

University of Windsor  
Chemistry and Biochemistry  
Chemistry 59-250, Fall Term 2005

Assignment 4

Question #1

Molecular Orbital Diagrams

Construct a valence MO diagram for the octahedral molecule  $\text{SF}_6$ ; to simplify the problem, you should only use the 2s orbitals on the F atoms. Write an acceptable normalized LCAO for ONE of the MO's that you have produced.

Question #2

Molecular Orbital Diagrams

Construct a valence MO diagram for the TBP molecule  $\text{SbF}_5$ ; to simplify the problem, you should only use the 2s orbitals on the F atoms. Write an acceptable normalized LCAO for ONE of the MO's that you have produced.

Question #3

Molecular Orbital Diagrams

- (a) Construct a valence MO diagram for the  $\sigma$  bonding in the trigonal planar molecule  $\text{BF}_3$ ; to simplify the problem, you should only use the 2s orbitals on the F atoms.  
(b) Write an acceptable pair of normalized LCAO's for the most stable of the doubly-degenerate pairs of SALC's that you have produced for the F atoms and draw a reasonable picture of this pair of SALC's. Indicate which AO on B can interact with each of the SALC's that you drew.  
(c) Construct a valence MO diagram for the  $\pi$  bonding in the trigonal planar molecule  $\text{BF}_3$ ; to simplify the problem, you should only use the  $2p_z$  orbitals on the F atoms.

Question #4

Use drawings and equations to estimate the values of the overlap integrals in the molecule  $\text{F}_2$  for the combination of the following orbitals:

- (a)  $2s$  and  $2p_x$  (b)  $2s$  and  $2p_z$  (c)  $2p_x$  and  $2p_x$  (d)  $2p_y$  and  $2p_x$

Question #5

Construct MO diagrams for (a) the cation  $[\text{HFH}]^{+1}$  and (b) the anion  $[\text{FHF}]^{-1}$ . Use all the available valence orbitals and be sure to indicate and justify your choice of point group for each ion.