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Chemistry 483

Final Examination December 10, 2008

1.(48 points) Define and/or Characterize the following. Each is worth 3 points

a. Photoelectric effect

b. de Broglie wavelength

c. Born-Oppenheimer approximation

d. Perturbation Theory

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e. Harmonic Oscillator

f. P and R branches

g. Radial distribution function for the 1s orbital in H

h. Variation Method

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i. Atomic unit of energy

j. Hund's three rules

k. Electronic angular momentum of the H atom

l. Antisymmetric wavefunction

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m. Franck-Condon principle

n. point group

o. degeneracy of an energy level

p. ionization energy

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2. (6 points) Given that the electron configuration of a zirconium atom is $[Kr]4d^2 5s^2$, determine the ground state term symbol of Zr.

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3. (10 points) Calculate the probability that an electron described by a hydrogen atomic 1s function will be found within one Bohr radius of the nucleus

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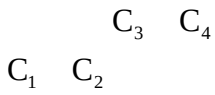
4. (10 points) Assume the skeletal π electron framework of butadiene has C_{2h} symmetry.



If we denote the $2p_z$ orbital on carbon atom *i* by φ_i determine the irreducible representations of

a. $\varphi_1 - \varphi_4$

and

b. $\varphi_2 + \varphi_3$

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5. (10 points) Use the formula

$$E_j = \alpha + 2\beta \cos\left(\frac{2\pi j}{N}\right) \; j = 0, \pm 1, \pm 2, \cdots, N/2 \,, \; N \; even$$

a. determine the Huckel energy levels of the Benzene molecule.

b. Express the delocalization energy in terms of β

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6. (6 points) Write the electron configuration for $N_2, N_2^+, \& N_2^-$ and predict the relative bond lengths and bond energies.

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7. (10 points) Suppose we have an approximate wavefunction for the He atom with the form $\phi(r_1, r_2) = \frac{\alpha^3}{\pi} e^{-\alpha(r_1+r_2)}$. Evaluating the energy results in the energy in atomic units

$$E(\alpha) = \langle \phi | \hat{H} | \phi \rangle = \alpha^2 - \frac{27}{8}\alpha \, .$$

a. What is the optimum value of α?
b. What is the corresponding energy?
c. The experimental energy is -2.9033 atomic units. How is this number determined?