Quiz 6

Chemistry 3BB3; Winter 2006

1. The non-crossing rule implies that

(a) In a diatomic molecule, potential energy curves corresponding to wave functions with the same symmetry do not intersect.

(b) In a diatomic molecule, potential energy curves corresponding to wave functions with the different symmetry do not intersect.

(c) In a triatomic molecule, potential energy surfaces corresponding to wave functions with the same symmetry do not intersect.

(d) In a triatomic molecule, potential energy surfaces corresponding to wave functions with the different 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 $\psi_{1s}^{(l)}(\boldsymbol{r})$, with the obvious generalization of notation to the other orbitals and the "right-hand" atom.

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

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(c) In a triatomic molecule, potential energy surfaces corresponding to wave functions with the same symmetry do not intersect.

(d) In a triatomic molecule, potential energy surfaces corresponding to wave functions with the different 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	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 $\psi_{1s}^{(l)}(\boldsymbol{r})$, with the obvious generalization of notation to the other orbitals and the "right-hand" atom.

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