

Atomic Energy Central School, Indore

Class XII Chemistry CO-ORDINATION COMPOUNDS

Handout 5/6

Bonding in Coordination Compounds

Crystal Field Theory

The crystal field theory (CFT) is an electrostatic model which considers

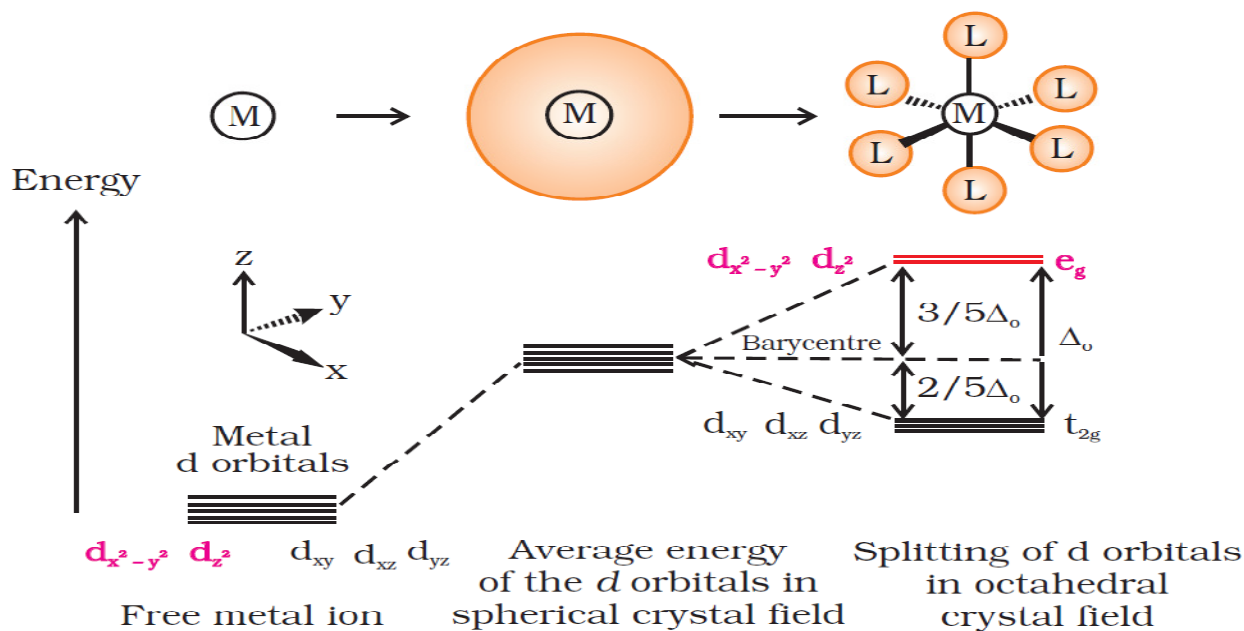
- the metal-ligand bond to be ionic
- Ligands are treated as point charges in case of anions or dipoles in case of neutral molecules.
- The five d orbitals in an isolated gaseous metal atom/ion are degenerate.
- However, in the presence of negative field is due to ligands, it becomes asymmetrical and the degeneracy of the d orbitals is lifted. It results in splitting of the d orbitals.
- The pattern of splitting depends upon the nature of the crystal field.

(a) Crystal field splitting in octahedral coordination entities

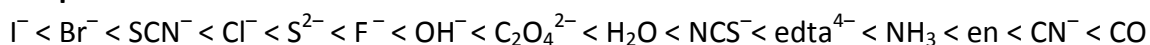
The six ligands surrounding the metal atom/ion octahedrally, will face repulsion with the electrons in metal d orbitals (e_g set), $d_{x^2-y^2}$ and d_{z^2} which point towards the axes.

These orbitals will experience more repulsion and will be raised in energy; and the (t_{2g} Set) d_{xy} , d_{yz} and d_{xz} orbitals which are directed between the axes will be lowered in energy relative to the average energy in the spherical crystal field.

This splitting of the degenerate levels due to the presence of ligands in a definite geometry is termed as crystal field splitting and the energy separation is denoted by Δ_o .



A series in which the ligands are arranged in a series in the order of increasing field strength is termed as **spectrochemical series**.



For d^4 ions, two possible patterns of electron distribution arise:

(i) If $\Delta_o < P$, the fourth electron enters one of the e_g orbitals giving the configuration $t_{2g}^3 e_g^1$

Ligands for which $\Delta_o < P$ are known as *weak field ligands* and form high spin complexes.

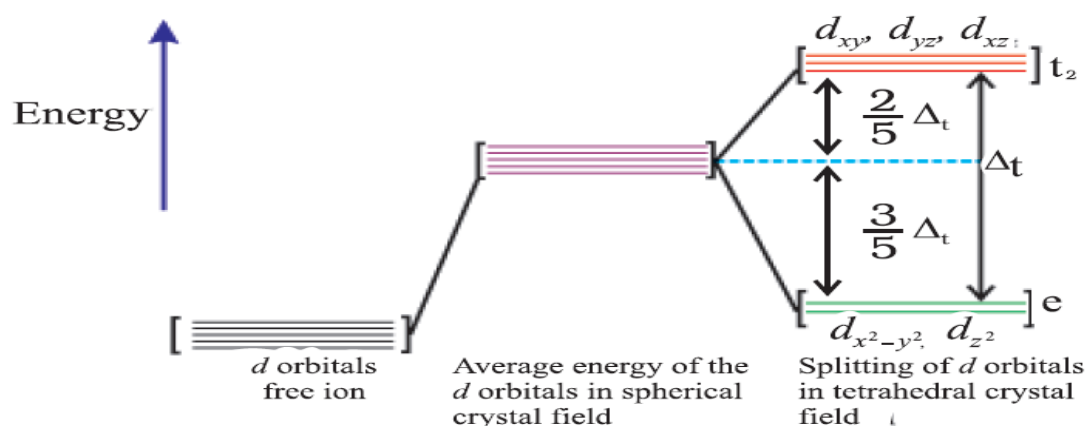
(ii) If $\Delta_o > P$, it becomes more energetically favourable for the fourth electron to occupy a t_{2g} orbital with configuration $t_{2g}^4 e_g^0$.

Ligands which produce this effect are known as *strong field ligands* and form low spin complexes.

(b) Crystal field splitting in tetrahedral coordination entities

In tetrahedral coordination entity formation, the (t_{2g} Set) d_{xy} , d_{yz} and d_{xz} orbitals which are directed along the axes will be higher in energy relative to the average energy in the spherical crystal field.

It is seen that $\Delta_t = (4/9) \Delta_o$. Consequently, the orbital splitting energies are not sufficiently large for forcing pairing and, therefore, low spin configurations are rarely observed.



Colour in Coordination Compounds

The crystal field theory attributes the colour of the coordination compounds to ***d-d transition*** of the electron. In an octahedral complex, the electron will excite from t_{2g} level to the e_g level on absorption of light energy and on returning back it emits radiation of complementary colour to the colour absorbed.

Limitations of Crystal Field Theory

The crystal field model is successful in explaining the formation, structures, colour and magnetic properties of coordination compounds to a large extent.

However, it could not explain:

- anionic ligands, though being negative, are found at the low end of the spectrochemical series.
- it does not take into account the covalent character of bonding between the ligand & the central atom.