CHEM 411/512 TakehomeTest 2 Spring 2008 (Delaney) NAME _____

Due Wednesday April 2, 2008

1. What are the term symbols for the free atoms and ions below? (10 points)

   a. Co^{+1}

   b. Ir^{+3}

   c. S

   d. O^{-}

   e. Ti^{3+}

   f. Mg^{+2}

   g. Ni^{+2}

   h. Pt^{+4}

   i. Ag^{+1}

   j. Cu^{+1}

2. For the compounds below, calculate the ligand fields using the data in the table below to determine Δ_o ($10\ Dq_o$) for the compounds and $B_{complex}$ for the compounds.

Determine the allowed transitions for each of the compounds below, tell whether the compound is high spin-low field or low spin-high field, and tell what absorptions occur and at what wavelength (in nanometers) they occur. (40 points)

a. $[VF_6]^{4-}$

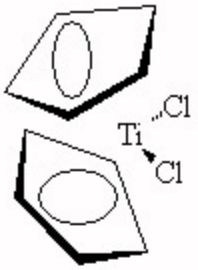
b. $[Mn(CN)_6]^{4-}$

c. $[Cr(H_2O)_6]^{3+}$

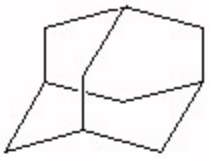
3. What colors would you expect the complexes above to appear to the eye? (Only absorbances in the visible region contribute to observed color.)(10 points)

4. What point group do the molecules below belong to? (20 points)

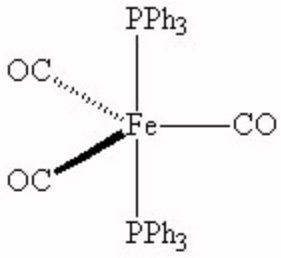
a.



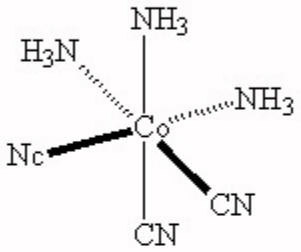
b.



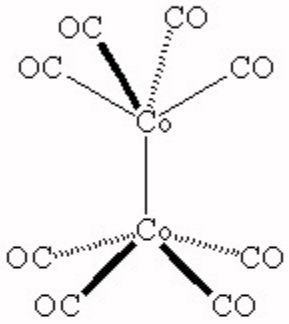
c.



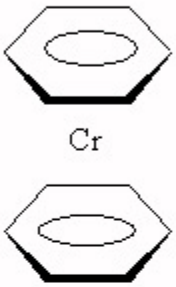
d.



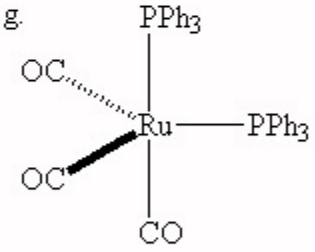
e.



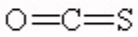
f.



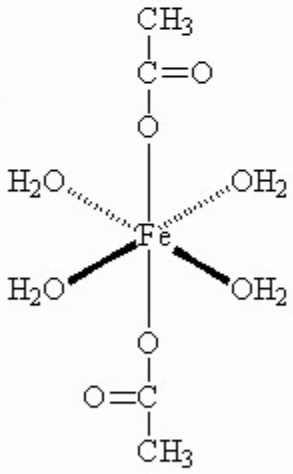
g.



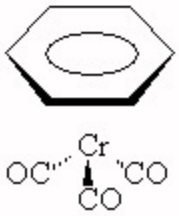
h.



i.



j.



5. Explain which types of normal modes are infrared active and which types are Raman active. (10 points)

6. For the compounds in problem 4, look up the character tables, and with the aid of online resources identify which modes within the character tables are IR active and which modes are Raman active.

7. For the compounds in problem 4, determine the oxidation state of the metal, and determine how many electons are around the metal center. (Apply the 18 electron rule!!) (10 points)

   a.

   b.

   c.

   d.

   e.

   f.

   g.

h.

i.

j.

8. Using table available on eithe Blackboard or Dr. Delaney's site at http://chemprof.tripod.com/spring08.htm for d-orbital energies in crystal fields of different symmetries determine the geometry with the highest CFSE (i.e. most stable) for each of the various high spin d configurations below. (20 points)

   a. d^3

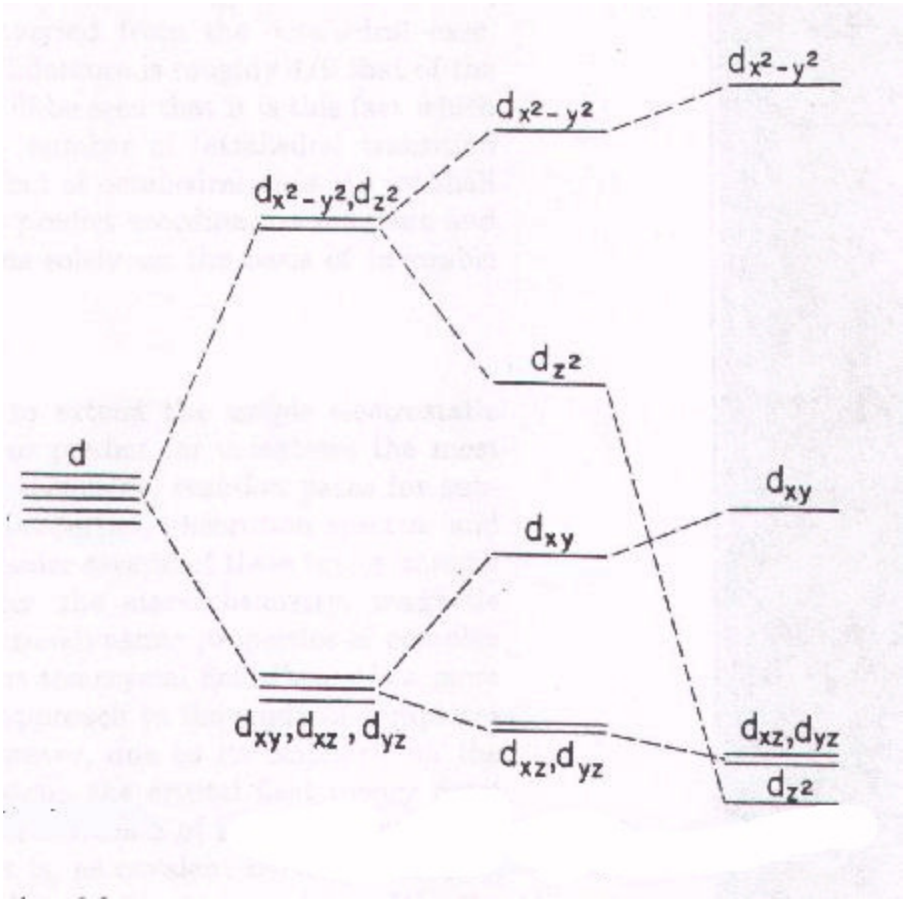
   b. d^7

   c. d^8

   d. d^4

   e. d^6

9. What does the diagram below represent? Explain. (10 points)



10. What is the advantage of a neutron diffraction structure of a single crystal compared to that of an X-ray diffraction structure of a single crystal? (10 points)

11. Electronic absorption spectra are typically taken in which wavelenghts of light? What instruments might be used for such measurements? (i.e. consider d-d transitions and π -->π^* transitions) (10 points)

12. What is the typical use for an X-ray photoelectron spectrometer? What type of orbitals are affected in this type of spectroscopy? What is another older name for this type of spectroscopy? (10 points)

13. What type of orbitals are usually examined via Ultraviolet photoelectron spectrscopy? What state must the sample be in? What is typically used for a source in such spectroscopy? (10 points)

14. In mass spectrometry the most common method of ionization is electron impact to make cations. Explain this process. (10 points)

15. What other types of ionization are used with mass spectrometry, and what types of materials are they especially suited for? (10 points)

16. Mass spectrometers are often combined with other instruments such as gas chromatographs, liqid chromatographs, and ion coupled plasma spectrometers. What are the advantages of combining a mass spectrometer with these instruments, what are their advatages and limitations, and what unique information can be obtained by combining a mass spectrometer with these instruments?

17. Atomic absorption spectrometry and ion coupled plasma spectrometry can be used to give very similar information. However, they work in fundmentally different ,ways. Explain how these two instruments work. (10 points)

18. Explain the concept of thermal analysis methods below. (15 points)

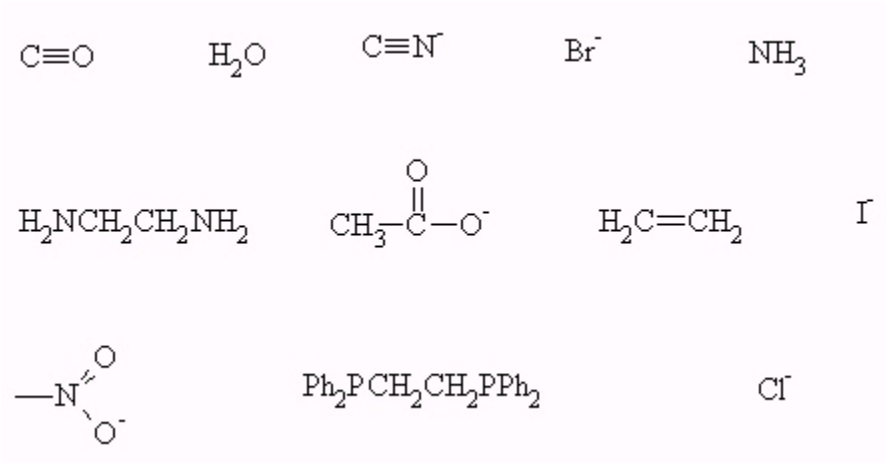
    a. thermogravimetric analysis

    b. differential thermal analysis

    c. differential scanning calorimetry

19. Classify the ligands below as i) σ-donor or π-acceptor, ii) neutral or anionic, iii) monodentate or

multidentate (chelate), and iv) by the number of electrons donated to the metal center. Each ligand should have four answers by it. (10 points)



20. In organic chemistry the cyanide ion, CN^-, is often considered a "pseudohalide." Would this be an appropriate type of designation in transition metal coordination chemistry for the cyanide ion? Why or why not? (10 points)