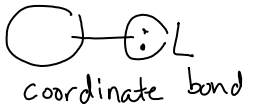
Notes 03/05

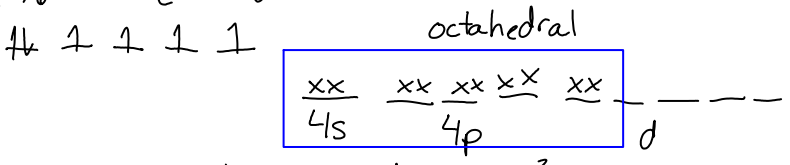
Wednesday, March 05, 2008
10:01 AM

Review session. March 15th Franz 1178 @ 3-4:50pm

- Bonding in Transition Metal Complexes
  - Valence Bond Theory
  - Concept of hybrid orbitals

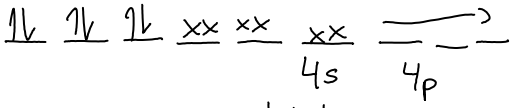


- $Fe(H_2O)_6^{2+}$ Fe^{2+} d^6



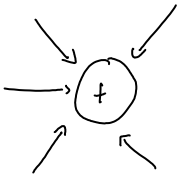
high spin outer orbital complex sp^2d^2

- $Fe(CN)_6^{4-}$ d^6

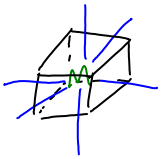


low spin inner orbital complex d^2sp^3

  - Drawbacks of VB theory:
    1. Does not explain low and high spin
    2. Does not explain why transition metal complex have colors
  - Crystal Field Theory
    - Electrostatic field created by ligands around metal ion.



octahedral:



Ti^{2+} 16

- Fe^{2+} d^6

  - H_2O ligand (weak field ligand) high spin

    ↑ ↑
    ↑ ↑ ↑

    pop energy < pairing energy

  - CN^- ligand (strong field ligand) low spin

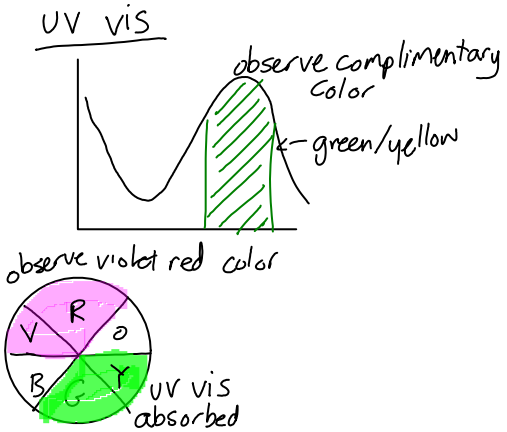
    ↓↑ ↓↑ ↑

    pop energy > pairing energy

- $Ti(H_2O)^{3+}$ Ti^{3+} d^1

  ↑ _ $\xrightarrow{h\nu}$ ↑ _

  ↑ _ _ _ _ _



Spectrochemical series will show strong and weak field ligands

The lower you go, the energy gap will become higher (ie 3d to 4d)

- Crystal field stabilization energy

  d^0 CFSE=0

  d^1 _ _ $-2/5\ \Delta_o$

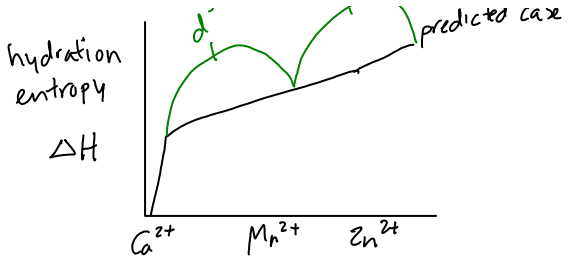
  ↑ ↑ ↑ $-4/5\ \Delta_o$

  d^4 ↑↑
  ↓↑ ↑

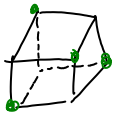
d^6 is most stable case.

High spin case

. . . | d^3 d^6 predicted case



Tetrahedral Field



ligands Δ_T d_{xy} d_{yz} d_{xz} T_2 d_{z^2} $d_{x^2-y^2}$ e_g

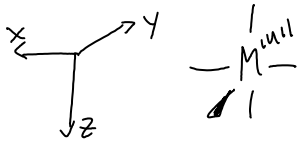
$\Delta t \approx \frac{4}{9}\Delta_o$

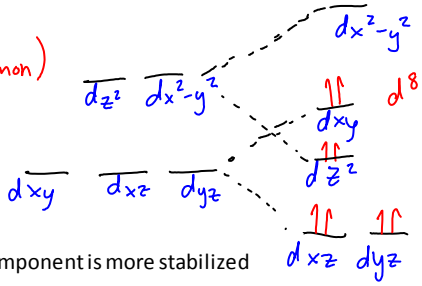
So always get high spin

- d^6 ↑ ↑ ↑

high spin ↑↓ ↑

Square Planar Field (d^8 very common)





Every z component is more stabilized