CHEM442-001/002
College of Charleston
Spring 2000
Exam III

1(25). Consider the H_2^+ molecule-ion in which the bond length is 106 pm. A trial wave function that describes the bonding orbital is

$$\phi(bonding) = (1/2)^{1/2}(\psi_{1sA} + \psi_{1sB})$$

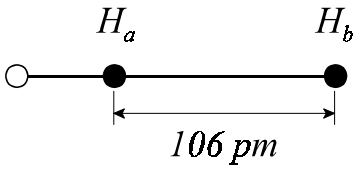
and the antibonding orbital is

$$\phi(antibonding) = (1/2)^{1/2}(\psi_{1sA} - \psi_{1sB})$$

where

$$\psi_{1s} = (1/\pi)^{1/2}(1/a_o)^{3/2}e^{-r/a_o}$$

and a_o = 52.92 pm. Calculate the ratio $\phi(bonding)/\phi(antibonding)$ at the position marked which lies 50 pm to the left of H_A.



2(25). Using the correct molecular orbital diagram for homonuclear diatomic molecules, write the complete electron configuration for C_2.

Describe the bonding in the molecule and calculate the bond order.

Describe the magnetic properties of the molecule.

Using the other (incorrrect) molecular orbital diagram, write the complete electron configuration for C_2. Based on this configuration, has the bond order changed? _____
Have the magnetic properties changed? _____

Returning to the correct molecular orbital diagram, write the complete electron configuration for C_2^-.

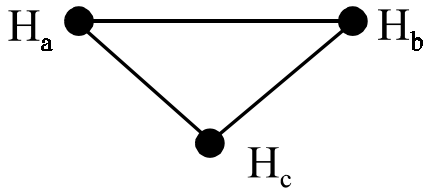
Which is more stable: C_2 or C_2^-? _____
Which molecule has the shorter bond length (1.2682 Å compared to 1.3117 Å)? _____

For the reaction

$$C_2(g) + e^- \rightarrow C_2^-(g) \qquad \Delta H = \pm 400 \text{ kJ}$$

which sign should appear for the enthalpy change? _____

3(25). Consider the H_3 molecule in which we will assume the three nuclei to form an equilateral triangle.

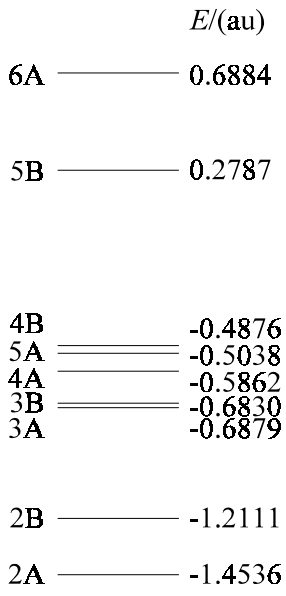


Write the complete internal hamiltonian for this system listing all terms (use no summation shortcut notation).

Using simple molecular orbital theory, write a trial wave function in terms of basis functions.

Following our derivation for H_2^+ and H_2 in class, write the LCAO basis functions using ψ_{1s} hydrogen-like atomic wave functions.

4(25). In laboratory we saw that only the valence electrons are important in describing the bonding in H_2O_2. Shown below are several (but not all) of the molecular orbitals drawn in scale and designated by the symmetry notation rather than σ, σ*, etc.



How many valence atomic orbitals were used in these calculations? _____

How many molecular orbitals are generated by these calculations? _____

How many of the molecular orbitals are completely filled? _____

Sketches of three of the molecular are shown. ***Circle*** the sketch which represents σ(OH) and ***box*** the sketch which represents σ*(OH).