

Crack CSIR-NET 2021

(Study Notes on CFT)



Crystal Field Theory (CFT)

This theory describes the interaction between transition metals and ligands. There is an attraction between the metal ion (having positive charge) and non-bonding electrons of ligands (having negative charge). When ligands tend to approach the central metal ion, degeneracy of d or f orbital is lifted due to the production of static electric field which is present due to surrounding charge distribution. This theory helps to explain certain characteristics like magnetic properties, color, and hydration energies. There occurs a repulsion between the electrons in d orbital of the central atom and those present in the ligand, as a result, electrons of d orbitals which are closer to the ligand will be higher in energy than those further away which results in splitting in energy of d orbitals. There are three factors on which splitting generally depends:

Nature of metal ion

Oxidation state of the metal ion

Arrangement of the ligands around central atom

Nature of ligands surrounding metal ion

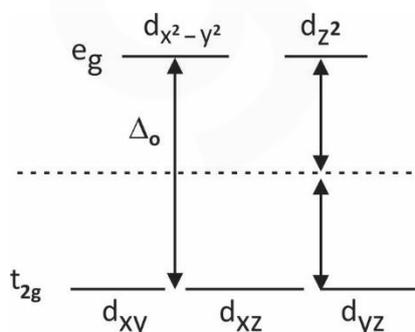
Splitting in octahedral complexes:

In an octahedral, six ligands are present around the central atom. The splitting of d orbital takes place into two levels:

Bottom three energy levels(t_{2g})- d_{xy} , d_{yz} , d_{xz}

Upper two energy levels(e_g)- $d_{x^2-y^2}$, d_{z^2}

In an octahedral complex, the attraction of electrons takes place towards the axis. An orbital having a lobe on the axis will move to a higher energy level. It means energy of e_g levels are higher as compared to t_{2g} levels.



Tetrahedral complexes:

In tetrahedral complexes, four ligands are present around the central atom. The splitting of d orbital takes place into two levels:

Top three energy levels(t_{2g})- d_{xy} , d_{yz} , d_{xz}

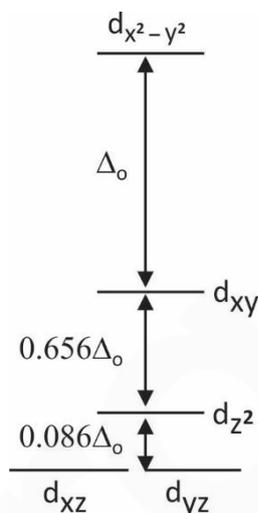
Bottom two energy levels(e_g)- $d_{x^2-y^2}$, d_z^2

The reason behind this splitting is due to poor overlapping of the orbital between metal and ligand. In this, orbitals are directed on the axes, but ligands are not.

Square planar complexes:

In square planar complexes, four ligands are present around the central atom. In this, electrons of ligands get attracted towards the xy plane only. The four different energy level for this complex are:

$d_{x^2-y^2}$, d_z^2 , d_{xy} and both d_{yz} , d_{xz} .



Crystal field stabilization energy:

It is the difference between the ligand field energy and energy in an isotropic field. There are mainly four factors on which CFSE depends:

Geometry

Number of d electrons

Spin pairing energy

Nature of the ligand

The complete detail of the splitting of d orbital along with nature of ligand in both octahedral and tetrahedral environment is given below:

Total d-electrons	CFSE(Octahedral)		CFSE(Tetrahedral)	
	High Spin	Low Spin	Configuration	Always High Spin*
d^0	$0 \Delta_o$	$0 \Delta_o$	e^0	$0 \Delta_t$
d^1	$-2/5\Delta_o$	$-2/5\Delta_o$	e^1	$-3/5\Delta_t$
d^2	$-4/5\Delta_o$	$-4/5\Delta_o$	e^2	$-6/5\Delta_t$
d^3	$-6/5\Delta_o$	$-6/5\Delta_o$	$e^2 t_2^1$	$-4/5\Delta_t$
d^4	$-3/5\Delta_o$	$-8/5\Delta_o + P$	$e^2 t_2^2$	$-2/5\Delta_t$
d^5	$0 \Delta_o$	$-10/5\Delta_o + 2P$	$e^2 t_2^3$	$0\Delta_t$
d^6	$2/5\Delta_o$	$-12/5\Delta_o + P$	$e^3 t_2^3$	$-3/5\Delta_t$
d^7	$-4/5\Delta_o$	$-9/5\Delta_o + P$	$e^4 t_2^3$	$-6/5\Delta_t$
d^8	$-6/5\Delta_o$	$-6/5\Delta_o$	$e^4 t_2^4$	$-4/5\Delta_t$
d^9	$-3/5\Delta_o$	$-3/5\Delta_o$	$e^4 t_2^5$	$-2/5\Delta_t$
d^{10}	0	0	$e^4 t_2^6$	$0\Delta_t$

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