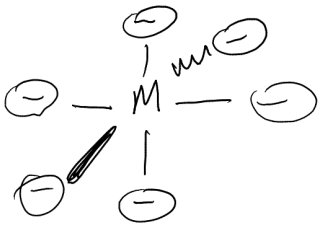
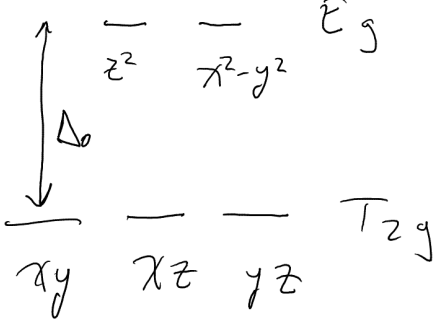
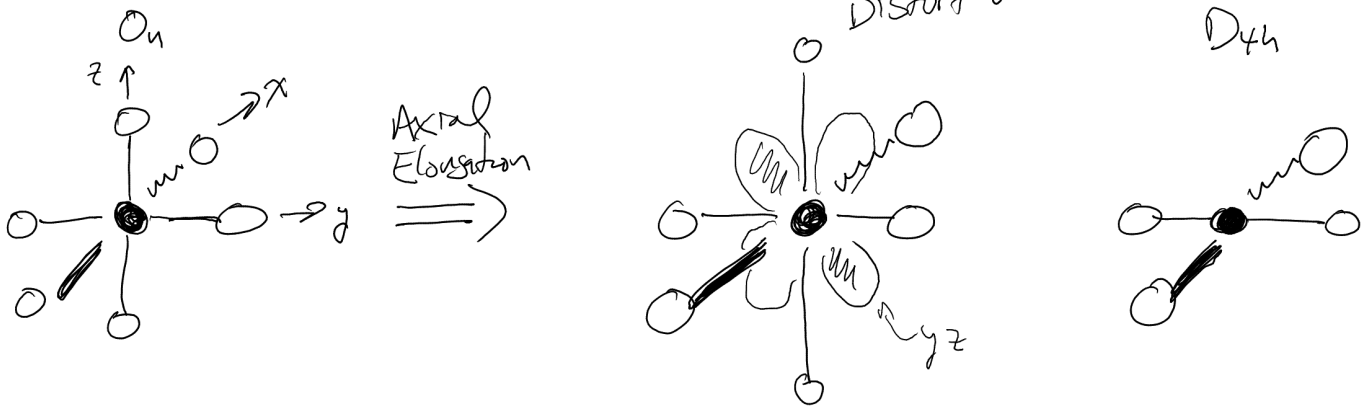
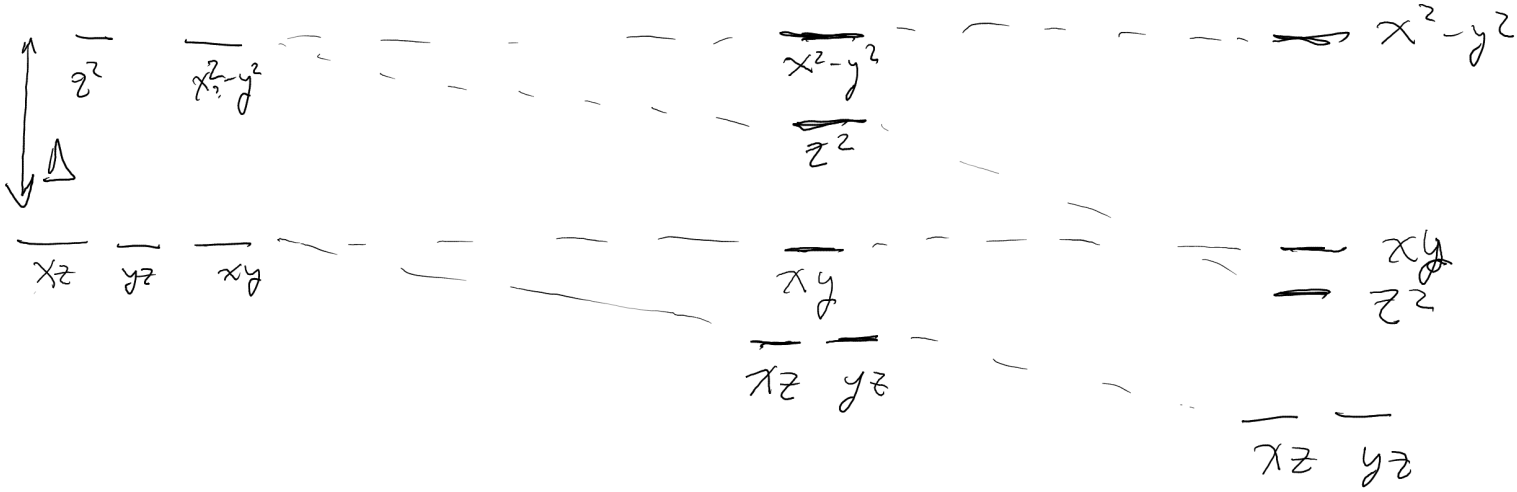
CFT









Walsh Diagram
(Arthur Walsh) J. Chem. Soc. 1953, 2266-66

Basic Assumptions based on CFT to determine HS vs. LS.

① Coulombic Repulsion (energy penalty of placing $2e^-$ in the same orbital) $\uparrow_C$

② Loss of $\uparrow_E$

① Coulombic Penalty is greatest for smallest d-orbitals

$3d \gg 4d > 5d$

First Row metals tend to be HS.

2nd + 3rd Row Metals found to be LS

② loss of exchange energy is greatest for d^5

Fe^{3+}, Mn^{2+} tend to be HS

Basic Trends that define Δ magnitude

① OS of Metal

$[CoF_6]^{2-}$ $\Delta_o = 20{,}600\ cm^{-1}$ (Co^{II})

$[CoF_6]^{3-}$ $\Delta_o = 13{,}100\ cm^{-1}$ (Co^{III})

As OS increases, so does Δ.

↳ Shorter M-L bonding drives greater electrostatic perturbation

② Number of ligands $\Delta_t < \frac{1}{2}\Delta_o$

③ Nature of the Ligands

Some ligands give large Δ (strong field)

Some ligands give small Δ (weak field)

Weak Field (Small Δ) ⟶ Spectrochemical Series ⟶ Strong Field (Large Δ)

$I^- < Br^- < S^{2-} < SCN^- < Cl^- < F^- < \boxed{OH^-} < ox < O^{2-} < \boxed{H_2O} < NCS < py, NH_3 <$

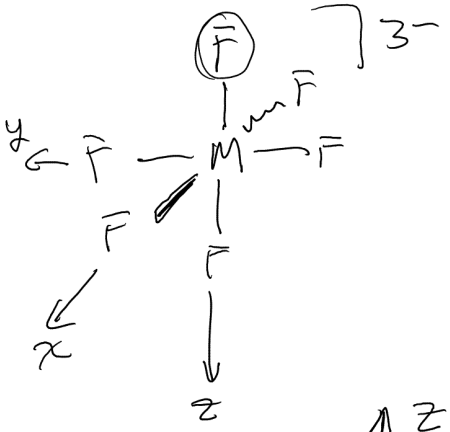
$bpy < NO_2^- < CH_3^- < C_6H_5^- < CN \sim CO < NO^+$

M-L bonding is highly <u>covalent</u>

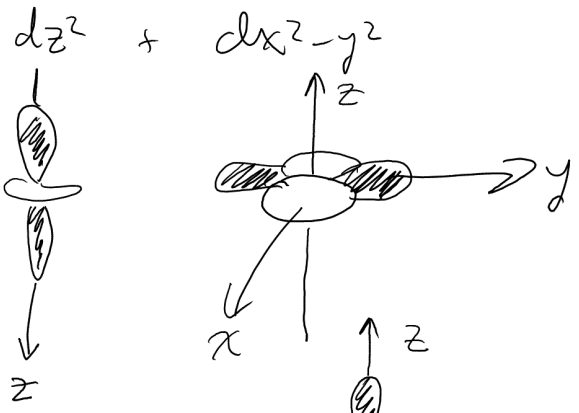
↳ Need MO theory

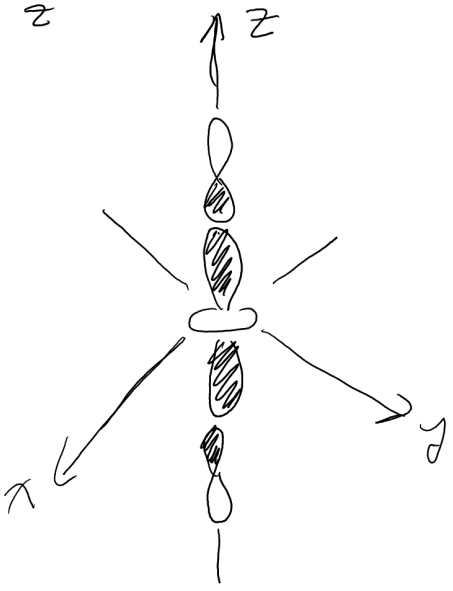
CFT + MO theory = LFT

Let's consider ML_6 Complex $[CoF_6]^{3-}$ Co^{III}



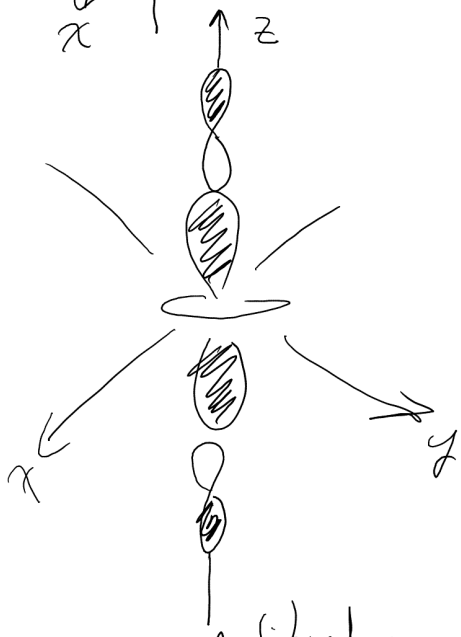
σ-bonding Frameword



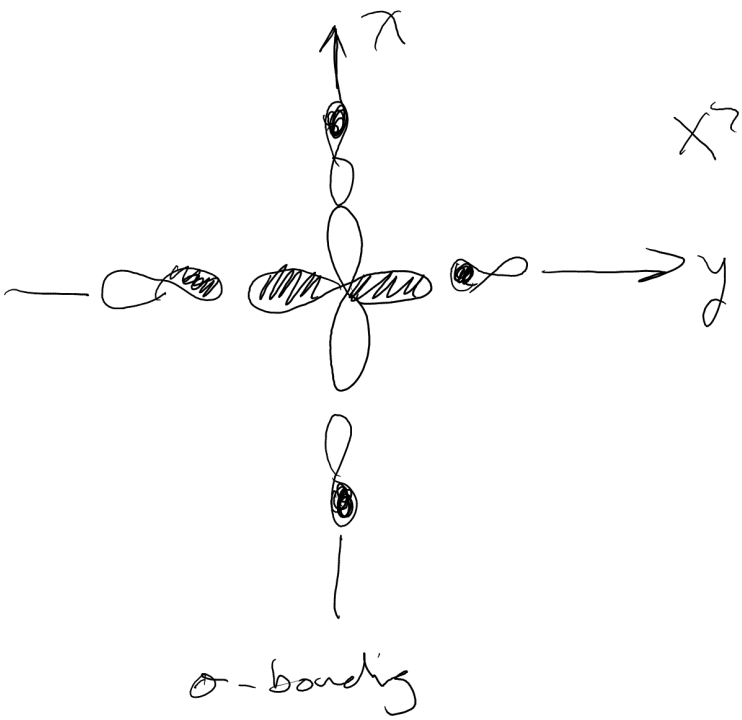


σ-bonding

z^2

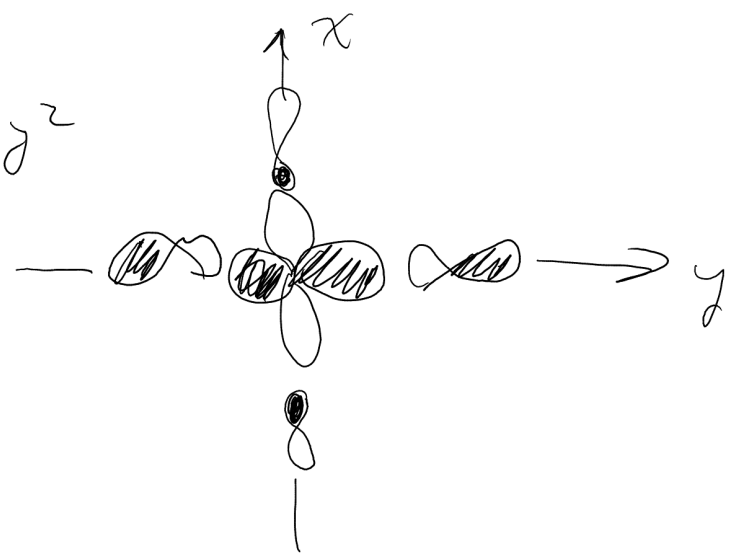


σ-Antibonding

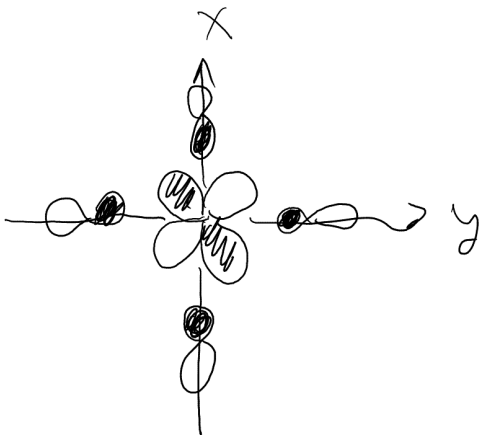


σ-bonding

x^2-y^2

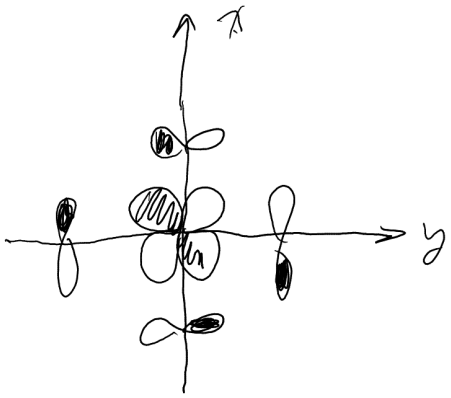


σ-Antibonding



Non-bonding

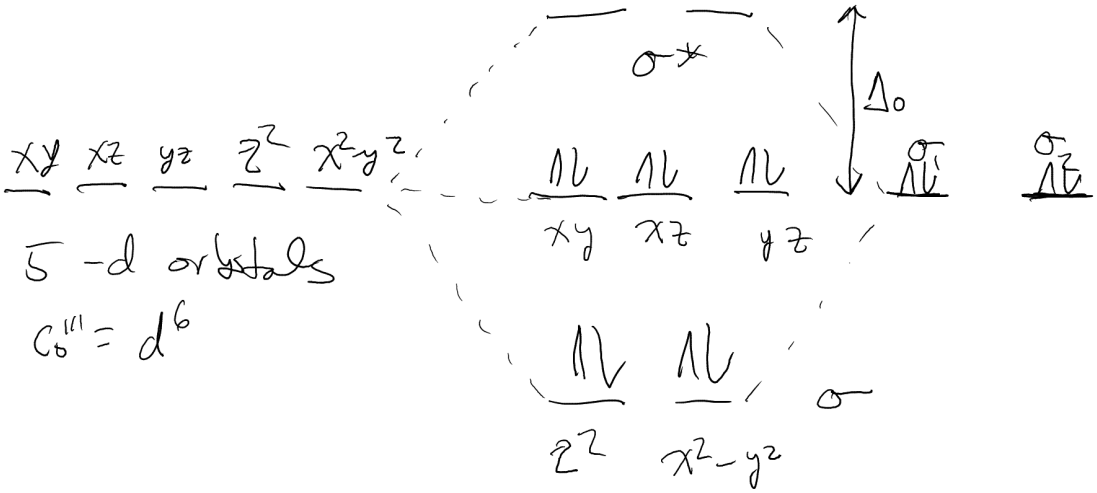
xy



π- bonding

ML_6 σ-bonding

σ - Bonding



π- Bonding