Chemistry 6011 (Fall 2016)
Advanced Inorganic Chemistry I: From Atoms to Coordination Compounds
Chapter 2, 3, 4 and Huheey Chapter 18 HW Set

How does metal chelation by a ligand help to maintain the metal bioavailable?

Chapter 2-

1. Which quantum numbers reveal:
a. Shape
b. Energy
c. Orientation
d. Size of orbitals

2. How many orbitals are possible for n=4? Define them.

3. What is the maximum number of electrons in a completely filled n=5 level. Give 4 possible quantum numbers for a 5f e^- of the hydrogen atom.

4. Draw an example for the following p^3 configuration.

a. A configuration in which exchange energy is maximized.

b. A configuration in which coulombic repulsion is maximized.

c. A configuration that is impossible.

d. Determine all of the term symbols for p^3 and arrange them in terms of energy following Hund's rules.

5. Determine all of the term symbols for Sc^+ and Ti and arrange them in terms of energy following Hund's rules.

6. Write out the electronic configuration for the free atoms and determine the number of unpaired e^- in the ground state.

B V Cu Lu

7. Write out the electronic configuration for the ions and determine the number of unpaired e^- in the ground state.

Ti^{3+} Mn^{2+} Cu^{2+} Gd^{3+}

8. Using Slater's rules, calculate Z^* for the following electrons:
a. a 3p e^- in P

b. a 4s e^- in Co

c. a 3d e^- in Mn

d. a valence e^- in Mg

9. Which has the higher first ionization energy:

Li or Cs? F or Br? Sc or Cu? Cu or Pt?

10. Plot the total ionization energies of the Al^{n+} as a function of n from n=1 to n=8. Explain the source of discontinuity in your curve.

n	Ionization Energy (MJ mol^{-1})
1	0.5776
2	1.8167
3	2.7448
4	11.578
5	14.831
6	18.378
7	23.295
8	27.459

11. Which has the highest e^- affinity:

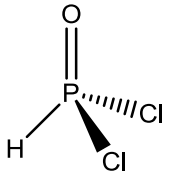
Li or Cs? F or Cl? Cl or Br? O or S?

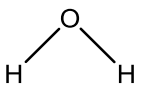
Chapter 18-

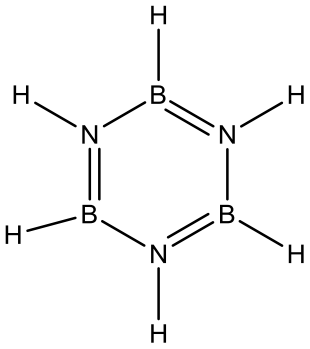
Huheey's questions 2, 4, 8, 9 (For problems 8 and 9 please refer to Figure 2.13 in the Miessler textbook), and 18 (For this problem think about how electronegativity differences can affect whether a bond is covalent or ionic).

Chapter 4-

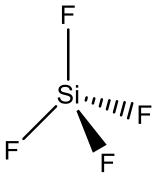
1. Assign the following molecules to their appropriate point groups.

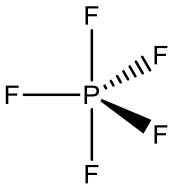


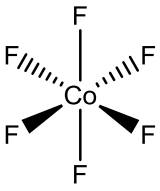


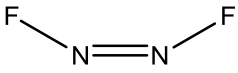

H
H
B
H
N
N
H
B
B
H
N
H
H


S
O


F
Si
F
F
F


F
F
P
F
F
F


F
F
F
Co
F
F
F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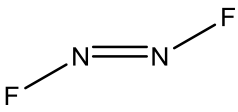
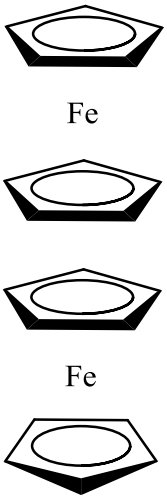
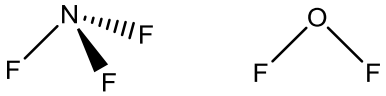
N
N
F

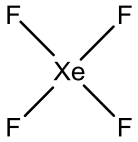

N
N
F
F



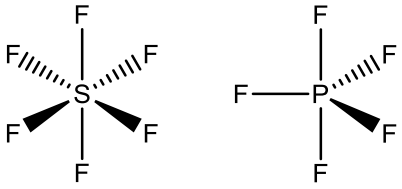
2. What are the symmetries of the normal modes of vibration of these molecules?



3. Derive the irreducible representations for the normal vibrations of XeF_4 and determine which are IR active, which are Raman active, and which are neither.



4. For each of the following molecules, determine what atomic orbitals on the central atom are allowed by symmetry to be used in the construction of sigma hybrid orbitals.



Chapter 3 and Valence Bond Theory-

1. Draw Lewis structures for the following molecules and predict the molecular geometry including expected distortions.

a. BCl_3

b. BeH_2

c. $SnBr_4$

d. TeF_6

e. AsF_5

f. XeO_4

g. $TeCl_4$

h. ICl_2^+

i. XeO_3

j. ClO_2F_3 (Cl is the central atom)

2. Write resonance structures, including formal charges for O_3, SO_3, NO_2.

3. The bond angles in fluoromethanes are:

Molecule	H-C-H	F-C-F
CH_3F	111°	
CH_2F_2	112°	108.3°
CHF_3		108.8°

a. Calculate the s character used by the carbon atom in the orbitals directed to the hydrogen and fluorine atoms.

b. Discuss the results in terms of Bent's rule.

4. In an sp^3d hybridized phosphorus atom in a trigonal bipyramidal molecule, will the atom have a greater electronegativity when bonding through equatorial or axial orbitals? Explain.

5. From what you know of the relationship between ionization energies, electron affinities, and electronegativities, would you expect the addition of some d character to a hybrid orbital to raise or lower the electronegativity; for example, will sulfur be more electronegative when hybridized sp^3 or sp^3d^2?