METAL LIGAND BONDING

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Three modern theories have been suggested to explain the nature of metal-ligand bonding in transition metal complexes.

➤ Valence Bond Theory, VBT (due to L. Pauling and J. L. Slater, 1935).

➤ Crystal Field Theory, CFT (due to H. Bethe, 1929 and J. Van Vleck, 1932)

➤ Ligand Field Theory, LFT or Molecular Orbital Theory, MOT (due to J. Van Vleck, 1935).

Valence Bond Theory (VBT)

Assumptions:

➤ The central metal atom provides a number of empty s, p and d atomic orbitals equal to it's co-ordination number for the formation of co-ordinate bond with ligand orbitals.

➤ Each ligand has at least one s-orbital containing a lone pair of electrons.

➤ The empty orbitals of the metal ion hybridise together to form hybrid orbitals which are equal in number as the atomic orbitals taking part in hybridisation. These are vacant, equivalent in energy and have definite geometry.

Different types of hybridisation in co-ordination compounds

C.N.	Hybridisation	Geometry	Examples
2	sp	Linear or diagonal	$[Ag(NH_3)_2]^+$
3	sp^2	Trigonal planar	$[HgI_3]^-$
4	sp^3	Tetrahedral	$[Ni(CO)_4]^0$, $\quad [NiX_4]^{2-}$, $(X= Cl^-, Br^-, I^-)$
4	$d\,sp^2$	Square planar	$[Ni(CN)_4]^{2-}$
5	$d\,sp^3$	Trigonal bipyramidal	$[Fe(CO)_5]^o$, $\quad [CuCl_5]^{3-}$
5	$sp^3\,d$	Square pyramidal	$[SbF_5]^{2-}$, $\quad IF_5$
6	$d^2\,sp^3$	Octahedral	$[Fe(CN)_6]^{3-}$, $[Co(NH_3)_6]^{3+}$
6	$sp^3\,d^2$	Octahedral	$[CoF_6]^{3-}$, $\quad [FeF_6]^{3-}$

- Empty hybrid orbital of the metal atom or ion overlap with the filled orbitals of the ligand to form ligand→metal coordinate bonds. $\left(L \overset{\sigma}{\longrightarrow} M\right)$

- The d-orbitals involved in the hybridisation may be either inner (n-1) d orbitals or the outer nd orbitals. The complexes thus formed are referred to as low spin or high spin complexes, respectively.

- If the complex has paired electrons, it is called diamagnetic while the complex containing one or more unpaired electrons is called paramagnetic.

- In complex formation, Hund's rule of maximum multiplicity is strictly followed.

(A) Complexes with co-ordination number 6:

These complexes have octahedral geometry due to $(n-1)$ d^2 ns np^3 (inner orbital) or ns np^3 nd^2 (outer orbital) hybridisation of central metal atom or ion.
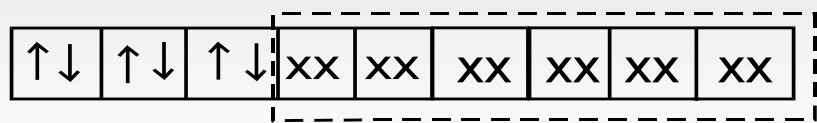
(i) d^2 sp^3 hybridisation in inner orbital octahedral complexes :

➢ This type of hybridisation takes place in those octahedral complexes which contain strong ligands. These are also called low spin or spin paired octahedral complexes due to lesser number of unpaired electrons. For the example.

• For the formation of octahedral complex through d^2sp^3 hybridization, the metal atom must have two 3d orbitals, one 4s and three 4p orbitals empty.

Hexaamine cobalt (III) ion, $[Co(NH_3)_6]^{3+}$

$3d^7$ $4s^2$ $4p$

$_{27}Co$, 18 [Ar] $3d^7 4s^2$

Co^{3+},   [Ar] $3d^6$

Co^{3+}, ion in $[Co(NH_3)_6]^{3+}$
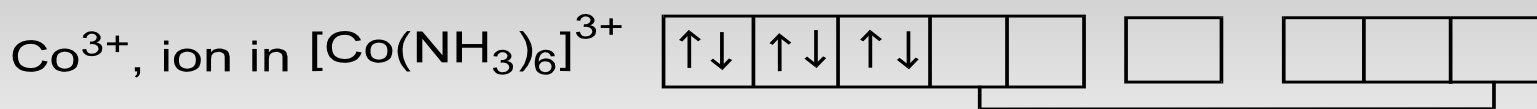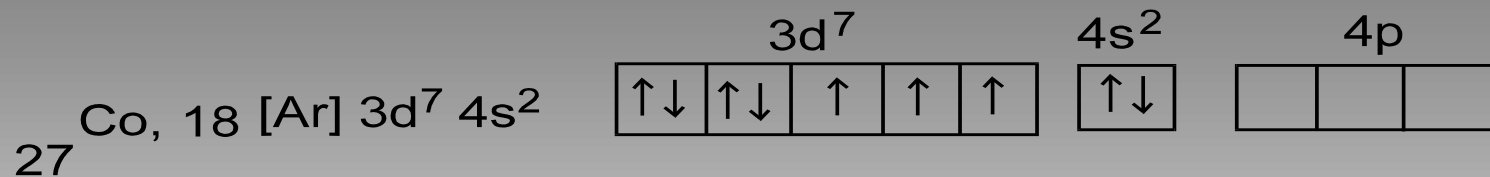
d^2sp^3 hybridisation

$[Co(NH_3)_6]^{3+}$

six d^2sp^3 hybrid orbitals

six coordinated bonds are formed by donating six electron pairs (xx) of six NH_3 molecules

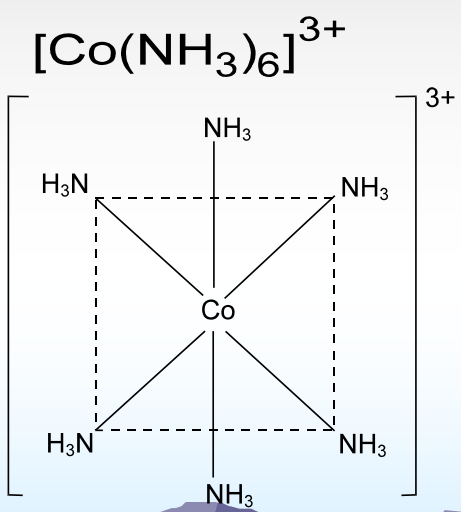Fig. 1: Octahedral shape of $[Co(NH_3)_6]^{3+}$ ion due to d^2sp^3 hybridisation
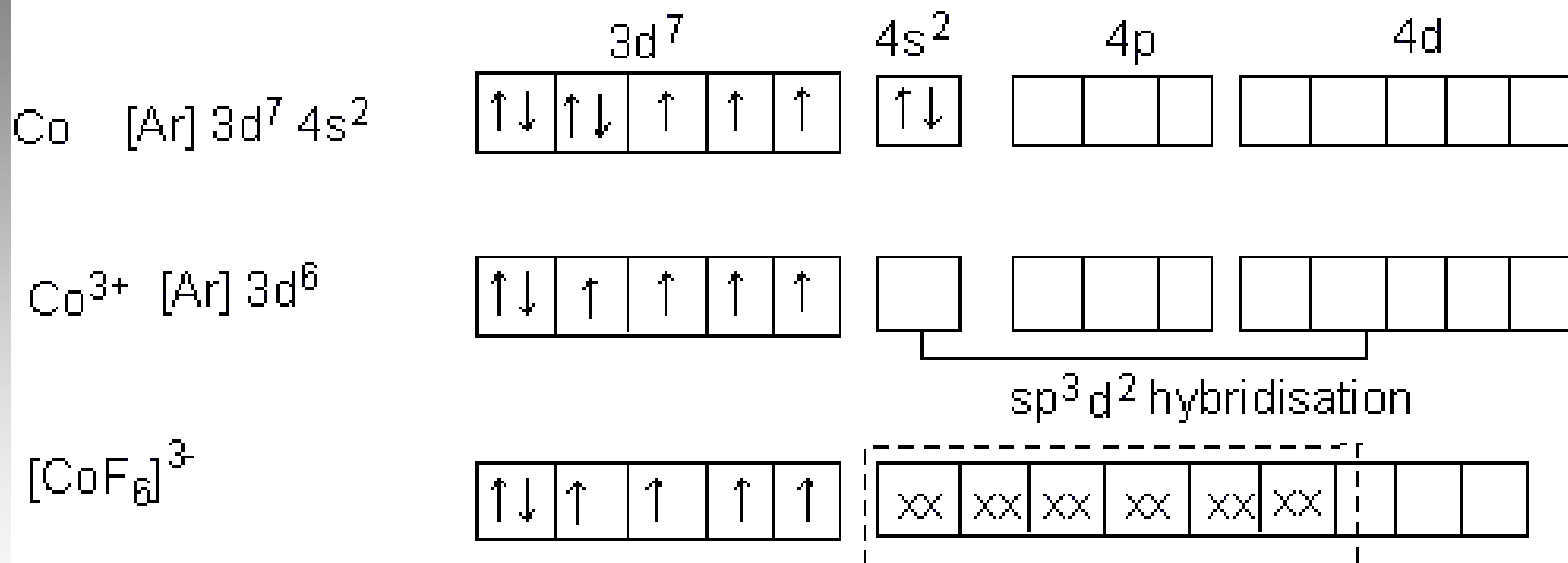
- Now Co^{3+} provides six empty orbitals to accommodate six pairs of electrons from six molecules of NH_3.

- This is achieved by the pairing of two 3d electrons as a result of the energy released due to the approach of strong ligands (NH_3).

- Since there are no unpaired electrons in the 3d orbitals in the complex, it is diamagnetic.

(ii) sp^3d^2 hybridisation in outer orbital octahedral complexes

Weak ligands containing octahedral complexes have sp^3d^2 hybridisation. These complexes are also called high spin or spin free octahedral complexes due to greater number of unpaired electrons. For example,

Hexafluoro cobaltate (III) ion, $[CoF_6]^{3-}$

Co $[Ar]\ 3d^7\ 4s^2$

$3d^7$ ↑↓ ↑↓ ↑ ↑ ↑ $4s^2$ ↑↓   4p   4d

Co^{3+} $[Ar]\ 3d^6$

$3d^6$ ↑↓ ↑ ↑ ↑ ↑

sp^3d^2 hybridisation

$[CoF_6]^{3}$

↑↓ ↑ ↑ ↑ ↑   xx xx xx xx xx xx

six sp^3d^2 hybrid orbitals

Six coordinate bonds are formed by donating six electron pairs (xx) of six F^- ions.

$[\ F^-\ F^-\ F^-\ Co\ F^-\ F^-\ F^-\ ]^{3-}$
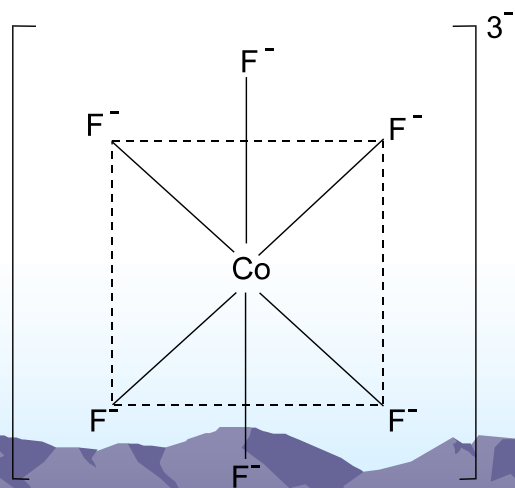
Fig. 2: Octahedral shape of $[CoF_6]^{3-}$ ion due to sp^3d^2 hybridisation

- Since weak ligands can not force the electrons of d_z^2 and $d_{x^2-y^2}$ orbitals in to the d_{xy}, d_{yz} and d_{zn} orbitals of the same shell. Thus we use nd^2 orbitals of outer shell.

- Now one 4s, three 4p and two 4d orbitals of cobalt ion are hybridised to give six sp^3d^2 hybrid orbitals, which accommodate six pairs of electrons from six F^- ions.

- This complex is found to be paramagnetic.
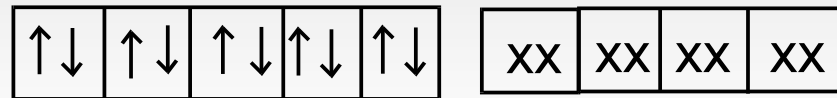
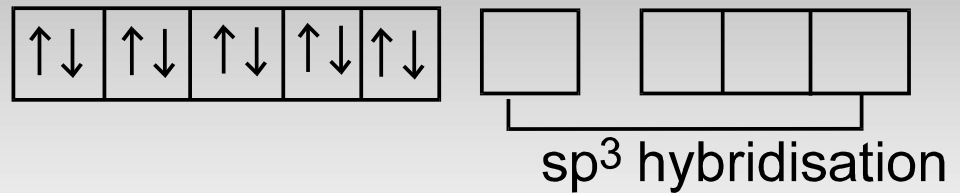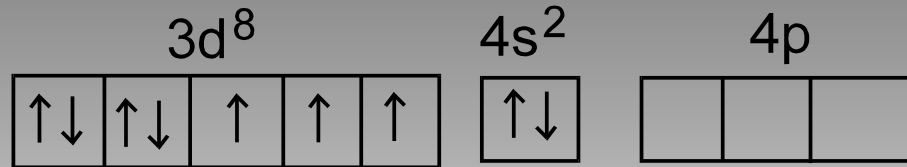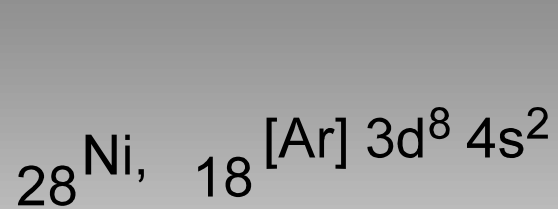**(B) Complexes with coordination number 4**

These complexes can be either tetrahedral or square planar depending upon hybridisation of central metal atom or ion.

(i) Tetrahedral complexes:

These complexes are formed by sp^3 hybridization, for example,

Tetracarbonyl nickel [Ni (CO)$_4$]

$3d^8$ $4s^2$ $4p$

$_{28}$Ni, $_{18}$[Ar] $3d^8$ $4s^2$

| ↑↓ | ↑↓ | ↑ | ↑ | ↑ | | ↑↓ | | | | |

Ni atom in Ni (CO)$_4$

| ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | | | | |

sp^3 hybridisation

[Ni (CO)$_4$]

| ↑↓ | ↑↓ | ↑↓ | ↑↓ | ↑↓ | | xx | xx | xx | xx |

Fig. 3: Tetrahedral shape of [Ni(CO)$_4$]

four sp^3 hybrid orbitals
four electron pairs (xx)
donated by 4CO molecules

- Due to the coordination No of Ni in tetracarbonyl nickel is 4, hence the complex can acquire either sp^3 or dsp^2 hybridisation.

- For sp^3 or dsp^2 hybridisation, 4s orbital must be made vacant.

- Since magnetic studies of $Ni(CO)_4$ have indicated that this complex is diamagnetic. Thus the two 4s electrons are forced to pair up with 3d orbitals.

- Now one 4s and three 4p orbitals are hybridised to form four sp^3 hybrid orbitals, which are accommodate 4 pairs of electrons from four CO molecules.

(II) Square planar complexes

These complexes are formed by either dsp^2 or sp^2d hybridisation.

(a) dsp^2 hybridisation :

Tetra cyano nickelate (II) ion, $[Ni(CN)_4]^{2-}$

	$3d^8$	$4s^2$	$4p$
Ni, [Ar] $3d^8 4s^2$	↑↓ ↑↓ ↑↓ ↑ ↑	↑↓	
Ni^{2+}ion [Ar] $3d^8$	↑↓ ↑↓ ↑↓ ↑ ↑		
Ni^{2+} ion in $[Ni(CN)_4]^{2-}$ for d sp^2 hybridisation	↑↓ ↑↓ ↑↓ ↑↓		

$d sp^3$ hybridisation

$[Ni(CN)_4]^{2-}$	↑↓ ↑↓ ↑↓ ↑↓ xx xx xx xx		

four dsp^2 hybrid orbitals

four electron pairs donated by four CN⁻ ions.
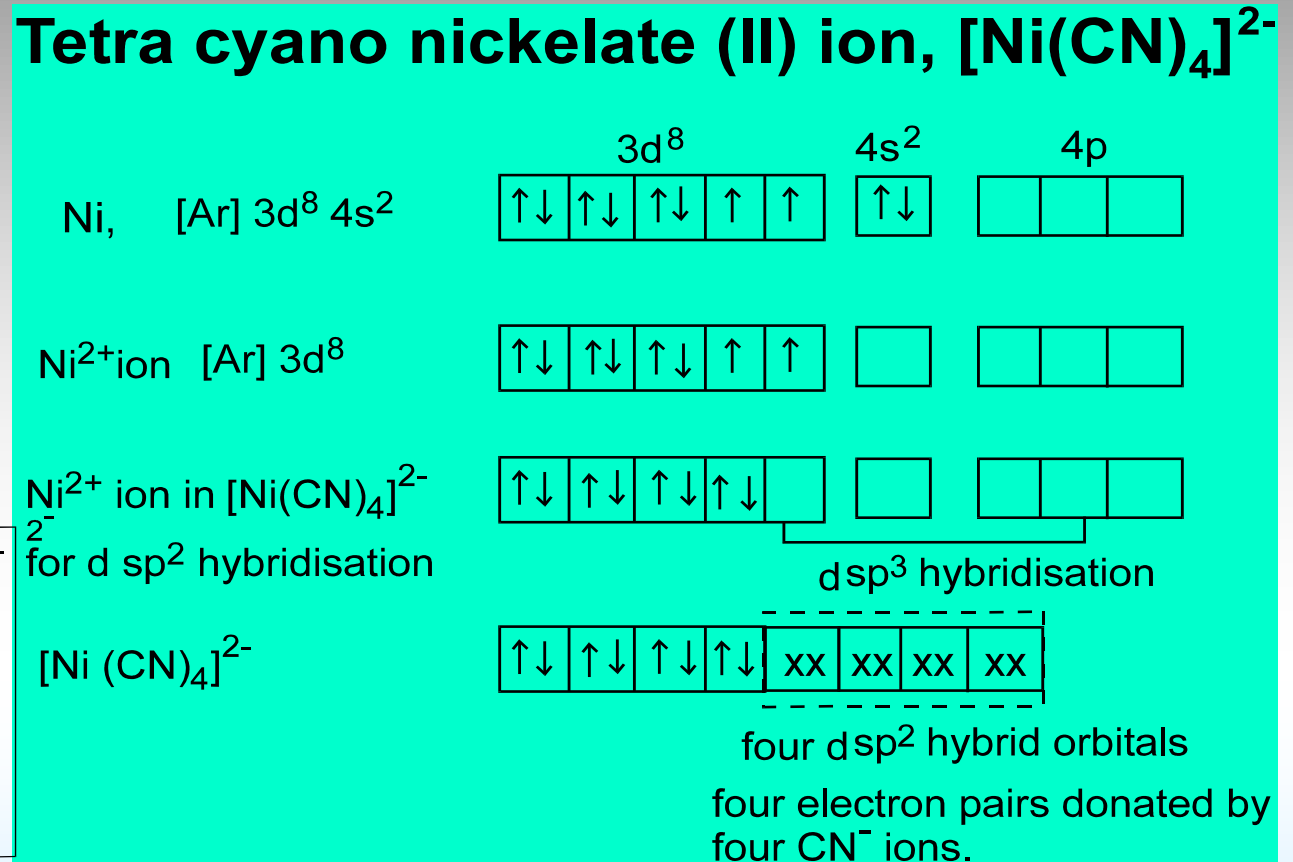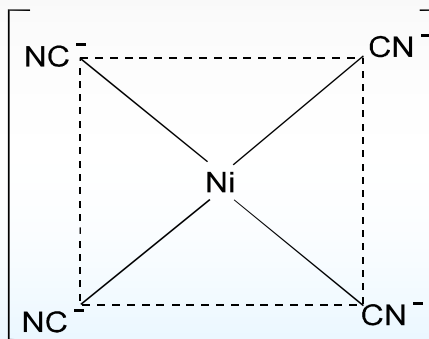
Fig. 4: Square planar shape of $[Ni(CN)_4]^{2-}$

NC⁻ — CN⁻

Ni

NC⁻ — CN⁻

- Due to co-ordination number 4 of Ni in this complex. It can acquire either sp^3 or dsp^2.

- It has been experimentally observed that the $[Ni(CN)_4]^{2-}$ complex is diamagnetic. This is possible only if two unpaired 3d-electrons are paired up.

- Since pairing makes one of the 3d-orbitals empty. Thus one 3d, one 4s and two 4p orbitals can be hybridised to form four dsp^2 hybrid orbitals.

- Now four cyanide ions donate lone pair of electrons to vacant dsp^2 hybrid orbitals to form metal-ligand co-ordinate bonds.

(b) sp²d hybridisation:

Tetramine copper (II) ion, $[Cu(NH_3)_4]^{2+}$

$3d^{10}$ $4s^1$ $4p$

$_{29}Cu, \ _{18}[Ar] \ 3d^{10} \ 4s^1$

Cu^{2+} ion $[Ar] \ 3d^9$

$4d$

$sp^2 d$ hybridisation

$[Cu \ (NH_3)_4]^{2+}$

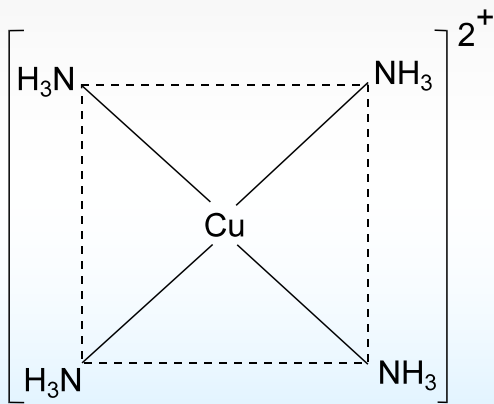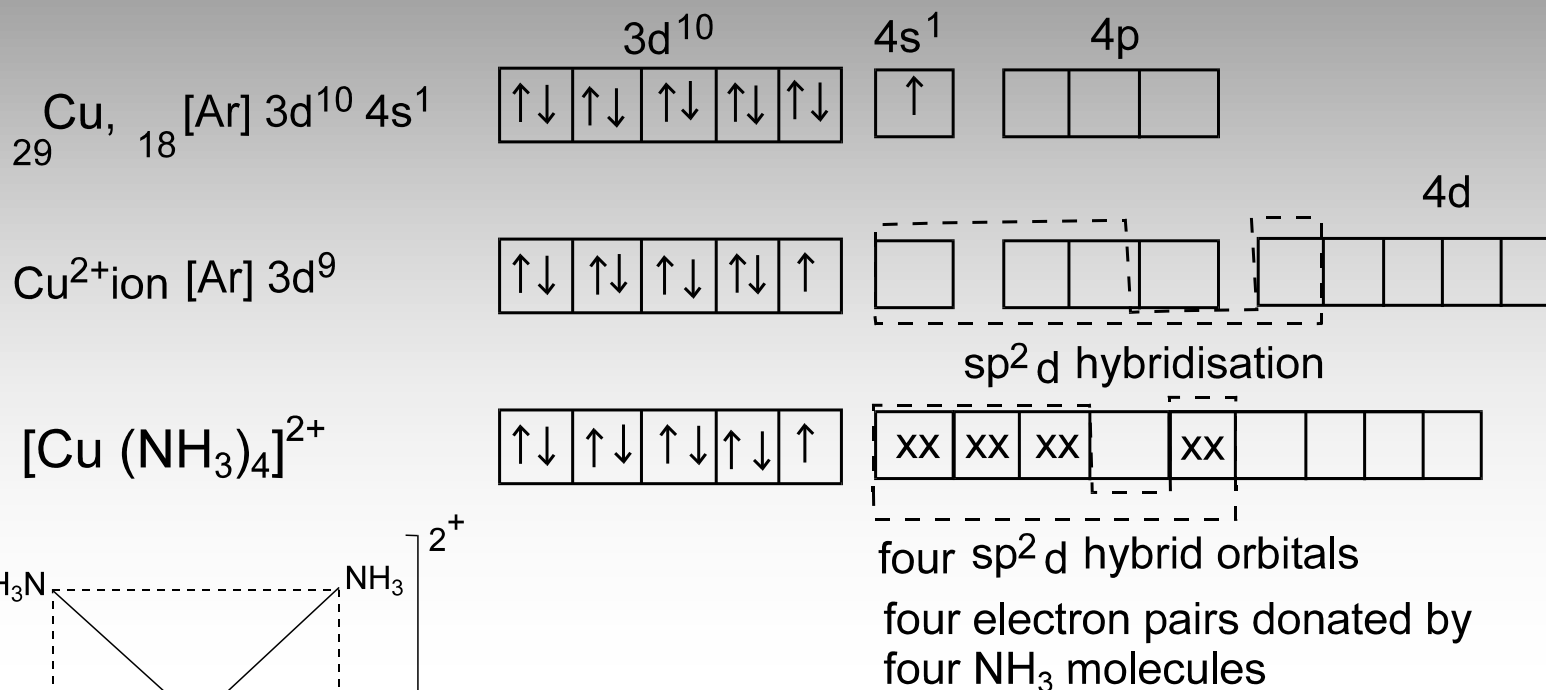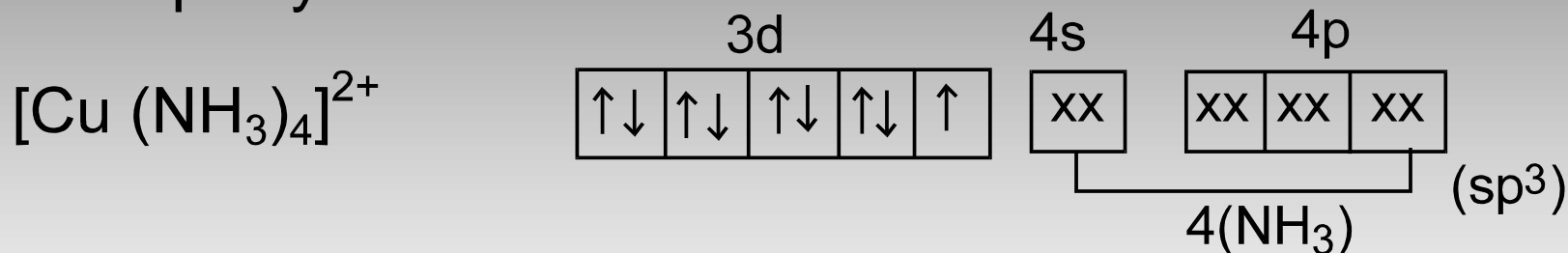four $sp^2 d$ hybrid orbitals

four electron pairs donated by four NH_3 molecules

Fig. 5: Square planar shape of $[Cu \ (NH_3)_4]^{2+}$

- Since the co-ordination number of Cu^{2+} ion in $[Cu(NH_3)_4]^{2+}$ is 4. It can be formed by sp^3 or dsp^2 as shown.

- For sp^3 hybridisation.

$[Cu (NH_3)_4]^{2+}$

3d					4s	4p		
↑↓	↑↓	↑↓	↑↓	↑	xx	xx	xx	xx

4(NH₃)   (sp3)

- For d sp^2 hybridisation (promoting the unpaired electron from 3d orbital to 4p orbital)

$[Cu (NH_3)_4]^{2+}$

3d					4s	4p		
↑↓	↑↓	↑↓	↑↓	xx	xx	xx	xx	↑

4(NH₃)   (dsp2)
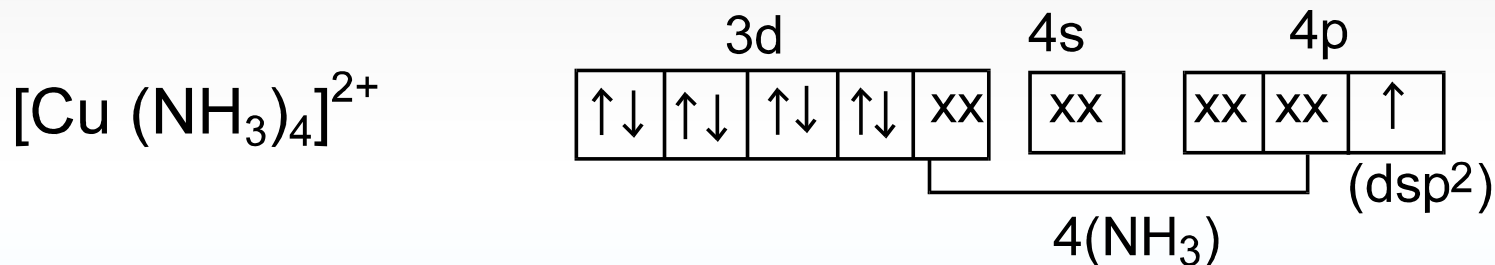
- Since both the configurations of $[Cu(NH_3)_4]^{2+}$ ion have one unpaired electron and hence the magnetic moment of this complex ion can not be used to predict it's geometry.

- Crystal structure determination has revealed that the complex has square planar structure. In this structure, the unpaired electron in 4p orbital belongs to higher energy level would be expected to be easily lost. i.e. the complex ion $[Cu(NH_3)_4]^{2+}$ could be easily oxidised to $[Cu(NH_3)_4]^{3+}$, which is not possible.

$$[Cu\ (NH_3)_4]^{2+} \xrightarrow[-e^-]{\text{Oxidation}} [Cu(NH_3)_4]^{3+}$$

(II)   (III)
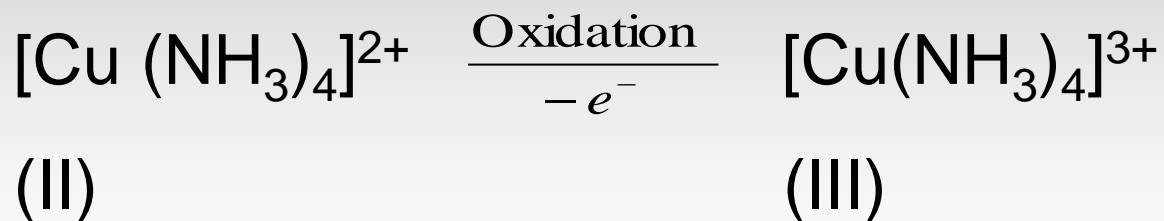
- Thus Huggin suggested that it has square planar geometry due to sp^2d hybridisation. This difficulty is removed in the crystal field theory.

LIMITATIONS OF VBT

- Octahedral (d^2sp^3 or sp^3d^2 hybridization), tetrahedral (sp^3) and square planar (dsp^2) complexes of d^1, d^2, d^3 and d^9 ion have the same number of unpaired electrons (i.e. 1,2,3, and 1 respectively) and hence can not be distinguished from each other.

- Outer orbital octahedral (sp^3d^2 hybridisation) and tetrahedral (sp^3) complexes of d^1 to d^9 ions have the same number of unpaired electron (i.e. 1, 2, 3, 4, 5, 4, 3, 2 and 1 respectively) can not be distinguished from each other.

- Complex formation of certain metal ions is totally unsatisfactory eg. dsp^2 hybridisation in Cu^{2+} ion is obtained by promoting one 3d electron to 4d orbital. Which occurs very rarely.

- This theory fails to explain why a particular structure is preferred e.g. d^8 ion form square planar complexes after maximum pairing. These ions may also form tetrahedral complexes.

- In this theory too much stress has been given to the metal ion while the importance of the ligand is not properly expressed.

- This theory does not predict magnetic behaviour quantitatively except the number of unpaired electrons in the complex.

- It does not explain thermodynamic properties of the complexes.

- This theory fails to explain the temperature dependent paramagnetism of the complexes.

- It can not explain why certain complexes are more labile than the other.

- This theory fails to explain why some metal complexes in a particular oxidation state are low spin, while some other complexes of the same metal ion in the same oxidation state are high spin. For example, $[Co(NH_3)_6]^{3+}$ and $[CoF_6]^{3-}$ in which cobalt is in +3 oxidation state, the former is low spin while the latter is high spin.

Crystal Field Theory (CFT)

Assumptions:

- The metal ion and ligands act as a point charges and bonding between them is purely electrostatic.

- There is no interaction between metal orbital and ligand orbitals.

- In the free metal atom or ion all the five d-orbitals possess the same energy (i.e. degenerate). Their degeneracy is destroyed by the ligands during complex formation.

Important features of CFT:

- A complex is considered to be a combination of central metal ion surrounded various ligands.

- The ligands in the complexes to be considered are either negatively charged ions e.g. F^-, Cl^-, CN^- etc. or neutral molecules e.g. H_2O and NH_3 etc. are regarded as dipole. If the ligand is neutral, the negative end of this ligand dipole is oriented towards the metal cation.

- This theory does not permit the electrons to enter the metal orbitals i.e. it does not consider any orbital overlap.

- CFT does not consider covalent bonding in complexes, but it is regarded as purely electrostatic or coulombic attraction between positively charged cation and negatively-charged ligands.

- The interaction between the electrons of the cation and those of ligands is purely repulsive. These repulsive forces cause the splitting of d-orbital of the metal cation into two groups.

- $d_{x^2-y^2}$ and d_{z^2} orbitals of e_g (higher energy)- Duplet.

- d_{xy}, d_{yz} and d_{zx} orbitals or t_{2g} (lower energy)-triplet.

- The splitting depends on whether the ligands are arranged in an octahedral, tetrahedral or square planar way around the central ion. This effect is known as crystal field splitting.

Crystal Field Splitting of d-orbitals

(A) Octahedral complexes

- Central metal ion is at the centre and the six ligands occupy the six corners of the octahedron (along the x, y and z axes).
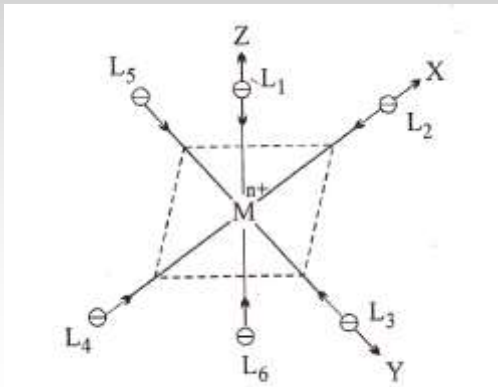

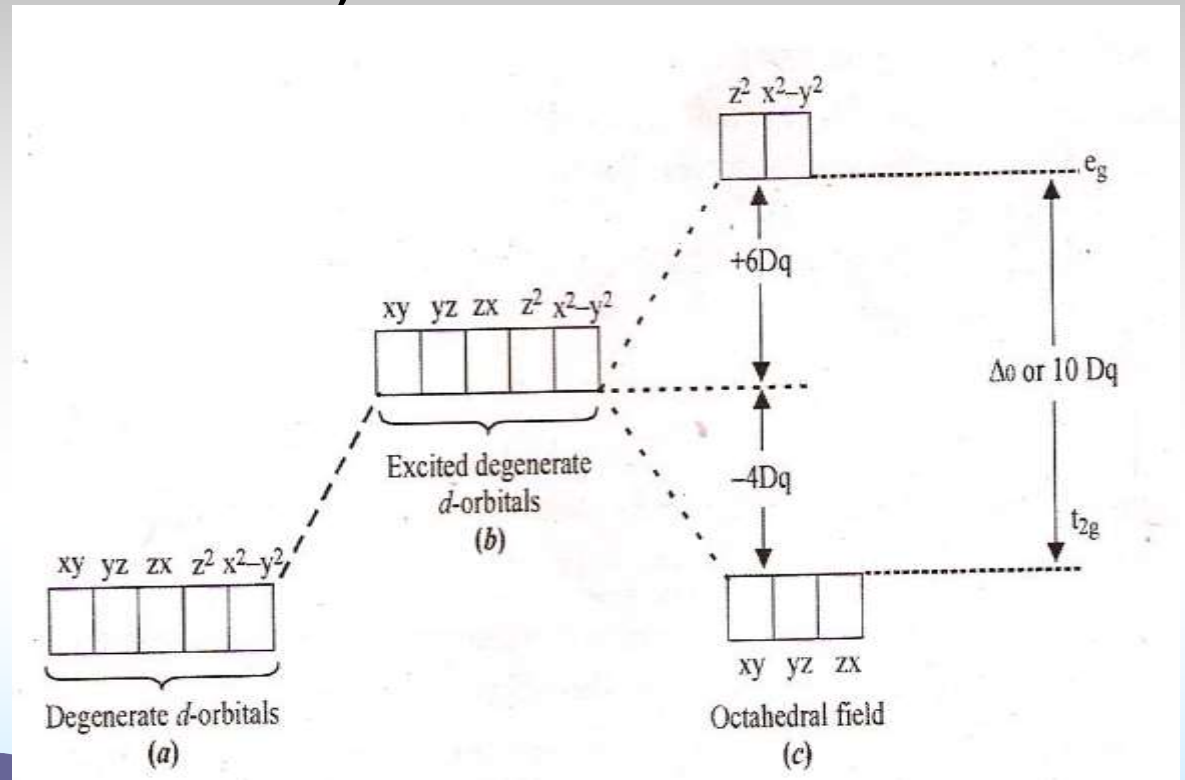Fig.6: Geometry of octahedral complex

Fig.7 : Crystal field splitting in an octahedral complex

- In an isolated gaseous metal ion, all the five d-orbitals are degenerate as shown at (a) of Fig.7

- When the six ligands approach the central metal ion, the electrons present in the d-orbitals are repelled by the lone pairs of the ligands. This repulsion will raise the energy of the d-orbitals to give five excited degenerate orbitals as shown at (b) of Fig.7

- The electrons present in d_{z^2} and $d_{x^2-y^2}$ orbitals (e_g set) experience greater repulsion than that present in d_{xy}, d_{yz} and d_{zx} orbitals (t_{2g}set) because the lobes of d_{z^2} and $d_{x^2-y^2}$ orbitals lie in the path of the approaching ligands.

- Hence under the influence of approaching ligands e_g set of orbitals is raised in energy while t_{2g} set is lowered in energy relative to the excited d-level as shown at (c) in Fig.7. The state C represents crystal splitting.

Crystal Field Stabilization Energy (CFSE)

The energy difference between eg and t_{2g} set of orbitals is measured in terms of Δ_o or 10Dq which is called crystal field stabilisation energy.

The geometry of an octahedral complex shows that

➢The energy of t_{2g} set is decreased by $2/5\Delta_o$ or $0.4\Delta_o$ (4Dq)

➢While the energy of e_g set is increased by $3/5\ \Delta_o$ or $0.6\Delta_o$(6Dq) that of exicted degenerated d-orbitals.

Strong and weak ligands and spectrochemical series

- Strong ligands have higher splitting power, while ligands have lower splitting power. Thus, strong ligands give higher value of Δ_o and weak ligands give smaller value of Δ_o .

- The common ligands can be arranged in order of their increasing splitting power and form a series which is called spectrochemical series as follows:

$I^- < Br^- < SCN^- < Cl^- < NO_3^- < F^- < OH^- = C_2O_4^{2-} < H_2O$
Weak field ligand
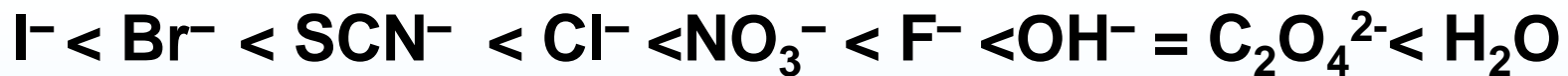
$< py < NH_3 < en < NO_2^- < CN^- < CO$
Strong field ligands

Table: Distribution of d-electrons in t_{2g} and e_g sets of orbitals of central metal ion surrounded by ligands in octahedral complexes.

No of electrons	Weak field ligand t_{2g} orbitals			e_g orbitals		CFSE	n	$s=\dfrac{n}{2}$	Strong field ligand t_{2g} orbitals			e_g orbitals		CFSE	n	$s=\dfrac{n}{2}$
$d^1(Ti^{3+})$	↑					-4Dq or -0.4Δ_o	1	$\dfrac{1}{2}$	↑					-4Dq or -0.4Δ_o	1	$\dfrac{1}{2}$
$d^2(Ti^{2+})$	↑	↑				-8Dq or -0.8Δ_o	2	1	↑	↑				-8Dq or -0.8Δ_o	2	1
$d^3(V^{2+})$	↑	↑	↑			-12Dq or -1.2Δ_o	3	$\dfrac{3}{2}$	↑	↑	↑			-12Dq or -1.2Δ_o	3	$\dfrac{3}{2}$
$d^4(Cr^{2+})$	↑	↑	↑	↑		-6Dq or-0.6Δ_o	4	2	↑↓	↑	↑			-6Dq or-0.6Δ_o	2	1
$d^5(Fe^{3+})$	↑	↑	↑	↑	↑	0	5	$\dfrac{5}{2}$	↑↓	↑↓	↑			0	1	$\dfrac{1}{2}$
$d^6(Co^{2+})$	↑↓	↑	↑	↑	↑	-4Dq + P or -0.4Δ_o+ P	4	2	↑↓	↑↓	↑↓			-4Dq + P or -0.4Δ_o+ P	0	0
$d^7(Co^{3+})$	↑↓	↑↓	↑	↑	↑	-8Dq + 2P or -0.8Δ_o+ 2P	3	$\dfrac{3}{2}$	↑↓	↑↓	↑↓	↑		-8Dq + 2P or -0.8Δ_o+ 2P	1	$\dfrac{1}{2}$
$d^8(Co^{2+})$	↑↓	↑↓	↑↓	↑	↑	-12Dq + 3P or -1.2Δ_o+ 3P	2	1	↑↓	↑↓	↑↓	↑	↑	-12Dq + 3P or -1.2Δ_o+ 3P	2	1
$d^9(Cu^{2+})$	↑↓	↑↓	↑↓	↑↓	↑	-6Dq + 4P or -0.6Δ_o+ 4P	1	$\dfrac{1}{2}$	↑↓	↑↓	↑↓	↑↓	↑	-6Dq + 4P or -0.6Δ_o+ 4P	1	$\dfrac{1}{2}$
$d^{10}(Zn^{2+})$	↑↓	↑↓	↑↓	↑↓	↑↓	0Dq + 5P	0	0	↑↓	↑↓	↑↓	↑↓	↑↓	0Dq + 5P	0	0

The following points may be concluded from the table:

(a) If the ligands are weak, Δ_o value will be small and all the five d-orbitals are singly occupied first and then pairing occurs. Thus, weak ligands gives higher number of unpaired electrons (n) or high spin value (S).(higher spin (HS) or spin free complexes).

(b) If the ligands are strong, Δ_o value will be higher and will first be paired in t_{2g} orbitals before going into e_g orbitals. Thus, strong ligands give minimum number of unpaired electrons (n) or smaller value of S (low spin (LS) or spin paired)

(i) The distribution of electrons of d^1, d^2, d^3, d^8, d^9 and d^{10} configurations in t_{2g} and e_g levels for both strong and weak field ligand is the same.

(ii) For each of d^4, d^5, d^6 and d^7 configurations there is a difference in the arrangement of electrons in weak and strong ligand fields.

(a) Tetrahedral Complexes

Let us consider a tetrahedral placed inside a cube as shown in Fig.8

➢ The four ligands occupy the alternate corners of a cube in the centre of which is placed the metal ion.
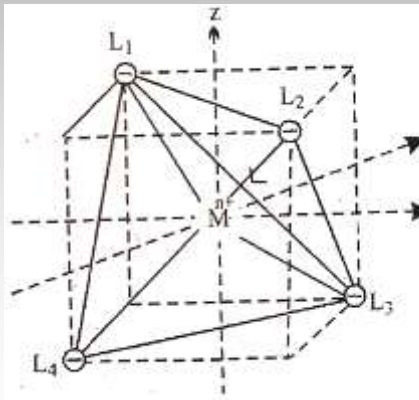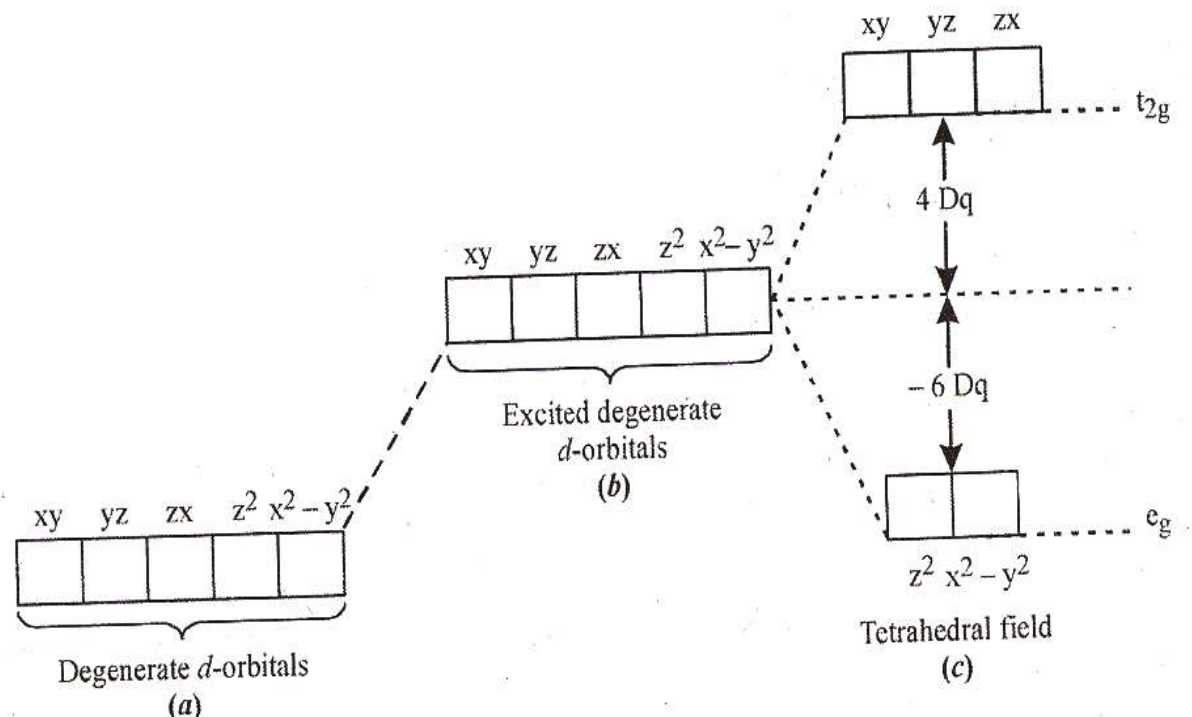

Fig.8: Geometry of tetrahedral c

Fig.9: Crystal field splitting in tetrahedral field.

- Since x, y and z axes pass through the centres of the six faces of the cube. Thus, these four ligands are lying between the axes x, y and z.

- Orbitals of t_{2g} set (d_{xy}, d_{yz} and d_{zx}) are also lying between the axes i.e., are lying directly in the path of the ligands. Thus these orbitals will experience greater force of repulsion than orbitals of e_g set (d_{z^2} and $d_{x^2-y^2}$).

- Thus the energy of t_{2g} orbitals will be increased while that of e_g orbitals will be decreased. Consequently, the d-orbitals split into two sets as shown in Fig.9.

- The order of energy of t_{2g} and e_g sets is the reverse of that observed in octahedral complexes. CFSE for tetrahedral complex is represented as Δ_t. It has been shown that Δ_t=0.45 Δ_0 i.e., $\Delta_t < \Delta_0$. The reason is as

a. Since in an octahedral complex there is a ligand along each axis while in a tetrahedral complex no ligand lies directly along any axis.

b. There are only four ligands in the tetrahedral complex while in an octahedral complex, there are six ligands. Thus the CFSE of tetrahedral complex (Δ_t) is less than octahedral complex (Δ_0).

Square Planar Complexes

If the two trans ligands on the z-axis are completely removed from octahedral geometry (Fig.6) we get a square planar geometry.
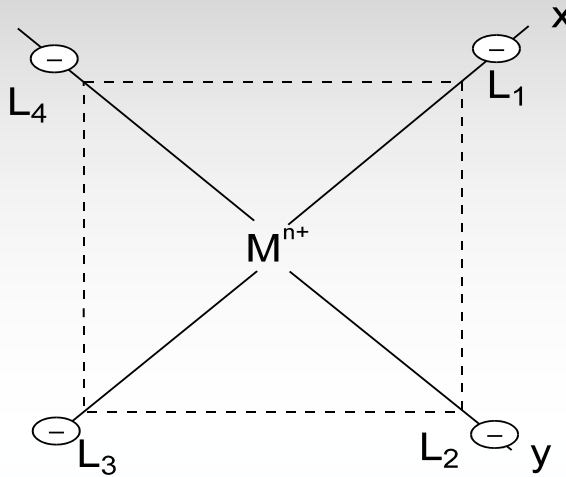

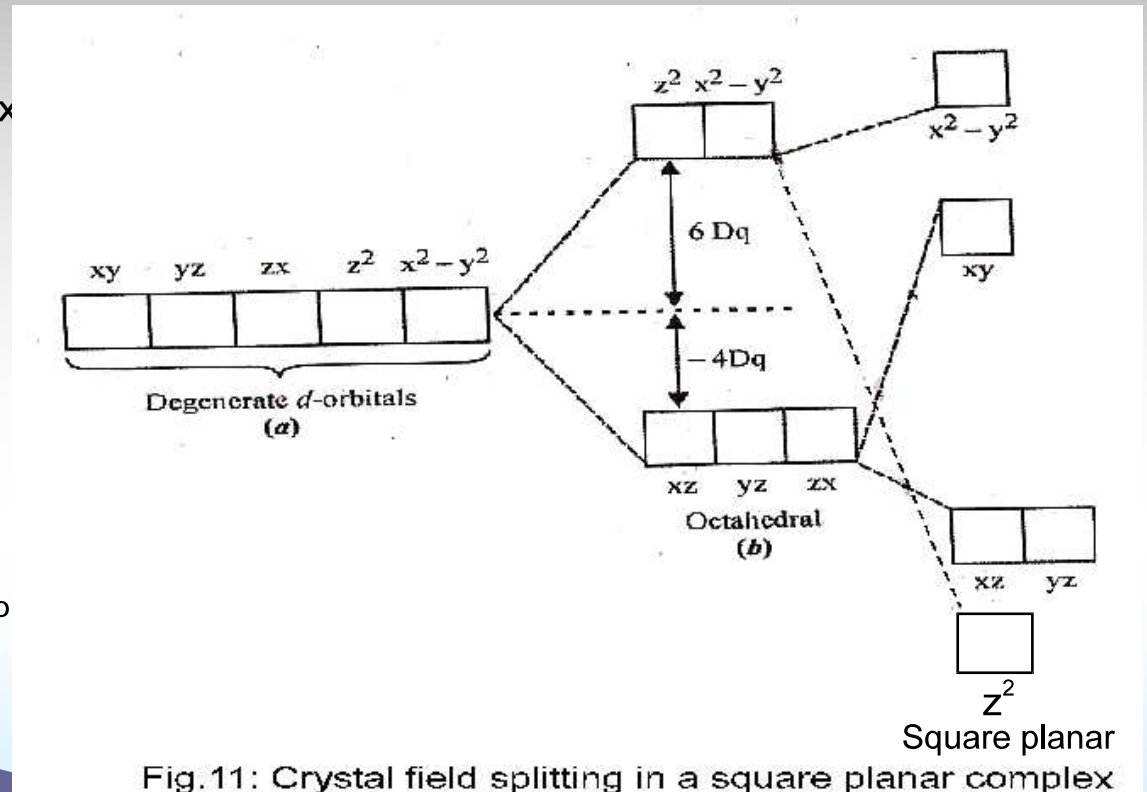Fig.10: Geometry of square planar comp

Square planar

Fig.11: Crystal field splitting in a square planar complex

- Since four ligands are lying in the x and y axis. Thus the increase in the energies of $d_{x^2-y^2}$ and d_{xy} orbitals and decrease in the energies of d_{xz}, d_{yz} and d_{z^2} orbitals are observed as shown in fig. 11.

- The crystal field splitting in a square planar complexes is donated by Δ_{sp}. It has been found that $\Delta_{sp} = 1.3\ \Delta_0$ i.e. $\Delta_{sp} > \Delta_0$.

Calculation of CFSE (Dq)

Let us consider d^{P+q} ion,

where   p= electrons in t_{2g} orbitals
               q = electrons in e_g orbitals.

Thus,

increase in energy due to q electrons in e$_g$ orbitals= 6Dq x q

loss in energy due to p electrons in t$_{2g}$ orbitals = - 4Dq x p

(+ and – signs indicate the increase and decrease in the energy of d-orbitals caused by their splitting).

Change in energy   = [-4Dq x p + 6Dq x q]
= (-4xp + 6 x q) Dq

If pairing of electrons in an orbital occurs then

crystal field stabilisation energy [(CFSE) for d^{p+q} ion
=(-4xp +6xq)Dq + mP
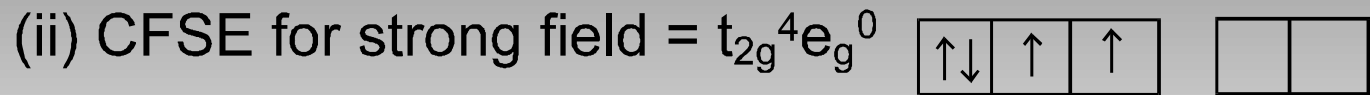
where   **P =   pairing energy** (i.e. the energy required to pair two   electrons   against   electron-electron repulsion in the   same orbital)

m = number of paired electrons.

for example, d^4 ion

(i) CFSE for weak field = $t_{2g}^3 e_g^1$

t_{2g} e_g

| ↑ | ↑ | ↑ | | ↑ | |

CFSE = $(-4 \times 3 + 6 \times 1)$ Dq + $0 \times$ P = -6Dq

(ii) CFSE for strong field = $t_{2g}^4 e_g^0$

| ↑↓ | ↑ | ↑ | | | |
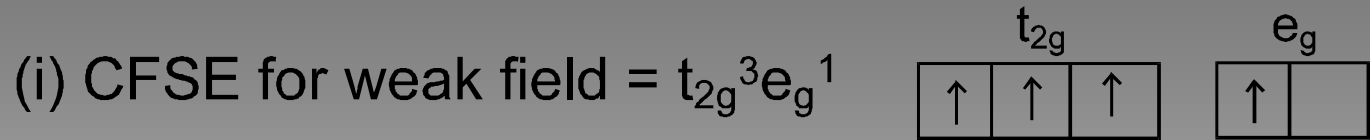
CFSE = $(-4 \times 4 + 6 \times 0)$ Dq + $1 \times$ P = -16Dq + P

Applications of crystal field theory

➢ **Colour of transition metal complexes:** The colour of transition metal complexes is due to d-d transitions between t_{2g} and e_g electrons.
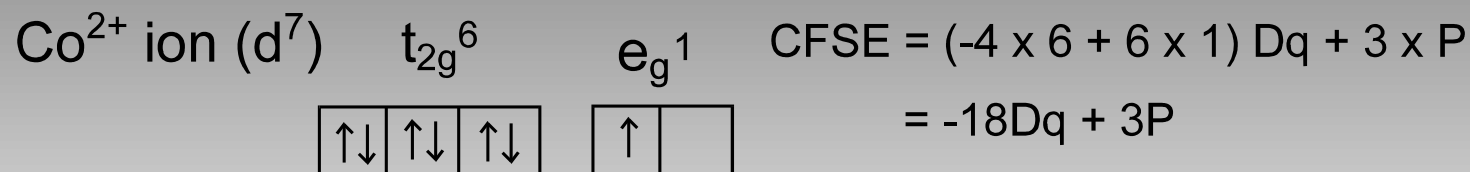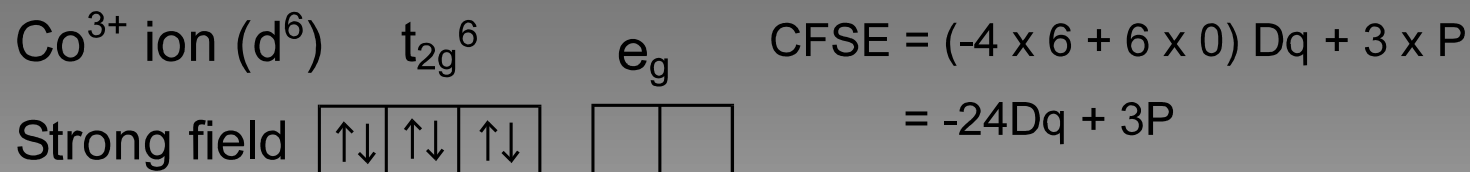
▪ If the energy difference between t_{2g} and e_g orbitals (i.e. D) for any complex is lower, the complex requires relatively low excitation energy and the complex is light in colour e.g. $[Co(H_2O)_6]^{2+}$ ion is pink in colour.

- If the Δ value for any complex is higher, i.e. the complex requires relatively large excitation energy and the complex is dark in colour e.g. $[Co(NH_3)_6]^{3+}$ ion is blue in colour.

➢ **Magnetic properties of complexes:** The crystal field theory is helpful in calculating the number of unpaired electrons in high and low spin complexes with the help of the following formula :

$$\mu_s = \sqrt{n(n+2)} \text{ B.M.}$$

where μ_s = Spin only moment and n= number of unpaired electrons.

➢ **Stabilisation of oxidation state:** CFSE values explains why certain oxidation states are stabilised by co-ordination with certain ligands. For example, If we consider the co-ordination of NH_3 molecule with Co^{2+} and Co^{3+} ions, it is seen that NH_3 molecule (a strong ligand) stabilises Co^{3+} ion by forming $[Co(NH_3)_6]^{3+}$ rather than Co^{2+} ion because Co^{3+} ion has much higher value of CFSE than Co^{2+} ion Co^{3+} ion.

Co^{3+} ion (d^6) t_{2g}^6 e_g CFSE = (-4 x 6 + 6 x 0) Dq + 3 x P

Strong field | ↑↓ | ↑↓ | ↑↓ | | | | = -24Dq + 3P

Co^{2+} ion (d^7) t_{2g}^6 e_g^1 CFSE = (-4 x 6 + 6 x 1) Dq + 3 x P

| ↑↓ | ↑↓ | ↑↓ | | ↑ | | = -18Dq + 3P

has much higher value of CFSE than Co^{2+} ion.

Limitations of CFT

- According to CFT, the metal ligand bonds are purely ionic. It gives no account of partial covalent character of the metal ligand bonds.

- It can not explain the relative strength of the ligands.

- CFT considers only d-orbitals of the metal ion and gives no consideration to other metal orbitals such as s, p_x, p_y and p_z.

- According to this theory π bonding is not possible in complexes while it exists in the complexes.