Name________________________________ Student #__________________________

Quiz 8
CHEM 3PA3; Fall 2019

1-2. What is the ground-state (a) wavefunction and (b) energy for the hydrogen molecule cation, H_2^+, in the united-atom limit?

$\psi_{g.s.}(\mathbf{r}) =$

$E_{g.s.} =$

3-4. What is the ground-state (a) wavefunction and (b) energy for the hydrogen molecule cation, H_2^+, in the separated-atom limit?

$\psi_{g.s.}(\mathbf{r}) =$

$E_{g.s.} =$

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5-10. **For each of the following orbitals, assign a symmetry label $\{\sigma,\pi,\delta,\ldots\},\{u,g\},\{+,-\}$. Assume that the orbitals are the atomic orbitals of the left and right atom in the separated-atom limit, and that the molecule is a homonuclear diatomic molecule. Assume that the bond axis is the *z* axis. Circle whether the orbital is bonding or antibonding.**

Orbital	**Symmetry-Label**	**Bonding/Antibonding** (circle one)
$\psi_{1s}^{(l)}(\mathbf{r})-\psi_{1s}^{(r)}(\mathbf{r})$		bonding antibonding
$\psi_{2p_z}^{(l)}(\mathbf{r})-\psi_{2p_z}^{(r)}(\mathbf{r})$		bonding antibonding
$\psi_{3p_x}^{(l)}(\mathbf{r})-\psi_{3p_x}^{(r)}(\mathbf{r})$		bonding antibonding
$\psi_{2p_y}^{(l)}(\mathbf{r})+\psi_{2p_y}^{(r)}(\mathbf{r})$		bonding antibonding
$\psi_{3d_{+2}}^{(l)}(\mathbf{r})-\psi_{3d_{+2}}^{(r)}(\mathbf{r})$		bonding antibonding
$\psi_{3d_0}^{(l)}(\mathbf{r})+\psi_{3d_0}^{(r)}(\mathbf{r})$		bonding antibonding
Bonus:		
$\psi_{3d_{xy}}^{(l)}(\mathbf{r})+\psi_{3d_{xy}}^{(r)}(\mathbf{r})$		bonding antibonding
$\psi_{3d_{xz}}^{(l)}(\mathbf{r})-\psi_{3d_{xz}}^{(r)}(\mathbf{r})$		bonding antibonding

Bonus: (5 points) How would these answers change if the molecule were a heteronuclear diatomic, that is, if the right- and left- atoms were different?

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1-2. What is the ground-state (a) wavefunction and (b) energy for the hydrogen molecule cation, H_2^+, in the united-atom limit?

$$\psi_{g.s.}(\mathbf{r}) = \psi_{1s}^{\mathrm{He}}(\mathbf{r})$$

$$E_{g.s.} = -2 \text{ a.u.}$$

3-5. What is the ground-state (a) wavefunction and (b) energy for the hydrogen molecule cation, H_2^+, in the separated-atom limit?

$$\psi_{g.s.}(\mathbf{r}) = \tfrac{1}{\sqrt{2}}\left(\psi_{1s}^{\mathrm{H_{left}}}(\mathbf{r}) \pm \psi_{1s}^{\mathrm{H_{right}}}(\mathbf{r})\right)$$

$$E_{g.s.} = -\tfrac{1}{2} \text{ a.u.}$$

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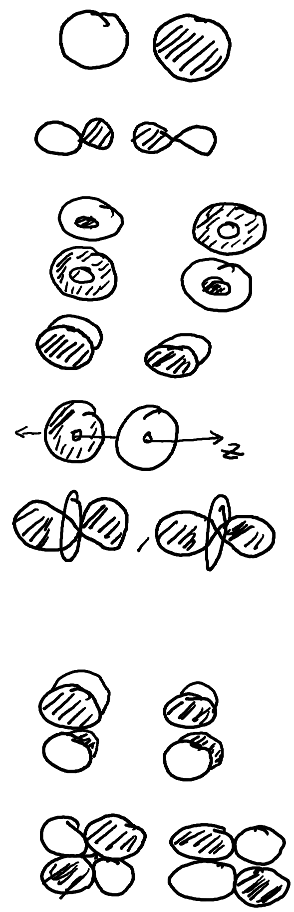
5-10. For each of the following orbitals, assign a symmetry label $\{\sigma, \pi, \delta, \ldots\}, \{u, g\}, \{+, -\}$. Assume that the orbitals are the atomic orbitals of the left and right atom in the separated-atom limit, and that the molecule is a homonuclear diatomic molecule. Assume that the bond axis is the *z* axis. Circle whether the orbital is bonding or antibonding.

I will include a “count” of how many orbitals there are of this symmetry before you get to this one but this is not essential.

Orbital	Symmetry-Label	Bonding/Antibonding (circle one)
$\psi_{1s}^{(l)}(\mathbf{r})-\psi_{1s}^{(r)}(\mathbf{r})$	$1\sigma_g^+$	bonding antibonding
$\psi_{2p_z}^{(l)}(\mathbf{r})-\psi_{2p_z}^{(r)}(\mathbf{r})$	$3\sigma_g^+$	bonding antibonding
$\psi_{3p_x}^{(l)}(\mathbf{r})-\psi_{3p_x}^{(r)}(\mathbf{r})$	$2\pi_g^+$	bonding antibonding
$\psi_{2p_y}^{(l)}(\mathbf{r})+\psi_{2p_y}^{(r)}(\mathbf{r})$	$1\pi_u^-$	bonding antibonding
$\psi_{3d_{+2}}^{(l)}(\mathbf{r})-\psi_{3d_{+2}}^{(r)}(\mathbf{r})$	$1\delta_u^+$	bonding antibonding
$\psi_{3d_0}^{(l)}(\mathbf{r})+\psi_{3d_0}^{(r)}(\mathbf{r})$	$6\sigma_g^+$	bonding antibonding
Bonus:		
$\psi_{3d_{xy}}^{(l)}(\mathbf{r})+\psi_{3d_{xy}}^{(r)}(\mathbf{r})$	$1\delta_g^-$	bonding antibonding
$\psi_{3d_{xz}}^{(l)}(\mathbf{r})-\psi_{3d_{xz}}^{(r)}(\mathbf{r})$	$5\pi_u^+$	bonding antibonding



Bonus: (5 points) How would these answers change if the molecule were a heteronuclear diatomic, that is, if the right- and left- atoms were different?

The “u” and “g” labels would be deleted. That’s the only change.