Concepts of Chemistry for Engineering
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Lecture No. 28
Predicting molecular structures: VSEPR model

Welcome to this segment, where we are going to discuss how we can use a model to predict the molecular structure of different compounds.

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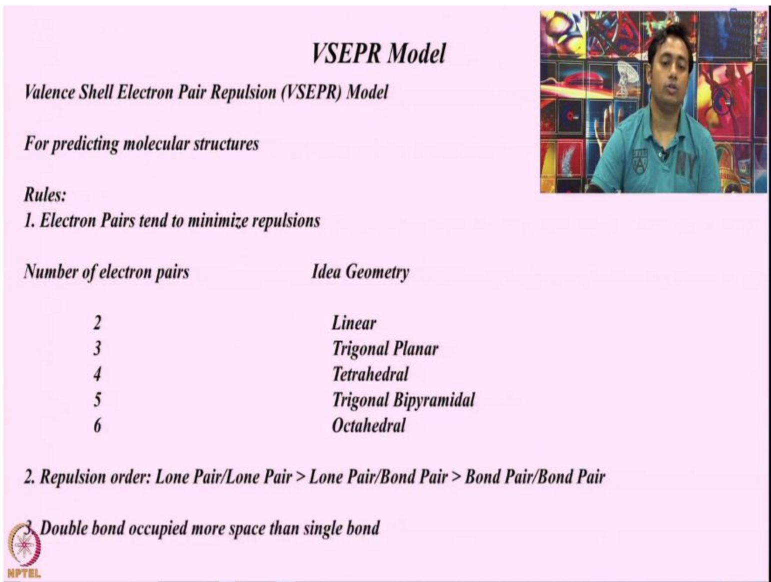

So, this particular model we are going to use is known as VSEPR model, which is an acronym for the valence shell electron pair repulsion model. So, what we are going to do over here that we will count how many electron pairs are actually present in a molecule, because during the forming of the bond, they actually created a bonding pair of electrons. And sometimes, some of the electron pair remains on particular atoms, which is not participating in the bond directly at all those are known as lone pairs.

So, this interaction between these lone pairs and the bond pairs and how we can distribute them in a 3-dimensional space that is going to help me to find out what will be the possible structure of the molecules. So, counting of the total electron pairs, distinguish them between bonding pairs and lone pairs and predicting the possible geometry is the backbone of this VSEPR model.

So, first, the thing that actually controls the structure following this model is that electron pairs are actually going to repel each other, because they are all negatively charged and over there, we try to go to a particular structure such a way that in 3 dimensions, the electron pairs are as far as possible present. So, in 3-dimensional space the electron pairs are situated as far as possible and with respect to that, this overall structure formation comes.

So, depending on the number of electron pairs, this is the ideal geometry, we can think about. If it is a 2-coordination system, where only two electron pairs are present, it should prefer a linear geometry, if it is a 3 electron pair present, then it is going to have a trigonal planar geometry, if it is a 4 electron pair present, it will be tetrahedral, if it is 5 electron pair, it will be trigonal bipyramidal structure and if it is a 6 electron pair present, it will prefer a geometry of octahedral.

Also, the repulsion, that lone pair lone pair repulsion is actually the strongest repulsion compared to this lone pair bond pair compared to the bond pair bond pair which face the least amount of repulsion. So, the actual structure of the molecule following this ideal geometry will differ a little bit to make sure the lone pair lone pair repulsion can be avoided in place of lone pair bond pair or bond pair bond pair.

So, that preference will be given during the formation of the structure. And also, if we have a double bond present that will cover more area compared to a single bond. So, that will create more repulsion with respect to a single bond.

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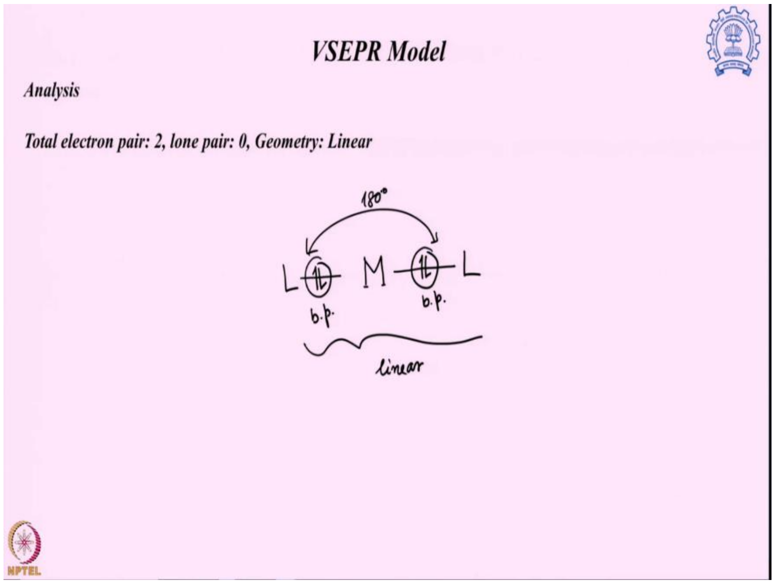

With that thing in mind, now, we are going to draw basic structures of different electron pairs present and what are the different possibility of their structures. So, we will start with the only two electron pair present and none of them are lone pair, so what kind of geometry we can expect.

So, it is pretty simple we have a metal ion present which is connected to two ligand and where in between the two-ligand metal bond, there is the bond pair coming. So, you have two bond pair, no lone pair present and that is going to create a linear geometry where they are 180 degrees apart. So, there is the least amount of repulsion between those two bond pairs. So, that is very easy to understand and that is what is actually happening.

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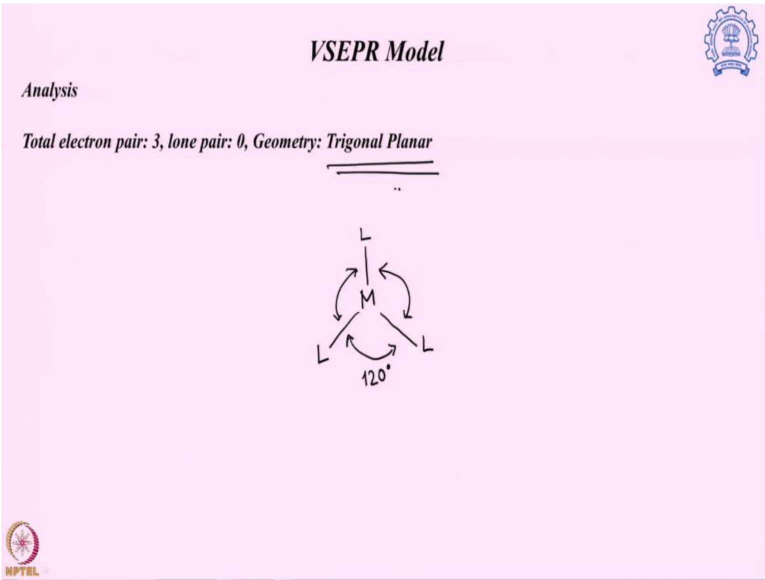

Now go to a system where we have total three electron pairs, none of them are lone pair, what will be the geometry? So, now we have three ligands, I am not drawing the electrons anymore, this line represents the bond pairs. So, over there in 3-dimensional space, I can move that ligand in such a way that they are in the same plane but they are apart by 120 degrees to each other. And that is known as that trigonal planar structure. And that is present, when we have a metal bound to three ligands and all the bond pairs, the only electron pairs present in the system, three electron pair, no lone pair.

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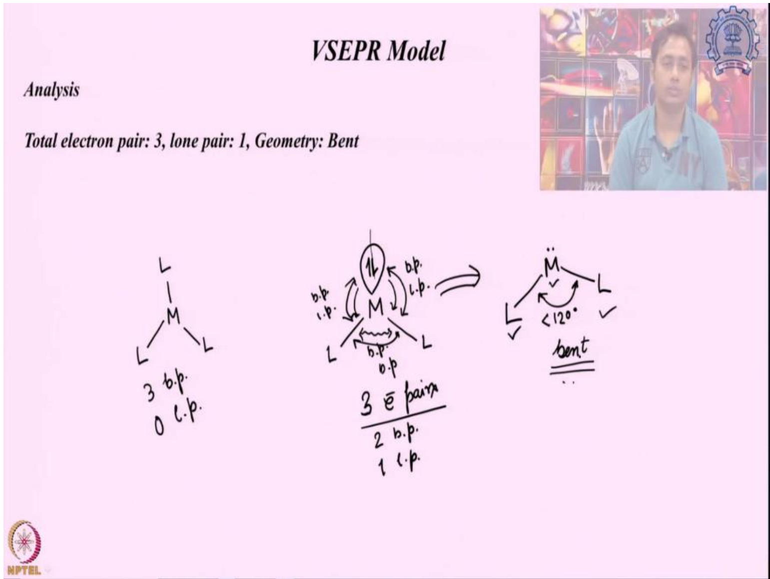

Now come to a system where we have three electron pairs, but now one of them is a lone pair. So, we will just draw the previous one just in case two ideas it is actually having three bond pair, but 0 lone pair, lp means lone pair, bp means bond pair. Now, over here I have total 3 electron pairs but out of them 2 bond pair and 1 lone pair. So, lone pair is generally shown in this way.

Now, what happens, they still will prefer this kind of trigonal geometry, trigonal planar geometry. So, it is a trigonal planar geometry. But generally, when you draw the molecule, we do not draw this lone pair, we are just going to draw the metals and ligands, we will draw some two dots like that to show here is my lone pairs, but we generally do not draw it.

So, the actual structure will be defined by the presence of the atoms over here. So, you can say it is going to be a bent structure. So, although inclusion of the lone pair gives me a trigonal planar, but when we generally discuss about a molecule of geometry, we generally discuss with respect to only the ligand and metal. So, that is why we say it is a bent structure.

And not only that, this lone pair bond pair repulsion is going to be more compared to this bond pair bond pair repulsion. And that will reflect on the bond angle over here. So, this bond angle is expected to be less than 120 degrees then, it is expected in a perfect planar geometry, because over there this bond pair lone pair repulsion is going to push these metal ligand bonds too close to each other, that will shrink down the angle which will go lower than 120 degree. So, that happens when you have three electron pairs and one of them is a lone pair.

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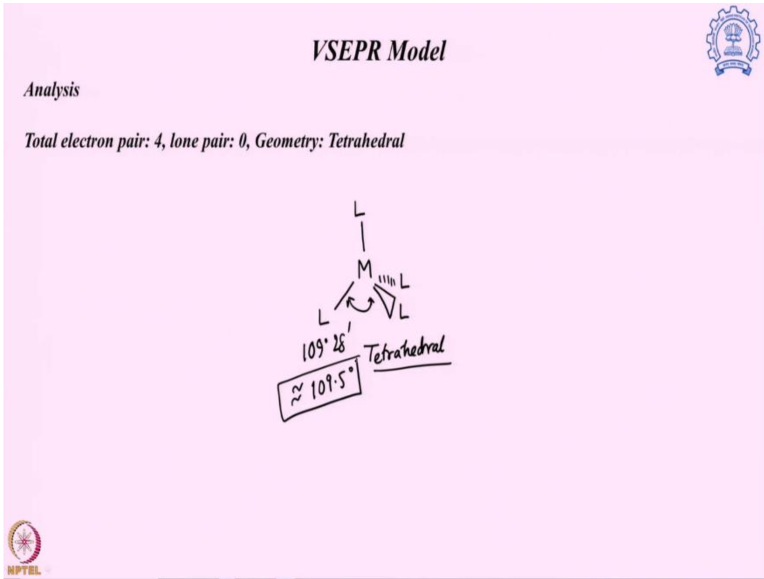

Next comes a system where we have 4 coordination system and we have only 4 bond pairs but no lone pair. So, that will be preferring this tetrahedral geometry, because over here, each of the bonds are separated by from each other by 109 degree 28 minutes or you can say 109.5 degrees, which is the maximum we can move in 3-dimensional space to create the maximum difference between them. So, they have the minimum electron-electron repulsion.

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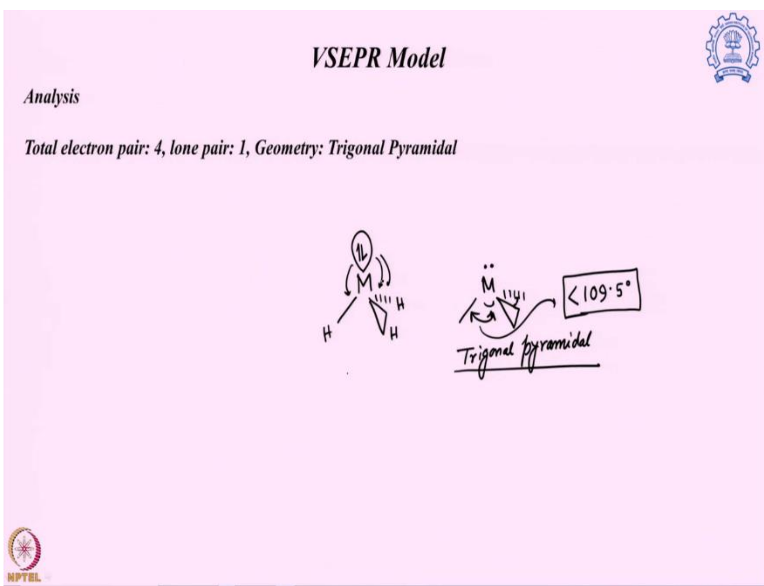

Now, what happens out of these 4 pairs, one of them is a lone pair. Let us now say I have a central metal ion, one of them is a lone pair now, so, they will still go for this overall tetrahedral geometry, but as I am not going to draw the lone pair, the actual system will look like something like that. Lone pairs are present there, but I am not going to show that in the actual structure. So, instead of a tetrahedral it is now, a trigonal pyramidal, so it is a trigonal system but not planar but pyramidal because it is showing you the reminiscence of the tetrahedral geometry.

And over there also, the lone pair is going to push this bond pair apart. So, this is going to create some change between the bond angles and this bond angles are expected to be less than 109.5 degrees that is expected for a perfect octahedral. That is again because the bond pair lone pair repulsion is stronger compared to bond pair bond pair. So, the bonds will come a little bit closer to each other so that it can create some space between lone pair and the bond pair.

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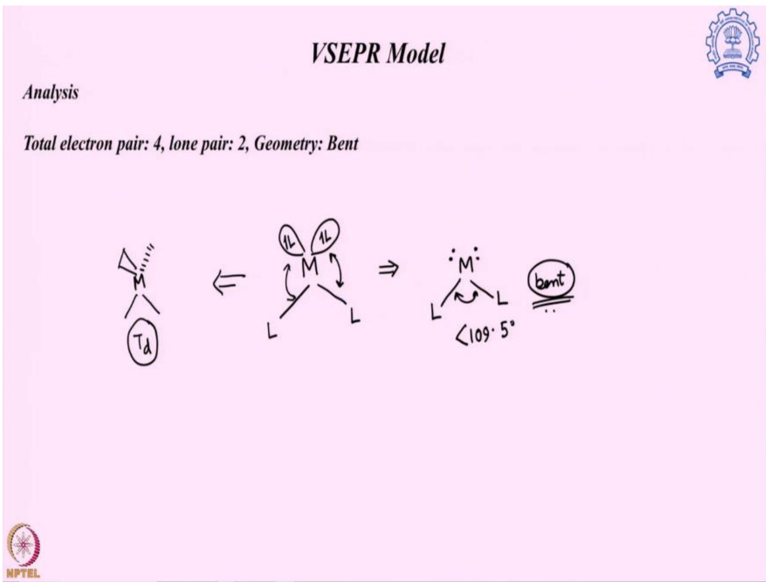

Now comes a 4-electron pair system. But now, two of them are actually lone pairs. So again, it will still follow its original geometry, such way so which is nothing but derived if say all of them are actually present, so it will be a perfect tetrahedral system, so instead of a tetrahedral I am showing you in this way, because I am not going to see the lone pairs, so I just draw the lone pairs like this. But I am going to show the molecule like this.

So, this is basically nothing but a bent structure molecule, because I am not going to show the lone pairs in the actual structures. However, this lone pair bond pair repulsion again will push this bond down and this bond will be less than it is expected for a perfect 109.5 degree that we expect for a tetrahedral system. So, that is going to happen when we have four pairs and two of them are lone pair.

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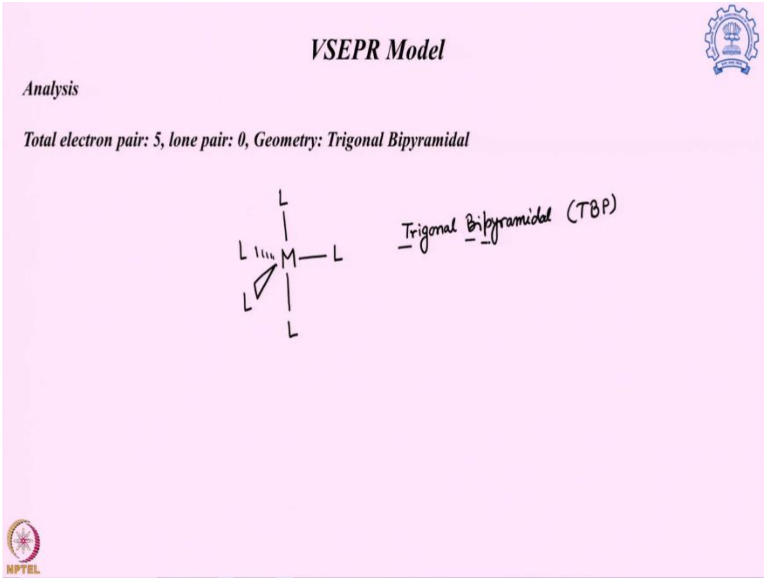

Now come to a 5 pair system where we have now 5 pairs. So, you have a perfect 5 pair system, the geometry preferred is this following trigonal bipyramidal. In short from, it is sometimes written as TBP structure trigonal bipyramidal structure. So, if you have total 5 bond pairs, no lone pairs at all, it will directly go to this trigonal bipyramidal, the preferred geometry with 5 pair system.

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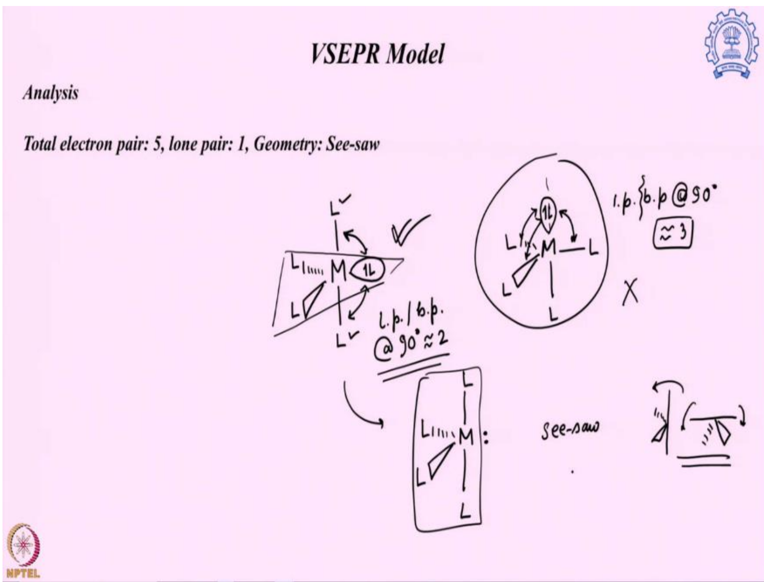

The problem begins when one of them now becomes lone pair. So, over here, what happens, it will still start with its original system where it prefers a trigonal bipyramidal structure, but instead of a bond pair now it has a lone pair sitting in one of the system. Now, over here, the question comes, why do I put this lone pair in the equatorial plane not in the axial plane? That is because the lone pair in this particular format is facing lone pair bond pair repulsion in 90 degree with two sets of ligands.

But now say if we have done that in the following way, where it is actually the lone pair is present in the axial plane, then what would happen? In that particular case that lone pair would face a lone pair bond pair repulsion at 90 degree, 3 of them it will face if it is in a axial position, it will face this interaction with 3 ligands present in the equatorial plane 90 degree.

Over here in the equatorial plane if I put that it is facing lone pair bond pair repulsion at 90 degree, only 2 of them and that is why this particular structure will be preferred not this one. And this structure if I draw that without showing the lone pair to show like this, in that condition, this particular structure is says a seesaw structure.

Because over here, if you look into this particular figure, we can say it is nothing but something like this, if we rotate 90 degree it is a seesaw we see in the parks during our childhood. So, that is why it is called a seesaw structure. That is found when you have total 5 electron pair and one of them is in lone pair.

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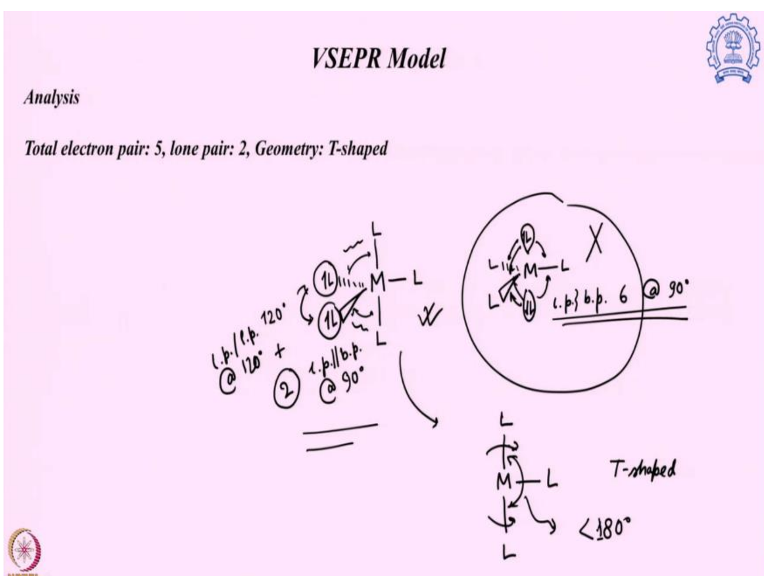

Now comes the next one. Where we have 5 electron pair and two of them are lone pairs. Now, what happens? So, here what it actually occurs there are the 3 ligands and 2 of them between the equatorial plane comes over here the two lone pairs. Why the two lone pairs are over here, so, that each of the lone pair can have 120 degree difference to each other. And at the same time, each of them are facing only two of the lone pair bond pair repulsion at 90 degree.

If imagine, if the lone pairs are actually present in each of the equatorial plane then what would happen? Obviously, there would be no lone pair lone pair repulsion, but there will be total 6 lone pair bond pair repulsion at 90 degree coming from each of them. So, which will be much stronger compared to two such lone pair bond pair repulsion plus one lone pair lone pair repulsion at 120 degree.

So, here if we add them together, this is actually going to be more stable. So, this is preferred compared to this one. And if I draw that without the lone pair, how it will look like it will look like this one, which we called them as a T shaped molecule. And over there this repulsion between the lone pair and bond pair will make sure these bonds are little bit bent. So, this angle over here which is supposed to be 180 degree, it will be a little less than 180 degree. This happens when you have 5 electron pairs and two of them are bond pairs.

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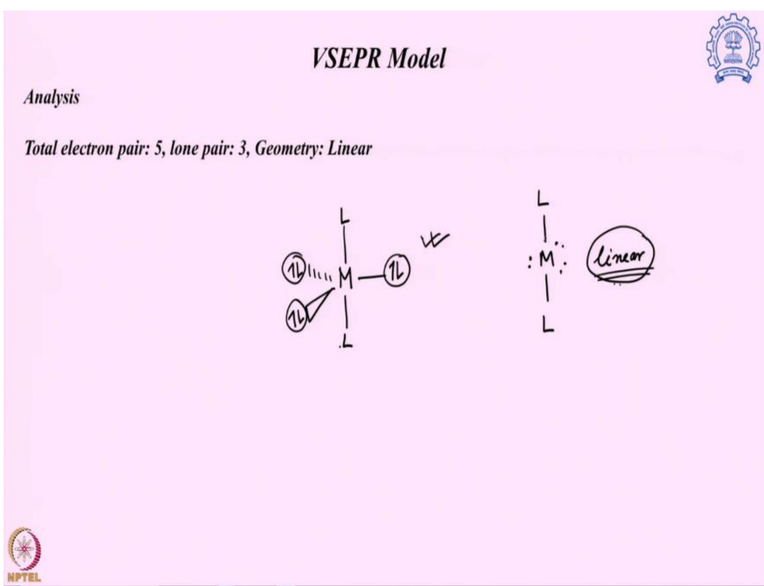

Now, go to the next one where we have 5 lone pairs, sorry, in this case, we have total 5 electron pairs and now 3 of them are lone pairs and this is found in the following way. These are the two bond pairs how it is found and the three lone pairs are all in the equatorial plane, because in the equatorial plane, they actually can keep the maximum distance between themselves.

And now, if we want to put one of them in the equatorial plane to axial plane, that will face a 90 degree repulsion between the lone pair lone pair. So, that is why this particular geometry is preferred. And if I remove the other electron pairs, it will look like a linear molecule because it has 3 lone pairs sitting around here in the equatorial plane. So, that is how it looks like.

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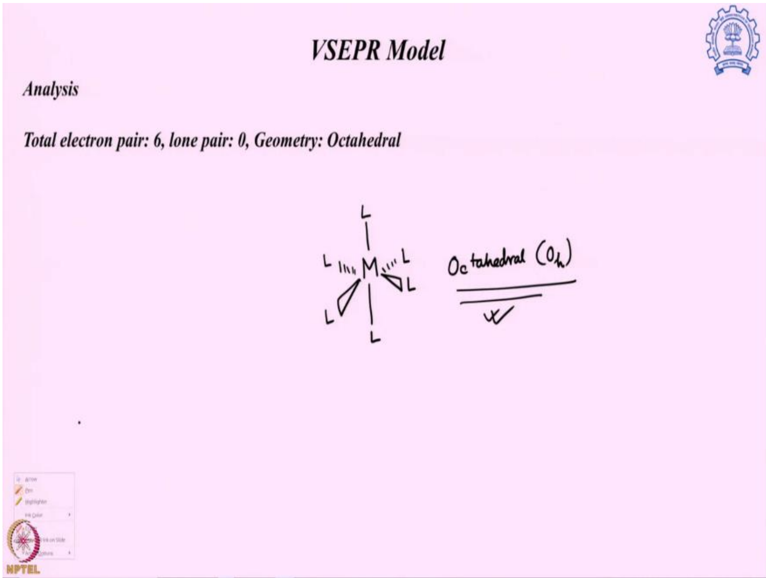

Now, come to 6 coordination system, where the basic system we can find with maximum distance between the electron pairs in the form of bond pairs is this octahedral geometry. So, that is found when you have 6 electron pairs.

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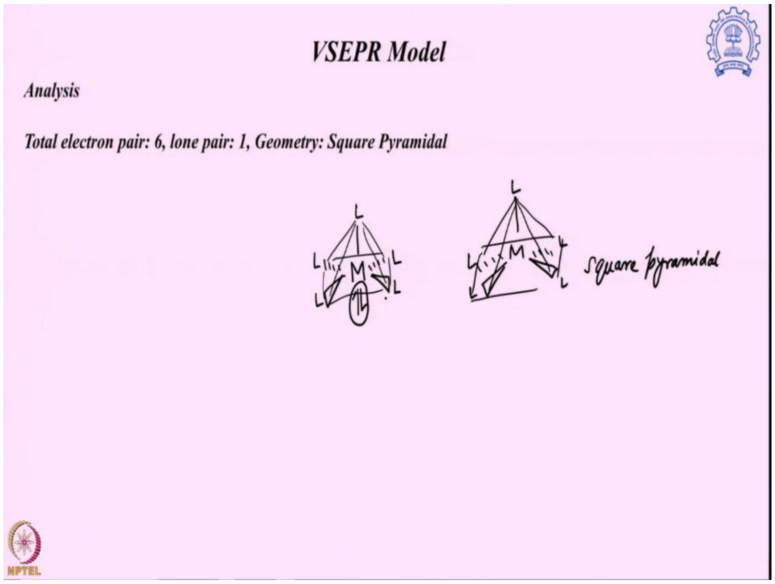

Now, say we have 6 electron pairs, but only one of them is a lone pair system then what happens? Then the system again, begin from the same way and over there one of the lone pair is going to sit in one of the plane somewhere here and the rest of them will be the ligand. So, it will be this particular structure which is known as the square pyramidal because the axial ligand shows it kind of a pyramid apex, but it is actually going to have a square base it is known as the square pyramidal.

And over here lone pair will go to one of the binding spot because all of them are equivalent in octahedral geometry. So, it does not matter where it goes the rest of the geometry will be a square pyramidal.

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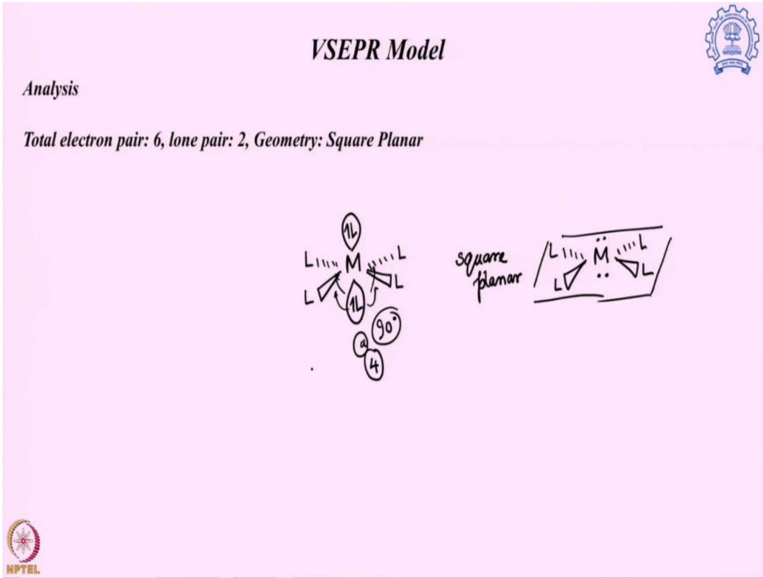

Now comes 6 electron pair system, but 2 of them are now the lone pair. So, over here the lone pairs will go exactly opposite to each other. And it will create this particular structure known as square planar. Here each of the lone pair bond pair is facing a 90 degree repulsion, 4 of them each, so, total 8 of them are facing, but it is still better orientation, because the lone pair lone pair is actually opposite to each other.

So, all the possible combination in this geometry, this one is the most feasible one and the most stable one. So, it is going to have a square planar geometry, all the atoms present in the same plane in a square geometry.

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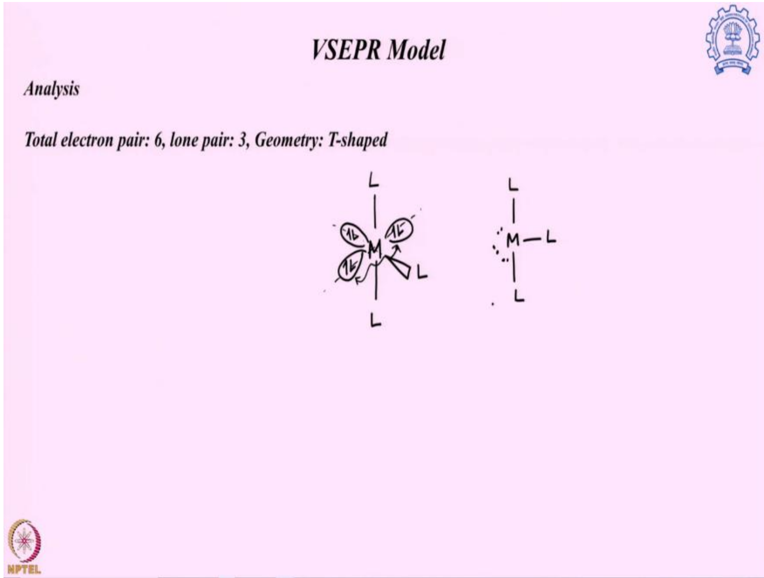

Then comes another 6 pair system, but now we have three of them are in lone pair. So, now the lone pairs will go in such a way 2 of them will be opposite to each other. But one of them will now come to the picture over here and the rest of them will be like this. So, it is nothing but a T shaped structure, if I just orient that a little bit with three lone pairs present around it. So, two of them was already 108 degree to avoid as much as lone pair repulsion possible, but now one of them has to come over here, no other possibility, so, that is why this T shaped structure will end up with.

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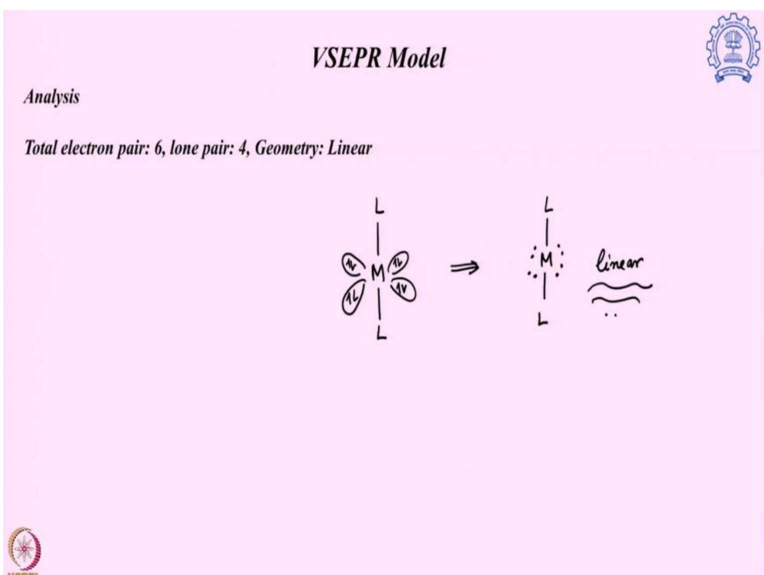

What happens if we have a system where there are 6 pairs and 4 of them are lone pairs. So, all of them will be in such a way that they are holding up the equatorial plane and two of the other ligand system present in this way, which is going to show you nothing but a linear structure. So, all the structures are like that, so, it is going to be a linear structure, so it can also happen. So, you can see starting from octahedral geometry we can follow from the perfect octahedral to square pyramidal to a T shaped to at the end a linear structure.

So, all the things we are going to follow. So, that is how the analysis has been done in VSEPR theory, first find out what is the total number of electron pair present bond pair plus lone pair and then find out what is the preferred geometry and then with respect to the number of lone pairs, draw the structure and predict the structure without considering the lone pair. So, we will go through a few examples to explain it better.

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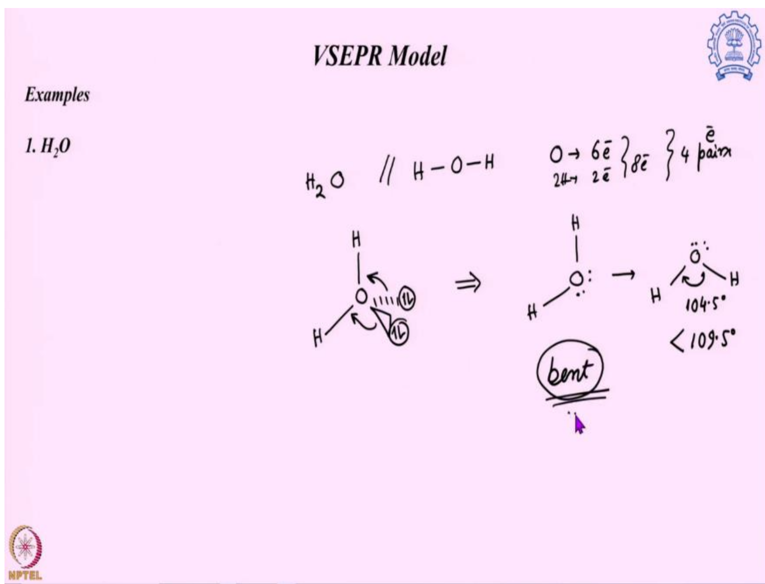

So, the first example is water. Now in water system, it is actually H_2O. So basically, it has two OH bonds, how many electrons present in water? So, oxygen has 6 electrons in his valence shell plus 2 electrons are coming from each of the hydrogen. So, altogether total 8 electrons. So total, we can say there 4 electron pairs. As we know 4 electron pairs, we can easily put them in the form of a tetrahedral geometry. So, in two of them, we are going to put the lone pairs and two of them we are going to put the bond pair the H_2O.

So now, if I redraw that, without showing the lone pairs, it will be like this. And if I just rotate it a little bit, this particular bent structure will be the structure of water. And as you have discussed earlier, this lone pairs will push the bond pairs. So, this particular bond angle over here is actually 104.5 degree, which is less than 109.5 degree which is expected for a perfect octahedral. So, which actually shows that this lone pair bond pair repulsion does exist over here. And that is why water is actually having a bent structure altogether.

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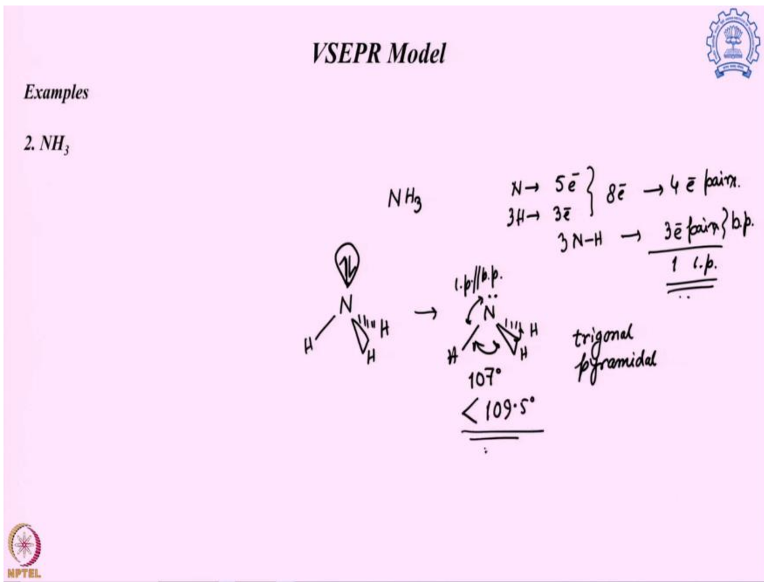

The next example we have in our mind is ammonia. Again, in ammonia, we have nitrogen, which gives 5 electrons in the valence shell, 3 hydrogens will give total 3 electrons, so total 8 electrons, again, 4 electron pairs, and out of these 4 electron pairs, you have only 3 nitrogen hydrogen bonds. So, 3 electron pairs will be actually bond pairs, and the rest 1 of them will be the lone pair system. So, it is a 4 pair system with 1 lone pair.

So again, we will go to a tetrahedral geometry because of these 4 pair present and 1 of them is going to be the lone pair. So, basically, the structure it will end up with is this following this lone pair. So, which is nothing but a trigonal pyramidal structure and over here, the bond angles are actually shrink down because of the repulsion between the lone pair and bond pair and the angle over here comes around 107 degree which is again lower than the 109.5 degree.

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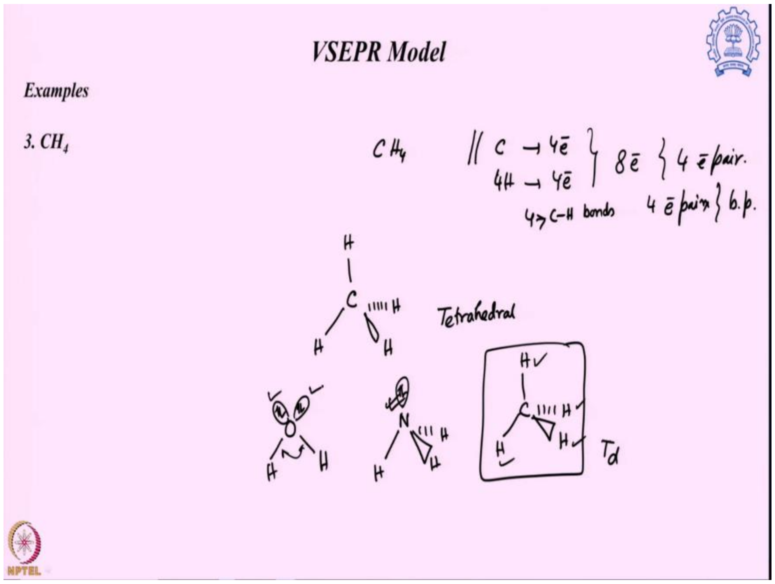

The next example comes to our mind is methane. So, in methane we have carbon which gives 4 electrons, we have 4 hydrogen that gives another 4 electron, 1 electron per each hydrogen. So, total 8 electrons it is again 4 electron pair system, we have 4 CH bonds over here. So, all of them will end up as bond pairs. So, that is a 4-bond pair system with no lone pair. So, the basic methane structure is nothing but a tetrahedral structure.

So, you can see over here from water to ammonia to methane all of them are actually having 4 electron pair systems. So, their underlying structure is basically tetrahedral structure, but only in methane we can say it is a tetrahedral structure, because all of them has atoms present. Over there the ammonia is nothing but a trigonal pyramidal structure, because one of them is actually electron pair and in water it is a bent structure although it is derived from the tetrahedral, because two of them are the bond pairs.

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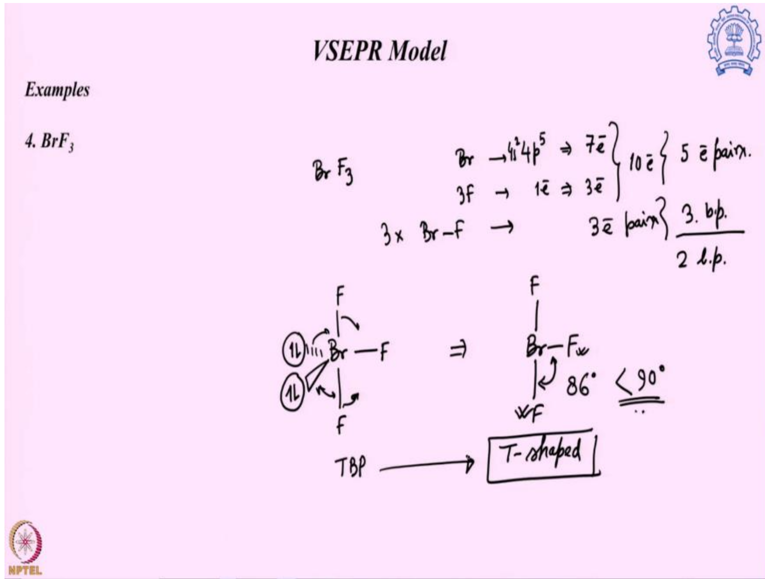

Now we go to another example, BrF_3, a BrF_3 system. Now bromine belongs to a system where they have four p^5 set of electrons at the end, along with two s electrons. So, altogether there are 7 electrons in its valence shell. And there are 3 fluorine coming is given one extra electron. So, total, 3 electrons. So, if we combine all these things together, we have 10 electrons, which is nothing but 5 electron pairs altogether we have.

And BrF bond, we have 3 of them. So, that will take care of 3 electron pairs. So, this will be the 3 bond pairs so we will have 2 of them as lone pairs. So, it is a 5-electron pair system with 2 lone pairs. So, as we know, for a system like this, it is going to show me a trigonal planar structure and I am going to put the lone pairs over here so that I can minimize that lone pair bond pair repulsion.

So, at the end, I am going to have this kind of structure which is nothing but we can say it is a T shaped structure. And over here, what will happen due to this bond pair lone pair repulsion these bonds will shrink down and this angle between this axial fluorine and the equatorial fluorine and the bromine comes down to 86 degree, whereas the 90 degree it is preferred for a perfect TBP structure.

So, we can say it is actually having a T shaped structure, although the original template is derived from the trigonal bipyramidal structure, but we talk always about the structure with respect to the atoms present without considering the lone pairs.

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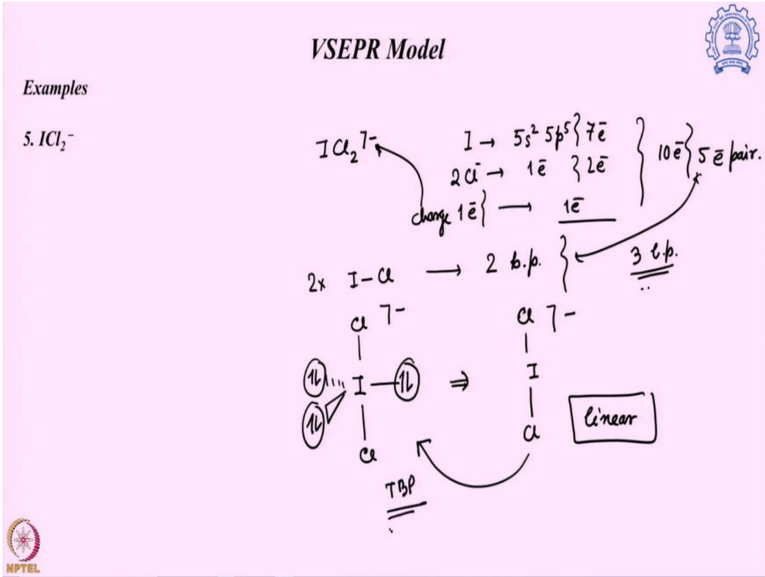

Next example, is ICl_2^-, so over here we have ICl_2 and there is an extra negative charge present. So, iodine is again is a halide system. So, it is $5s^2$ $5p^5$ so, 7 electrons it has in the valence shell. We have two chlorines, so, which is giving me 1 electron at a time, so total 2 electrons and there is 1 extra charge over there. So, that is giving me the 1 electron this charge over here.

So, all together if we add, it is again coming to 10 electrons. So, it is again a 5-electron pair system. Now, look into how many ICl bonds I have only 2 of them. So, you will have only 2 bond pairs out of this 5 and the rest 3 of them will be the lone pair system. So, it is 3 lone pair 2 bond pair and out of total 5 electron pairs.

So, as we know it will go to a TBP original structure first and the chlorides will be present on the axial, so that it can have the maximum distance from this lone pairs, so at the end the structure we can say linear structure or although it is derived from again TBP original structure.

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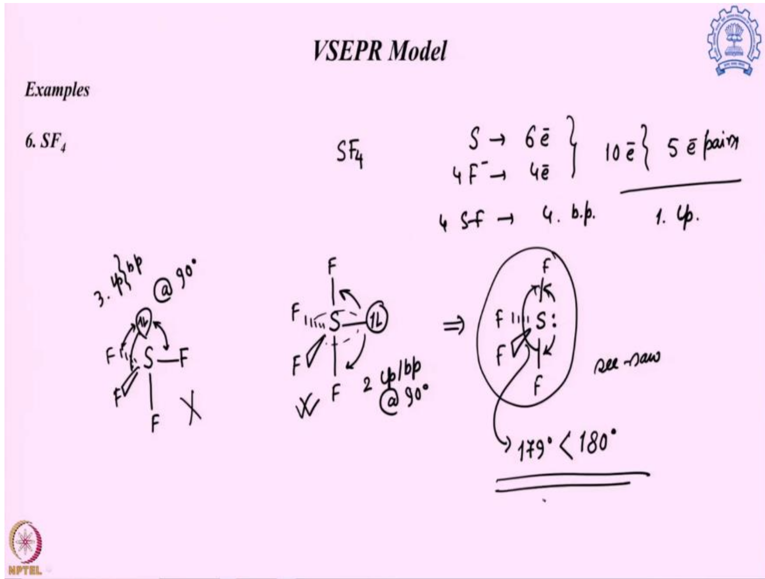

Now, one of the last examples of this system, it is the SF_4, sulfur is present in the oxygen group which has 6 electrons present in its valence shell and 4 of the fluoride is providing the extra 4 electrons altogether I have 10 electrons or again 5 electron pairs. I have 4 sulfur fluoride bonds. So, I have 4 bonding pairs. So, the rest of them 1 of them will be one lone pair. So, SF4 with 5 electron pairs it will start from a system with TBP structure.

So, it will start from a trigonal planar structure to start with. And over there, the question is, where the lone pair should go? So, the lone pair generally sits over here and 4 fluorides present over here. So, it is basically a seesaw structure that is going to form at the end, like this. Now, the question comes, is it possible? What happens if I put one of the lone pair actually in the equatorial position to that in the axial position, what will happen to there?

So, now you can see the lone pair is pushing 3 lone pair bond pair interaction, whereas, in this case, it has only 2 lone pair bond pair interaction, which is happening at 90 degree, because at 90 degree it has more repulsion compared to when it is seeing them in the 120 degree. So, that is why this structure is preferred not this one.

So, at the end, we are going to go out this particular seesaw kind of structure and because of the presence of the lone pair over here, these bonds are going to get back a little bit and that is why this particular angle is not going to be exact 180 degree and this particular molecule it is found to be 179 degree, which is less than 180 degree.

So, in this way, we can use VSEPR model to predict molecular structure; first, find out how many electron pairs are there and with respect to the number of pairs, we can find what is the geometry they would like to prefer. For 2 electron pairs it is linear, 3 trigonal planar, 4 tetrahedral, 5 trigonal bipyramidal, 6 octahedral.

This will be the basic structure and depending on how many lone pairs they have, and minimize a lone pair lone pair, a lone pair bond pair and bond pair bond pair repulsion the actual structure will be defined when only atoms are present, not connecting with respect to the lone pair. So even with the octahedral structure in water, the actual structures can be in a bent structure.

Similarly, ammonia although it derived from a tetrahedral structure, the actual structure we can see it is a trigonal pyramidal. So, that is the end of this segment where we learned how to use VSEPR theory to predict the structure of molecules. Thank you.