Quiz 7

Chemistry 3BB3; Winter 2006

1-3. List three things that are favorable for covalent bonding.

4. Consider the π-bonding and π-antibonding orbitals in O_2. Along the internuclear axis (the line between the two atomic nuclei that represents the "bond"), the amount of electron density in a π-antibonding orbital is _____ the amount of electron density in the associated π-bonding orbital.

(a) greater than
(b) less than
(c) the same as

5. Consider the σ-bonding and σ-antibonding in the the Helium molecule cation, He_2^+. Along the internuclear axis (the line between the two atomic nuclei that represents the "bond"), the amount of electron density in a σ-antibonding orbital is _____ the amount of orbital density in the associated σ-bonding orbital.

(a) greater than
(b) less than
(c) the same as

6-10. Label the following approximate (unnormalized) molecular orbitals using the σ, π, δ, u, g, and $+, -$ designations. Here, we denote the $1s$ orbital on the "left-hand" atom as $\psi_{1s}^{(l)}(\boldsymbol{r})$, with the obvious generalization of notation to the other orbitals and the "right-hand" atom.

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

Quiz 7

Chemistry 3BB3; Winter 2006

1-3. List three things that are favorable for covalent bonding.

-- orbitals that are similar in size.

-- orbitals that are similar in energy.

-- good overlap between orbitals. (Orbitals in similar regions of space.)

-- "directionality" in orbitals (so that they "point at" each other).

-- smaller orbitals are (usually) better than bigger orbitals.

....

4. Consider the π-bonding and π-antibonding orbitals in O_2. Along the internuclear axis (the line between the two atomic nuclei that represents the "bond"), the amount of electron density in a π-antibonding orbital is _____ the amount of electron density in the associated π-bonding orbital.

(a) greater than
(b) less than
(c) the same as

5. Consider the σ-bonding and σ-antibonding in the the Helium molecule cation, He_2^+. Along the internuclear axis (the line between the two atomic nuclei that represents the "bond"), the amount of electron density in a σ-antibonding orbital is _____ the amount of orbital density in the associated σ-bonding orbital.

(a) greater than
(b) less than
(c) the same as

6-10. Label the following approximate (unnormalized) molecular orbitals using the σ, π, δ, u, g, and $+, -$ designations. Here, we denote the $1s$ orbital on the "left-hand" atom as $\psi_{1s}^{(l)}(\boldsymbol{r})$, with the obvious generalization of notation to the other orbitals and the "right-hand" atom.

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^+	$\psi_{3d_{z^2}}^{(l)}(\boldsymbol{r}) - \psi_{3d_{z^2}}^{(r)}(\boldsymbol{r})$