

DISTRIBUTION OF d-ELECTRONS IN d_{xy} & d_{yz} ORBITALS IN OCTAHEDRAL COMPLEXES

The distribution of d-electrons in d_{xy} and d_{yz} orbital takes place on the basis of the nature of the ligands, i.e. whether the ligands are weaker or stronger.

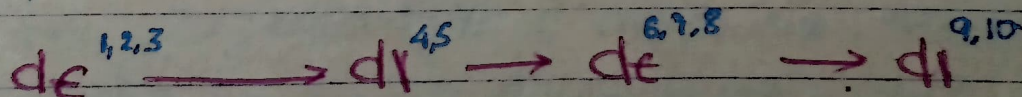
Thus two cases arise:—

P Δ_0 (i) ^{Weak field} When the ligands are weaker: \rightarrow (High spin complex.)

It has been that under the influence of weaker ligands the energy difference, Δ_0 between d_{xy} and d_{yz} orbitals is comparatively small and so, all the five d-orbitals of these two orbitals may be supposed to be degenerate. i.e. in presence of weaker ligands all the d-orbitals have the same energy, and consequently the distribution of d-electrons in d_{xy} & d_{yz} sets takes place according to Hund's rule, which states, electron will pair up only when each of the five d-orbitals is at least singly filled.

It may be clearly understood by means of the following example.

The d-orbital contains 10 electrons, hence in this case electron nos. 1, 2, 3 go to d_{xy} level, and 4, 5 go to the d_{yz} level, then 6, 7, 8 (three electrons) go to d_{xy} level and the remaining two electrons 9 & 10 will occupy d_{yz} sets.



For example, if we consider the octahedral complex i.e. $[\text{CoF}_6]^{3-}$, which contains weaker ligands, the distribution of six d-electrons of Co^{3+} ion ($\text{Co}^{3+} - 3d^6$) in d_{xy} & d_{yz} sets will be d_{xy}^4, d_{yz}^2 . This complex which contains weaker field

Ligands are referred as weak field or low field complex.

In the formation of such type of complex $\Delta_o < P$, where P is average pairing energy, which is the energy required to pair two electrons in the same orbital, & Δ_o is Octahedral Crystal field splitting Energy.

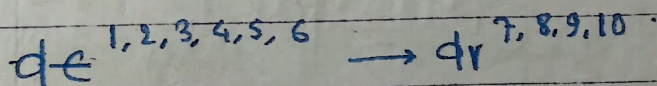
(ii) When the ligands are stronger \rightarrow (Strong field) or high spm complex.

$P > \Delta_o$

Now we consider the octahedral complexes containing stronger ligands, the distribution of d -electrons in d_e and d_f sets does not obey Hund's rule.

Thus in stronger field the first six electrons numbered as 1, 2, 3, 4, 5 & 6, these electrons will go to d_e set and the remaining four electrons numbered as 7, 8, 9 & 10 enters into d_f set.

This can be shown as:—



Let us consider on the distribution of six d electrons of Co^{+3} ion ($Co^{+3} \rightarrow 3d^6$) in the complex ion $[Co(NH_3)_6]^{3+}$

which contains stronger ligand, thus it is quite obvious that the

distribution will be taken as $d_e^6 d_f^0$ i.e. $t_{2g}^6 e_g^0$

(where t_{2g} stands for triply degenerate and e_g stands for doubly degenerate orbitals).

The complex which contains stronger field ligand like NH_3 is called strong field complex or high field complex.

For these complex, $\Delta_o > P$
i.e. the C.F. splitting in octahedral complex is greater than the pairing energy.