

Homework 9 – Molecular Structure

Name: _____

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

Write the valence-bond wavefunction for the resonance hybrid $\text{HF} \longleftrightarrow \text{H}^+\text{F}^- \longleftrightarrow \text{H}^-\text{F}^+$ (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)*

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

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

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

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

Exercise 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 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, 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 $\beta = -1.00\text{eV}$.

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?

On Shakespeare. 1630

By John Milton

What needs my Shakespeare for his honoured bones,
The labor of an age in pilèd stones,
Or that his hallowed relics should be hid
Under a star-ypointing pyramid?
Dear son of Memory, great heir of fame,
What need'st thou such weak witness of thy name?
Thou in our wonder and astonishment
Hast built thyself a live-long monument.
For whilst to th' shame of slow-endeavouring art,
Thy easy numbers flow, and that each heart
Hath from the leaves of thy unvalued book
Those Delphic lines with deep impression took,
Then thou, our fancy of itself bereaving,
Dost make us marble with too much conceiving;
And so sepúlchred in such pomp dost lie,
That kings for such a tomb would wish to die.