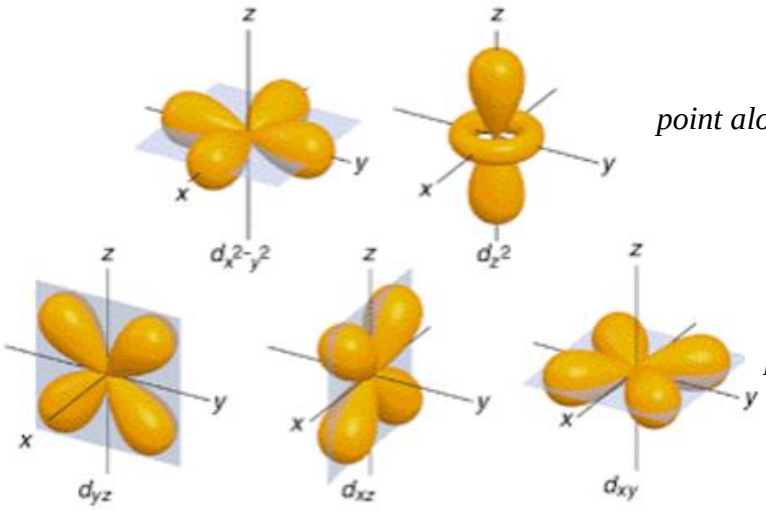
CRYSTAL FIELD THEORY (CFT)

BASIC CONCEPT OF CFT

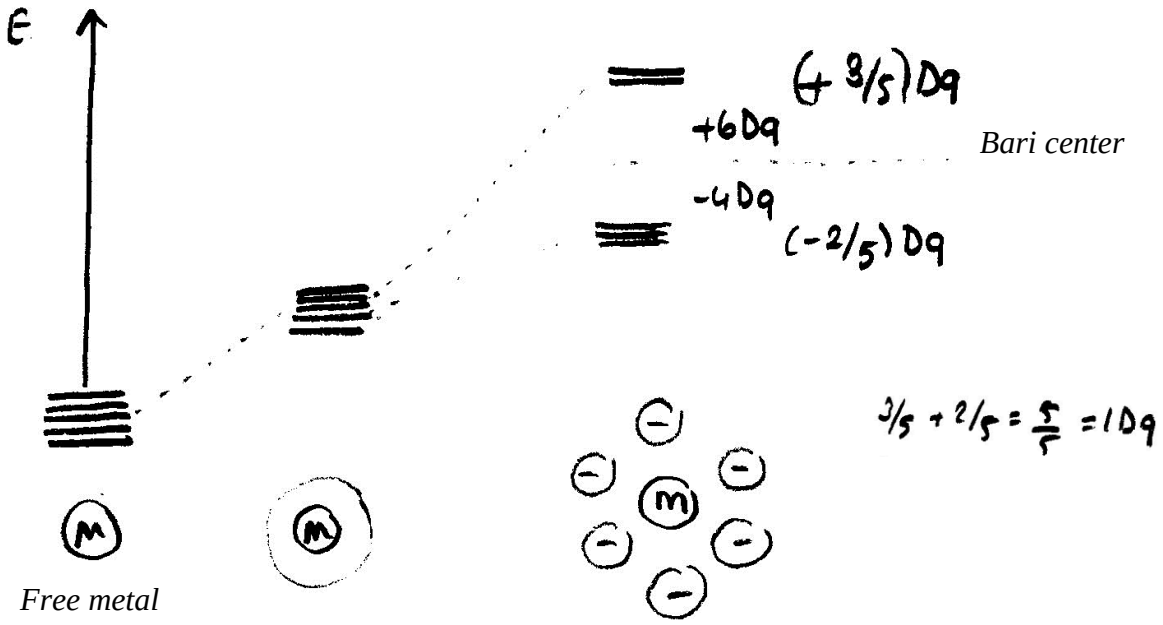
According to the CFT, each ligand creates a negative electrical field around itself. The cleavage of d orbitals to different energy levels is due to the different interaction of d orbitals with ligands. In the free metal ion, the (n-1)d orbitals of the metal have equal energies. The lobes of two of these orbitals ($d_{x^2-y^2}$ ve d_{z^2}) point along the x-, y-, z-axes, while the lobes of the other three (d_{xy}, d_{xz}, d_{yz}) point in between the axes.



point along the axes

point along in between the axes

THE ORBITAL SPLITTING DIAGRAM FOR OCTAHEDRAL COMPLEXES



Free metal ion M

Global field (a)

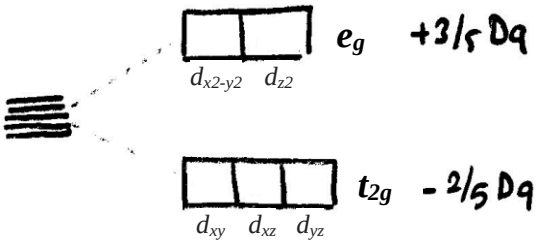
This happens when we put the center atom at the center of the sphere loaded with electricity

Octahedral field (b)

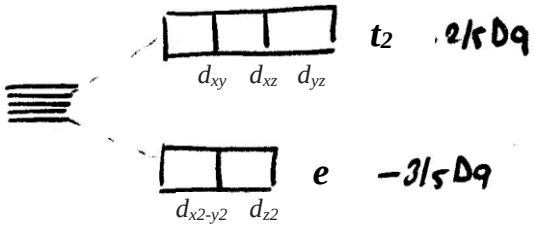
In the octahedral field, ligands approach the central atom in the direction of the x, y, z axes. Therefore, the ligands interact more with d-orbitals (d_{x2-y2} and d_{z2}) on the x, y, z axes. As a result, the d_{x2-y2} and d_{z2} orbitals on the axes increase their energies as they interact more with ligands (negative charges). The splitting between the orbitals is called crystal field splitting (Δ_o). $_o$ at Δ_0 indicates that the split is in the octahedral field. Crystal field splitting energy or crystal field stabilizing energy (CFSE) is indicated by Δ_o=10Dq.

THE ORBITAL SPLITTING DIAGRAM FOR TETRAHEDRAL COMPLEXES

In the tetrahedral field, ligands approach the central atom in between x, y and z directions. Therefore, the ligands interact more with d-orbitals (d_{xy}, d_{xz} and d_{yz}) between the axes. As a result, the energy of t_2 orbitals (d_{xy}, d_{xz} and d_{yz}) increases compared to the energy of e orbitals (d_{x2-y2} and d_{z2}). Thus, d orbitals split into two sets.



Octahedral field



Tetrahedral field

THE ORBITAL SPLITTING DIAGRAM FOR SQUARE PLANAR COMPLEXES