Name:

Quiz 3

Chemistry 3BB3; Winter 2006

When we performed the Born-Oppenheimer approximation for the Hydrogen molecule, we separated the Schrödinger equation for the molecule into an electronic Schrödinger equation and a nuclear Schrödinger equation.

1. **Write the electronic Schrödinger equation for the Helium <u>atom</u> in SI units, showing the dependence on $\hbar$, *e*, m_e, etc..**

The ionization potential is defined as "the amount of energy it takes to remove one electron from a system." The second ionization potential is defined as "the amount of energy it takes to remove the second electron from the system." (E.g., for a neutral molecule, the second ionization potential is the amount of energy it takes to remove an electron from the cation.) The energy of the neutral Helium atom is -2.9037 Hartree.

2. **What is the first ionization potential of the Helium atom?**

3. **What is the second ionization potential of the Helium atom?**

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4. **Which of the following statements is true. There may be more than one answer.**
   (a) The energy of the Lithide ion Li^- is <u>less than</u> the energy of the Beryllium atom, Be.
   (b) The energy of the Beryllium atom, Be, is <u>less than</u> the energy of the Boron cation, B^+.
   (c) The energy of the Lithide ion Li^- is <u>greater than</u> the energy of the Beryllium atom, Be.
   (d) The energy of the Beryllium atom, Be, is <u>greater than</u> the energy of the Boron cation, B^+.

5. **Which of the following statements is true. There may be more than one answer.**
   (a) The energy of the Lithium atom, Li, is <u>greater than</u> three times the energy of the Lithium dication, Li^{2+}.
   (b) The energy of the Lithium atom, Li, is <u>less than</u> three times the energy of the Lithium dication, Li^{2+}.
   (c) The energy of the Lithium atom, Li, is <u>equal to</u> three times the energy of the Lithium dication, Li^{2+}.

6. **Which of the following commutators are <u>zero</u>; there may be more than one answer.**
   (a) $\left[\hat{S}^2, \hat{S}_x\right]$ (d) $\left[\hat{S}_x, \hat{S}^2\right]$ (g) $\left[\hat{S}_y, \hat{S}_x\right]$
   (b) $\left[\hat{S}^2, \hat{S}_y\right]$ (e) $\left[\hat{S}_y, \hat{S}^2\right]$ (h) $\left[\hat{S}_y, \hat{S}_y\right]$
   (c) $\left[\hat{S}^2, \hat{S}_z\right]$ (f) $\left[\hat{S}_z, \hat{S}^2\right]$ (i) $\left[\hat{S}_y, \hat{S}_z\right]$

7. **The spin-magnetic moment of an electron is related to the operator for the spin-angular momentum of the electron by the formula $\boldsymbol{\mu}_S = g \cdot \frac{-e}{2mc}\hat{\boldsymbol{S}}$. The potential energy of interaction between the spinning electron and a magnetic field, $\boldsymbol{B}$, is expressed using the operator:**
   (a) $\hat{V}_{mag} \equiv \hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}$ (d) $\hat{V}_{mag} \equiv -\hat{\boldsymbol{\mu}} \times \boldsymbol{B}$ (g) $\hat{V}_{mag} \equiv i\hbar\hat{\boldsymbol{\mu}} \times \boldsymbol{B}$
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   (c) $\hat{V}_{mag} \equiv \hat{\boldsymbol{\mu}} \times \boldsymbol{B}$ (f) $\hat{V}_{mag} \equiv -i\hbar\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}$

8. **The "g factor" for an electron is approximately**
   (a) 1.0 (c) 2.0 (e) ln(2)
   (b) 0.5 (d) π (f) $\ln\ \hbar$

9. **The quantity $\beta_e = \dfrac{e\hbar}{mc}$ is called the**
   (a) Hartree magneton. (c) Bohr magneton. (e) Gauss magneton.
   (b) Landau factor. (d) Hartree factor. (f) Schrödinger factor.

10. **Consider the Beryllium atom. ($Z = 4$ with 4 electrons.) The effective nuclear charge felt by one of the electrons when it is very, very far from the nucleus is**
    (a) $Z_{eff} = -1$ (c) $Z_{eff} = 1$ (e) $Z_{eff} = 3$
    (b) $Z_{eff} = 0$ (d) $Z_{eff} = 2$ (f) $Z_{eff} = 4$

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1. **Write the electronic Schrödinger equation for the Helium <u>atom</u> in SI units, showing the dependence on $\hbar$, *e*, m_e, etc..**

$$\left(-\frac{\hbar^2}{2m_e}\nabla_1^2-\frac{\hbar^2}{2m_e}\nabla_2^2-\frac{Ze^2}{4\pi\varepsilon_0 r_1}-\frac{Ze^2}{4\pi\varepsilon_0 r_2}+\frac{e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_1-\boldsymbol{r}_2\right|}\right)\Psi\ \boldsymbol{r}_1,\sigma_1;\boldsymbol{r}_2,\sigma_2\ =E\Psi\ \boldsymbol{r}_1,\sigma_1;\boldsymbol{r}_2,\sigma_2$$

The ionization potential is defined as "the amount of energy it takes to remove one electron from a system." The second ionization potential is defined as "the amount of energy it takes to remove the second electron from the system." (E.g., for a neutral molecule, the second ionization potential is the amount of energy it takes to remove an electron from the cation.) The energy of the neutral Helium atom is -2.9037 Hartree.

2. **What is the first ionization potential of the Helium atom?**

.9037 Hartree = E(He^+) – E(He)

3. **What is the second ionization potential of the Helium atom?**

2 Hartree = - E(He^+)

Note that since it always requires energy to remove electrons, ionization potential are always positive.

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