HW # 8, Chem 2430

1. Consider the H_3 molecule in an equilateral triangular geometry. Sketch the MOs that derive from an s orbital on each of the H atoms and label these according to their symmetry representations (the relevant point group is D_{3h}). Now consider the distortion of the molecule to an isosceles triangular structure. What point group is this and what are the symmetry representations of the orbitals.
2. Write the integral (in cartesian coordinates) for the overlap of two 1s orbitals separated a distance R. No need to actually evaluate the integral. (I have not been able to get Wolfram Alpha to do it.)
3. Benzene belongs to the D_{6h} point group. The π orbitals belong to the a_{2u}, e_{1g}, e_{2u}, and b_{2g} representation, in order of increasing energy. What is the symmetry of the ground state? What states (give their representations) result from exciting an electron from the HOMO to the LUMO? Which of these are dipole allowed?