Quiz 6

Chemistry 3BB3; Winter 2006

1. **The non-crossing rule implies that**
   (a) In a <u>diatomic</u> molecule, potential energy curves corresponding to wave functions with the <u>same</u> symmetry do not intersect.
   (b) In a <u>diatomic</u> molecule, potential energy curves corresponding to wave functions with the <u>different</u> symmetry do not intersect.
   (c) In a <u>triatomic</u> molecule, potential energy surfaces corresponding to wave functions with the <u>same</u> symmetry do not intersect.
   (d) In a <u>triatomic</u> molecule, potential energy surfaces corresponding to wave functions with the <u>different</u> symmetry do not intersect.

2-7. **Complete the following table by filling in the appropriate properties for the molecular ground states.**

Molecule	Bond Order	Multiplicity
LiBe		
LiB		
CN		
CN⁻		
CO		
HF		

8-10. **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 $\psi_{1s}^{l}\ r$, with the obvious generalization of notation to the other orbitals and the "right-hand" atom.**

Orbital Symmetry Label	Molecular Orbital
	$\psi_{2p_x}^{l}\ r + \psi_{2p_x}^{r}\ r$
	$\psi_{2p_x}^{l}\ r - \psi_{2p_x}^{r}\ r$
	$\psi_{2p_y}^{l}\ r + \psi_{2p_y}^{r}\ r$
	$\psi_{2p_y}^{l}\ r - \psi_{2p_y}^{r}\ r$
	$\psi_{2p_z}^{l}\ r + \psi_{2p_z}^{r}\ r$
	$\psi_{2p_z}^{l}\ r - \psi_{2p_z}^{r}\ r$

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2-7. **Complete the following table by filling in the appropriate properties for the molecular ground states.**

Molecule	Bond Order	Multiplicity
LiBe	½	2
LiB	0	1
CN	2 ½	2
CN⁻	3	1
CO	3	1
HF	1	1

8-10. **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 $\psi_{1s}^{l}\ r$, with the obvious generalization of notation to the other orbitals and the "right-hand" atom.**

Orbital Symmetry Label	Molecular Orbital
π_u^+	$\psi_{2p_x}^{l}\ r + \psi_{2p_x}^{r}\ r$
π_g^+	$\psi_{2p_x}^{l}\ r - \psi_{2p_x}^{r}\ r$
π_u^-	$\psi_{2p_y}^{l}\ r + \psi_{2p_y}^{r}\ r$
π_g^-	$\psi_{2p_y}^{l}\ r - \psi_{2p_y}^{r}\ r$
σ_u^+	$\psi_{2p_z}^{l}\ r + \psi_{2p_z}^{r}\ r$
σ_g^+	$\psi_{2p_z}^{l}\ r - \psi_{2p_z}^{r}\ r$