Quiz 5

Chemistry 3BB3; Winter 2006

1. Write the electronic Schrödinger equation for the hydrogen molecule cation, H_2^+, in SI units, showing the dependence on $\hbar$, *e*, m_e, etc..

2,3. What is the ground state electronic energy of the hydrogen molecule cation, H_2^+, in the <u>united atom limit</u>? What is the ground state wave function? (You can use atomic units in this problem.)

4,5. What is the ground state electronic energy of the hydrogen molecule cation, H_2^+, in the <u>separated atom limit</u>? What is the ground state wave function? (You can use atomic units in this problem.)

6-10. Complete the following table by filling in the appropriate properties for the molecular ground states.

Molecule	Bond Order	Multiplicity
H_2		
He_2		
Li_2		
Be_2		
B_2		
C_2		
N_2		
O_2		
F_2		
Ne_2		

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1. Write the electronic Schrödinger equation for the hydrogen molecule cation, H_2^+, in SI units, showing the dependence on $\hbar$, *e*, m_e, etc..

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r_l} - -\frac{e^2}{4\pi\varepsilon_0 r_r}\right)\psi(r_l, r_r, \phi) = E\psi(r_l, r_r, \phi)$$

where r_l and r_r are the distances from the "left" and "right" nuclei, respectively

2,3. What is the ground state electronic energy of the hydrogen molecule cation, H_2^+, in the <u>united atom limit</u>? What is the ground state wave function? (You can use atomic units in this problem.)

$E_{u.a.} = -\frac{2^2}{2} = -2$ Hartree
$\psi_{u.a.} \propto e^{-2r}$

4,5. What is the ground state electronic energy of the hydrogen molecule cation, H_2^+, in the <u>separated atom limit</u>? What is the ground state wave function? (You can use atomic units in this problem.)

$E_{sep.a.} = -.5$ Hartree
$\psi_{\text{sep.a.}} \propto \left(ce^{-\eta} \pm \sqrt{1-|c|^2}e^{-r_r}\right)$

where r_l and r_r are the distances from the "left" and "right" nuclei, respectively.

6-10. Complete the following table by filling in the appropriate properties for the molecular ground states.

Molecule	Bond Order	Multiplicity
H_2	**1**	**1**
He_2	**0**	**1**
Li_2	**1**	**1**
Be_2	**0**	**1**
B_2	**1**	**3**
C_2	**2**	**1**
N_2	**3**	**1**
O_2	**2**	**3**
F_2	**1**	**1**
Ne_2	**0**	**1**