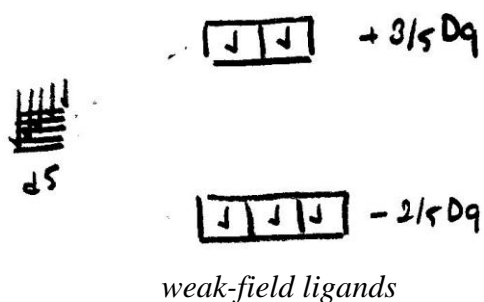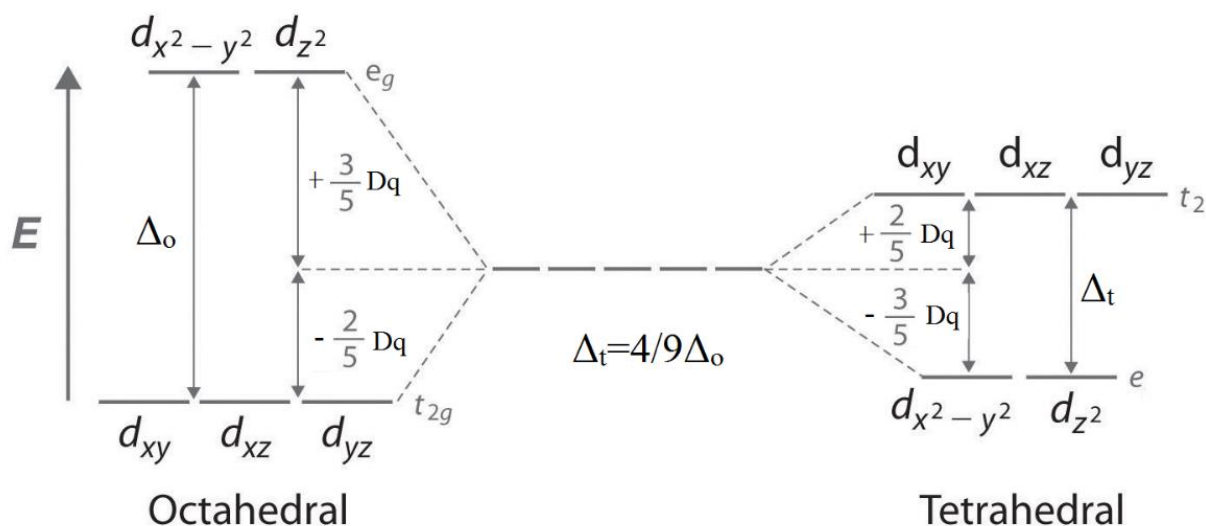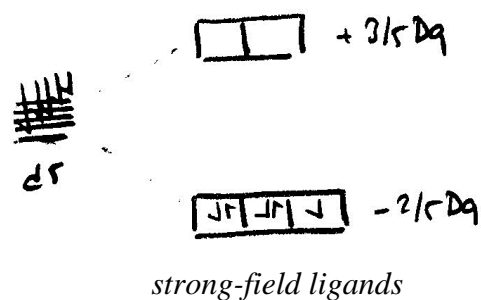---

CRYSTAL FIELD THEORY (CFT)

CALCULATION OF CRYSTAL FIELD STABILIZATION ENERGY OR CRYSTAL FIELD SPLITTING ENERGY (CFSE) IN OCTAHEDRAL, TETRAHEDRAL AND SQUARE PLANAR COMPLEXES

Octahedral $\Delta_t = 4/9\Delta_o$ Tetrahedral

weak-field ligands   *strong-field ligands*

$$CFSE = 3 \cdot \left(-\tfrac{2}{5} Dq\right) + 2\left(+\tfrac{3}{5} Dq\right) + 4\Pi e$$

$$CFSE = 0 Dq + 4\Pi e$$

$$CFSE = 5 \cdot \left(-\tfrac{2}{5} Dq\right) + 2\Pi c + 4\Pi e$$
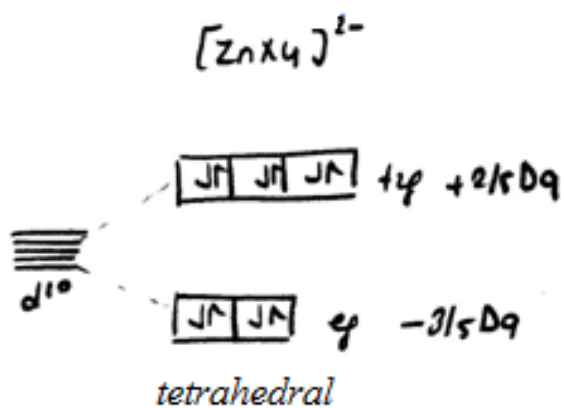
$$CFSE = -2 Dq + 2\Pi c + 4\Pi e$$

Coulomb pushing energy (Π_c) is the energy that occurs when two electrons in an orbital push each other because of their loads. It increases the energy of the system (+ marked). The exchange energy (Π_e) is the displacement energy of two electrons with the same spins. It decreases the energy of the system (- marked).

$[ZnX_6]^{4-}$

$$\boxed{\uparrow\downarrow \mid \uparrow\downarrow} \quad e_g \quad +3/5\,Dq$$

d^{10}

$$\boxed{\uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\downarrow} \quad t_{2g} \quad -2/5\,Dq$$

octahedral
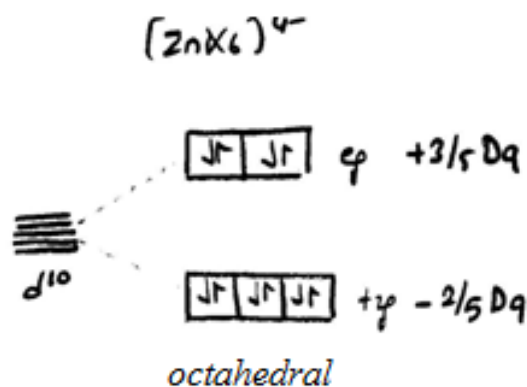
$$CFSE = 6\cdot\left(-\frac{2}{5}Dq\right) + 4\left(+\frac{3}{5}Dq\right) + 8\Pi e + 5\Pi c$$

$$CFSE = 0\,Dq + 8\Pi e + 5\Pi c$$

$[ZnX_4]^{2-}$

$$\boxed{\uparrow\downarrow \mid \uparrow\downarrow \mid \uparrow\downarrow} \quad t_2 \quad +2/5\,Dq$$

d^{10}

$$\boxed{\uparrow\downarrow \mid \uparrow\downarrow} \quad e \quad -3/5\,Dq$$

tetrahedral

$$CFSE = 4\cdot\left(-\frac{3}{5}Dq\right) + 6\cdot\left(+\frac{2}{5}Dq\right) + 8\Pi e + 5\Pi c$$

$$CFSE = 0\,Dq + 8\Pi e + 5\Pi c$$

THE ORBITAL SPLITTING DIAGRAMS FOR OTHER COMPLEXES

$\overline{d_{z^2}}$ a'

$\overline{dx^2}$ $\overline{dy^2}$

$\overline{dxy}$ $\overline{dx^2y^2}$ e'

$\overline{dxy}$ $\overline{dx^2y^2}$

$\overline{dxz}$ $\overline{dyz}$ e''

$\overline{d_{z^2}}$

Trigonal bipyramide

Square antiprism

$\overline{dx^2y^2}$ b_1

$\overline{d_{z^2}}$ a_1

$\overline{dxy}$ b_2

$\overline{dxz}$ $\overline{dyz}$ e

Square pyramide