ORTH CAROLINA STATE UNIVERSITY
Department of Chemistry Name_____
Physical Chemistry CH437 Problem Set #5
Due Date: September 29, 2015

Part I.

1. A. Construct SALCs for trigonal planar BH_3, using the H 1s orbitals as a basis. Call these orbitals h_1, h_2, and h_3, as an abbreviation. B. Use the character table to determine which 2s and 2p orbitals on the B atom can give rise to SALCs that will bond with the hydrogen atoms.

3. Compare the energies of butadiene and cyclobutadiene. What can you say about the stabilization of the π-electrons in a 4-membered ring? Comment on how this result relates to the aromatic stabilization of π-systems.

4. CH_4 belongs to the T_d point group. What irreducible representations do the 4 1s orbitals of H span in the molecule CH_4? Are there any matching irreducible representations spanned by the 2s and 2p orbitals on the central carbon atom? Based on this analysis list the possible irreducible representations of MOs of methane.

5. Determine the irreducible representations of the vibrations of pyridine. Separate the translational and rotational degrees of freedom from the vibrational degrees of freedom. Which modes are infrared active? What are the polarizations of the transitions? Which modes are Raman active? Which elements of the Raman tensor contribute?

Part II.

Work the following Problems in Atkins and DePaula, 12.2a, 12.9a, 12.10b