

HW 7
CHEM 362

Due: November 5, 2019

1. What is the difference between crystal field theory and ligand field theory?

CFT assumes that bonds between the metal atom and the ligands are totally ionic – in other words, point charges, and purely electrostatic interactions

LFT is a modification of CFT that allows for the effects of covalent character in the bonds, but the two theories are used in essentially the same manner.

2. Determine if the following molecular orbitals are symmetric with respect to an inversion center, and assign the appropriate g (gerade, symmetric) or u (ungerade, antisymmetric) labels:
 - a. Sigma bonding M.O. between two s orbitals
g
 - b. Anti-bonding sigma M.O. between two s orbitals
u
 - c. Pi Bonding M.O. between two p orbitals
u
 - d. Pi anti-bonding M.O. between two p orbitals
g
 - e. Delta bonding M.O. between two d orbitals
u
 - f. Anti-bonding delta M.O. between two d orbitals
g

3. Using a crystal field theory approach, determine the d-orbital splitting pattern for each of the following geometries.
 - a. Octahedral

4.
 - a.
 - i. Distorted Octahedral – elongation of ligands in the z direction
 - ii. Distorted Octahedral – shortening of ligands in the z direction
 - b. Tetrahedral
 - c. Square Planar
 - d. Linear

e. Trigonal Bipyramidal

HINT: In order to receive full credit for this question, you must show ALL of your work. Your answer should comprise diagrams/figures as well as written explanations. Your answer may/should include (but is not limited to):

- Drawing d-orbital diagrams
- Drawing d-orbital interactions with ligands in their respective geometries
- Describing and explaining such interactions and showing why some d-orbitals are raised or lowered in energy

15 points each. 5 point sfor correct orbital splitting, 5 points for describing in words the differences in energy, 5 points for SHOWING that (ie. It is not sufficient to simply say that the orbitals with a z component are raised in energy, if you don't give an explanation why, and show how the geometry affects that)

