Due: November 12, 2019

1. What is the crystal field stabilization energy? For an octahedral complex, how is the CFSE calculated?

    The crystal field stabilization energy (CFSE) is the stability that results from placing a transition metal ion in the crystal field generated by a set of ligandsThe Crystal Field Stabilization Energy is defined as the energy of the electron configuration in the ligand field minus the energy of the electronic configuration in the isotropic field.
    To calculate CFSE for an octahedral field, one must consider both the contribution of the eg set (+3/5 Δ_o) and the contribution from the t2g set (-2/5 Δ_o), in addition to the pairing energy

2. Why is Δ_o typically greater than Δ_t? *Hint: you may want to include diagrams in your answer*

    Interactions are weaker in tetrahedral geometries as ligands do not point to orbitals on the metal. Therefore, the magnitude of stabilization/destabilization is decreased compared to octahedral geometries.

3. Classify the following as strong field or weak field ligands Is there a relationship between ligand type and field strength?
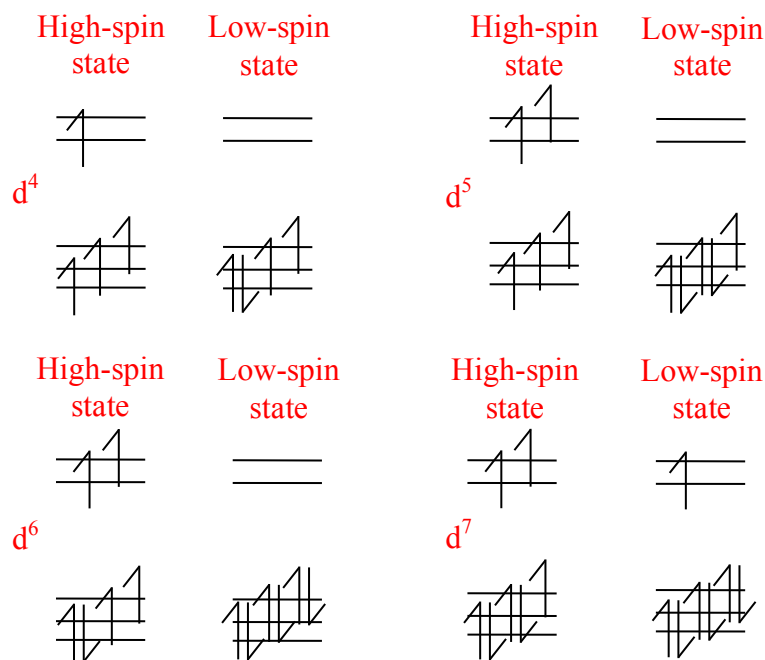   a. H_2O **weak**
    b. CN^- **strong**
    c. Br^- **weak**
    d. CO **strong**
    e. NH_3 **strong**
    Weak field ligands tend to be pi-donors, while strong field ligands tend to be pi-acceptors. Note the trend of decreasing field strength pi acceptor>sigma donor>pi donor

4. Calculate the crystal/ligand field stabilization energy for the following: *Note that the way in the notes does not subtract the energy of the isotropic field from the energy of the ligand field. If you DID do that based on what you read on the internet, that's fine too.*
    a. d^2
        -4/5 Δ_o
    b. d^4 (Low-spin)
        -8/5 Δ_o +PE
    c. d^4 (High spin)
        -3/5 Δ_o
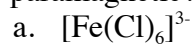   d. d^8
        -6/5 Δ_o + 3P
    e. d^{10}
        5P

5. Which d electron counts are capable of giving rise to both low spin and high spin configurations? Show using orbital diagrams.

High-spin state Low-spin state   High-spin state Low-spin state

d^4 d^5

High-spin state Low-spin state   High-spin state Low-spin state

d^6 d^7

6. When can one expect a high spin configuration? Low spin configuration? Discuss this in the context of crystal field splitting energy and pairing energy.

A high spin configuration can be expected if the pairing energy is greater than the crystal field energy. A low spin configuration can be expected if the pairing energy is less than the crystal field energy.
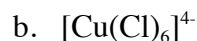
7. For the following compounds: a) Draw the orbital splitting diagram b) If applicable, explain why you chose a LS or HS configuration c) Predict the magnetic properties (diamagnetic or paramagnetic?)
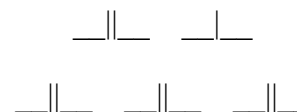   a. $[Fe(Cl)_6]^{3-}$
        Fe(III): d^5
        HS because Cl is weak field
        5 unpaired electrons - paramagnetic

    b. $[Cu(Cl)_6]^{4-}$
        Cu(II): d^9
        1 unpaired electron – paramagnetic

    c. $[CoF_6]^{3-}$
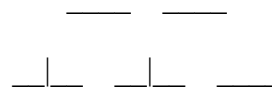   **Co(III): d^6**
        HS because F is weak field
        4 unpaired electrons- paramagnetic
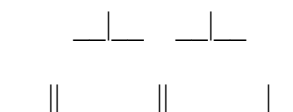
d. $[Ti(H_2O)_6]^{2+}$
Ti(II): d²
2 unpaired electrons – paramagnetic

           ___ ___
        _↿_ _↿_ ___

e. $[CoCl_4]^{2-}$
Co(II): d⁷
3 unpaired electrons – paramagnetic

        _↿_ _↿_ _↿_
        _⇅_ _⇅_
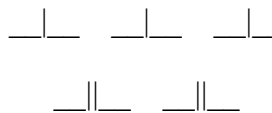
8. Give the ground state term symbols for the following free ions. *To receive full credit, you must show all your work.*

a. Ti^{2+}
   d²: _↿_ _↿_ ___ ___ ___
         +2   +1   0   -1   -2
   L=3 → F
   2S+1 = 2(1)+1 = 3
   ³F

b. Mn^{3+}
   d⁴: _↿_ _↿_ _↿_ _↿_ ___
         +2   +1   0   -1   -2
   L=2 → D
   2S+1 = 2(2)+1 = 5
   ⁵D

c. Fe^{3+}
   d⁵: _↿_ _↿_ _↿_ _↿_ _↿_
         +2   +1   0   -1   -2
   L=0 → S
   2S+1 = 2(2.5)+1 = 6
   ⁶S

d. Cu^{2+}

   d⁹: _⇅_ _⇅_ _⇅_ _⇅_ _↿_
         +2   +1   0   -1   -2
   L=2 → D
   2S+1 = 2(0.5)+1 = 2
   ²D

   Zn^{2+}

   d¹⁰: _⇅_ _⇅_ _⇅_ _⇅_ _⇅_
         +2   +1   0   -1   -2
   L=0 → S
   2S+1 = 2(0)+1 = 1
   ¹S