Good day students. A warmwelcome to this chemistry class. Your paper code is CHC106 inorganic chemistry. The title of the topic, bonding in coordination compounds the module that I will be taking up is molecular orbital diagrams for hexa aguo titanium + 3. And hexacyanoiron - 3. I'm Cheryl Alvares, associate professor. Camel College for Women Nuvem, Goa. The outline of the module will flow as follows. We will construct the molecular orbital diagram for these two complexes. Then we shall show the electron distribution in the molecular orbitals and based on these MO diagrams we shall decide the value of O whether these are high or low spin complexes Δ and we will also know something about the magnetic nature. Of these complexes. The learning objective is to discuss the relationship between ligand binding in an octahedral metal complex and the degeneracy of the d orbital. The MOT allows overlap between metal and ligand. Therefore it is quantitatively more accurate than the crystal field theory and the ligand field theory. Let us begin with the first complex hexa aquo titanium + 3. Titanium belongs to the first transition series. The atomic number is 22, so distribution of

electron goes Ar 18, 3d2, 4s2 in this complex, titanium exhibits a + 3oxidation state, so therefore the associated electron configuration with titanium + 3 is Argon 18,3d1. It d1 ion having outer electronic configuration 3d 4s0 4p0 so thus this complex has a total of 13 electrons 12 which would be contributed by the 6 aquo ligands and one which will be contributed by the Ti + 3 Titanium ion. Out of the 13 electrons, students, 12 electrons will be placed in the lower 6 bonding molecular orbitals and one electron will be placed in the nonbonding T2g orbital. So the distribution of electrons, the12 electrons in the bonding molecular orbitals will be as A1g T1U6 Eg 4, whereas the 13th electron is placed in nonbonding T2g as in 3d X Y1 3dYZ0 And 3dXZ0. So on your screen students you have the molecular orbital energy level diagram for hexaaquo titanium +3. Considering only Sigma interaction an showing the distribution of these 13electrons. Please note that every metal ion orbital will overlap with its matching ligand

symmetry orbital to give you a bonding, and antibonding

molecular orbital. So if you look at the diagram a A1g

bonding, T1U bonding. Occupy lowest energy. Likewise A1g antibonding and T1U antibonding Occupy highest

level of energy in the order of molecular orbitals.

The Eg set of metal ion orbitals overlaps with its matching ligand group orbitals to give you a bonding and an antibonding MO. This overlap is a little weaker, therefore the energy gap between Eg bonding and Eg antibonding is a little less. So the Eg molecular orbital is displaced less from its barycenter. The T2g orbitals of the metal ion are considered to be non bonding with respect to Sigma interaction. Therefore they remain unchanged in energy. Students please look at the diagram properly again. The energy gap between T2g nonbonding and Eg antibonding is given in terms of a parameter called ΔO the value of ΔO here is lower. Why is it lower students? because of the poor overlap between the Eg orbitals of metal and the matching ligand orbitals. When the overlap is poor, the energy gap automatically becomes small. Now this could be attributed to the fact that the Aquo ligand is a weak ligand. Because of the weak Ligand and the overlap between Eg orbitals of metal and the matching ligand orbitals is a little weaker. Consequently, the

value of ΔO is small, so he distribution of 13 electrons goes as follows. 12 electrons are occupied in the bonding molecular orbitals. Students.Please note that these bonding molecular orbitals A1g T1U Eg lie closer to the ligand orbital so they will be preferentially filled by ligand electrons. The antibonding molecular orbitals, lie closer to the metal ion orbital, so obviously they will be preferentially filled by metal ion electrons, whereas the electrons in non bonding T2g will be purely metal ion electrons. So of the 13 electrons 12 are placed in the lower bonding molecular orbitals and one occupies the nonbonding T2g molecule orbital. So this hexa aquo titanium +3 ion has one unpaired electron as you've seen in the molecular orbital diagram, thus it is paramagnetic. The absorption spectrum of this ion shows you, an absorption Maxima at 500 nanometers or 5000. Aº This is because of the transition of the single electron from nonbonding T2g to Eg antibonding. There's a transition of that one single electron from Nonbonding T2g to Eg antibonding molecular orbitals. CFT gives us a similar explanation. Transition of the

single electron takes place.

From lower T2g orbitals to higher energy EG orbitals.

We will next see the next complex now. Hexacyanoiron- 3. Iron again belongs to 1stTransition series, atomic number 26 distribution of electrons goes Ar 18 3d6 4S2 in the

complex ion it exhibits a + 3oxidation state. So the

associated electron configuration goes argon 18

3d5. So in this complex students there are a total of 17

electrons to be filled up in the molecular orbitals 12 which will

be contributed by the 6 cyano ligands. And five, which would be contributed by the Fe

+3 ion.Sso out of the17 electrons, 12 electrons will

be placed in the lower bonding molecule orbitals. 5 electrons

will go up to the nonbonding T2g orbital. The distribution of

electrons in the bonding molecular orbitals will be as in

A1g2 TIU6 Eg4and the nonbonding T2g5 as in 3d X Y23dY

Z2. And 3d XZ 1. On your screen students what you see now is the

molecule are orbital energy level diagram for hexacyanoiron -3

considering only sigma interaction. Kindly look

at the diagram closely.

The value of ΔO is the energy gap between T2g nonbonding and

Eg anti bonding. It is a higher value. This is due to a

stronger overlap between the Eg orbitals of metal and the

corresponding ligand orbitals. Now why is the overlap stronger? This could be attributed to the fact that the cyano ligand is a stronger ligand, stronger the overlap, stronger will be the covalent nature of the metal ligand bond. Out of the 17 electron students. The first 12 will be. placed in the lower bonding molecular orbitals, the other five will be placed in nonbonding T2g so the electrons prefer to pair up in T2g orbitals rather than go to the Eg antibonding because of the energy gap. The gap between the T2g non bonding and Eg anti bonding is large. This high value of Δ is attributed to the larger extent of overlapping between metal Eg and the ligand orbitals. Therefore it indicates a stronger covalent character of the metal ligand bond and owing to the presence of this one single unpaired electron as you've seen in the diagram, there is one single unpaired electron in non bonding T2g. This makes this complex ion {Fe(CN)6}- 3 weakly paramagnetic.Since maximum number of electrons are paired and minimum number are unpaired, It is an example of a low spin complex. A very similar explanation is given to us by the crystal field theory. That is electrons pair up in lower T2g orbital, instead of going to the higher

Eg because of a higher value of Δ O. And how do we get this high value of Δ O? This high value of Δ O was attributed to the strong ligand field exerted by the cyano ligand. So in conclusion, molecular orbital diagram of an octahedral complex containing only Sigma bonds.Show us that T1U antibonding A1g antibonding has higher energy than Eg. Antibonding molecular orbitals. Just like the crystal field theory, MOT can also predict the number of unpaired electrons in low spin and high spin octahedral complexes. Thus,

magnetic properties of complexes are retained in the same manner in both these theories i.e. molecular orbital theory as well as the crystal field theory.

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Devi and others. Have a good day. Students thank you.