

Quiz 4

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 Lithium atom in SI units, showing the dependence on \hbar , e , m_e , etc..

- 2,3. Write a Slater determinant for an excited state of the Lithium atom with $M_S = \frac{1}{2}$ and $M_L = 1$. Do not use shorthand notation. (That is, write out every element in all three columns and all three rows.) Make sure you include the normalization factor.

- 4-5. For an atom, you start by measuring the expectation value of \hat{J}_z , which gives you M_J . The wavefunction associated with this value of M_J is clearly an eigenfunction of \hat{J}_z . The wavefunction could also be chosen to be an eigenfunction of which of the following operators. [Circle all that apply.]

- | | | | | |
|-----------------|-----------------|-----------------|-----------------------------------------------|-----------------|
| (a) \hat{J}^2 | (d) \hat{J}_y | (g) \hat{J}_x | (k) $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ | (n) \hat{L}_z |
| (b) \hat{L}^2 | (e) \hat{S}_y | (h) \hat{S}_x | (l) \hat{H} | |
| (c) \hat{S}^2 | (f) \hat{L}_y | (i) \hat{L}_x | (m) \hat{S}_z | |

Name:

The ground state electron configuration of the Protactinium atom is $\text{Rn } 7s^2 5f^2 6d^1$ where Rn is a shorthand for the electron configuration of the Radon atom,

$$\text{Rn} \equiv 1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^6 5s^2 4d^{10} 5p^6 6s^2 4f^{14} 5d^{10} 6p^6$$

The L-S coupling scheme we used in class is not especially appropriate here, but let's pretend there is no problem and determine the term symbols for Proactinium. You may find the following information helpful

- The ground state electron configuration of the Protactinium atom is $\text{Rn } 7s^2 5f^2 6d^1$.
- The ground state term symbol for Radon is 1S .
- The term symbols corresponding to a $5f^2$ electron configuration are $^1S, ^3P, ^1D, ^3F, ^1G, ^3H, ^1I$.

6-7. What are the term symbols for the ground state of the Protactinium atom. You do not need to denote the “ J ” values.

Assume that Hund's Rules are accurate in this setting. The ground state of this system has

- 8. Total orbital angular momentum, $L =$ _____**
- 9. Total spin angular momentum, $S =$ _____**
- 10. If Hund's third rule is valid, the total angular momentum of the ground state is, $J =$ _____**

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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 Lithium atom in SI units, showing the dependence on \hbar , e , m_e , etc..

$$\left(\sum_{i=1}^3 \left(-\frac{\hbar^2}{2m_e} \nabla_i^2 - \frac{3e^2}{4\pi\epsilon_0 r_i} \right) + \sum_{i=1}^2 \sum_{j=i+1}^3 \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} \right) \Psi(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2; \mathbf{r}_3, \sigma_3) = E \Psi(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2; \mathbf{r}_3, \sigma_3)$$

- 2,3. Write a Slater determinant for an excited state of the Lithium atom with $M_S = \frac{1}{2}$ and $M_L = 1$. Do not use shorthand notation. (That is, write out every element in all three columns and all three rows.) Make sure you include the normalization factor.

$$\frac{1}{\sqrt{6}} \begin{vmatrix} \psi_{1s}(\mathbf{r}_1) \alpha 1 & \psi_{1s}(\mathbf{r}_1) \beta 1 & \psi_{2p+1}(\mathbf{r}_1) \alpha 1 \\ \psi_{1s}(\mathbf{r}_2) \alpha 2 & \psi_{1s}(\mathbf{r}_2) \beta 2 & \psi_{2p+1}(\mathbf{r}_2) \alpha 2 \\ \psi_{1s}(\mathbf{r}_3) \alpha 3 & \psi_{1s}(\mathbf{r}_3) \beta 3 & \psi_{2p+1}(\mathbf{r}_3) \alpha 3 \end{vmatrix}$$

- 4-5. For an atom, you start by measuring the expectation value of \hat{J}_z , which gives you M_J . The wavefunction associated with this value of M_J is clearly an eigenfunction of \hat{J}_z . The wavefunction could also be chosen to be an eigenfunction of which of the following operators. [Circle all that apply.]

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| (c) \hat{S}^2 | (f) \hat{L}_y | (i) \hat{L}_x | (m) \hat{S}_z | |

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6-7. What are the term symbols for the ground state of the Protactinium atom. You do not need to denote the “J” values.

from the 1S ; we get a 2D term

from the 3P we get $^2P, ^4P, ^2D, ^4D, ^2F, ^4F$ terms

from the 1D we get $^2S, ^2P, ^2D, ^2F, ^2G$ terms

from the 3F we get $^2P, ^4P, ^2D, ^4D, ^2F, ^4F, ^2G, ^4G, ^2H, ^4H$ terms

from the 1G we get $^2D, ^2F, ^2G, ^2H, ^2I$ terms

from the 3H we get $^2F, ^4F, ^2G, ^4G, ^2H, ^4H, ^2I, ^4I, ^2J, ^4J$

from the 1I we get $^2G, ^2H, ^2I, ^2J, ^2K$

The ground state is 4J . This is $S = \frac{3}{2}$ and $L = 7$.

J values range from $7 + \frac{3}{2} = \frac{17}{2}$ to $7 - \frac{3}{2} = \frac{11}{2}$ and since the shell is less than half filled, the smaller value of J is favorable.

Assume that Hund's Rules are accurate in this setting. The ground state of this system has

8. Total orbital angular momentum, $L = 7$

9. Total spin angular momentum, $S = 3/2$

10. If Hund's third rule is valid, the total angular momentum of the ground state is, $J = 11/2$