Homework 9 – Molecular Structure

Name: _____

Excercise 9A.2(a) (5 points)

White the valence-bond wavefunction for the resonance hybrid HF $\longleftrightarrow$ H^+F^- $\longleftrightarrow$ H^-F^+ (allow for different contributions of each structure)*(For this problem you may neglect the Pauli principle, which is always followed by taking a simple wavefunction and making it more complicated in a rather banal way)*

Excercise 9A.4(a) (5 points)

Account for the ability of Nitrogen to form four bonds, as in NH_4^+

Excercise 9A.5(a) (5 points)

Describe the bonding in 1,3-butadiene using hybrid orbitals

Excercise 9A.7(a) (5 points)

Show that the linear combinations $h_1 = s + p_x + p_y + p_z$ and $h_2 = s - p_x - p_y + p_z$ are mutually orthogonal

Excercise 9B.4(a) (5 points)

Identify the g or u character of bonding and antibonding π orbitals formed by side-by-side overlap of p atomic orbitals

Excercise 9C.1(a) (5 points)

Give the ground-state electron configurations ad bond orders of (i) Li_2, (ii) Be_2, and (iii) C_2.

Excercise 9C.3(a) (5 points)

Which has the higher dissociation energy, F_2 or F_2^+?

Excercise 9D.1(a) (5 points)

Give the ground-state electron configurations of (i) CO, (ii) NO, and (iii) CN^-

Excercise 9D.5(a) (5 points)

Estimate the orbital energies to use in a calculation of the molecular orbitals of HCl. For data, see Tables 8B.4 and 8B.5 (The full tables, in the appendix). Take $\beta = -1.00eV$.

Excercise 9D.6(a) (5 points)

Use the values derived in Exercise 9D.5(a) to estimate the molecular orbital energies in HCl; use $S = 0$

Excercise 9E.1(a) (5 points)

Set up the secular determinants for (i) linear H_3, (ii) cyclic H_3 within the Hückel approximation.

Excercise 9E.3(a) (5 points)

What is the delocalization energy and π-bond formation energy of (i) the benzene anion, (ii) the benzene cation?