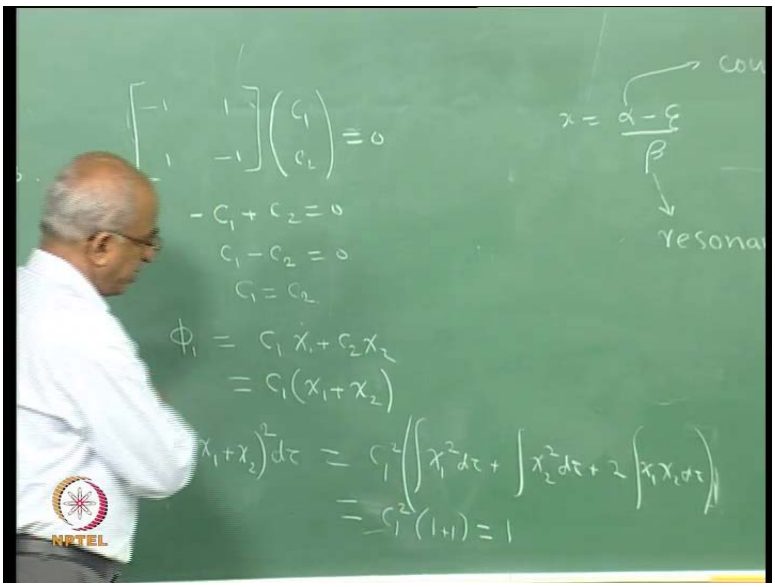

So, if you put x is equal to minus 1 what will you get? The matrix equation will look like this. And, if you multiplied what are you going to get? You find minus c 1 plus c 2 is equal to 0. And, the second equation that you get is not deferent, you will find that that says c 1 minus c 2 is equal to 0 both the equations are the same. So, essentially when though have matrix equations essentially, I have only one equation. And, what is this mean? This makes at c 1 is equal to c 2. And, therefore; what is my expression for the

corresponding molecular orbital right, Phi. Phi would be actually c 1 chi 1 plus c 2 chi 2, but c 2 is equal to c 1. So, therefore; I can write this as c 1 into chi 1 plus chi 2. So, this is my first molecular orbital. And, therefore what I will do is; I will put subscript here to indicate that this is the first molecular orbital.

And, then I have to determine c 1, how will you determine c 1; answer is very simple, I have to ensure that the orbital is normalized so; that means, I just take the square of it, squaring is enough. It is not necessary to multiplied by it is own complex conjugate because; complex conjugate is the function itself. So, d tau it should be equal to 1 right. So, now suppose I expand this what is going to happen; I will get chi 1 square d tau plus integral chi 2 square d tau plus 2 chi 1 chi 2 d tau integrated the whole thing must be equal to 1; this all thing should be equal to 1. But then chi 1 is normalize chi 2 is normalized; chi 1 into chi 2 integrated over the entire space is actually the overlap integral, but remember in Huckel theory you neglect the overlap integral. You say that it is equal to 0.

So, to be consisting with that this is to going to be taken to be 0. So, we are going to get c 1 square into 1 plus 1 equal to 1 which is a normalization condition. Implies that c 1 must be equal to how much? c 1 must be equal to 1 by root 2. So, therefore this orbital phi 1 is actually, 1 by root2 times chi 1 plus chi 2. On the other hand; if you had put x is equal to minus 1, you are going to get this as the energy. And, if you substituted sorry, we have just now done the case where x is equal to minus1. So, let me put x is equal to plus 1. So, if we put x is equal to plus 1 the same kind of analysis can be carried out it is pretty straight forward. What will happen is that you will get 1, 1, 1, 1 that is the value of the matrix. And, so this into c 1 c 2 must be equal to 0 which imply is that c 1 must be equal to minus c 2 right.

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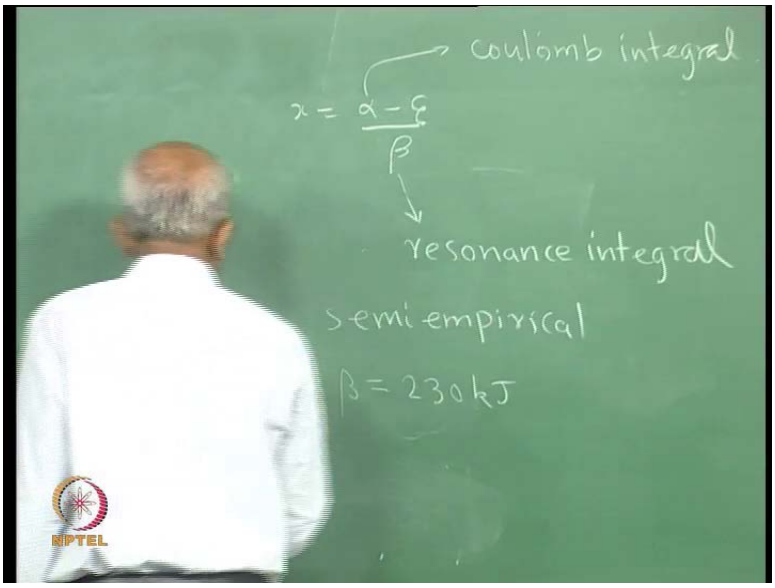

And, then you can go ahead and find the orbital without any difficulty you will find that that orbital is phi 2 equal to 1 by root 2 chi 1 minus chi 2 right. So, as expected actually this is a bonding molecular Orbital of will that is an anti molecular orbital. So, how will I represent these orbitals pictorially; well, these are the p orbitals remember this lob is plus, that also is plus, this is minus, that is minus. So, if we added that 2 up; you are going to get orbital. How it will look like, it will look like roughly; it will look like this. These are the 2 atoms correct, that 2 lobs are equivalent.

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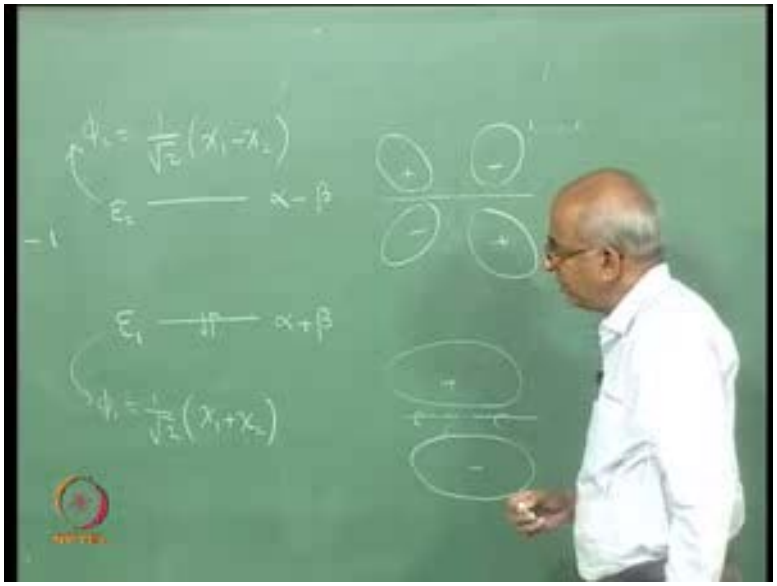

And, you should also remember that this orbital has a nodal plane, this is the nodal plane. Then to get the other orbital what you should do is you have to multiply the second 1 with a minus 1. So, therefore; this lob will become negative and that will become plus and then we just add, you will get the second orbital. And, obviously; the second orbital would look like this. And, in addition to the node that the p orbitals have this particular orbital has a nodal plane which is perpendicular to the plane of the molecules something like that. And, further if you like; you can say in the case of ethane there are 2 electrons sitting in this molecular orbital, so therefore the total phi electron energy of ethane which we will denote as E chi.

E chi appropriate for ethane; how much will it be you will have 2 times alpha plus beta as the energy. Now, this you may make you unhappy; the reason is that I have just added you see alpha plus beta is the energy of 1 electron. So, you multiply that by 2 I am saying that you will get the pi electron energy; you may ask what about electron repulsions? Because we know that electrons actually ripple each other we should be worrying about that. But you see Huckel theory is very approximate, very crowd and it simply neglects electron repulsions. Now, further what it does is; they approximate so many approximations have been made, that it is practically impossible to calculate any of these things using regress quantum mechanics.

So, what is done is this alpha and beta are taken to be parameters which are to be determined from experiment. And, you adjust their values in such a fashion that there is best agreement with experimental values. And, because of this is actually known as semi empirical theory and in most applications that one makes the value alpha itself is not needed. Because you see mostly what will happen is that you will calculate the energy differences and compare with experiments. So, if we calculate and differentiate between this and that then you will find that that does not involve alpha.

Let the difference actually is minus 2 beta right. And, suppose you can spectroscopically measure the frequency of the radiation which will bring about this transition then you can estimate the value of beta. And, there are other ways of estimating the value of beta, but; again this is a little bit problematic because depending upon the method that used the values of beta that you get are somewhat different. And, we will assume the value of beta to be 230 kilo joules per mole. So, now suppose I think of the next system when I would like to think of a system which contains 3 carbon atoms.

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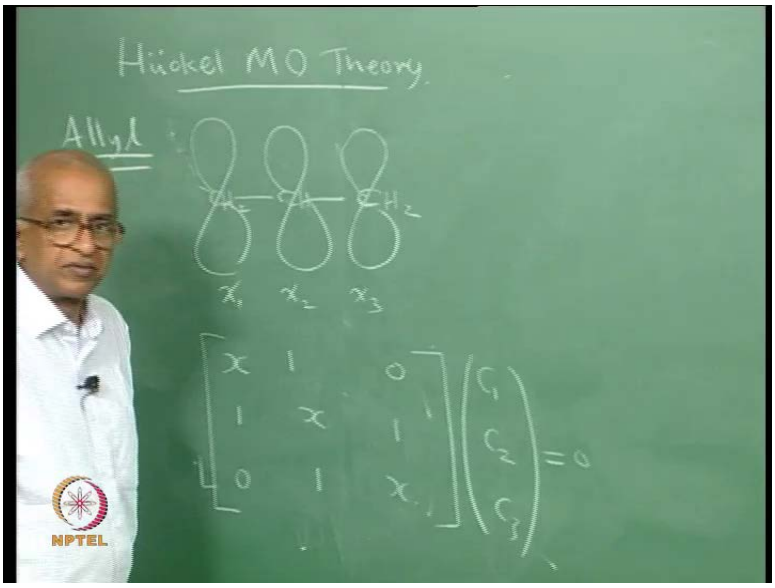

So, I will say that I have 3 carbon atoms; the system will be Allyl. For example, it could be Allyl radical or it could be Allyl cat ion or Allyl anion. So, you will have C H 2 here C H and C H 2. And, you will have 3 U N hybridize p Orbitals; you can call them Chi 1, chi 2, chi 3. And, what will be the Huckel matrix? Naturally, the Huckel matrix will be a 3by 3 matrix. How will you write it down, the diagonal elements are all equal to x, you will have a 1 here, because; atoms 1 and 2 neighbors. You will have a 0 here, because; atoms 1 and 3 are not neighbors here. Again, you will have a 1 because 2 and 1 are neighbour's. Then here you will have a 0 because they are not neighbour's then this is 1 and that also is 1. So, this is the structure of the Huckel matrix c 1 c 2 c 3 must be equal to 0.

And, then what will say? You will say that the determinant of this matrix must be equal to 0. The determinant of this matrix must be equal to 0. Now, this matrix is easy to expand and you will find that the answer is x cube minus 2 x is equal to 0. If expanded that the matrix sorry, if you expanded the determinant you will find that it is x cube minus 2 x, which may written as x into x square minus 2 is equal to 0. This implies that I have 3 possible values of x. x being minus root 2 is one possibility; the next possibility is x is equal to 0. And, while let me put x is equal to plus root 2 first then x being equal to minus root. So, then I will have to say that alpha minus script e by beta is minus root 2 which you can easily find.

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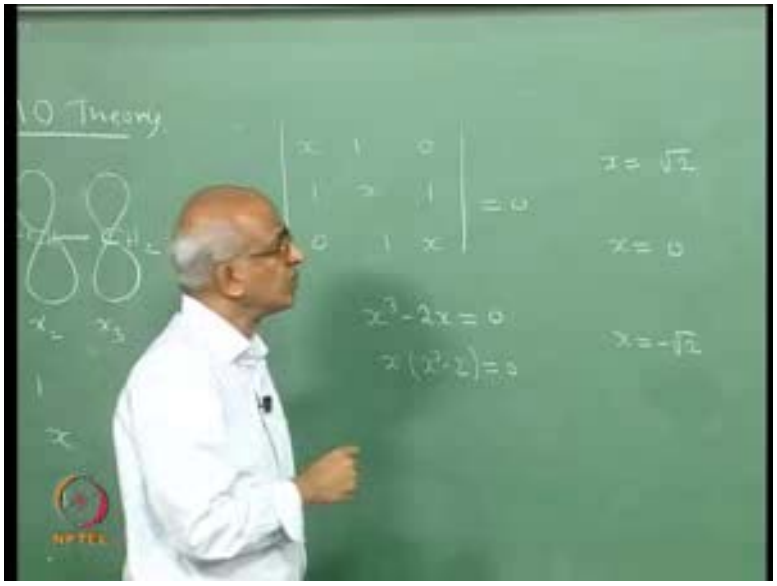

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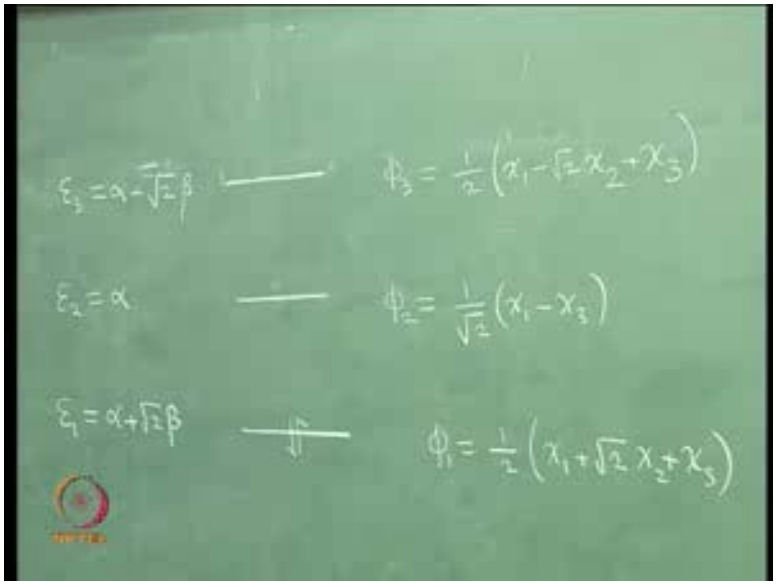

The solution you will find that the corresponding energy is script e 1 which is alpha plus root 2 beta. Right, you just put this minus root 2 in here and then rearrange and you will find that script e must be equal to so much. If x is equal to 0; you will find that the energy level is actually epsilon script e 2 which is equal to alpha. And, if x is equal to root 2 you will find the next energy level script e 3 which is alpha plus. Sorry, alpha minus root 2 beta. So, you will find that these are the 3 allowed the energy levels of the system. So, you can represent them in a picture. So, these are the 3 allowed energy levels. And, then you ask the question, how many electrons are there in the system? If it

is Allyl radical there are 3 electrons, because each carbon will contribute 1 electron to the phi system.

Allyl cat ion means; you have only 2electrons. So, if I thinking of Allyl cat ion what I will do is I will put electrons here. And, they will paired while if I had Allyl radical the third electron will go there and if I had Allyl anion there will be 1 more electron. So, let me say I am thinking of Allyl cat ion this is the structure or this is how the electrons are distributed. And, then you will ask what about the corresponding expressions for molecular orbital's that will take a little bit of time, because; what I will have to do is I will have to put x is equal to minus root 2; right. I will have to put x is equal to minus root 2 then solve for c 1, c 2, c 3 find c 1, c 2, c 3 then normalize the orbital. And, similarly; you can do with x is equal to 0 as well as x is equal to plus root 2.

So, let me just write the expression; you will get the first molecular orbital that you will find actually is 1 by 2 chi 1 plus root 2 chi 2 plus chi 3. This is the first molecular orbital that you will find. Then the second molecular orbital that you will find is psi 2 which is actually 1by root 2 times. And, third ho sorry, I made a mistake. So, these are the 3 molecular orbitals of the system; they are not difficult to find, it needs a little bit of time to the analysis. So, I do not go into the details of the analysis, but this is what happens. And, then how will you represent these molecular orbitals.

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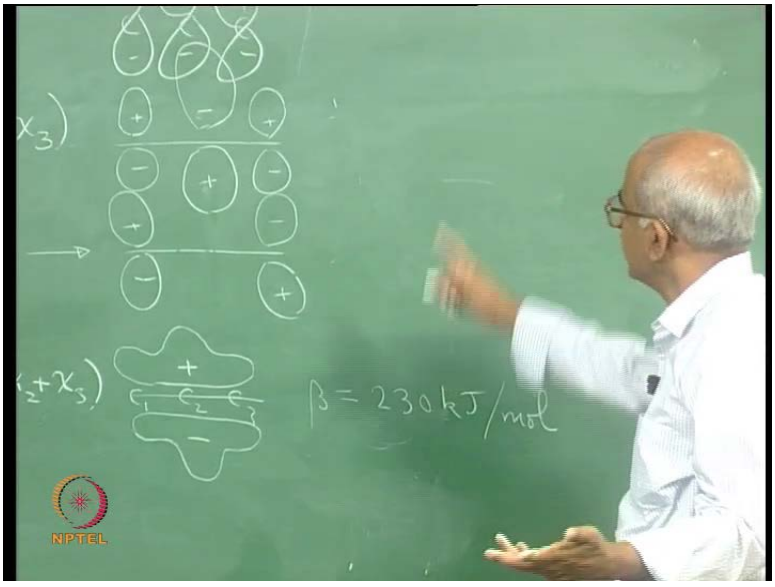

While, you have 3 carbon atoms 1, 2, 3 you have p orbitals on each one of them. And, if you are concerned with the first molecular orbital; you can see that they are simply being added up. But you also notice that the second orbital has a lot of impotence, because; it is co efficient is square root of 2 while, the coefficient of the other are just unity. Therefore, this is more important, this orbital is more important. And, therefore; what will the molecular orbital will have more value, it near that atom, near that the second carbon atom. So, if I want to represent it in a figure; these are the 3 carbon atoms c 1, c 2, c 3 the way to represent this orbital will be something like this. Notice that I have put more the size for the second carbon atom right, this assistantly because; the coefficient is root 2 there, from that carbon atom.

Now, if you looked at the second one; you find again something very surprising, why because; there is no contribution from the second carbon. So, how will you represent this while Chi 3 occurring with the negative sign so naturally this plus, but; that is minus. But Chi 3 locates with the negative sign. So, you have minus and plus; obviously, there is a node here, the lowest one you see it has only one node which is the plane of the molecule. This has 2 nodes; one is the plane of the molecule and other is plane like that. And, there is no contribution from the second carbon atom and it is you see you have to separate atomic orbitals this actually resembles 2 separate atomic orbital's. And, you would expect that there is actually no stability for the system cost by the formation of this molecular orbital, because you see if there was a contribution from the second carbon atom. Then you would put off throughout that may that is the system getting more stable or less stable, but; that does not happen.

And, that is the reason why the energy of this orbital is just alpha. What is alpha? Alpha is the energy; remember alpha was our H 1 1. For example; that is just energy of an atomic orbital right. So, there is no interaction essentially between these 2 lobes. And, therefore; the energy is unaffected; the energy is just equal to alpha. While, here of course, there are interactions there are attractive or stabilizing interactions and that is why the orbital has a low energy. Now, if you look at this orbital; you will conclude that this is not a stabilized orbital. In fact, this is a bonding, this one is anti bonding and the middle one you referred it as a known bonding. This is not actually, involved in any bond formation.

And, now if I do the third one; how will you represent it? Well, there is in the contribution of the second atom is more, but; it locates with a negative sign. So, therefore; how will you represent it? Well, this is plus that is minus this is also is plus here is minus, but; the middle one. You have to multiplied by a minus root 2. And, therefore; that is how it would appear this value of beta, let me keep it somewhere else. So, this is the Allyl system.

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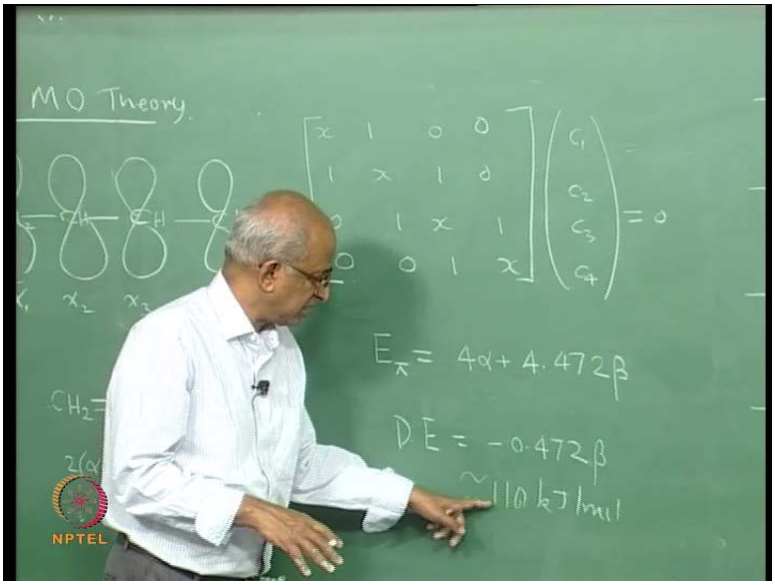

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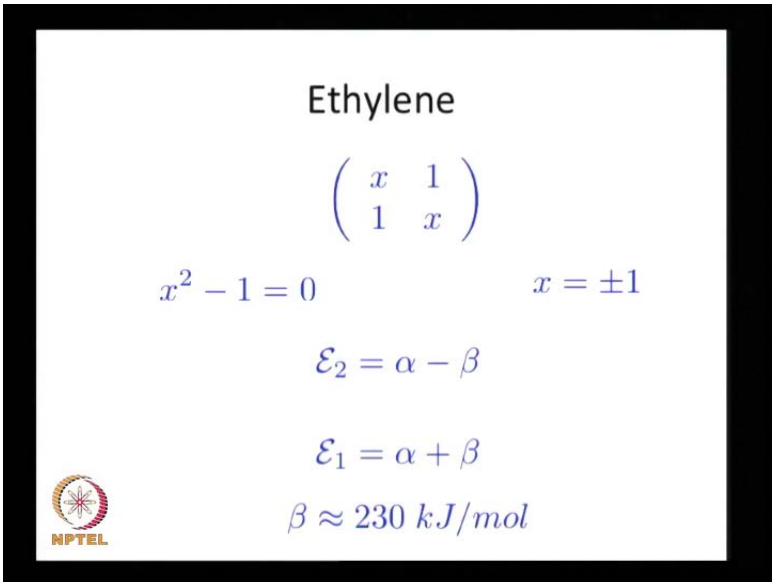

Now, another interesting system is butadiene; all that happens is you have one more carbon. And, so the Huckel matrix I will just continue here would have the form. This will be the Huckel matrix this into c 1, c 2, c 3, c 4 is equal to 0. And, then you have to expand the determinant evaluate the determinant when I will just show you my power point presentation on this on the things that I have been saying. Well, this has lots of information this power point presentation.

First is ethylene; we have already discussed it that is the Huckel matrix, x square minus 1 is equal to 0 is the determinant being put equal to 0. Then x is equal to plus or minus 1. This means that you will get epsilon 1 which is equal to alpha plus beta. Then you will also get epsilon 2 which is alpha minus beta. And, as I told you beta is approximately 230 kilo joules per mole.

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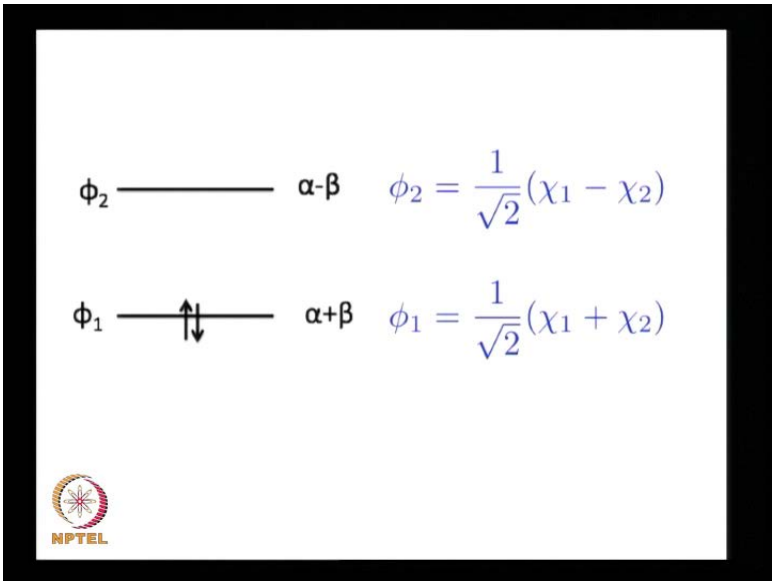

These are the molecular orbital's phi 1 and phi 2 and the expressions for them are also here psi 1 given by that while, phi 2 given by that expression, we have already done this.

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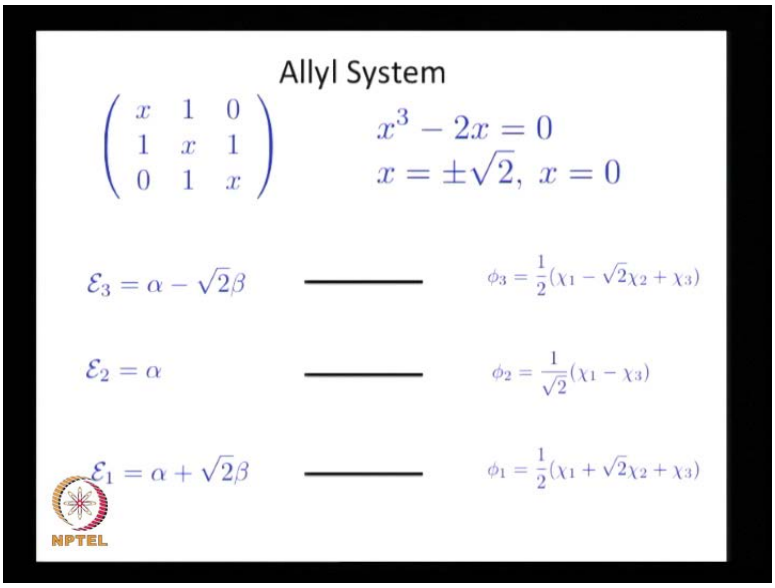

Then, Allyl system again, that is the Huckel matrix; if you put the determinant is equal to 0 you will get the solutions which are shown here. You have 3 solutions and corresponding to that you have 3 energy levels. First energy level and the corresponding molecular orbital or shown here, second energy level and the corresponding molecular orbital, third energy level and the corresponding molecular orbital we have again discussed all these.

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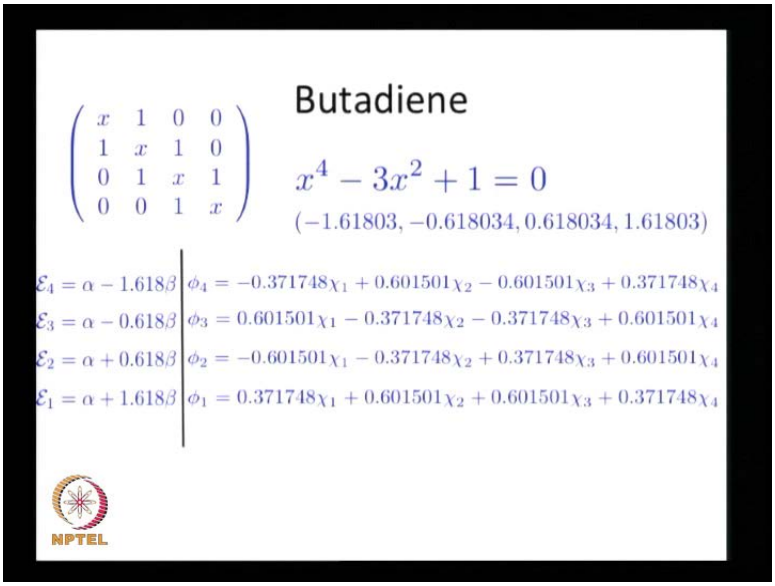

Then, if you think of butadiene this is the Huckel matrix. Expand the Huckel matrix you will get this equation x to the power of 4 minus 3 square plus 1 is equal to 0. You can solve for the values of x. You will find that these are the vales of x. Let minus 1.618, minus 0.618, plus 0.618, and 1.618. So, these actually will give you for energy levels which may be denoted as epsilon 1 epsilon 2 epsilon 3 and epsilon 4. What are their values? They are actually, alpha plus 1.618 beta, alpha plus 0.618 beta, alpha minus 0.618 beta and alpha minus 1.618 beta. And, the corresponding molecular orbital's; you can calculate you will find that these are the corresponding molecular orbitals.

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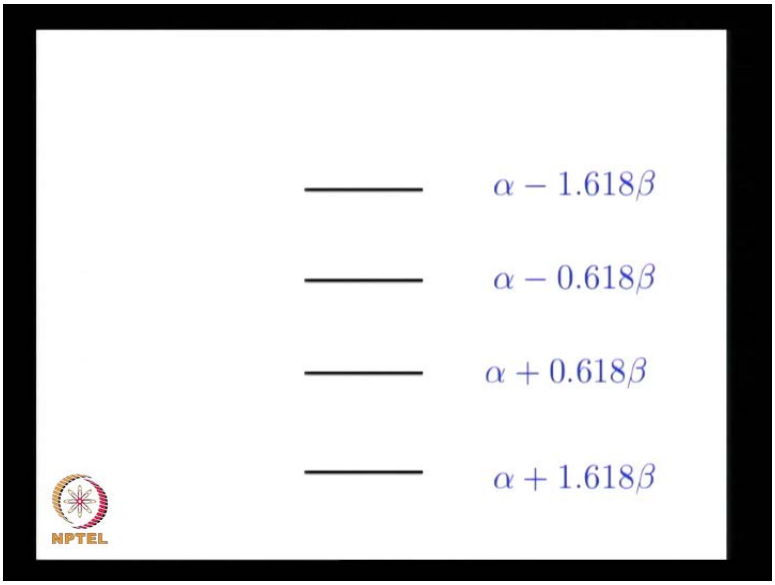

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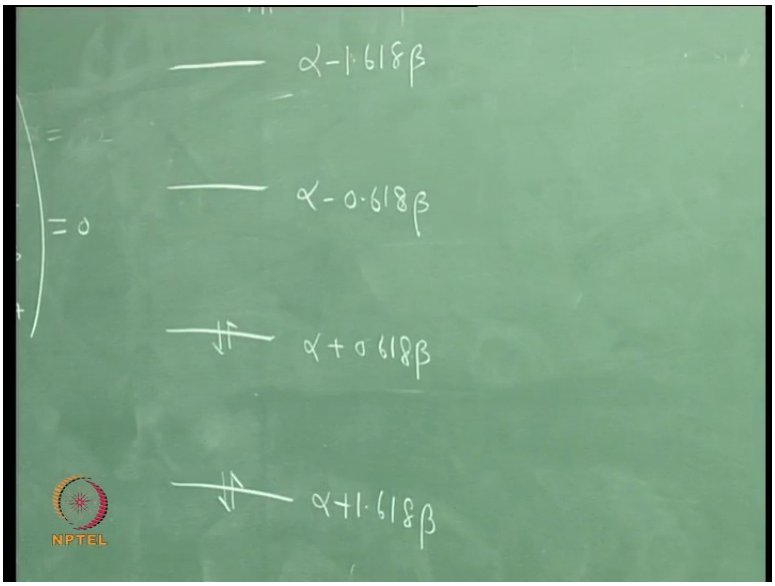

We will look at the molecular orbitals in a second, but; before we do that, let us look at the energy levels of the system; these are the 4 allowed energy levels. And, in the case of butadiene that 4 energy levels are shown here.

These are the energies of the molecular orbitals. Butadiene has how many phi electrons? Well, each carbon contributes 1 phi electron to the system. So, therefore it has 4 phi electrons. What will they do? They will go and sit in these bonding molecular orbitals. Correct, this orbital has energy of alpha plus 1.618 beta, this has an energy of alpha plus 0.618 beta. The other orbitals are not occupied, but they have energy is which are given by this expressions. So, if this 2 orbital's occupied what will be the phi electron energy of butadiene? Well, you will have to multiply this by 2, this also by 2 and then add them up, if you did that addition you will find that the answer is 4 alpha plus, how much? Well, maybe I should do the addition 0.618 and 4. So, it will work out be 4.472 beta. So, this we says the phi electron energy of butadiene.

Now, I shall assume that you know little bit of organic chemistry. So, this is one of the way is of writing the structure of butadiene suppose, I have written a structure like this. So, if you say that this is the structure of butadiene, a chemical structure written this way actually, means that there is an ethane like double bond here and an ethane like double bond there. Now, if had an ethane like bond here, and if you used Huckel theory this is in like bond would have a phi electron energy of alpha plus beta into 2 right. And, this is the like bond also would have energy of alpha, 2 times alpha plus beta.

And, therefore; if you have 2 separate ethane like bonds; how much will be the total energy of the system? It would have been 4 alpha plus 4 beta, but; in the case of butadiene the phi electron energy is not this. The actual phi electron energy is how much why this is happening? The reason is actually simple; if you had 2 separate ethane like systems which were not interacting then that would have been the energy. But what you actually have is not to separate ethane like entities, but; you have molecular orbital's this molecular orbital's are actually delocalized over the entire system, we will look at the shapes of the molecular orbital's in a few seconds. You will see that the molecular orbitals are d localized. And, therefore; what is happen you see this is the energy if they were localized right the bonds where localize between these atoms and those atoms.

But because the molecular orbitals are delocalized what is happened the energy has changed from here to there. Now, which one of these 2 energies is lower? The answer is that this is lower, because; beta is negative. So, this change we say is because of delocalization and people usually denote it by the symbol D E, just write a notation for delocalization, how much is the delocalization energy? It is this energy minus that energy. So, it is actually minus 0.472 beta. And, I realize that I had a slight mistake here beta should have been, I mean strictly speak this is just the magnitude of beta actual value would be minus 230 ok.

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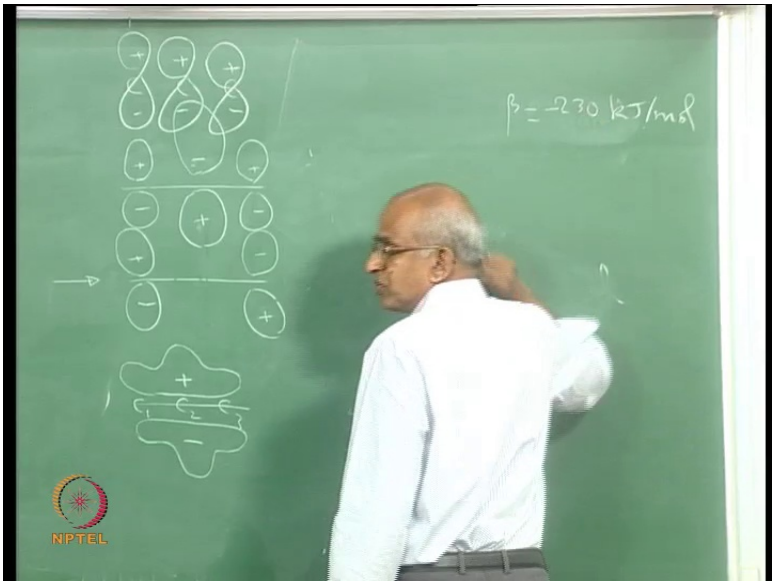

So, therefore you can use that and estimate the delocalization energy of butadiene, you are find that will be approximately 110 kilo joules per mole. So, this is the reason why organic chemistry that delocalization actually lowest the energy of the system. There is also another way of thinking about it which is in times of resonance, but we will not go into the details of that. We will just stick to the molecular orbital theory and according to molecular orbital theory there is a lowering of energy, because; of delocalization energy. And, the roughly speaking in the case of butadiene this is the amount of energy.

Now, we will discuss the most important system; that is of interest to the chemist that which is actually benzene. So, how will benzene be? Well, before I go into benzene I did promise that I shall take about the molecular orbitals of butadiene. So, let me just look at the molecular orbitals. The expressions are shown there, because; I would like to finish

this topic today. I shall not write these those expressions on the board, but; I will just draw the molecular orbitals.

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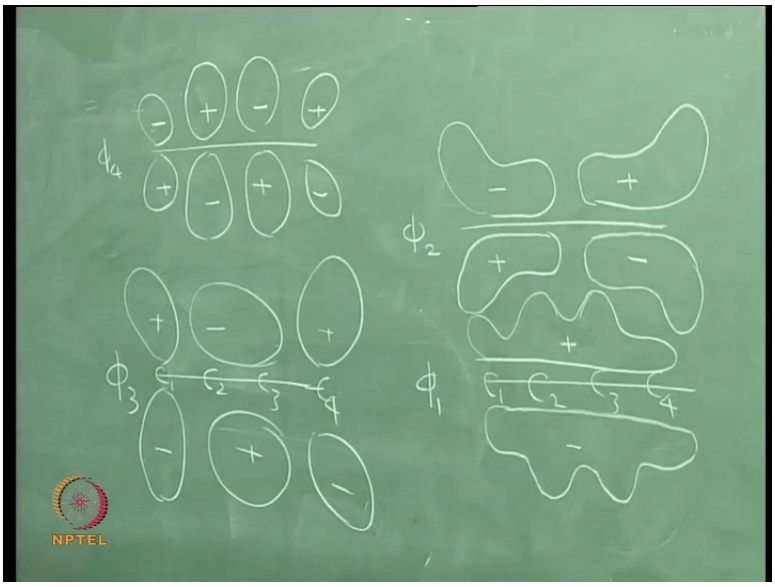

The molecular orbital phi 1; for example, if you look at this you see this is carbon 1, carbon 2, carbon 3 and carbon 4. And, if you look that the expression, you will find that all the orbitals are occurring with positive sign, not only that the middle 2 atomic orbitals have a larger weight age. So, how will you draw this? Answer is actually quite simple. So, this is the way this will be plus and that is minus, this is phi 1. In a simpler fashion you can look at the coefficients and make plots of the other molecular orbitals. Let me just draw them. So, that is phi 2 then phi 3. So, this is phi 3 I mean this you can draw by just looking at coefficients and then making appropriate analysis and finally, phi 4. So, that is phi 4 I mean these things can be easily do not by just looking at the expressions for the molecular orbital's in times of the atomic orbitals.

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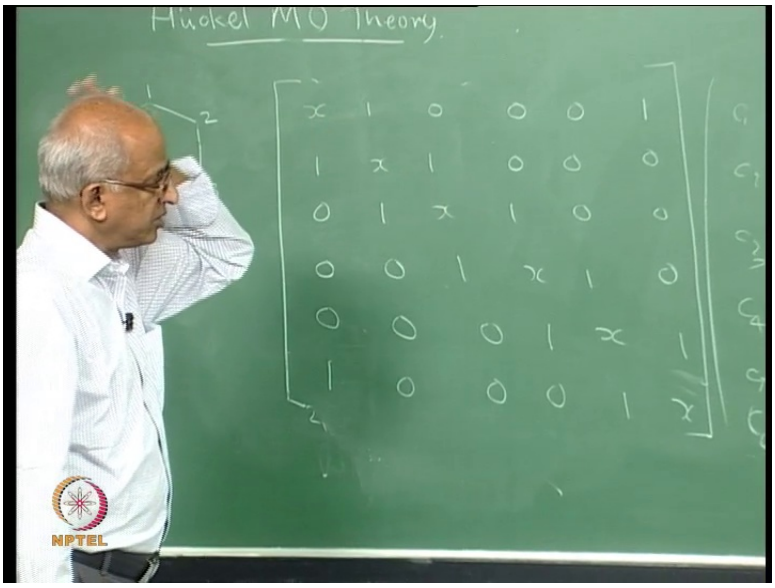

So, having seen that we will discuss benzene; so in the case of benzene you will say, let me number the carbon atoms. Let me say this is carbon atom 1, 2, 3, 4, 5, 6. So, naturally the Huckel matrix will be a 6 by 6 matrix. So, you will have x here, you will have 1 because; 1 and 2 are neighbour's right. So, we will have 1 then 1 and 3 are not neighbour's so you will have 0. 1 and 4 are not neighbour's so that means; another 0. 1 and 5 again not neighbour's, but; you think of 1 and 6 they are neighbour's. And, therefore; you are going to get a 1 here. Then you can continue like this you will get 1 x 1 0 0 0, 0 1 x 1 0 0, 0 0 1 x 1 0 and 0 0 0 1 x 1 and finally, 1 0 0 0 1 x this is the Huckel matrix fine.

And, you of course, you will say that this multiplying c 1 c 2 c 3 c 4 c 5 c 6 is 0. And, then you will have to put the determinant of the matrix equal to 0. So, if you did that you will get an equation. This is the Huckel matrix; that is the Huckel matrix you expand the determinant of the matrix put it equal to 0. Then you will find that this equation it looks complex, but; it can be determine this simple factored form. And, what is this mean? This means that you have different solutions. What are the solutions x is equal to minus 2 is a possible solution, x is equal to minus 2 is a solution, x is equal to minus 2 implies energy is alpha plus 2 beta. And, the way this equation is you will find that x is equal to 1 occurs 2 times. Because it is occurring with x minus 1 is occurring with a square. So, x is equal to 1 occurs 2 times that actually means orbital is doubly degenerates.

When x is equal to minus 1 occurs 2 times, x is equal to minus 2 occurs only once. So, this is actually having an energy of alpha plus beta that has energy of alpha minus beta and this one has energy of alpha minus 2 beta. And, in the ground state of benzene; how many electrons are there, how many pi electrons are there? The answer is 6. So, you will have to put 2 electrons here, 2electrons there, and 2 electrons there. So, if you looked at this, you can calculate the phi electron energy of benzene. What is the phi electron energy? You multiply this by 2, because; there are 2 electrons here, you multiply alpha plus beta by 4 and then add.

If you did that you are going to get 6 alpha plus 8 beta as the phi electron energy of benzene. So, this is the phi electron energy of benzene. Now, in comparison suppose; I say I have a chemical structure where I shall represent the structure something like that. And, this means what? 3 separate ethane like units, each ethane like unit has an energy phi electron energy of alpha plus 2 times of alpha plus beta. This is the energy of one ethane like system. So, you multiply this by 3, you are going to get 6 alpha plus 6 beta. So, if you had separate ethane like units which are not interacting with one another. Then the energy would have been 6 alpha sorry, it would have in 6 alpha plus 6 beta.

And, if we compared these 2 what is the conclusion? The conclusion is that delocalization of the molecular orbital's right; delocalization caused by the formation of molecular orbitals actually has lowest phi electron energy of benzene. And, what how much is the lowering as they find the difference between the 2? And, you conclude that the lowering is actually minus 2 beta and beta has a minus 230 kilo joules per mole. So, this works out to be roughly 460 kilo joules per mole. And, this value is quite large and this is the reason why benzene you say is extras stable and in fact, this is a molecule that you referred to as being aromatic. Now, the molecular orbital so benzene I shall just show the expressions.

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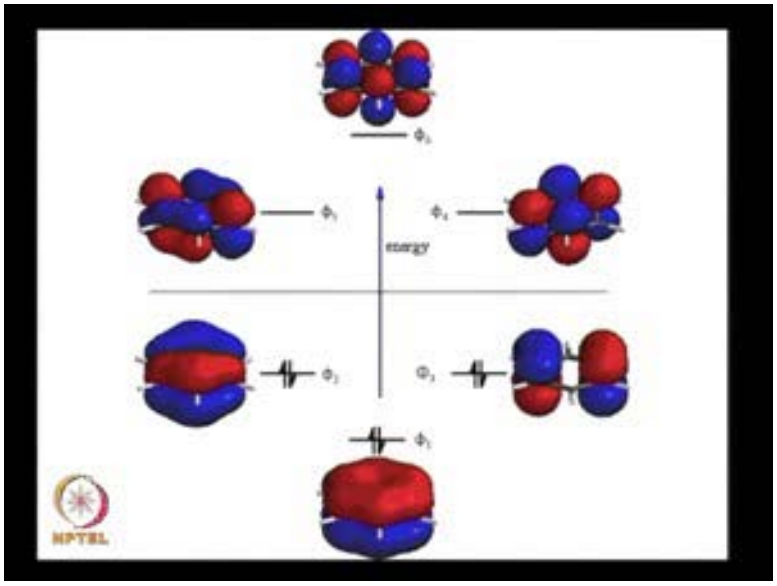

The expressions are here, they will take time to compute. So, will not do the computation, but; I will show you a nice picture which shows this molecular orbitals. So, this is where the molecular orbitals are in fact I should say that this particular picture is taken from the web.

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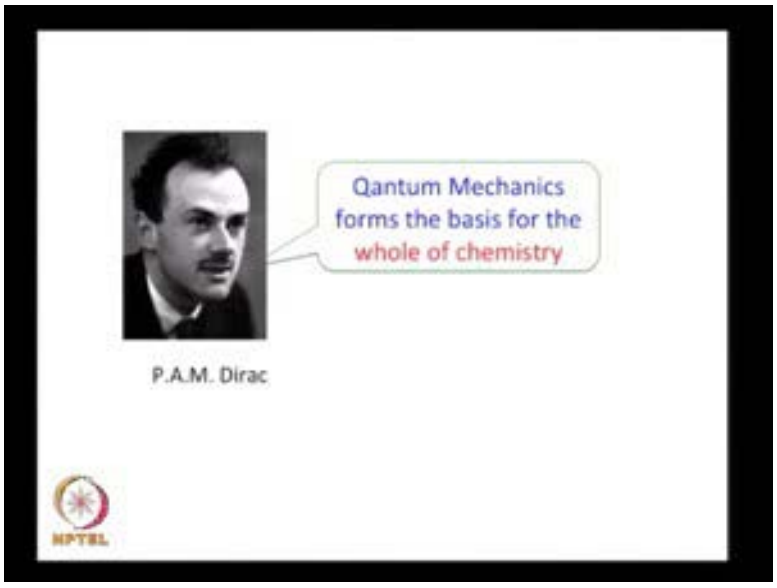

And, I think with this I shall conclude this course, but; before I actually conclude, I would like to leave you with quotation. The quotation actually says that quantum mechanics forms the basis for the whole of chemistry. I hope the lecture's that have

given convinces you that quantum mechanics is very useful for the chemise. And, this quotation actually is due to a physics is very famous one and the quotation is actually from Dirac.

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Now, I would like to adds a acknowledge, the NPTAL of in fact, professor Mangala sunder, who ask me to give this set of lecture's. He has been very nice and in addition I would of course, like to thank to this staff of the NPTAL program here in Madras I I T, they have been very cordial and helpful. And, I would like thanks students of I I T Madras who have attended my lectures. And, finally; I would of course, like to thank the department of inorganic chemistry which is my department; department of inorganic and physical chemistry; Indian institute of science which is in Bangalore. And, to conclude I shall leave you with this question.

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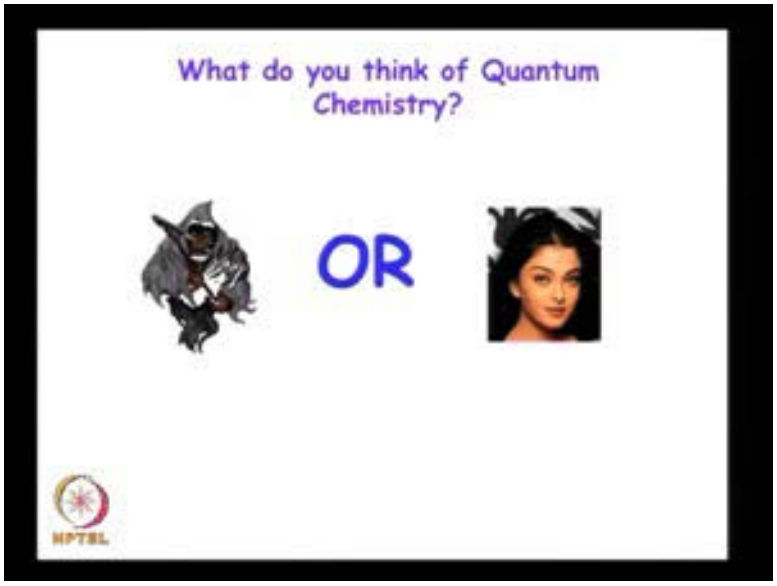

So, thank you very much. Thanks to all of you.