Introductory Quantum Chemistry Prof. K. L. Sebastian Department of Inorganic and Physical Chemistry Indian Institute of Science, Bangalore

Lecture - 47 Di-atomics – Continued

(Refer Slide Time: 00:24)

So, we continue what we were discussing in the case where the energy separation between 2 s and 2 p is large, the molecular orbitals found to have this order as far as their energies are concerned. But if the separation between 2 s and 2 p x is 2 s and 2 p is not that large, then what happens is that the order of the orbitals change, and what happens is that this is sigma g 2 p actually goes above the pi orbitals, and that is what is shown in this picture. But then of course, you should realize that this sigma g 2 p as it is written it has contributions from 2 s as well as 2 p, and therefore strictly speaking it is not completely correct to call it sigma g 2 p.

But we will continue to use this notation; I mean more recently people have changed the notation, but we will not worry about that. We will still continue to use sigma g 2 p, right. What I am saying is that there is appreciable contribution from 2 s also, therefore you cannot really say that this sigma g 2 p and that is sigma u the sigma u star 2 s and this is sigma g 2 s, because there is appreciable contribution from the 2 p orbitals also for these orbitals.

(Refer Slide Time: 01:50)

Now for analyzing this diatomic molecules let me start with this picture, right, because this is the situation where 2 p and 2 s are not that much separated, and that will happen in the case of lithium, then in the case of Ba 2, C 2, and so on. So, let me write this orbital order.

(Refer Slide Time: 02:08)

 $-(\sigma_{21}$ $(\sigma^*_{423})^2(\pi_{42p})$ B

That orbital order is actually sigma g 2 s less than sigma u star 2 s which is less than pi u 2 p which is less than sigma g 2 p which is less than pi g star 2 p which is less than sigma u star 2 p. Now going back to Li 2 lithium has the electronic configuration 1 s 2 2 s 1. So, it has one valance electron.

Student: Sir, it is sigma g 2 s.

Professor: Thank you.

So, it has only one valance electron, and remember we are not going to be interested in 1 s 2 electrons. So, we will consider only the valance electrons. These valance orbitals are the ones which form these molecular orbitals. So, therefore, in Li 2 what will happen is that there are two electrons among these molecular orbitals. So, therefore, you will say ok, the electronic configuration of Li 2 molecule is nothing but sigma g 2 s with two electrons, right; there is many few you would like to have, I can also write 1 s 2 1 s 2. These are actually the lithium 2 lithium atoms, right; the 2 lithium nuclei have 1 s orbitals and their two electrons, each are sitting. So, four electrons are accounted for here, and the remaining two electrons go to sigma g 2 s. So, there are two electrons sitting in a bonding molecular orbital; naturally the bond order will be unity, ok.

The bond order in this case is unity. Let me denote it as bond order. It is equal to 1, and the bond length you find is 2.67 angstroms which is actually surprisingly large. If you compare this with the case of hydrogen molecule the bond length in the case of hydrogen molecule is 0.74 angstroms. So, one may ask why is that this bond length is very large? The reason is actually quite simple. You have these 1 s electrons; they form the core, right, and these 1 s electrons actually repel each other. So, with repulsion between the two 1 s core orbitals I mean the electrons occupying the core orbitals is the one that causes the bond length to be large, and in addition to that the 2 s orbital is rather diffuse; diffuse meaning that it extends into space, and therefore, the overlap between the 2 s is not very effective.

That is the reason why is the bond length is very large, and because the bond length is very large the bond energy is actually low. It is only 105 kilojoules per mol; just to compare maybe I should write h 2 here. H 2 has two electrons in sigma g 1 s, right, h 2 has two electrons in sigma g 1 s; bond order actually is 1, bond length is 1 is 0.74 angstroms, and the bond energy is how much? It is 431 kilojoules just to compare the two. Now thinking of Be 2; Be 2 means you have just added two more electrons. Okay, let me remove this part. I do not need this anymore, and if you have maybe I will write this here Li 2, then Be 2; you have added two more electrons. So, you would have sigma g you will of course have 1 s 2 1 s 2 which I will not worry about.

I will not write them down, sigma g 2 s with two electrons and sigma u star 2 s with two electrons. So, two electrons in a bonding orbital, two electrons in an anti-bonding orbital; so bond order if you calculate you will find it is 0. That is the bond order, and this predicts that Be 2 will not be stable, and this is in agreement with the experiment, right. This is what is nice about molecular orbital theory; most of it productions are in full agreement with experiments. Then if you think of B 2, well, you will have sigma g 2 s with two electrons sigma u star 2 s with two electrons, and you have to add two more electrons to the pi u 2 p, right; pi u 2 p is actually w degenerate, right, because you have pi u 2 p x and pi u 2 p y, and so if we have w degenerate orbitals and if you put two electrons into them, what will happen? They will go and occupy the two separate orbitals.

They will not get paired up, because pairing means electron-electron repulsion is larger. So, they will not pair; they will not get paired up if you want to represent it in this picture, then maybe I should do that. I have two electrons here, I have two electrons there; I have one electron here and one electron there. So, therefore, you have two unpaired electrons, and so you predict that the molecule will not be diamagnetic, but instead it will be paramagnetic, and this is in agreement with experiments. And then what about the bond order? Well, the bonding due to this is cancelled by the bonding due to that, but these are bonding orbitals, and there are two electrons sitting in these bonding orbitals. So, therefore, bond order is going to be how much? It is going to be 1, and bond energy you can measure. It is found to be 289 kilojoules per mol, ok.

Then you think of C 2; C 2 what will happen? You will just add two more electrons. So, you would have sigma g 2 s with two electrons, sigma u star 2 s with two electrons, pi u 2 p with four electrons. So, there are no unpaired electrons; now in the case of C 2 calculate the bond order you will find that bond order is actually equal to 2. This means that in the case of molecule C 2 there is a double bond between the two carbon atoms, and naturally the bond length will be short. It is found to be 1.31 angstroms. That is the bond length, and the bond energy is 627.6 kilojoules per mol rather high; that is because there is double bond. Then coming to N 2, you just add two more electrons. So, therefore, you would have sigma g 2 s sigma u star 2 s pi u 2 p 4, and then the next one which is the orbital; it is sigma g 2 p with two electrons.

So, remember you see this and that they cancel each other, because this is bonding, that is anti-bonding, but these are all bonding orbitals. And therefore, you have six electrons sitting in them; that means the bond order actually is three, which means that there is a triple bond in the case of N 2 molecule; nitrogen molecule has a triple bond, and the bond length is short. It is 1.01 angstroms, and the bond energy is 941.4 kilojoules, and notice that the highest occupied molecular orbital is sigma g 2 p. Now this can be experimentally verified; you see there is this technique called photoelectron spectroscopy where we can remove an electron from the molecule by allowing it to interact with electromagnetic radiation, right.

For example, UV radiation can cause emission of electrons from this orbital from which you can actually find out whether it is a sigma type or a pi type orbital, ok. So, the experiments indicate what electron spectroscopic experiments indicate that, see this is a sigma orbital, the highest occupied orbital is a sigma orbital. Then you come to O 2; as you go down this separation in energy between the 2 s and 2 p atomic orbitals increase, as a result of which what will happen the orbital order gets interchanged. In the case of oxygen what happens is that the orbital order is actually this one, right. This is the orbital order and therefore, what will happen it is the case that sigma g 2 p has a lower energy in comparison with pi u 2 p. So, therefore, the electronic configuration of oxygen will be sigma g 2 s with two electrons sigma u star 2 s with two electrons; the orbital order is this. So, therefore, the next orbital is sigma g 2 p with two electrons.

(Refer Slide Time: 13:10)

And pi u 2 p with how many electrons? With four electrons and pi g star 2 p will contain how many electrons? It will contain two electrons; have I got something interchanged? It is actually this orbital order that you have to follow now essentially because the energy separation between 2 s and 2 p is large, right, and therefore, you have this order, and if that is the way it is you would find that there are two unpaired electrons in the case of oxygen molecule which again is in agreement with experiment.

Oxygen molecule has a bond order of two, and bond length actually is 1.21 angstroms. It is predicted to be a double bond, because if we calculate the bond order you get two, and the bond energy is actually 493.7 kilojoules per mol. So, oxygen is predicted to be paramagnetic, because there are two electrons sitting in pi g 2 p; pi g 2 p is w degenerate. So, therefore, the two electrons are unpaired. Now suppose I remove an electron from oxygen to get O 2 plus, ok, I do not have any space.

(Refer Slide Time: 15:05)

Let me just write here; suppose I make O 2 plus then what are you actually doing? You are removing one electron from this orbital, and this orbital is actually anti-bonding; this orbital pi g star 2 p is anti-bonding. So, if you remove one electron what you are doing is you are increasing the bond order, because you see one electron has been removed from anti-bonding orbitals. So, the system actually requires more bonding. If you calculated the bond order you will find that it is 2.5, right. So, instead of 2, for oxygen it will become 2.5, and as a result of that if you are able to measure the bond length you will find that it the bond length is 1.227 angstroms.

Oxygen molecule itself has a higher bond length; if it is 1.21 in the case of oxygen molecule while O 2 plus the bond length is shorter, because the bond length has increased, because the bond order has increased. On the other hand if you made O 2 minus; that means you are adding one more electron, what will happen? The bond order will actually decrease; it will become 1.5, because you are putting one electron into an anti-bonding orbital as a result of which the bond length will actually increase. It will decrease to 1.26 angstroms. Finally, if you think of F 2, well you will have just one more electron.

So, all these things remain as they are, but the last orbital pi g star 2 p now has four electrons; that means there are no unpaired electrons. See everything else remains the same; you put two more electrons. So, this will become pi g star 2 p. If you calculated the bond order you will find that is equal to unity, and the bond length is 1.42 angstroms, and bond energy is 151 kilojoules per mol. So, this way I mean all the homo-nuclide diatomic molecules can be their existence, their magnetic nature, their bond energy, bond length, everything can be very satisfactorily explained using the molecular orbital theory, and regarding hetero-nuclide diatomics I shall very briefly indicate you how the molecule orbital theory is applied; the discussion will be very brief.

In fact, these days it is possible for you to calculate; it is possible for you to make molecular orbital calculations for not only diatomic molecules but triatomic or any big system; I mean bigger systems it is not very difficult these days, because the computer power available is tremendous these days. As a result of which even if you had a big system may be you have 60 carbon atoms or even larger number of carbon atoms and equally large number of hydrogen or oxygen atoms. It is not very difficult to do calculations using molecule orbital theory. Let us now think of simple hetero-nuclide atom; again this is the only example that I shall discuss.

(Refer Slide Time: 19:01)

The molecule that I have chosen is LiH. In the case of LiH what happens? You have the 1 s orbital on lithium, ok; this is the 1 orbital on lithium, and then you have the 2 s and the 2 p. These are on the lithium, ok, and now you think of the 1 s orbital on the hydrogen; relatively speaking you see its energy will be higher than that of 1 s on the lithium, because you see lithium nucleus is having three positive charges, and the 1 s orbital which is centered around that nucleus will have very low energy. So, relative to that you see the 1 s orbital on hydrogen will have a much higher energy in comparison with this, right, and in fact, the energy of this 1 s will be lower than 2 s on the lithium, right.

So, what will happen? This is very much low in energy. In fact, in this picture maybe I should move it even further down. As a result of which what will happen? This orbital is not involved in the bond formation; this has little overlap with the 1 s at the bonding geometry, and therefore, it is not going to interact. So, effectively what will happen? It is the 1 s interacting with 2 s. It will also have some interaction with appropriately oriented 2 p orbital which is actually 2 p z, ok, and what will happen? The 2 p x and 2 p y will not interact with the 1 s. So, therefore, they will remain non-interacting in the molecules. So, therefore, if this is your molecule the 2 p orbitals 2 p x and 2 p y they will not interact, and they have to be classified as pi type orbitals in the molecule, because if you rotated about the z axis; you see if you rotate by 180 degrees the orbitals change sign, ok, and there are two of them.

So, this is not involved in the bond formation. Now 2 s and 1 s will interact, but this 1 s can also interact with 2 p z there. So, therefore, what will happen is that the 1 s, 2 s and the 2 p z all will mix together; three orbitals will combine together. If three atomic orbitals combine together what do you expect to get? You would expect to get three molecular orbitals. So, therefore, you will have an orbital which is a bonding orbital which maybe something like this, and notice that it is in fact close to 1 s, right; the energy wise it is close to 1 s, why? Because the 2 s is having a higher energy, and then you will have an orbital which will be again a sigma type orbital which will be having an energy like that; as I told you 1 s from the hydrogen and 2 s and 2 p z from the lithium are combining. So, three atomic orbitals are combining.

When three atomic orbitals combine you will get three new orbitals which are molecular orbitals. So, you will have an orbital of roughly that energy, and you will have one more orbital of energy roughly that much, and we need notation. What do we do? These are all sigma type orbitals. So, therefore, you will say this is a sigma type orbital; this is another sigma type, and this is the third sigma type, ok, and to distinguish between them what do you do? You put a 1 here. So, you call it 1 sigma; this you will call 2 sigma. It just simply means that it is the next sigma type orbital; that is all, and this you will call 3 sigma.

And this one to be correct I will call it 1 pi, because it is the first pi type molecular orbital in the molecule, ok, and how many valance electrons does lithium hydride; I mean they are there in the molecule. Lithium has one valance electron, hydrogen has one valance electron. So, there are only two electrons. So, naturally those two electrons they will sit in this bonding molecular orbital, and that is why the bond is formed, but then if you think of that orbital you see it is rather close to the 1 s which means that this 1 s actually makes a fairly large contribution to that bonding orbital, right.

(Refer Slide Time: 24:01)

So, therefore, if I try to represent it pictorially what will happen? I would have lithium and the hydrogen, but this is essentially having little contribution from the 2 s, and majority of the contribution will come from the 2 s; sorry not the 2 s but the 1 s; 2 s will have a small contribution. 2 s and 2 p together will make small contributions, and 1 s will make the largest contribution. So, therefore, if you put two electrons into this orbital these two electrons will be mostly spending their time near the hydrogen, right, and therefore, in the case of LiH you will find that there is a sizable negative charge on the hydrogen and with an equal resizable positive charge on the lithium, right.

In fact, the bond length is actually 1.60; in the case of lithium hydride 1.60 angstroms. You can actually measure the dipole moment, and you find that the dipole moment of the molecule is 5.9 Debye which is fairly large dipole moment, and that is because what has happened is that when the molecule is formed there is charge transfer from lithium to the hydrogen, and that is why the hydrogen has negative charge, and lithium has positive charge. So, the bond is actually almost ionic because you see ionic bond, what do you mean by ionic bond? Ionic bond is a situation where charge is transferred from one of the bonding specious to the other, and there is almost 80 percent ionic nature as far as this bond is concerned. Sizable charge transfer is there from lithium to the hydrogen, and that is why you say it is ionic, ok.

This is all that I will discuss as far as hetero-nuclide diatomics are concerned, but you can think of other hetero-nuclide diatomics. They are not difficult to consider, but we will not do it, and the next topic that I shall discuss is actually the ideas of hybridization. In fact, hybridization also would be taught in inorganic chemistry, but what I will do is I will give a brief description constructing what are known as the hybrid orbitals, so that you will have a clear idea of the mathematics that is involved in the construction of hybrid orbitals.

(Refer Slide Time: 26:45)

So, hybridization I shall illustrate this concept using the molecule Be H 2, ok. Now what is the electron configuration of Be? It is actually 1 s 2 2 s 2, right, and well, if you think of beryllium atom, what happens is that you have 2 s 2; it is a colossal system, and therefore, there are no unpaired electrons, and therefore, a chemist would have difficulty in understanding how bonds are formed, because you see the atom has no unpaired electrons. So, usually chemist will say that ok, if there are unpaired electrons you will have the possibility of forming an electron pair bond, but the answer to that is not difficult because the 2 p orbitals are there; the 2 p orbitals are close in energy to 2 s. So, therefore, imagine that one electron is from order from 2 s to 2 p; let me say 2 p z.

So, that you have one electron here; you have one electron there. Now you have two unpaired electrons, and therefore, you can form two bonds; one with this hydrogen and the other with that hydrogen, ok. But if that is the way it is see if you have 2 s one electron in 2 s which is going to pair with the electron of hydrogen sitting in 1 s, and this is going to pair with the electron of the other hydrogen, right. So, that you have two electron pair bonds; this is essentially a valance bond way of thinking. So, if that happens, ok, then what would I expect? You see one bond is formed because of pairing with 2 s; the other bond is formed because of pairing with 2 p z, and you would expect that the two bonds are not equivalent, because one is formed using 2 s, the other is formed using 2 p z but then when you do an experiment measuring the bond length.

So, the bonds in Be H 2 you find that the two bonds are having the same bond length, and any experiment that you perform indicates to you that the two bonds are completely equivalent, and then to explain this equivalence the concept of hybridization was introduced by Pauline. So, what I said was this. Imagine that this 2 s and the 2 p z orbitals; these two orbitals imagine they are mixed together. So, how are they going to get mixed together? Well, what would happen is that you have 2 s and the 2 p z. Imagine you have some coefficient a 1 with which you multiply 2 s and some other coefficient B 1 with which you multiply 2 p z and add the two together. This is how I will mix the two orbitals, and the result I will say is an orbital which is a hybridized orbital which I will denote by the symbol pi 1.

And in a similar fashion I can say ok, I will take 2 s multiplied by a 2, add to it 2 p z multiplied by B 2, and I shall get another hybrid orbital. So, therefore, we say we are adding linearly 2 s and 2 p z. Now I shall also put the condition that these orbitals they should have the same kind of nature, right. They have to be completely equivalent to one another, maybe they can be oriented differently in space, but except for that they should be completely equivalent, correct. I will have to put that condition, and in addition any

orbital that I use I would like it to be normalized. I would also like these two orbitals to be orthogonal to one another, because that is a property of orbitals.

(Refer Slide Time: 31:18)

So, therefore, if I impose the condition that the orbital is normalized what would that mean? Integral of phi 1 square d 2 over the entire space must be equal to unity. That actually means I mean strictly speaking again I should say phi 1 star phi 1, but these orbitals are all real. So, it is not necessary to put the star. So, if you applied these two this condition to that orbital what it says is you take a 1 2 s plus b 1 2 p z; take the square, integrate over the entire space. The answer must be equal to 1, right; that is what is means. So, suppose we took the square what is the result? You are going to get a 1 square 2 s square plus b 1 square 2 p z square plus 2 a 1 b 1 2 s into 2 p z, and you are going to multiply by d 2 and integrate over the entire space. Each term you are going to; this is B 1 square of course, d 2 you have to put integrate over the entire space.

Here again you have to put d 2 integrate over the entire space. So, this integral is equal to that, and that should be equal to unity, correct. Now remember your atomic orbitals are already normalized. A 1 is just a constant which I want to determine, and this a 1 can be taken out of the integral sign. So, you have 2 s square integrated over the entire space; if your orbital is normalized that has to be equal to unity. So, therefore, this will become a 1 square, and in a similar fashion 2 p z also is normalized. So, therefore, you will get plus B 1 square, and further remember that 2 s and 2 p z are atomic orbitals on the same

atom; they are not on different atoms, because I am thinking of atomic orbitals on beryllium; they are on the same atom. So, atomic orbitals belonging to the same atom are actually orthogonal to one another, and therefore, this integral is going to be equal to 0, and therefore, what is the result that I get? A 1 square plus b 1 square must be equal to 1, fine.

And if we impose the condition that phi 2 is normalized, what is that you get? You get the result that a 2 square plus b 2 square must be equal to 1, fine. Then suppose I multiplied the two orbitals I multiply phi 1 into phi 2 and integrate over the entire space, what would be the answer? The answer is actually right, I mean if you multiplied these two you are going to get terms like a 1 a 2 2 s the whole square, right, d tau; that will be one term if you multiplied the two, and you will get b 1 b 2 2 s 2 p z; sorry not 2 s 2 p z, but 2 p z square d 2; this is another term that you will get, right, and you will also get terms which involving 2 s into 2 p z integrate it over the entire space, but that integral 2 s into 2 p z integrated over the entire space is actually zero. So, it is not necessary for me to consider the cross terms.

So, effectively what will happen is that you are going to get 0 here on the right hand side, because the two orbitals I want them to be orthogonal, but this integral is how much? This integral is unity that integral also is unity. So, effectively the condition becomes a 1 b 1; yeah a 1 b 1 plus a 2 b 2 must be equal to 0, ok. So, therefore, our orbitals hybrid orbitals phi 1 and phi 2 I want to determine them, and I want them to satisfy these conditions, ok. Now if you look at this expression see phi 1 is given by a 1 plus a 1 into 2 s plus b 1 into 2 p z, ok, and further I also found that a 1 square is actually the coefficient of 2 s square, and b 1 square is actually the coefficient of 2 p z square if you think of phi square.

And this means that the importance of the 2 s orbital in the orbital phi 1 is actually determined by a 1 square wherein the charge density of phi 1 square the importance of 2 s orbital is determined by a 1 square, right. So, therefore, you can say ok, a 1 square is the contribution of the 2 s; b 1 square is the contribution of the 2 p z to the orbital phi 1, and similarly a 2 square is the contribution of the 2 s, and b 2 square is the contribution of 2 p to the orbital phi 2, right. So, if that is the way it is I can say that ok, I want the two orbitals to be equivalent, fine. I want the two orbitals two hybrid orbitals to be equivalent and that means that magnitude wise a 1 square must be equal to a 2 square, and also that means that b 1 square must be equal to b 2 square, right.

I want a 1 b 1 square to be equal to b 2, because you see the orbitals should have the same p contribution. They should also have the same s contribution, and to ensure that you can say these two have to be equal; you should have these two also equal, right. So, using all these equations you see it is a fairly straight forward matter to solve for a 1 and b 1 and a 2 and b 2. If you solved them what is the answer that you get? You find that a 1 must be equal to 1 by square root of 2; you can choose b 1 to be equal to 1 by square root of 2, a 2 to be 1 by root 2 and b 2 to be minus 1 by root 2.

The easiest thing to do will be I claim that these are the solutions, and what you can do is we can substitute these things in here, and see that all these equations are satisfied if I chose a 1 b 1 a 2 b 2 to be having these values, right, and therefore, I have found two hybrid orbitals; what are the hybrid orbitals? The first hybrid orbital is phi 1; phi 1 actually has 1 by root 2 here 1 by root 2 there. So, you get 1 by root 2 times 2 s plus 2 p z, and phi 2 would be 1 by root 2 times 2 s minus 2 p z, fine, and so if these are the hybrid orbitals let me try to draw them.

(Refer Slide Time: 40:01)

See this is my 2 s which I represent by sphere, and that is my 2 p z. The 2 s is positive; you can say the 2 s orbital is having a positive value let us say, and so if you added the two up; suppose you add the 2 s with the 2 p z what will happen? Well, in these regions

both 2 s and 2 p z are positive. So, therefore, you will have a positive region which may be represented by a lobe of this shape, and in this region what will happen is that the 2 s has a positive sign while 2 p z has a negative sign. So, therefore, they will tend to cancel each other, but the 2 s is actually extending in this direction. So, therefore, you will be left with a negative lobe something like that, but it will be much smaller, and somewhere here you will say is your beryllium nucleus, ok.

Then if you construct with the other hybrid orbital which is phi 2, how will you construct that? Well, you have to multiply 2 p z with minus 1 and then add. So, if you multiply 2 p z with minus 1 this will become negative, and that will become positive, and then if you added them up what is the result? The result is you will have the beryllium nucleus here, and you will have a positive lobe which is pointing in this direction and a smaller negative lobe on the other side. So, if you have the beryllium atom what happens is that one hybrid points in that direction, and the other hybrid points in the reverse direction, right. So, that the angle between the two hybrids is actually exactly 180 degrees, because they are pointing in different directions along the same line which is the z direction.

So, then what will happen? This may be used from a bond with the hydrogen on this side, and this will be used from a bond with the other hydrogen on the other side. And therefore, if you had beryllium hydride Be H 2 these two bonds are formed by hybrid orbitals which point exactly in the opposite direction; as a result of which the bond angle works out to be 180 degrees, and you can see that the two hybrid orbitals are completely equivalent to one another.

(Refer Slide Time: 43:27)

Here I have a Mathematica file which shows the shape of these orbitals. Fortunately it has become too big; ok now it is become too small. This is the one of the hybrid orbitals which is pointing towards one of the hydrogen's. You can see it from different angles; somewhere here is the beryllium atom, and you can actually rotate it and view it from different angles if you like.

(Refer Slide Time: 44:16)

Similarly this is the other hybrid orbital which is pointing in exactly the opposite direction. This is only one way of representing the orbitals. I can think of other ways of representing the orbital, and this for example is another way of representing the orbital, ok.

(Refer Slide Time: 44:40)

So, this is a hybrid orbital which is represented using contour diagrams, and you will see that this orbital this hybrid orbital is pointing in this direction, and you have another hybrid which is shown down here I believe.

(Refer Slide Time: 44:57)

Yeah, here it is, and it is pointing in exactly the opposite direction, ok. So, these are the two orbitals; one is this one, and this is the other one. Unfortunately I should also find out that this is the labeling here is not correct; this is called as x, but it should have been called z, because the orbitals are pointing in the z direction, and this type of hybridization actually is referred to as SP hybridization, because in this case 1 s orbital that is the 2 s and 1 p orbital that is actually the 2 p z. These two combine and give you equivalent two equivalent hybrid orbitals, ok. So, therefore, this is referred to as SP hybridization, but you would already know that there are other systems.

(Refer Slide Time: 46:24)

For example, if you have the molecule B Cl 3 a molecule involving boron; if you have B Cl 3 how is it you have boron with the electronic configuration 1 s $22s2p1$, but it is able to form three bonds three equivalent bonds, and therefore, just as in this case what you will say is ok, one electron is from order from here, and so you have two unpaired electrons; one sitting in 2 p orbitals and one unpaired electron sitting in the 2 s, and then these three orbitals one 2 s and the two 2 p orbitals may be mixed together to give you hybrid orbitals, ok.

So, let us try to do that. I will say that I have my boron here in this at the centre of my coordinate systems this is my x axis, and that I will say is my y axis, ok. So, I would have the 2 s orbital; I would also have 2 p x, and I would have 2 p y. So, what is the problem now? The problem is that I would like to mix these three orbitals 2 s, 2 p x and 2 p y and to get hybrid orbitals three of them which I would denote as phi 1, phi 2, phi 3, and they should all be completely equivalent to one and another. Thank you for listening.