Homework 9 – Molecular Structure

Name:
Excercise 9A.2(a) (5 points)
Write 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)
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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 and 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, ${\rm F_2}$ or ${\rm F_2}^+?$

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Excercise 9D.1(a) (5 points) Give the ground-state electron configurations of (i) CO, (ii) NO, and (iii) CN	
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Excercise 9D.5(a) (5 points)	
Estimate the orbital energies to use in a calculation of the molecular orbitals of HCl. For data, see (The full tables, in the appendix). Take $\beta=-1.00eV$.	e Tables 8B.4 and 8B.5

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)
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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?