

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” ($\sigma, \pi, \delta \dots$; u or g , $+$ or $-$).

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!)

$$\begin{aligned}\Psi_{VB} &\propto \phi_{1s}^l(\mathbf{r}_1) \phi_{1s}^r(\mathbf{r}_2) + \phi_{1s}^r(\mathbf{r}_1) \phi_{1s}^l(\mathbf{r}_2) \quad \alpha(1) \beta(2) - \alpha(2) \beta(1) \\ &\propto \left| \phi_{1s}^l \alpha \quad \phi_{1s}^r \beta \right| + \left| \phi_{1s}^r \alpha \quad \phi_{1s}^l \beta \right|\end{aligned}$$

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!)

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

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

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

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

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__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.

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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” ($\sigma, \pi, \delta \dots$; u or g , $+$ or $-$).

