Name____________________________________ Student #_____________________________

Quiz 10
CHEM 3PA3; Fall 2018

This quiz has 10 problems worth 10 points each. There are 30 bonus points….

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

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

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

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

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

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

BONUS: (5 pt) What is the first excited-state wavefunction for the hydrogen molecule cation in the separated-atom limit?

There are many choices. Two of them are:

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

Any combination of *2s* or *2p* orbitals on the separated atoms is acceptable however.

Bonus (5 pt) What is the degeneracy of the first excited state for the hydrogen molecule cation in the separated-atom limit?

There are 8 degenerate spatial orbitals (1 2*s* and 3 2*p*'s on each atom). This is a total of 8 spatial orbitals that you can combine. Plus spin-symmetry gives a total degeneracy of 16. (I will give credit for 8 also, however.)

Bonus (5 pt) What is the degeneracy of the first excited state for the hydrogen molecule cation in the united-atom limit?

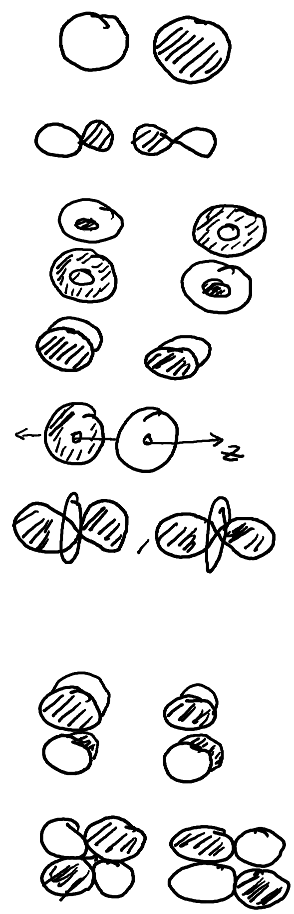
In the united atom limit you have He+, which as degenerate 2s and 2p states. So there are 4 degenerate spatial orbitals and including spin a total degeneracy of 8.

Name______________________________ Student #__________________________

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.

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

$E_{g.s.} =$

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

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

$E_{g.s.} =$

BONUS: (5 pt) What is the first excited-state wavefunction for the hydrogen molecule cation in the separated-atom limit?

Bonus (5 pt) What is the degeneracy of the first excited state for the hydrogen molecule cation in the separated-atom limit?

Bonus (5 pt) What is the degeneracy of the first excited state for the hydrogen molecule cation in the united-atom limit?

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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?