CHEM442-001/002 Name _____
College of Charleston
Spring 2001
Exam III Score _____ /100

1(25). Consider the ground state of the negatively charged dihydrogen molecule ion, H_2^-.
Write the ***complete*** hamiltonian operator (including any nuclear kinetic energy terms). Expand any summation terms to show each contribution.

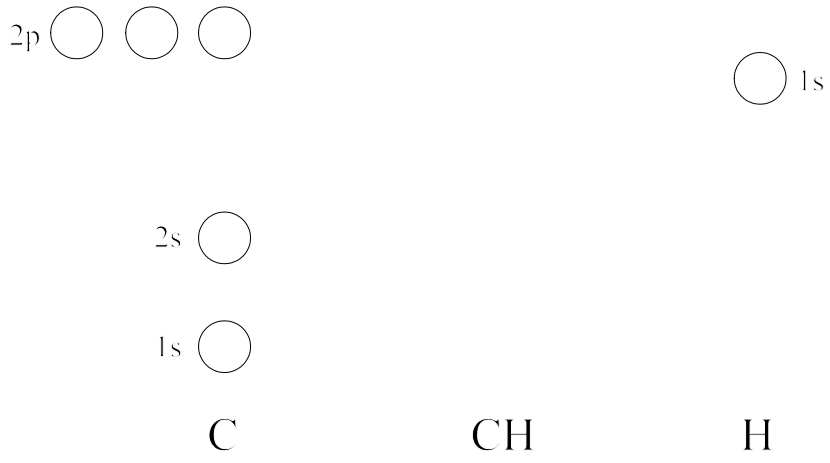
Write the hamiltonian operator after application of the Born-Oppenheimer approximation.

Write the expression for the trial wave function using the molecular orbital theory. Assuming LCAO of hydrogen-like wave functions, write the expressions for the wave functions of each electron that would be used in this trial wave function.

What type of molecular orbital is the HOMO?

Is this molecule-ion paramagnetic?

2(20). Complete the following simple (i.e., no hybridization) molecular orbital diagram for the heteronuclear diatomic molecule CH. Show electrons and label the orbitals.



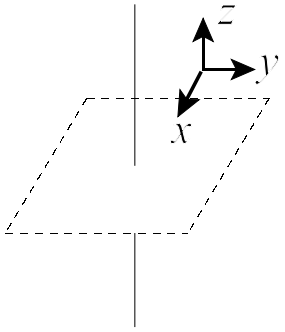
In a few words describe the bond that is formed and make a simple valence bond sketch of the bond.

3(10). In the sketch show what happens to x, y, and z after the $\hat{i}$ operation is performed. If the coordinate system after the operation is x', y', and z', relate the two systems.

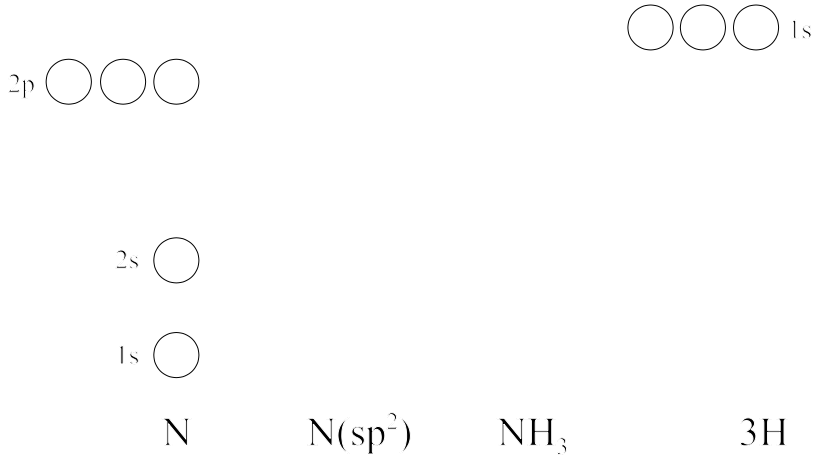
$x' = (\ )\, x$

$y' = (\ )\, y$

$z' = (\ )\, z$

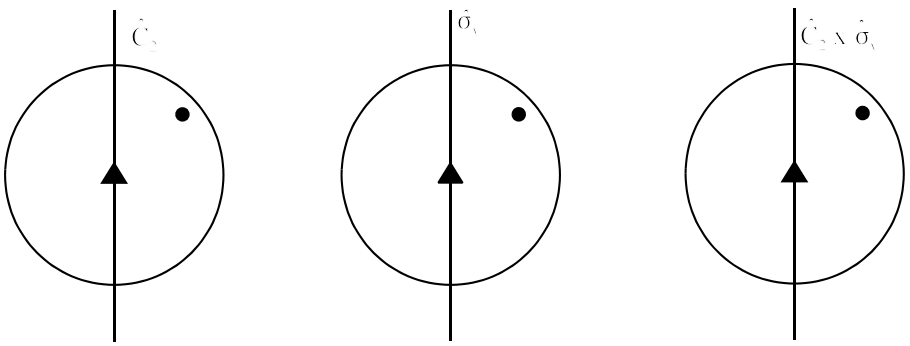


4(25). Let's pretend that the nitrogen atom in NH_3 is sp^2 hybridized and that the molecule is trigonal planar.
Complete the following molecular orbital diagram. Show electrons and label the orbitals.



List all the symmetry elements present in this form of the molecule and determine the point group.

Complete the orthographic projections for the two symmetry operations shown and for the "multiplication of operators" shown.



Identify the result of $\hat{C}_2 \times \hat{\sigma} =$

5(20). Consider the noble-gas fluoride XeF_4.

Construct the Lewis diagram.

Assume that all of the atoms undergo hybridization in this molecule. Determine the hybridization for each type of atom and construct a valence-bond (puff-ball) sketch showing the bonding. Identify the shape of the molecule:

List the symmetry elements present in this molecule and determine the point group.