## Quiz 7

## Chemistry 3BB3; Winter 2006

1-3.	List three	things	that are	favorable	for	covalent h	onding
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- 4. Consider the  $\pi$ -bonding and  $\pi$ -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  $\pi$ -antibonding orbital is \_\_\_\_\_\_ the amount of electron density in the associated  $\pi$ -bonding orbital.
  - (a) greater than
  - (b) less than
  - (c) the same as
- 5. Consider the  $\sigma$ -bonding and  $\sigma$ -antibonding in the Helium molecule cation,  $\text{He}_2^+$ . Along the internuclear axis (the line between the two atomic nuclei that represents the "bond"), the amount of electron density in a  $\sigma$ -antibonding orbital is \_\_\_\_\_\_ the amount of orbital density in the associated  $\sigma$ -bonding orbital.
  - (a) greater than
  - (b) less than
  - (c) the same as
- 6-10. Label the following approximate (unnormalized) molecular orbitals using the  $\sigma,\pi,\delta$ , u,g, and +,- designations. Here, we denote the 1s orbital on the "left-hand" atom as  $\psi_{1s}^{l}$  r, with the obvious generalization of notation to the other orbitals and the "right-hand" atom.

Orbital Symmetry Label	Molecular Orbital
	$\psi^{\;l}_{3d_{xz}}\;\;oldsymbol{r}\;-\psi^{\;r}_{3d_{xz}}\;\;oldsymbol{r}$
	$\psi^{\;l}_{3d_{yz}}\;m{r}\;+\psi^{\;r}_{3d_{yz}}\;m{r}$
	$\psi^{\;l}_{3d_{x^2-y^2}}\;m{r}\;+\psi^{\;r}_{3d_{x^2-y^2}}\;m{r}$
	$\psi^{~l}_{3d_{xy}}$ $m{r}$ $-\psi^{~r}_{3d_{xy}}$ $m{r}$
	$\psi^{\;l}_{3d_{z^2}}$ $oldsymbol{r}$ $-\psi^{\;r}_{3d_{z^2}}$ $oldsymbol{r}$

## Quiz 7

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- 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.

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4. Consider the  $\pi$ -bonding and  $\pi$ -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  $\pi$ -antibonding orbital is \_\_\_\_\_\_ the amount of electron density in the associated  $\pi$ -bonding orbital.

(a) greater than (b) less than

- (c) the same as
- 5. Consider the  $\sigma$ -bonding and  $\sigma$ -antibonding in the Helium molecule cation, He<sub>2</sub><sup>+</sup>. Along the internuclear axis (the line between the two atomic nuclei that represents the "bond"), the amount of electron density in a  $\sigma$ -antibonding orbital is \_\_\_\_\_ the amount of orbital density in the associated  $\sigma$ -bonding orbital.
  - (a) greater than(b) less than

(c) the same as

6-10. Label the following approximate (unnormalized) molecular orbitals using the  $\sigma,\pi,\delta$ , 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
$\pi_u^+$	$\psi^{~l}_{3d_{xz}}$ $oldsymbol{r}$ $-\psi^{~r}_{3d_{xz}}$ $oldsymbol{r}$
$\pi_g^-$	$\psi^{}_{3d_{yz}}$ $m{r}$ $+$ $\psi^{r}_{3d_{yz}}$ $m{r}$
$\delta_g^+$	$\psi^{~l}_{3d_{x^2-y^2}} ~~ m{r} ~ + \psi^{~r}_{3d_{x^2-y^2}} ~~ m{r}$
$\delta_u^-$	$\psi^{~l}_{3d_{xy}}$ $oldsymbol{r}$ $-\psi^{~r}_{3d_{xy}}$ $oldsymbol{r}$
$\sigma_u^+$	$\psi^{}_{3d_{z^2}}$ $oldsymbol{r}$ $-\psi^{}_{3d_{z^2}}$ $oldsymbol{r}$