Name:

Quiz 5

Chemistry 3BB3; Winter 2005

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

2. Which of the following diatomic molecules *do not* have a singlet ground state?

(a) Li_2
(b) B_2
(c) C_2
(d) N_2
(e) O_2
(f) F_2

3. The non-crossing rule states that

(a) Potential energy curves associated with states of the same symmetry never cross; potential energy curves associated with states of different symmetry always cross.
(b) Potential energy curves associated with states of the same symmetry always cross; potential energy curves associated with states of different symmetry never cross.
(c) Potential energy curves associated with states of the same symmetry never cross; potential energy curves associated with states of different symmetry sometimes cross.
(d) Potential energy curves associated with states of the same symmetry sometimes cross; potential energy curves associated with states of different symmetry never cross.

4. You are given a heteronuclear diatomic molecule, AB. Which of the following properties are most strongly associated with the presence of a strong ionic bond (with minimal covalent character)?

(a) Strong orbital overlap between the bonding orbitals.
(b) Weak orbital overlap between the bonding orbitals.
(c) A large difference in orbital energies of the bonding orbitals.
(d) A small difference in the orbital energies of the bonding orbitals.
(e) Both of the bonding orbitals have orbital energies that are very small (extremely negative).
(f) Both of the bonding orbitals have orbital energies that are rather large (barely negative).

5-9. What is the orbital symmetry label for each of the following molecular orbitals? (Assume that both atoms are the same, so we have a homonuclear diatomic molecule like H_2).

Orbital Symmetry Label	Molecular Orbital
	$\psi_{3d_{xz}}^{(l)}(\boldsymbol{r}) - \psi_{3d_{xz}}^{(r)}(\boldsymbol{r})$
	$\psi_{3d_{yz}}^{(l)}(\boldsymbol{r}) + \psi_{3d_{yz}}^{(r)}(\boldsymbol{r})$
	$\psi_{3d_{x^2-y^2}}^{(l)}(\boldsymbol{r}) + \psi_{3d_{x^2-y^2}}^{(r)}(\boldsymbol{r})$
	$\psi_{3d_{xy}}^{(l)}(\boldsymbol{r}) - \psi_{3d_{xy}}^{(r)}(\boldsymbol{r})$
	$\psi_{3d_{z^2}}^{(l)}(\boldsymbol{r}) - \psi_{3d_{z^2}}^{(r)}(\boldsymbol{r})$

10. How would your answer change if the left atom (whose orbitals are denoted with a superscript (l) and the right atom (whose orbitals are denoted with a superscript (r) were different? (In this case we have a heteronuclear diatomic molecule like LiH.)

Name:

Quiz 5 (Key)

Chemistry 3BB3; Winter 2005

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

$$\Psi_{H_2}^{HL}(\boldsymbol{r}_1,\boldsymbol{r}_2) \propto \left(\phi_{1s}^{(l)}(\boldsymbol{r}_1)\phi_{1s}^{(r)}(\boldsymbol{r}_2)+\phi_{1s}^{(r)}(\boldsymbol{r}_1)\phi_{1s}^{(l)}(\boldsymbol{r}_2)\right)\left(\alpha(1)\beta(2)-\alpha(2)\beta(1)\right)$$

$$\propto \begin{vmatrix}\phi_{1s}^{(l)}\alpha & \phi_{1s}^{(r)}\beta\end{vmatrix} + \begin{vmatrix}\phi_{1s}^{(r)}\alpha & \phi_{1s}^{(l)}\beta\end{vmatrix}$$

2. Which of the following diatomic molecules *do not* have a singlet ground state?

(a) Li_2
(b) B_2
(c) C_2
(d) N_2
(e) O_2
(f) F_2

3. The non-crossing rule states that

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4. You are given a heteronuclear diatomic molecule, AB. Which of the following properties are most strongly associated with the presence of a strong ionic bond (with minimal covalent character)?

(a) Strong orbital overlap between the bonding orbitals.
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(e) Both of the bonding orbitals have orbital energies that are very small (extremely negative).
(f) Both of the bonding orbitals have orbital energies that are rather large (barely negative).

Note: (e) and (f) can't be relevant because they would depend on the choice of the energy zero. The zero of energy can be arbitrarily assigned; so no chemical properties can depend on any particular choice of energy zero and, by implication, on the value of the orbital energy. Only relative energies (e.g., choice (c)) are relevant.

5-9. What is the orbital symmetry label for each of the following molecular orbitals? (Assume that both atoms are the same, so we have a homonuclear diatomic molecule like H_2).

Orbital Symmetry Label	Molecular Orbital
π_u^+	$\psi_{3d_{xz}}^{(l)}(\boldsymbol{r})-\psi_{3d_{xz}}^{(r)}(\boldsymbol{r})$
π_g^-	$\psi_{3d_{yz}}^{(l)}(\boldsymbol{r})+\psi_{3d_{yz}}^{(r)}(\boldsymbol{r})$
δ_g^+	$\psi_{3d_{x^2-y^2}}^{(l)}(\boldsymbol{r})+\psi_{3d_{x^2-y^2}}^{(r)}(\boldsymbol{r})$
δ_u^-	$\psi_{3d_{xy}}^{(l)}(\boldsymbol{r})-\psi_{3d_{xy}}^{(r)}(\boldsymbol{r})$
σ_u^+	$\psi_{3d_{z^2}}^{(l)}(\boldsymbol{r})-\psi_{3d_{z^2}}^{(r)}(\boldsymbol{r})$

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10. How would your answer change if the left atom (whose orbitals are denoted with a superscript (l) and the right atom (whose orbitals are denoted with a superscript (r) were different? (In this case we have a heteronuclear diatomic molecule like LiH.)

There is no "u" or "g" designation for a heteronuclear diatomic molecule. All the other portions of the term symbol are identical.

For practice, you might want to consider which of the orbitals in parts 5-9 are binding and antibinding. (Answer: the π_u^+ and δ_g^+ are binding. Can you explain why?)