

❖ Jahn-Teller Effect

The Jahn-Teller theorem essentially states that any nonlinear molecule system possessing electronic degeneracy will be unstable and will undergo distortion to form a system of lower symmetry as well as lower energy and thus the degeneracy will be removed.

This effect describes the geometrical distortion of molecules and ions that is associated with electronically degenerate configurations. A configuration is said to be electronically degenerate if more than one sites are available for the filling of a single electron. The Jahn-Teller effect is generally encountered in octahedral transition metal complexes. The phenomenon is much more common in hexacoordinated complexes of bivalent copper. The d^9 configuration of Cu^{2+} ion yields three electrons in the doubly degenerate e_g orbitals set, leading to a doubly degenerate electronic state as well. Such complexes distort along one of the molecular four-fold axis (always labeled the z -axis), which has the effect of removing the orbital and electronic degeneracies and lowering the overall energy. The distortion usually occurs via the elongation the metal-ligand bonds along the z -axis, but sometimes also occurs as a shortening of the same bonds instead. Moreover, the Jahn-Teller theorem predicts the presence of an unstable geometry only and not the direction of the distortion. When distortion involving elongation occurs to decrease the electrostatic repulsion between the electron-pair on the ligand-attached and any extra electrons in metal orbitals with a z -component; and hence lowering the energy of the metal complex. Inversion center is retained after z -out as well as z -in the distortion. Symmetrical configurations possess electronic degeneracy while the unsymmetrical ones do not. Various symmetrical and unsymmetrical configurations are given below.

Table 10. Symmetrical and Unsymmetrical t_{2g} and e_g orbitals.

Symmetrical configurations	Unsymmetrical configurations
$t_{2g}^0, t_{2g}^3, t_{2g}^6$	$t_{2g}^1, t_{2g}^2, t_{2g}^4, t_{2g}^5$
e_g^0, e_g^4, e_g^2 (high-spin)	e_g^1, e_g^3, e_g^2 (low-spin)

Now, the conditions for different kinds of distortion can be summed up as:

Table 11. Conditions for Jahn-Teller distortion.

Type of distortion	Configuration required
No distortion	t_{2g} (symmetrical) + e_g (symmetrical)
Slight distortion	t_{2g} (unsymmetrical)
Strong distortion	e_g (unsymmetrical)

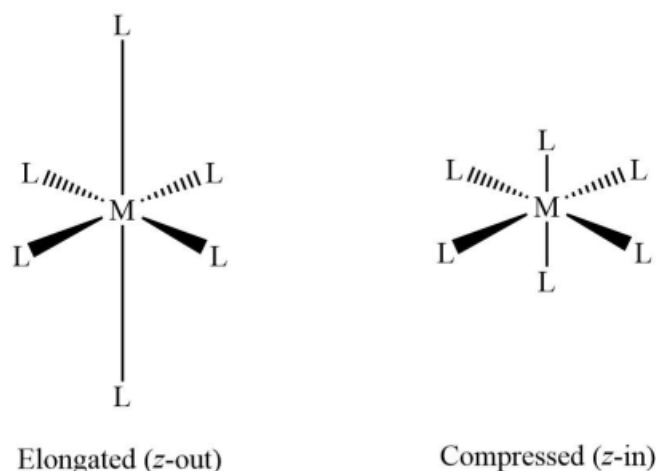


Figure 57. The Jahn-Teller distortions for an octahedral complex.

Let the case of the low-spin Co^{2+} octahedral complex. The corresponding electronic configuration is $t_{2g}^6 e_g^1$. Owing to the electronically degenerate state, the Jahn-Teller distortion is expected. Now suppose that the single electron of e_g set is present in d_{z^2} orbital; the ligands approaching from z -axis will feel more repulsion than the ligands coming from x and y -axis. Therefore, the bonds along z -axis will be weaker in comparison to the bond along x and y -axis. This results in a tetragonal elongation about z -axis with two longer and four shorter bonds. This is formally called as z -out distortion. On the other hand, if the single electron of e_g set is present in $d_{x^2-y^2}$ orbital; the ligands approaching from x and y -axis will feel more repulsion than the ligands coming from z -axis. Therefore, the bonds along x and y -axis will be weaker in comparison to the bond along z -axis. This results in a tetragonally flattened octahedral geometry about z -axis with two shorter and four longer bonds. This is formally called as z -in distortion.

Consider the following examples

1. $[\text{Co}(\text{CN})_6]^{4-}$: It is a low-spin complex with $t_{2g}^6 e_g^1$ electronic configuration and will undergo strong Jahn-Teller distortion.
2. $[\text{Cr}(\text{NH}_3)_6]^{3+}$: It is a high-spin complex with $t_{2g}^3 e_g^0$ electronic configuration which is completely symmetrical; and therefore, will not show any Jahn-Teller distortion.
3. $[\text{FeF}_6]^{4-}$: It is a high-spin complex with $t_{2g}^4 e_g^2$ electronic configuration and will undergo slight Jahn-Teller distortion.

➤ Energetics of Jahn-Teller Distortion

The Jahn-Teller distortion results in a system of lower symmetry and lower energy. This is actually the opposite of what is expected. Generally, symmetry leads to stability; but the Jahn-Teller effect is actually an exception to this statement. Therefore, it is necessary to discuss the driving force responsible for this behavior. The magnitude of Jahn-Teller effect is larger where the electron density associated with the

degenerate set orbitals is more concentrated. Hence, Jahn-Teller effect plays a significant role in determining the structure of transition metal complexes with active 3d-orbitals. The whole energetics of the Jahn-Teller can be understood by the case study of d^9 and d^1 complexes.

1. Cu^{2+} complexes: The electronic configuration of free Cu^{2+} ion is d^9 ; and in an octahedral environment, it is $t_{2g}^6 e_g^3$. Before we put any conclusive remark on the direction or nature of the distortion, we shall find the crystal field stabilization energy for z-out as well as for z-in case.

i) Crystal field stabilization energy for z-out distortion:

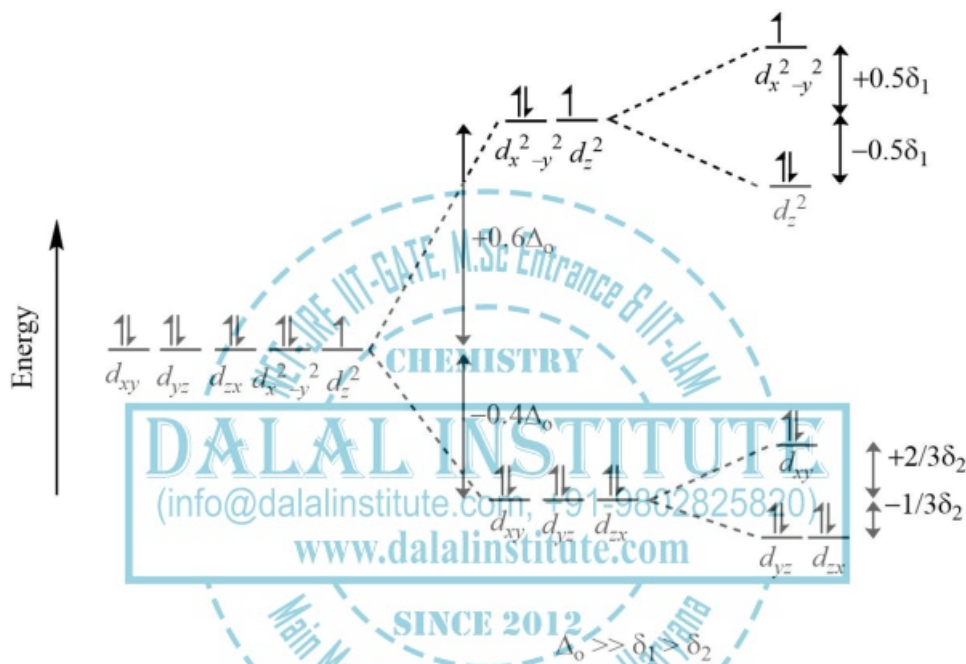


Figure 58. The splitting pattern and filling of d -orbital set of Cu^{2+} in octahedral and subsequently in the tetragonally elongated complex due to Jahn-Teller effect.

CFSE due to distortion = Energy of the distorted complex (E_2) – Energy of the complex without distortion (E_1)

$$E_1 = 6(-0.4\Delta_o) + 3(+0.6\Delta_o)$$

$$E_1 = -0.6\Delta_o$$

$$E_2 = 4(-0.4\Delta_o - \delta_2/3) + 2(-0.4\Delta_o + 2\delta_2/3) + 2(+0.6\Delta_o - \delta_1/2) + 1(+0.6\Delta_o + \delta_1/2)$$

$$E_2 = -0.6\Delta_o - \delta_1/2$$

$$\text{CFSE due to distortion} = E_2 - E_1 = -\delta_1/2$$

Hence, the crystal field stabilization due to z-out distortion is $-\delta_1/2$.

ii) Crystal field stabilization energy for z-in distortion:

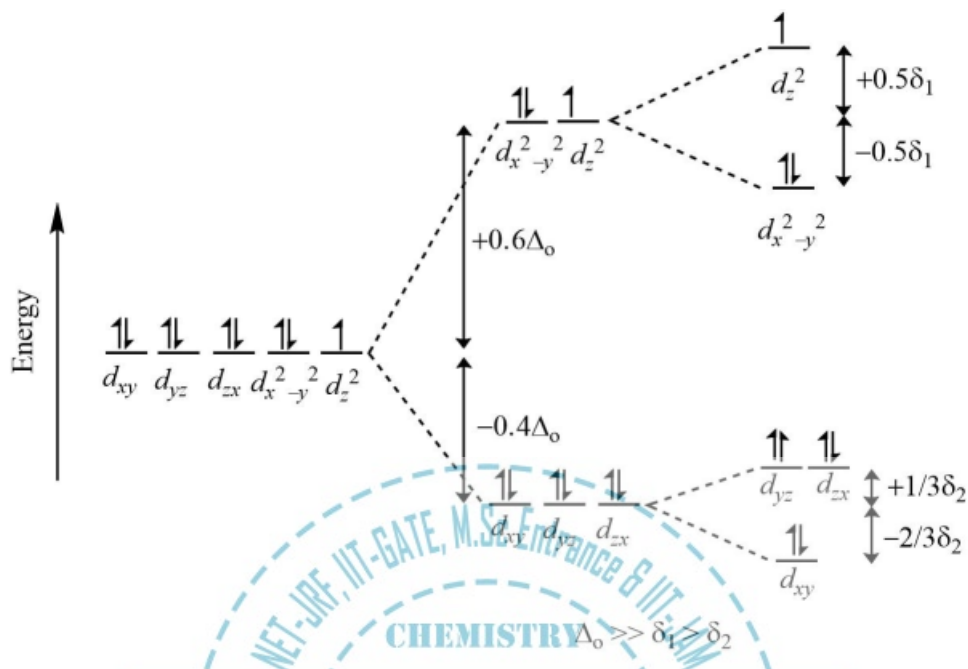


Figure 59. The splitting pattern and filling of d -orbital set of Cu^{2+} in octahedral and subsequently in the tetragonally compressed complex due to Jahn-Teller effect.

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CFSE due to distortion = Energy of the distorted complex (E_2) – Energy of the complex without distortion (E_1)

$$E_1 = 6(-0.4\Delta_o) + 3(+0.6\Delta_o)$$

$$E_1 = -0.6\Delta_o$$

$$E_2 = 4(-0.4\Delta_o - 2\delta_2/3) + 2(-0.4\Delta_o + \delta_2/3) + 2(+0.6\Delta_o - \delta_1/2) + 1(+0.6\Delta_o + \delta_1/2)$$

$$E_2 = -0.6\Delta_o - \delta_1/2$$

$$\text{CFSE due to distortion} = E_2 - E_1 = -\delta_1/2$$

Hence, the crystal field stabilization due to z-in distortion is $-\delta_1/2$.

Hence, the magnitude of crystal field stabilization in z-out case is same as that is present in z-in complex. This implies that Jahn-Teller effect cannot predict the direction of the distortion. However, it has been observed that it is the z-out case that dominates in most of the cases. It may depend on the repulsive forces between the d -electrons and the ligands, so the odd electron will prefer d_z^2 -orbital more than $d_{x^2-y^2}$ due to the lesser number of ligands it will repel with. Moreover, when a z-in distortion occurs, one can also view it terms of equatorial elongation while z-out will mean the weakening of two axial metal-ligand bonds. In other words, it is easier to weaken two bonds rather stretching four metal-ligand bonds.

2. Ti^{3+} complexes: The electronic configuration of free Ti^{3+} ion is d^1 ; and in an octahedral environment, it is $t_{2g}^1 e_g^0$. Before we put any conclusive remark on the direction or nature of the distortion, we shall find the crystal field stabilization energy for z -out as well as for z -in case.

i) Crystal field stabilization energy for z -out distortion:

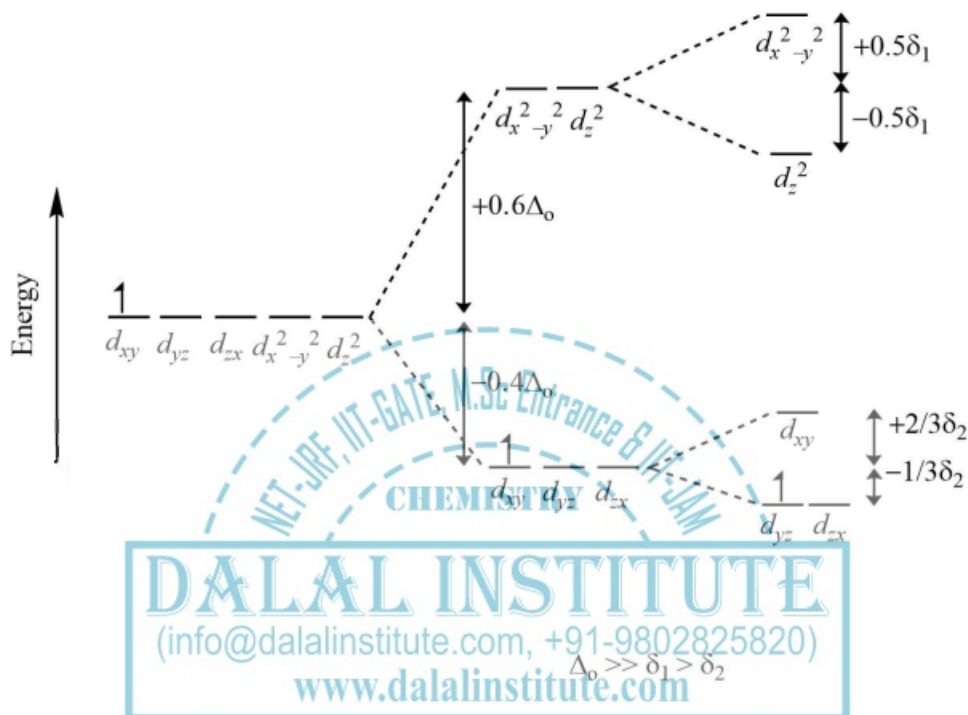


Figure 60. The splitting pattern and filling of d -orbital set of Ti^{3+} in octahedral and subsequently in the tetragonally elongated complex due to Jahn-Teller effect.

CFSE due to distortion = Energy of the distorted complex (E_2) – Energy of the complex without distortion (E_1)

$$E_1 = 1(-0.4\Delta_o)$$

$$E_1 = -0.4\Delta_o$$

$$E_2 = 1(-0.4\Delta_o - \delta_2/3)$$

$$E_2 = -0.4\Delta_o - \delta_2/3$$

$$\text{CFSE due to distortion} = E_2 - E_1 = -\delta_2/3$$

Hence, the crystal field stabilization due to z -out distortion is $-\delta_2/3$. Moreover, it is worthy to note that this type of Jahn-Teller distortion is unable to remove the electronic degeneracy completely (the single electron can still be filled in two degenerate orbitals namely d_{yz} and d_{zx}). Therefore, homoleptic octahedral complexes of d^1 -configuration undergoing z -in distortion are quite rare.

ii) Crystal field stabilization energy for z-in distortion:

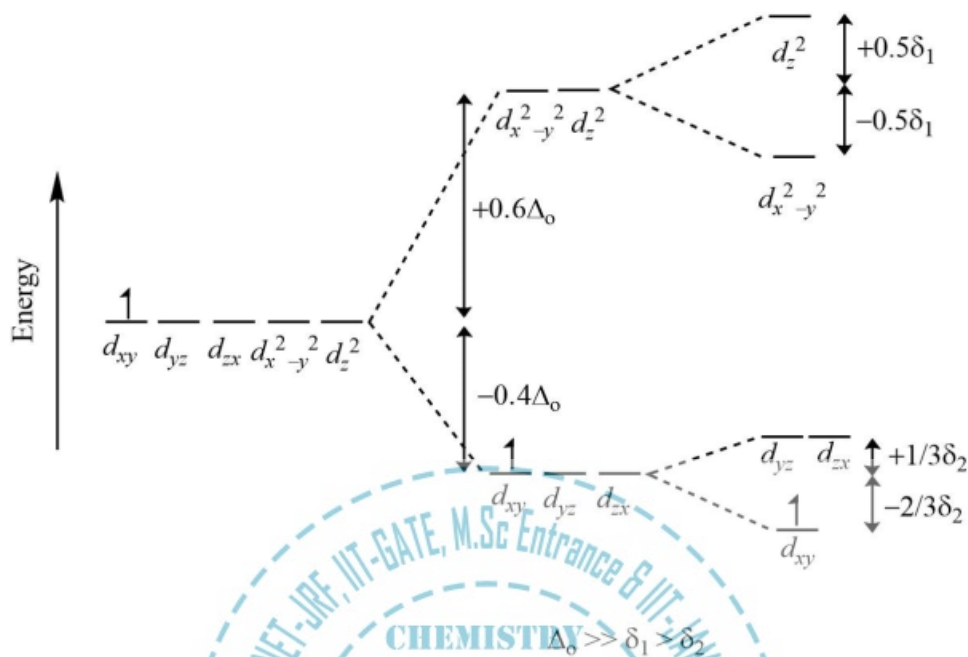


Figure 61. The splitting pattern and filling of d -orbital set of Ti^{3+} in octahedral and subsequently in the tetragonally compressed complex due to the Jahn-Teller effect.

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CFSE due to distortion = Energy of the distorted complex (E_2) – Energy of the complex without distortion (E_1)

$$E_1 = 1(-0.4\Delta_o)$$

$$E_1 = -0.4\Delta_o$$

$$E_2 = 1(-0.4\Delta_o - 2\delta_2/3)$$

$$E_2 = -0.4\Delta_o - 2\delta_2/3$$

$$\text{CFSE due to distortion} = E_2 - E_1 = -2\delta_2/3$$

Hence, the crystal field stabilization due to z-in distortion is $-2\delta_2/3$.

Hence, the magnitude of crystal field stabilization in z-out case is half of what is observed in z-in complex. This implies that Jahn-Teller effect can predict the direction of the distortion. However, it is the d^1 -configuration that has been observed to show z-in distortion; otherwise, the z-out case dominates in most of the cases. It may be explained in terms of the repulsive forces between the d -electrons and the ligands, so the odd electron will prefer d_z^2 -orbital more than $d_{x^2-y^2}$ due to the lesser number of ligands it will repel with. Nevertheless, Ti^{3+} octahedral complexes prefer to undergo z-in due to the greater value of crystal field stabilization energy.

➤ **Effect of Jahn-Teller Distortion on Electronic Spectra**

Jahn-Teller distortions affect the UV-visible spectra of many transition metal complexes in a significant manner and sometimes it is almost impossible to find out the values of the Racah parameter and crystal splitting energy if we do not take it into account. In UV-visible absorption spectroscopy, distortion causes the splitting of bands in the spectrum due to a reduction in symmetry (O_h to D_{4h}). The complexes undergoing Jahn-Teller distortion show an increased number of bands. Consider the following examples:

1. $[\text{Cr}(\text{H}_2\text{O})_6]^{2+}$: The Cr^{2+} ion in aqueous solutions is pale blue and its UV-visible absorption spectrum consists of a weak broad band with a maxima 14000 cm^{-1} . In normal conditions, this band is expected to provide the value of crystal field splitting value directly (from Orgel-diagram of d^4 -configuration); however, the actual value of Δ_o is considerably different. The electronic configuration for high-spin Cr^{2+} in the octahedral field is $t_{2g}^3 e_g^1$; and therefore, this complex is bound to undergo strong Jahn-Teller distortion. The energy level diagram and main transitions are shown below.

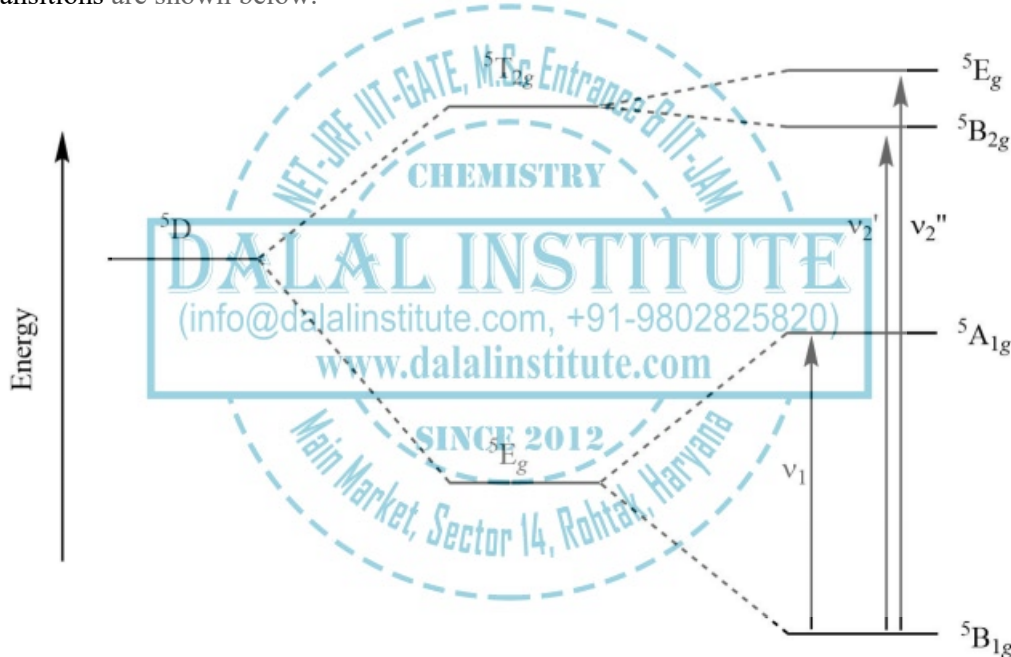
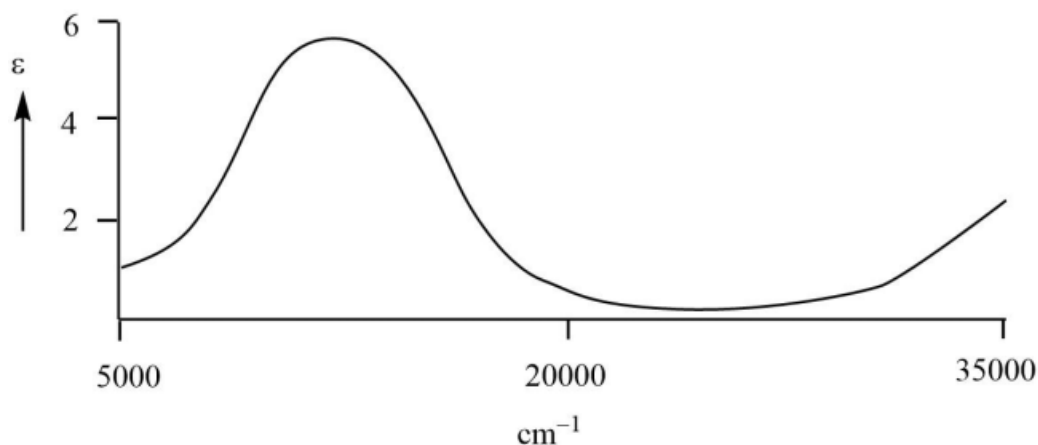


Figure 62. The schematic energy level diagram and prominent transitions in $[\text{Cr}(\text{H}_2\text{O})_6]^{2+}$.

The ground state term for a regular octahedral $[\text{Cr}(\text{H}_2\text{O})_6]^{2+}$ complex would be $5E_g$ but the ground as well as excited electronic state will undergo a Jahn-Teller distortion. It is worthy to note that the former state shows strong while splitting of later one is weak. Hence, the Tanabe-Sugano diagram cannot be used to describe the energy levels in the complex. The gaussian deconvolution of the overall spectrum has shown that the transition between the split components of the $5E_g$ level ($5B_{1g} \rightarrow 5A_{1g}$) occurs at around 10000 cm^{-1} and contributes to the low-energy tail of the broad band in aqueous solution.

Figure 63. UV-visible spectra of $[\text{Cr}(\text{H}_2\text{O})_6]^{2+}$.

The transitions from the ${}^5\text{B}_{1g}$ ground state to the components of the ${}^5\text{T}_{2g}$ state are unresolved and together give rise to the band at around 14000 cm^{-1} . Now, suppose that the Jahn-Teller effect produces a symmetrical splitting of the ${}^5\text{E}_g$ state, we can obtain the d -orbital splitting of the parent octahedral complex from the energy of the ${}^5\text{B}_{1g} \rightarrow {}^5\text{T}_{2g}$ transition minus half the energy of the ${}^5\text{B}_{1g} \rightarrow {}^5\text{A}_{1g}$ transition. This gives the estimated value of crystal field splitting value as follows:

$$\Delta_o = [v_2({}^5\text{B}_{1g} \rightarrow {}^5\text{T}_{2g})] - [v_1({}^5\text{B}_{1g} \rightarrow {}^5\text{A}_{1g})]/2$$

$$\Delta_o = 14000 - 10000/2 = 9000\text{ cm}^{-1}$$

Similar results have been observed in the low-temperature spectra of other hydrate complexes with Jahn-Teller distortion.

2. $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$: The Fe^{2+} ion in aqueous solutions is pale green and its UV-visible absorption spectrum is consisted of a weak broad band with a maxima 10000 cm^{-1} . The electronic configuration for high-spin Fe^{2+} in octahedral field is $t_{2g}^4 e_g^2$; and therefore, this complex is bound to undergo slight Jahn-Teller distortion. The ground state term for a regular octahedral $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$ complex would be ${}^5\text{T}_{2g}$ but the ground as well as excited electronic state will undergo a Jahn-Teller distortion. It is worthy to note that the former state shows strong while splitting of later one is weak.

Hence, the Orgel-diagram can be used to describe the energy levels in the complex. Moreover, as the band is obviously a doublet, we don't need gaussian deconvolution the overall spectrum. The transition from ${}^5\text{T}_{2g}$ to the split components of the ${}^5\text{E}_g$ level (${}^5\text{B}_{1g}$ and ${}^5\text{A}_{1g}$) are split by an energy difference of around 2000 cm^{-1} . This contributes to the broadening of the band in aqueous solution. The energy level diagram and main transitions are shown below.

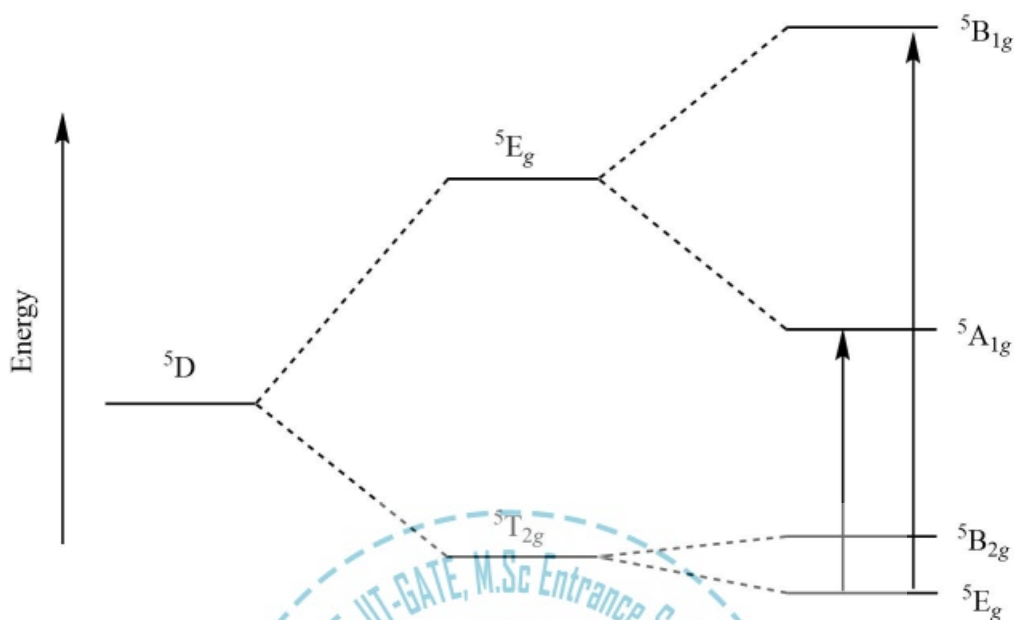


Figure 64. The schematic energy level diagram and prominent transitions in $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$.

The corresponding spectrum is given below.

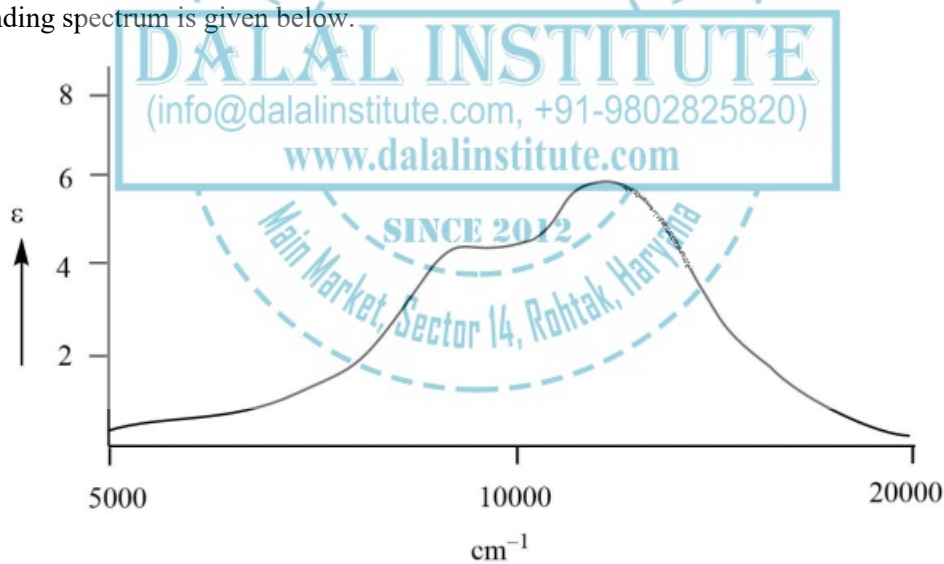


Figure 65. UV-visible spectra of $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$.

Now, suppose that the Jahn-Teller effect produces a symmetrical splitting of the 5E_g state, we can obtain the d -orbital splitting of the parent octahedral complex from the energy of the ${}^5T_{2g} \rightarrow {}^5E_g$ transition, and that value, in this case, is 10000 cm^{-1} . These results are rather similar to what we have observed in $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$. Both complexes possess Jahn-Teller distortion associated with the electronic degeneracy of t_{2g} orbital.

➤ **Static and Dynamic Jahn-Teller Distortion**

On the basis of the observed geometry, the Jahn-Teller distortion can be classified in two types as given below.

1. Static Jahn-Teller distortion: Some molecules show tetragonal shape under all conditions i.e., in solid state and in solution state; at lower and relatively higher temperatures. This is referred to as static Jahn-Teller distortion. Hence the distortion is strong and permanent. For example, in CuF_2 lattice

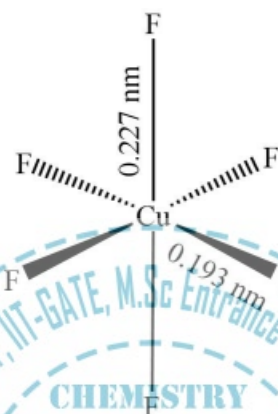


Figure 66. Static Jahn-Teller distortion in CuF_2 lattice.

2. Dynamic Jahn-Teller distortion: If the energy gap between z-out and z-in is smaller than the available thermal energy, the complex ions tend to attain both states, i.e., compressed and elongated. This is known as the "Dynamic Jahn Teller Effect". For examples, consider $\text{K}_2\text{Pb}[\text{Cu}(\text{NO}_2)_6]$ complex:

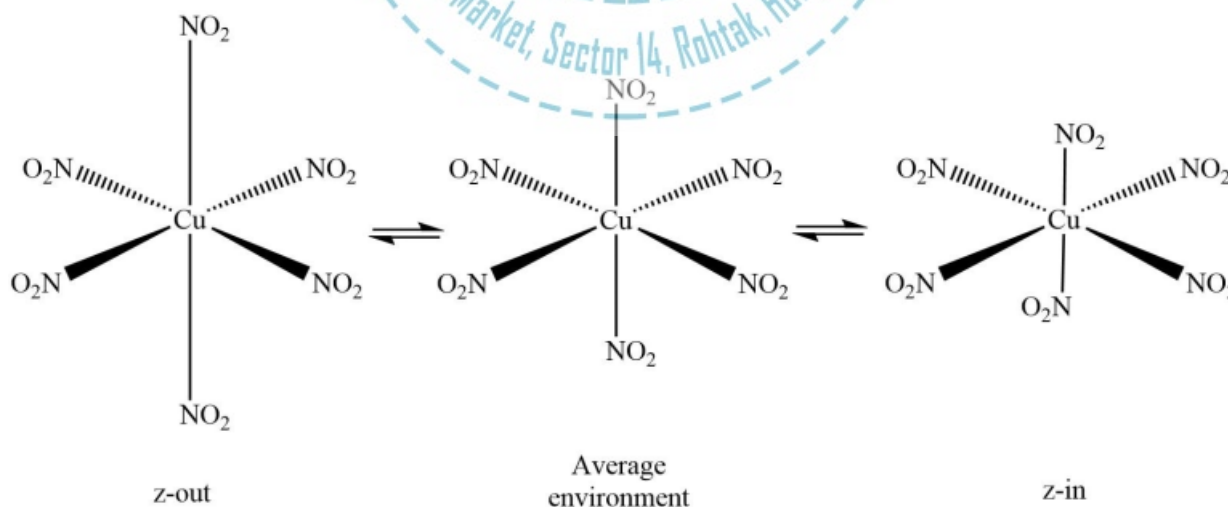


Figure 67. Dynamic Jahn-Teller distortion in $\text{K}_2\text{Pb}[\text{Cu}(\text{NO}_2)_6]$.

➤ **Consequences of Jahn-Teller Distortion**

Some of the main consequences of the Jahn-Teller effect in the field of chemical science are given below.

1. Irving-William series: Stability of metal complexes with a given ligand follows the order $\text{Mn}^{2+} < \text{Fe}^{2+} < \text{Co}^{2+} < \text{Ni}^{2+} < \text{Cu}^{2+} > \text{Zn}^{2+}$. The increase in the stability of the complexes from Mn^{2+} to Zn^{2+} is the increase effective nuclear charge. However, the exceptionally greater stability of Cu^{2+} complexes is the Jahn-Teller distortion.

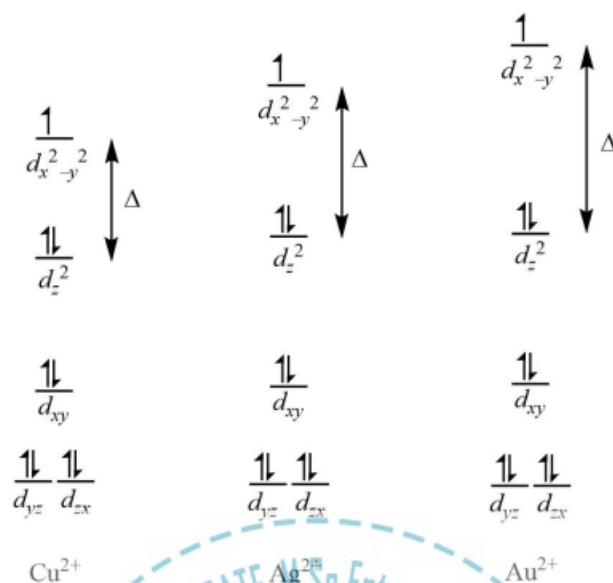


Figure 68. Variation of $\log K_1$ for the addition of first ethylenediamine.

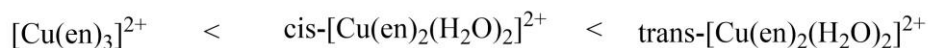
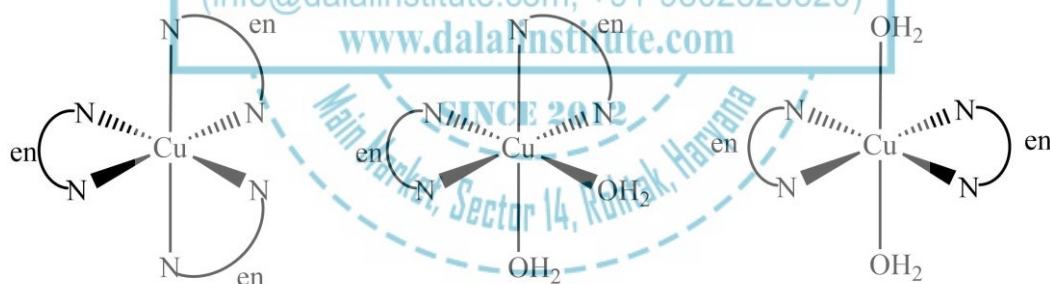
The sequence is generally quoted only for Mn(II) to Zn(II) as there is little or no data available for the other 3d series transition metal ions as their M(II) oxidation states are not very much stable. Crystal field theory is based on the idea that the interactions between the metal centre and the ligands-attached are purely ionic in nature; this suggests that the stability of the complexes should be related to the charge to radius ratio (ionic potential).

2. Disproportionation of Au^{2+} salts: Bivalent gold is less stable and undergoes disproportionation to form Au^{1+} and Au^{3+} . On the other hand, bivalent salts of Cu and Ag ions are quite common and relatively more stable. However, as far as the electronic configuration is concerned, all of the three belong to the same group and are d^9 systems.

Thus, a strong Jahn-Teller distortion is expected. The disproportion of Au^{2+} can be explained in terms of increasing Δ value down the group. Therefore, bivalent salts of gold would have the maximum magnitude of crystal field splitting, which results high destabilization associated with the filling of last electron (in $d_{x^2-y^2}$). This makes Au^{2+} to undergo either to form Au^{3+} , a d^8 system; or reduction to Au^{1+} , a d^{10} system. The d^8 system (Au^{3+}) is usually square-planar in geometry and quite stable as the electron from the $d_{x^2-y^2}$ is removed. The d^{10} system (Au^{1+}) is of linear geometry and stable due to fully filled configuration.

Figure 69. Variation of crystal field splitting energy for tetragonal Cu^{2+} , Ag^{2+} and Au^{2+} .

3. Stability order of ethylenediamine complexes of Cu^{2+} : Jahn-Teller distortion is responsible for the stability order of $[\text{Cu}(\text{en})_3]^{2+}$, $\text{cis-}[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$, $\text{trans-}[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$.

Figure 70. Stability order of $[\text{Cu}(\text{en})_3]^{2+}$, $\text{cis-}[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$, $\text{trans-}[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$.

Bivalent copper cannot form $[\text{Cu}(\text{en})_3]^{2+}$ because the Jahn-Teller distortion induces strain into the ethylenediamine molecule that is added along z-axis. Therefore, the only complex that exists is $[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$. Similarly, $\text{cis-}[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$ is less stable in comparison than $\text{trans-}[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$. The extra stability of $\text{trans-}[\text{Cu}(\text{en})_2(\text{H}_2\text{O})_2]^{2+}$ is because of the non-involvement of longer bonds in chelation.

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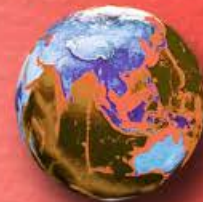
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Table of Contents

CHAPTER 1	11
Stereochemistry and Bonding in Main Group Compounds:.....	11
❖ VSEPR Theory	11
❖ $d\pi-p\pi$ Bonds	23
❖ Bent Rule and Energetic of Hybridization.....	28
❖ Problems	42
❖ Bibliography	43
CHAPTER 2	44
Metal-Ligand Equilibria in Solution:.....	44
❖ Stepwise and Overall Formation Constants and Their Interactions	44
❖ Trends in Stepwise Constants.....	46
❖ Factors Affecting Stability of Metal Complexes with Reference to the Nature of Metal Ion and Ligand.....	49
❖ Chelate Effect and Its Thermodynamic Origin.....	56
❖ Determination of Binary Formation Constants by pH-metry and Spectrophotometry.....	63
❖ Problems	68
❖ Bibliography	69
CHAPTER 3	70
Reaction Mechanism of Transition Metal Complexes – I:.....	70
❖ Inert and Labile Complexes.....	70
❖ Mechanisms for Ligand Replacement Reactions	77
❖ Formation of Complexes from Aquo Ions.....	82
❖ Ligand Displacement Reactions in Octahedral Complexes- Acid Hydrolysis, Base Hydrolysis....	86
❖ Racemization of Tris Chelate Complexes	89
❖ Electrophilic Attack on Ligands	92
❖ Problems	94
❖ Bibliography	95

CHAPTER 4	96
Reaction Mechanism of Transition Metal Complexes – II:	96
❖ Mechanism of Ligand Displacement Reactions in Square Planar Complexes.....	96
❖ The Trans Effect.....	98
❖ Theories of Trans Effect.....	103
❖ Mechanism of Electron Transfer Reactions – Types; Outer Sphere Electron Transfer Mechanism and Inner Sphere Electron Transfer Mechanism.....	106
❖ Electron Exchange.....	117
❖ Problems.....	121
❖ Bibliography.....	122
CHAPTER 5	123
Isopoly and Heteropoly Acids and Salts:	123
❖ Isopoly and Heteropoly Acids and Salts of Mo and W: Structures of Isopoly and Heteropoly Anions.....	123
❖ Problems.....	152
❖ Bibliography.....	153
CHAPTER 6	154
Crystal Structures:	154
❖ Structures of Some Binary and Ternary Compounds Such as Fluorite, Antifluorite, Rutile, Antirutile, Cristobalite, Layer Lattices - CdI_2 , BiI_3 ; ReO_3 , Mn_2O_3 , Corundum, Pervoskite, Ilmenite and Calcite.....	154
❖ Problems.....	178
❖ Bibliography.....	179
CHAPTER 7	180
Metal-Ligand Bonding:	180
❖ Limitation of Crystal Field Theory.....	180
❖ Molecular Orbital Theory – Octahedral, Tetrahedral or Square Planar Complexes.....	184
❖ π -Bonding and Molecular Orbital Theory.....	198
❖ Problems.....	212
❖ Bibliography.....	213

CHAPTER 8	214
Electronic Spectra of Transition Metal Complexes:	214
❖ Spectroscopic Ground States	214
❖ Correlation and Spin-Orbit Coupling in Free Ions for 1st Series of Transition Metals.....	243
❖ Orgel and Tanabe-Sugano Diagrams for Transition Metal Complexes ($d^1 - d^9$ States).....	248
❖ Calculation of Dq , B and β Parameters	280
❖ Effect of Distortion on the d -Orbital Energy Levels	300
❖ Structural Evidence from Electronic Spectrum	307
❖ Jahn-Teller Effect	312
❖ Spectrochemical and Nephelauxetic Series	324
❖ Charge Transfer Spectra	328
❖ Electronic Spectra of Molecular Addition Compounds.....	336
❖ Problems	340
❖ Bibliography	341
CHAPTER 9	342
Magnetic Properties of Transition Metal Complexes:	342
❖ Elementary Theory of Magneto-Chemistry	342
❖ Guoy's Method for Determination of Magnetic Susceptibility	351
❖ Calculation of Magnetic Moments	354
❖ Magnetic Properties of Free Ions.....	359
❖ Orbital Contribution: Effect of Ligand-Field	362
❖ Application of Magneto-Chemistry in Structure Determination	370
❖ Magnetic Exchange Coupling and Spin State Cross Over	375
❖ Problems	384
❖ Bibliography	385
CHAPTER 10	386
Metal Clusters:	386
❖ Structure and Bonding in Higher Boranes.....	386
❖ Wade's Rules.....	401

❖ Carboranes.....	407
❖ Metal Carbonyl Clusters- Low Nuclearity Carbonyl Clusters.....	412
❖ Total Electron Count (TEC).....	417
❖ Problems.....	424
❖ Bibliography.....	425
CHAPTER 11.....	426
Metal-II Complexes:	426
❖ Metal Carbonyls: Structure and Bonding.....	426
❖ Vibrational Spectra of Metal Carbonyls for Bonding and Structure Elucidation.....	439
❖ Important Reactions of Metal Carbonyls.....	446
❖ Preparation, Bonding, Structure and Important Reactions of Transition Metal Nitrosyl, Dinitrogen and Dioxygen Complexes.....	450
❖ Tertiary Phosphine as Ligand.....	463
❖ Problems.....	469
❖ Bibliography.....	470
INDEX.....	471



Mandeep Dalal

(M.Sc, Ph.D, CSIR UGC - NET JRF, IIT - GATE)

Founder & Director, Dalal Institute

Contact No: +91-9802825820

Homepage: www.mandeepdalal.com

E-Mail: dr.mandeep.dalal@gmail.com

Mandeep Dalal is an Indian research scholar who is primarily working in the field of Science and Philosophy. He received his Ph.D in Chemistry from Maharshi Dayanand University, Rohtak, in 2018. He is also the Founder and Director of "Dalal Institute", an India-based educational organization which is trying to revolutionize the mode of higher education in Chemistry across the globe. He has published more than 40 research papers in various international scientific journals, including mostly from Elsevier (USA), IOP (UK) and Springer (Netherlands) .

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Main Market, Sector 14, Rohtak, Haryana 124001, India

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