Name:

Quiz 3

Chemistry 3BB3; Winter 2004

1. **Write the electronic Schrödinger Equation for the Beryllium (Z=4, N=4) atom, showing the dependence on $\hbar$, e, ε_0, and m_e. (Do not use atomic units. You may use the Born-Oppenheimer approximation.)**

2. **Write a Slater determinant wave function for the $1s^2 4s^1$ excited state of the Lithium atom. Do not use the "shorthand" notation. Denote the spatial part of the 1s orbital with $\psi_{1s}(\boldsymbol{r})$ and the spatial part of the 2s orbital with $\psi_{4s}(\boldsymbol{r})$.**

Using separation of variables, the wave function for the hydrogen atom can be written as

$$\Psi_{n,l,m}(\boldsymbol{r}) = R_{n,l}(r) Y_l^m(\theta,\phi).$$

3. **Write the Schrödinger equation for radial wave function, $R_{n,l}(r)$, in the hydrogen atom. You may use atomic units.**

4. **Is** $\Psi(\boldsymbol{r}_1,\sigma(1),\boldsymbol{r}_2,\sigma(2)) \propto e^{-\zeta r_1} e^{-\zeta r_2}\left(1 + b|\boldsymbol{r}_1 - \boldsymbol{r}_2| + c|\boldsymbol{r}_1 - \boldsymbol{r}_2|^2\right)\left(\alpha(1)\beta(2) - \alpha(2)\beta(1)\right)$
an acceptable approximate wave function for the Helium atom?

(a) yes

(b) no

Name:

5. **Which of the following operators commute with the electronic Hamiltonian for an atom. (There may be more than one answer.)**

(a) $\hat{L}_x$	(d) $\hat{L}^2$	(g) $\hat{J}_x$
(b) $\hat{L}_y$	(e) $\hat{S}^2$	(h) $\hat{S}_y$
(c) $\hat{L}_z$	(f) $\hat{J}^2$	(i) $\hat{S}_x$

6. **Which of the following operators commute with $\hat{L}_x$. (There may be more than one answer.)**

(a) $\hat{L}_x$	(e) $\hat{J}_y$	(g) $\hat{S}_x$
(b) $\hat{L}_y$	(f) $\hat{L}^2$	(h) $\hat{S}_y$
(c) $\hat{L}_z$	(g) $\hat{S}^2$	(i) $\hat{S}_z$
(d) $\hat{J}_x$	(h) $\hat{J}^2$	

7. **Which of the following operators commute with $\hat{S}_x$. (There may be more than one answer.)**

(a) $\hat{L}_x$	(e) $\hat{J}_y$	(g) $\hat{S}_x$
(b) $\hat{L}_y$	(f) $\hat{L}^2$	(h) $\hat{S}_y$
(c) $\hat{L}_z$	(g) $\hat{S}^2$	(i) $\hat{S}_z$
(d) $\hat{J}_x$	(h) $\hat{J}^2$	

Below, there is a table with three term symbols.

8. **What are the possible values of J?**
9. **What are the possible values for M_S?**
10. **What are the possible values of M_L?**

	Term Symbol		
Values of	^6D	^3G	^1S
J			
M_S			
M_J			

Name:

Quiz 3

Chemistry 3BB3; Winter 2004

1. **Write the electronic Schrödinger Equation for the Beryllium (Z=4, N=4) atom, showing the dependence on $\hbar$, e, ε_0, and m_e. (Do not use atomic units. You may use the Born-Oppenheimer approximation.)**

$$\sum_{i=1}^{4}\left(\frac{-\hbar^2}{2m_e}\nabla_i^2-\frac{Ze^2}{4\pi\varepsilon_0 r_i}\right)+\sum_{i=1}^{3}\sum_{j=i+1}^{4}\frac{e^2}{4\pi\varepsilon_0\left|\boldsymbol{r}_i-\boldsymbol{r}_j\right|}$$

2. **Write a Slater determinant wave function for the $1s^2 4s^1$ excited state of the Lithium atom. Do not use the "shorthand" notation. Denote the spatial part of the 1s orbital with $\psi_{1s}(\boldsymbol{r})$ and the spatial part of the 2s orbital with $\psi_{4s}(\boldsymbol{r})$.**

$$\Phi_{1s^2 4s^1}(\boldsymbol{r}_1,s_1;\boldsymbol{r}_2,s_2;\boldsymbol{r}_3,s_3)=\frac{1}{\sqrt{3!}}\begin{vmatrix}\psi_{1s}(\boldsymbol{r}_1)\alpha(1) & \psi_{1s}(\boldsymbol{r}_1)\beta(1) & \psi_{4s}(\boldsymbol{r}_1)\alpha(1)\\ \psi_{1s}(\boldsymbol{r}_2)\alpha(2) & \psi_{1s}(\boldsymbol{r}_2)\beta(2) & \psi_{4s}(\boldsymbol{r}_2)\alpha(2)\\ \psi_{1s}(\boldsymbol{r}_3)\alpha(3) & \psi_{1s}(\boldsymbol{r}_3)\beta(3) & \psi_{4s}(\boldsymbol{r}_3)\alpha(3)\end{vmatrix}$$

Using separation of variables, the wave function for the hydrogen atom can be written as

$$\Psi_{n,l,m}(\boldsymbol{r})=R_{n,l}(r)Y_l^m(\theta,\phi).$$

3. **Write the Schrödinger equation for radial wave function, $R_{n,l}(r)$, in the hydrogen atom. You may use atomic units.**

$$\left(-\frac{1}{2r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{l(l+1)}{2r^2}-\frac{Z}{r}\right)R_{n,l}(r)=E_{n,l}R_{n,l}(r)$$

4. **Is** $\Psi(\boldsymbol{r}_1,\sigma(1),\boldsymbol{r}_2,\sigma(2))\propto e^{-\zeta r_1}e^{-\zeta r_2}\left(1+b\left|\boldsymbol{r}_1-\boldsymbol{r}_2\right|+c\left|\boldsymbol{r}_1-\boldsymbol{r}_2\right|^2\right)\left(\alpha(1)\beta(2)-\alpha(2)\beta(1)\right)$
an acceptable approximate wave function for the Helium atom?

(a) yes (b) no

5. **Which of the following operators commute with the electronic Hamiltonian for an atom. (There may be more than one answer.)**

(a) $\hat{L}_x$ **(d)** $\hat{L}^2$ **(g)** $\hat{J}_x$

(b) $\hat{L}_y$ **(e)** $\hat{S}^2$ **(h)** $\hat{S}_y$

(c) $\hat{L}_z$ **(f)** $\hat{J}^2$ **(i)** $\hat{S}_x$

Name:

6. **Which of the following operators commute with $\hat{L}_x$. (There may be more than one answer.)**

(a) $\hat{L}_x$
(b) $\hat{L}_y$
(c) $\hat{L}_z$
(d) $\hat{J}_x$
(e) $\hat{J}_y$
(f) $\hat{L}^2$
(g) $\hat{S}^2$
(h) $\hat{J}^2$
(g) $\hat{S}_x$
(h) $\hat{S}_y$
(i) $\hat{S}_z$

7. **Which of the following operators commute with $\hat{S}_x$. (There may be more than one answer.)**

(a) $\hat{L}_x$
(b) $\hat{L}_y$
(c) $\hat{L}_z$
(d) $\hat{J}_x$
(e) $\hat{J}_y$
(f) $\hat{L}^2$
(g) $\hat{S}^2$
(h) $\hat{J}^2$
(g) $\hat{S}_x$
(h) $\hat{S}_y$
(i) $\hat{S}_z$

Below, there is a table with three term symbols.

8. **What are the possible values of J?**
9. **What are the possible values for M_S?**
10. **What are the possible values of M_L?**

	Term Symbol		
Values	^6D	^3G	^1S
J	$\lvert L-S\rvert = \frac{1}{2} \le J \le \frac{9}{2} = L+S$ $J = \frac{1}{2},\frac{3}{2},\frac{5}{2},\frac{7}{2},\frac{9}{2}$	$\lvert L-S\rvert = 3 \le J \le 5 = L+S$ $J = 3,4,5$	$\lvert L-S\rvert = 0 \le J \le 0 = L+S$ $J = 0$
M_S	**2S+1=6, so S=$\frac{5}{2}$. Thus** $M_S = -\frac{5}{2},\frac{-3}{2},\ldots,\frac{5}{2}$	**2S+1=3, so S=1. Thus** $M_S = -1,0,1$	**2S+1=0, so S=0. Thus** $M_S = 0$
M_J	**L=2 so** $M_L = -2,-1,0,1,2$	**L=4 so** $M_L = -4,-3,-2,-1,0,1,2,3,4$	**L=0 so** $M_L = 0$