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) $\left[\hat{S}^2,\hat{S}_x\right]$
(b) $\left[\hat{S}^2,\hat{S}_y\right]$
(c) $\left[\hat{S}^2,\hat{S}_z\right]$
(d) $\left[\hat{S}_x,\hat{S}^2\right]$
(e) $\left[\hat{S}_y,\hat{S}^2\right]$
(f) $\left[\hat{S}_z,\hat{S}^2\right]$
(g) $\left[\hat{S}_y,\hat{S}_x\right]$
(h) $\left[\hat{S}_y,\hat{S}_y\right]$
(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) $\hat{V}_{mag} \equiv \hat{\boldsymbol{\mu}}\cdot\boldsymbol{B}$
(b) $\hat{V}_{mag} \equiv -\hat{\boldsymbol{\mu}}\cdot\boldsymbol{B}$
(c) $\hat{V}_{mag} \equiv \hat{\boldsymbol{\mu}}\times\boldsymbol{B}$
(d) $\hat{V}_{mag} \equiv -\hat{\boldsymbol{\mu}}\times\boldsymbol{B}$
(e) $\hat{V}_{mag} \equiv i\hbar\hat{\boldsymbol{\mu}}\cdot\boldsymbol{B}$
(f) $\hat{V}_{mag} \equiv -i\hbar\hat{\boldsymbol{\mu}}\cdot\boldsymbol{B}$
(g) $\hat{V}_{mag} \equiv i\hbar\hat{\boldsymbol{\mu}}\times\boldsymbol{B}$
(h) $\hat{V}_{mag} \equiv -i\hbar\hat{\boldsymbol{\mu}}\times\boldsymbol{B}$

8. The "g factor" for an electron is approximately

(a) 1.0
(b) 0.5
(c) 2.0
(d) π
(e) ln(2)
(f) $\ln(\hbar)$

9. The quantity $\beta_e = \dfrac{e\hbar}{mc}$ is called the

(a) Hartree magneton.
(b) Landau factor.
(c) Bohr magneton.
(d) Hartree factor.
(e) Gauss magneton.
(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) $Z_{eff} = -1$
(b) $Z_{eff} = 0$
(c) $Z_{eff} = 1$
(d) $Z_{eff} = 2$
(e) $Z_{eff} = 3$
(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..**

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

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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(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) $\left[\hat{S}_y, \hat{S}_z\right]$

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(b) $\hat{V}_{mag} \equiv -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}$ (e) $\hat{V}_{mag} \equiv i\hbar\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}$ (h) $\hat{V}_{mag} \equiv -i\hbar\hat{\boldsymbol{\mu}} \times \boldsymbol{B}$

(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.

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(b) $Z_{eff} = 0$ (d) $Z_{eff} = 2$ (f) $Z_{eff} = 4$