Name:

Quiz 8,9

Chemistry 3BB3; Winter 2006

1. Write the Heitler-London Valence-Bond Wave Function for the Hydrogen molecule, H_2.

2. Write a the simplest molecular-orbital wave function for the ground state of the Hydrogen molecule, H_2.

3,4. Write the form of the sp hybrid orbitals we used to describe BeH_2.

Name:

5-10. For each of the following, indicate whether the statement pertains to molecular orbital (MO) or valence bond (VB) theory.

_____ In the simplest form, this theory gives a poor description of molecular dissociation.

_____ This theory is associated with orbital hybridization.

_____ This theory is associated with the theory of resonance.

_____ Using this theory, it is difficult to predict the results of electronic spectroscopy.

_____ In this theory, the pairing of electrons to form lone pairs and chemical bonds is of primary importance.

_____ Using this method, it is easy to predict the multiplicity and bond order of diatomic molecules.

_____ This method is easier computationally.

_____ In order to turn this theory into an exact description of molecular phenomena, we must add contributions from ionic electron configurations.

_____ In order to turn this theory into an exact description of molecular phenomena, we must mix excited-state Slater determinants into the ground state.

_____ In this theory, a simple wave function can usually be written as a single Slater determinant.

_____ In this approach, it is rare that the simplest wave functions are single Slater determinants.

_____ The Heitler-London wave function is associated with this theory.

Name:

11-20. Sketch the *all* molecular orbitals of the BeH_2 molecule that are associated with the *2s* and *2p* orbitals of the Beryllium atom and the *1s* orbitals of the hydrogen atoms. (You can omit the molecular orbital due to the *1s* orbitals of Beryllium) Draw the "orbital energy diagram" like we did in class, so that the order of the orbital energies is clear. Assign each orbital a "symbol" ($\sigma, \pi, \delta \ldots$; u or g, + or –).

Name:

Quiz 8,9 (Key)

Chemistry 3BB3; Winter 2006

1. Write the simplest valence-bond wave function for the Hydrogen molecule, H_2. (A more complicated form is acceptable—but not required—but it must be correct!)

$$\Psi_{VB} \propto \left(\phi_{1s}^{(l)}(\boldsymbol{r}_1)\phi_{1s}^{(r)}(\boldsymbol{r}_2) + \phi_{1s}^{(r)}(\boldsymbol{r}_1)\phi_{1s}^{(l)}(\boldsymbol{r}_2)\right)\left(\alpha(1)\beta(2) - \alpha(2)\beta(1)\right)$$

$$\propto \left|\phi_{1s}^{(l)}\alpha \quad \phi_{1s}^{(r)}\beta\right| + \left|\phi_{1s}^{(r)}\alpha \quad \phi_{1s}^{(l)}\beta\right|$$

2. Write a the simplest molecular-orbital wave function for the ground state of the Hydrogen molecule, H_2. (A more complicated form is acceptable—but not required—but it must be correct!)

$$\Psi_{MO} \propto \left(\psi_{1s}^{(l)}(\boldsymbol{r}_1) + \psi_{1s}^{(r)}(\boldsymbol{r}_1)\right)\left(\psi_{1s}^{(l)}(\boldsymbol{r}_2) + \psi_{1s}^{(r)}(\boldsymbol{r}_2)\right)\left(\alpha(1)\beta(2) - \alpha(2)\beta(1)\right)$$

3,4. Write the form of the sp hybrid orbitals we used to describe BeH_2.

$$\psi_{2s}(\boldsymbol{r}) + \psi_{2p_z}(\boldsymbol{r})$$

$$\psi_{2s}(\boldsymbol{r}) - \psi_{2p_z}(\boldsymbol{r})$$

Name:

5-10. For each of the following, indicate whether the statement pertains to molecular orbital (MO) or valence bond (VB) theory.

__**MO**___ In the simplest form, this theory gives a poor description of molecular dissociation.

__**VB**___ This theory is associated with orbital hybridization.

__**VB**___ This theory is associated with the theory of resonance.

__**VB**___ Using this theory, it is difficult to predict the results of electronic spectroscopy.

__**VB**___ In this theory, the pairing of electrons to form lone pairs and chemical bonds is of primary importance.

__**MO**___ Using this method, it is easy to predict the multiplicity and bond order of diatomic molecules.

__**MO**___ This method is easier computationally.

__**VB**___ In order to turn this theory into an exact description of molecular phenomena, we must add contributions from ionic electron configurations.

__**MO**___ In order to turn this theory into an exact description of molecular phenomena, we must mix excited-state Slater determinants into the ground state.

__**MO**___ In this theory, a simple wave function can usually be written as a single Slater determinant.

__**VB**___ In this approach, it is rare that the simplest wave functions are single Slater determinants.

__**VB**___ The Heitler-London wave function is associated with this theory.

Name:

11-20. Sketch the *all* molecular orbitals of the BeH_2 molecule that are associated with the *2s* and *2p* orbitals of the Beryllium atom and the *1s* orbitals of the hydrogen atoms. (You can omit the molecular orbital due to the *1s* orbitals of Beryllium) Draw the "orbital energy diagram" like we did in class, so that the order of the orbital energies is clear. Assign each orbital a "symbol" ($\sigma, \pi, \delta \ldots$; u or g, + or –).