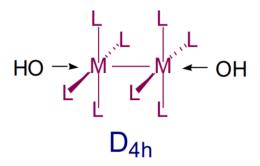
Problem Set 6

- (1) Use the MO diagram you constructed for Bis(cyclobutadiene)nickel in Problem Set 6. Assume that the complex is reduced by two electrons to yield the 2⁻ ion.
 - (a) Derive the symmetries of the ground state, dipole moment operator and the two lowest lying excited states.
 - (b) Assign the electronic transitions. Are these electronic transitions allowed?
 - (c) I. What type of transitions are these? II. What intensities would you expect?
 - (d) Assuming that the metal is now Zn, to yield the 2⁻ Bis(cyclobutadiene)zinc(II), repeat questions (a) (c).
- (2) Use the MO diagrams that you derived for square planar complexes with d⁸ electronic configuration in Problem Set 5. Assign the low-lying allowed transitions you would expect for the following types of complexes. Comment on the types of transitions and intensities.
 - (a) σ -donor ligands
 - (b) π -acceptor ligands
 - (c) π -donor ligands
- (3) Consider the metal-metal MO diagram on the reverse side of the page for the $D_{4\rm h}$ complex $M_2\,(L)_8$.
 - (a) Assign the lowest energy allowed transitions.
 - (b) What changes would you expect in the MO diagram of the complex when two hydroxide ligands bind in the axial positions (consider σ-only) as shown below.



- (c) How would you expect such axial binding to affect the electronic spectrum of the complex?
- (d) Would you expect the use of a better σ -donor to affect the spectrum? How? And a weaker σ -donor?
- (e) Assuming a d^4 metal is used in the M₂ (L)₈ complex, assign the allowed d-d transitions.

