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Quiz 8
CHEM 3PA3; Fall 2018

This quiz has 10 problems worth 10 points each. The first four problems go together and the last three problems go together.

1-7. Evaluate the following commutators.

$\left[\hat{H},\hat{L}_x\right]=$

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

$\left[\hat{S}^2,\hat{S}_y\right]=$

$\left[\hat{J}^2,\hat{L}^2\right]=$

$\left[\hat{L}_y,\hat{L}_x\right]=$

$\left[\hat{L}_x,\hat{S}_y\right]=$

$\left[\hat{J}_x,\hat{S}_y\right]=$

8-9. The term symbols for the $1s^2 2s^2 2p^1 3p^1$ excited state of the Carbon atom are ${}^1D, {}^1P, {}^1S, {}^3P, {}^3P, {}^3S$.

8. What is the predicted order of the states according to Hund's rules.

9. What is the predicted ground state according to the Kutzelnigg-Morgan and Russell-Meggers rules?

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10. What are the term symbols for the [Ar]$4s^2 3d^1 4p^1$ excited state (Titanium)?

Bonus (10 points): What are the term symbols for the [Ar]$4s^2 3d^3$ configuration (Scandium)?

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Quiz 8
CHEM 3PA3; Fall 2018

This quiz has 10 problems worth 10 points each. The first four problems go together and the last three problems go together.

1-8. Evaluate the following commutators.

$$\left[\hat{H},\hat{L}_x\right]=0$$

$$\left[\hat{S}_y,\hat{S}_z\right]=i\hbar\hat{S}_x$$

$$\left[\hat{S}^2,\hat{S}_y\right]=0$$

$$\left[\hat{J}^2,\hat{L}^2\right]=0$$

$$\left[\hat{L}_y,\hat{L}_x\right]=-\left[\hat{L}_x,\hat{L}_y\right]=-i\hbar\hat{L}_z$$

$$\left[\hat{L}_x,\hat{S}_y\right]=0$$

$$\left[\hat{J}_x,\hat{S}_y\right]=\left[\hat{L}_x+\hat{S}_x,\hat{S}_y\right]=\left[\hat{L}_x,\hat{S}_y\right]+\left[\hat{S}_x,\hat{S}_y\right]=0+i\hbar\hat{S}_z=i\hbar\hat{S}_z$$

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8-9. The term symbols for the $1s^2 2s^2 2p^1 3p^1$ excited state of the Carbon atom are $^1D, ^1P, ^1S, ^3D, ^3P, ^3S$.

8. What is the predicted order of the states according to Hund's rules.

$^3D, ^3P, ^3S, ^1D, ^1P, ^1S$

Really we should add J indices. Then

$^3D_1, ^3D_2, ^3D_3, ^3P_0, ^3P_1, ^3P_2, ^3S_1, ^1D_2, ^1P_1, ^1S_0$

9. What is the predicted ground state according to the Kutzelnigg-Morgan and Russell-Meggers rules?

The parity of the states is $(-1)^{L+l_1+l_2}$ so the *P* states (*L* = 1) are odd-parity and the *S* and *D* states are even parity. The optimal angular momentum is $L_{opt} = \frac{1+1}{\sqrt{2}} = \sqrt{2} \approx 1.414$.

So with the odd-parity singlet states, then triplets, then even-parity singlet states, with the *D* states being closer to optimal angular momentum than the *S* states, we have $^1P, ^3P, ^3D, ^3S, ^1D, ^1S$ in increasing order of energy.

10. What are the term symbols for the [Ar]$4s^2 3d^1 4p^1$ excited state (Titanium)?

The 3d electron has *L* = 2 and *S* = ½ and the 4p electron has *L* = 1 and *S* = ½. The possible choices of orbital angular momentum then range from $L = |L_1 - L_2|, \ldots, L_1 + L_2 = 1, 2, 3$ and the choices of spin-angular momentum range from $S = |S_1 - S_2|, \ldots, S_1 + S_2 = 0, 1$. So the states are $^3F, ^3D, ^3P, ^1F, ^1D, ^1P$ in Hunds rule order. If we add on the *J* values, we have $^3F_2, ^3F_3, ^3F_4, ^3D_1, ^3D_2, ^3D_3, ^3P_0, ^3P_1, ^3P_2, ^1F_3, ^1D_2, ^1P_1$.

According to the Kutzelnigg-Morgan and Russell-Meggers rules, the *L* = 2 states have odd parity and the *L* = 1 and *L* = 3 states have even parity. Moreover, $L_{\text{opt}} = \frac{2+1}{\sqrt{2}} = 2.12$. So the predicted order of states is $^1D, ^3D, ^3F, ^3P, ^1F, ^1P$.

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Bonus (10 points): What are the term symbols for the [Ar]4s^{2}3d^3 configuration (Scandium)?

	M_L=5	M_L=4	M_L=3	M_L=2	M_L=1	M_L=0
$M_S=\frac{3}{2}$			$\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\uparrow}3d_{0}^{\uparrow}\rangle$	$\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\uparrow}3d_{-1}^{\uparrow}\rangle$	$\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\uparrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{0}^{\uparrow}3d_{-1}^{\uparrow}\rangle$	$\lvert 3d_{+2}^{\uparrow}3d_{0}^{\uparrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+1}^{\uparrow}3d_{0}^{\uparrow}3d_{-1}^{\uparrow}\rangle$
$M_S=\frac{1}{2}$	$\lvert 3d_{+2}^{\uparrow}3d_{+2}^{\downarrow}3d_{+1}^{\uparrow}\rangle$	$\lvert 3d_{+2}^{\uparrow}3d_{+2}^{\downarrow}3d_{0}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\uparrow}3d_{+1}^{\downarrow}\rangle$	$\lvert 3d_{+2}^{\downarrow}3d_{+1}^{\uparrow}3d_{0}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\downarrow}3d_{0}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\uparrow}3d_{0}^{\downarrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+2}^{\downarrow}3d_{-1}^{\uparrow}\rangle$	$\lvert 3d_{+2}^{\downarrow}3d_{+1}^{\uparrow}3d_{-1}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\downarrow}3d_{-1}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\uparrow}3d_{-1}^{\downarrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+2}^{\downarrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+1}^{\uparrow}3d_{+1}^{\downarrow}3d_{0}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{0}^{\uparrow}3d_{0}^{\downarrow}\rangle$	$\lvert 3d_{+2}^{\downarrow}3d_{+1}^{\uparrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\downarrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{+1}^{\uparrow}3d_{-2}^{\downarrow}\rangle$ $\lvert 3d_{+2}^{\downarrow}3d_{0}^{\uparrow}3d_{-1}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{0}^{\downarrow}3d_{-1}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{0}^{\uparrow}3d_{-1}^{\downarrow}\rangle$ $\lvert 3d_{+1}^{\uparrow}3d_{+1}^{\downarrow}3d_{-1}^{\uparrow}\rangle$ $\lvert 3d_{+1}^{\uparrow}3d_{0}^{\uparrow}3d_{0}^{\downarrow}\rangle$	$\lvert 3d_{+2}^{\downarrow}3d_{0}^{\uparrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{0}^{\downarrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{0}^{\uparrow}3d_{-2}^{\downarrow}\rangle$ $\lvert 3d_{+1}^{\downarrow}3d_{0}^{\uparrow}3d_{-1}^{\uparrow}\rangle$ $\lvert 3d_{+1}^{\uparrow}3d_{0}^{\downarrow}3d_{-1}^{\uparrow}\rangle$ $\lvert 3d_{+1}^{\uparrow}3d_{0}^{\uparrow}3d_{-1}^{\downarrow}\rangle$ $\lvert 3d_{+1}^{\uparrow}3d_{+1}^{\downarrow}3d_{-2}^{\uparrow}\rangle$ $\lvert 3d_{+2}^{\uparrow}3d_{-1}^{\uparrow}3d_{-1}^{\downarrow}\rangle$

^{2}H, ^{2}G, ^{4}F, ^{2}F, ^{2}D, ^{2}D, ^{4}P, ^{2}P