ATOMS, MOLECULES & REACTIONS

QUANTUM MECHANICS, WEEK 3, SPRING 2006

Chapter 13

(33) $\frac{\uparrow\downarrow}{1s}$ $\frac{\uparrow\downarrow}{2s}$

$$\psi_{Be}(1s^2 2s^2) = \frac{1}{\sqrt{4!}} \begin{vmatrix} 1s(1)\alpha(1) & 1s(1)\beta(1) & 2s(1)\alpha(1) & 2s(1)\beta(1) \\ 1s(2)\alpha(2) & 1s(2)\beta(2) & 2s(2)\alpha(2) & 2s(2)\beta(2) \\ 1s(3)\alpha(3) & 1s(3)\beta(3) & 2s(3)\alpha(3) & 2s(3)\beta(3) \\ 1s(4)\alpha(4) & 1s(4)\beta(4) & 2s(4)\alpha(4) & 2s(4)\beta(4) \end{vmatrix}$$

(36) C $1s^2 2s^2 2p^1 3p^1$

The text has worked out the possible terms arising from this configuration to be

^3D, ^1D, ^3P, ^1P, ^3S and ^1S (Page 744 of Raff)

Of these, the ~~ground~~ lowest energy state is $\underline{\underline{^3D}}$

(38) – (40)

These ~~was~~ were assigned in error. Don't have to do these.

Hw Sheet

(29)

$$\psi = \begin{vmatrix} \psi_A(1) & \psi_A(2) \\ \psi_B(1) & \psi_B(2) \end{vmatrix} = \psi_A(1)\psi_B(2) - \psi_A(2)\psi_B(1)$$

(a)
if we ~~interage~~ interchange the rows we get

$$\psi_1 = \begin{vmatrix} \psi_B(1) & \psi_B(2) \\ \psi_A(1) & \psi_A(2) \end{vmatrix} = \psi_B(1)\psi_A(2) - \psi_B(2)\psi_A(1)$$

$$= -\psi$$

(b)
if we interchange the columns we get

$$\psi_2 = \begin{vmatrix} \psi_A(2) & \psi_A(1) \\ \psi_B(2) & \psi_B(1) \end{vmatrix} = \psi_A(2)\psi_B(1) - \psi_B(2)\psi_A(1)$$

$$= -\psi.$$

∴ Interchanging the columns or the rows changes the sign of the wavefunction.

(c) If two electrons have the same spin orbital (say electron 2 has the spin orbital ~~ψ_B~~ ψ_A

$$\text{then } \psi = \begin{vmatrix} \psi_A(1) & \psi_A(2) \\ \psi_A(1) & \psi_A(2) \end{vmatrix} = \psi_A(1)\psi_A(2) - \psi_A(1)\psi_A(2)$$

$$= 0$$

∴ wavefunction ceases to ~~exist~~ exist if the 2 electrons have the same spin orbital.

(39) C $^1S_0$ $^3P_0$ $^3P_1$ $^3P_2$ $^1D_2$ $\frac{\uparrow\downarrow}{1s}$ $\frac{\uparrow\downarrow}{2s}$ $\frac{\uparrow}{}\frac{\uparrow}{2p}\frac{}{}$

according to Hund's rules, the ground state is $\underline{\underline{^3P_0}}$

Term symbols

$Z = 11$ Na [Ne] $3s^1$ $\frac{\uparrow}{3s}$ $M_L = 0$ $M_S = \frac{1}{2}$

$\Rightarrow L = 0$ $S = \frac{1}{2}$

$\Rightarrow J = 1/2$

$\underline{\underline{^2S_{1/2}}}$

Mg ($Z=12$) [Ne] $3s^2$ $\frac{\uparrow\downarrow}{3s}$ $M_L = 0$ $M_S = 0$ $\Rightarrow L = 0, S = 0$

$\Rightarrow J = 0$

$\underline{\underline{^1S_0}}$

Al ($Z=13$) [Ne] $3s^2 3p^1$ $\frac{\uparrow}{+1}\frac{}{\overset{0}{3p}}\frac{}{-1}$ $M_L = 1$ $M_S = 1/2 \Rightarrow L = 1, S = 1/2$

$\Rightarrow J = 3/2, 1/2$

$\underline{\underline{^2P_{1/2}}}$ $^2P_{3/2}$

Si ($Z=14$) [Ne] $3s^2 3p^2$ $\frac{\uparrow}{+1}\frac{\uparrow}{\underset{3p}{0}}\frac{}{-1}$ $M_L = 1$ $M_S = \sout{3/2}$ 1

$L = 1$ $S = \sout{3/2}$ 1

~~$^4P_{1/2}$~~ $J = 2, 1, 0$ ~~$J = 5/2, 3/2, 1/2$~~

$\underline{\underline{^3P_0}}$ $^3P_1$ $^3P_2$

P (Z = 15) [Ne] $3s^2\ 3p^3$

$\underset{+1}{\uparrow}\ \underset{0}{\uparrow}\ \underset{-1}{\uparrow}$ (3p)

$M_L = 0 \quad M_S = 3/2$

$L = 0 \quad S = 3/2$

$J = 3/2$

$^4S_{3/2}$

S (Z = 16) [Ne] $3s^2\ 3p^4$

$\underset{+1}{\uparrow\downarrow}\ \underset{0}{\uparrow}\ \underset{-1}{\uparrow}$ (3p)

$M_L = 1 \quad M_S = 1$

$L = 1 \quad S = 1$

$J = 2, 1, 0$

$^3P_0 \quad ^3P_1 \quad ^3P_2$

Cl (Z = 17) [Ne] $3s^2\ 3p^5$

$\underset{+1}{\uparrow\downarrow}\ \underset{0}{\uparrow\downarrow}\ \underset{-1}{\uparrow}$ (3p)

$M_L = 1 \quad M_S = 1/2$

$L = 1 \quad S = 1/2$

$J = 3/2, 1/2$

$^2P_{1/2} \quad ^2P_{3/2}$

Ar (Z = 18) [Ne] $3s^2\ 3p^6$ ~~closed~~

$\underset{+1}{\uparrow\downarrow}\ \underset{0}{\uparrow\downarrow}\ \underset{-1}{\uparrow\downarrow}$ (3p)

$M_L = 0 \quad M_S = 0$

$L = 0 \quad S = 0$

$J = 0$

$^1S_0$

K (Z = 19) [Ar] $3s^1$ $\underset{3s}{\uparrow}$ $M_L = 0 \quad M_S = 1/2 \Rightarrow L = 0 \quad S = 1/2$

$J = 1/2$

$^2S_{1/2}$

Ca (Z=20) [Ar] $4s^2$ $\frac{1\!\downarrow}{4s}$ $M_L = 0$ $M_s = 0$ $L = 0$ $S = 0$

$J = 0$

$^1S_0$

Sc (Z=21) [Ar] $4s^2 3d^1$ $\underset{+2}{1}$ $\underset{+1}{\_}$ $\underset{0}{\_}$ $\underset{-1}{\_}$ $\underset{-2}{\_}$ $M_L = 2$ $M_s = 1/2$

$L = 2$ $S = 1/2$

$J = 5/2, 3/2$

$^2D_{3/2}$

Ti (Z=22) $3d^2$ $\underset{+2}{1}$ $\underset{+1}{1}$ $\underset{0}{\_}$ $\underset{-1}{\_}$ $\underset{-2}{\_}$ $M_L = 3$ $M_s = 1$

$L = 3$ $S = 1$

$J = 4, 3, 2$

$^3F_4$ $^3F_3$ $^3F_2$

V (Z=23) $3d^3$ $\underset{+2}{1}$ $\underset{+1}{1}$ $\underset{0}{1}$ $\underset{-1}{\_}$ $\underset{-2}{\_}$ $M_L = 3$ $M_s = 3/2$

$L = 3$ $S = 3/2$

$J = 9/2, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}$

$^4F_{9/2}$ $^4F_{7/2}$ $^4F_{5/2}$ $^4F_{3/2}$

Cr (Z=24) $4s^1 3d^5$ $\underset{0}{1}$ (4s) $\underset{+2}{1}$ $\underset{+1}{1}$ $\underset{0}{1}$ $\underset{-1}{1}$ $\underset{-2}{1}$ (3d) $M_L = 0$ $M_s = 3$

$L = 0$ $S = 3$

$J = 3$

$^7S_3$

Mn (Z=25) $4s^2 3d^5$ $\underset{+2}{1}$ $\underset{+1}{1}$ $\underset{0}{1}$ $\underset{-1}{1}$ $\underset{-2}{1}$ $M_L = 0$ $M_s = 5/2$

$L = 0$ $S = 5/2$

$J = 5/2$

$^6S_{5/2}$

Fe ($Z = 26$) $3d^6$ $\underset{+2}{\uparrow\downarrow}\ \underset{+1}{\uparrow}\ \underset{0}{\uparrow}\ \underset{-1}{\uparrow}\ \underset{-2}{\uparrow}$ $M_L = 2$ $M_S = 2$

$L = 2$ $S = 2$

$J = 4, 3, 2, 1, 0$

$\underline{\underline{^5D_4}}$ $^5D_3$ $^5D_2$ $^5D_1$ $^5D_0$

Co ($Z = 27$) $3d^7$ $\underset{+2}{\uparrow\downarrow}\ \underset{+1}{\uparrow\downarrow}\ \underset{0}{\uparrow}\ \underset{-1}{\uparrow}\ \underset{-2}{\uparrow}$ $M_L = 3$ $M_S = 3/2$

$L = 3$ $S = 3/2$

$J = \frac{9}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}$

$\underline{\underline{^4F_{9/2}}}$

Ni ($Z = 28$) $3d^8$ $\underset{+2}{\uparrow\downarrow}\ \underset{+1}{\uparrow\downarrow}\ \underset{0}{\uparrow\downarrow}\ \underset{-1}{\uparrow}\ \underset{-2}{\uparrow}$ $M_L = 3$ $M_S = 1$

$L = 3$ $S = 1$

$J = 4, 3, 2$

$\underline{\underline{^3F_4}}$

Cu ($Z = 29$) $4s^1 3d^{10}$ $\underset{4s}{\uparrow}$ $\underset{3d}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow}$ $M_L = 0$ $M_S = 1/2$

$L = 0$ $S = 1/2$

$J = 1/2$

$\underline{\underline{^2S_{1/2}}}$

Zn ($Z = 30$) $4s^2 3d^{10}$ $\underset{3d}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow}$ $M_L = 0$ $M_S = 0$

$L = 0$ $S = 0$

$J = 0$

$\underline{\underline{^1S_0}}$

Ga ($Z = 31$) $4s^2 3d^{10} 4p^1$ $\underset{4p}{\underset{+1}{\uparrow}\ \underset{0}{\_}\ \underset{-1}{\_}}$ $M_L = 1$ $M_S = 1/2$

$L = 1$ $S = 1/2$

$J = 3/2, 1/2$

$\underline{\underline{^2P_{1/2}}}$ $^2P_{3/2}$

Ge $(Z = 32)$ $4s^2 4p^2$

↑	↑	
+1	0	−1

4p

$M_L = 1$ $M_S = 1$

$L = 1$ $S = 1$

$J = 2, 1, 0$

$\mathbf{{}^3P_0}$ ${}^3P_1$ ${}^3P_2$

As $(Z = 33)$ $4p^3$

↑	↑	↑
+1	0	−1

$M_L = 0$ $M_S = 3/2$

$L = 0$ $S = 3/2$

$J = 3/2$

$\mathbf{{}^4S_{3/2}}$

Se $(Z = 34)$ $4p^4$

↑↓	↑	↑
+1	0	−1

$M_L = 1$ $M_S =$ ~~3/2~~ 1

$L = 1$ $S = 1$

$J = 2, 1, 0$

${}^3P_0$ ${}^3P_1$ $\mathbf{{}^3P_2}$

Br $(Z = 35)$ $4p^5$

↑↓	↑↓	↑
+1	0	−1

$M_L = 1$ $M_S = 1/2$

$L = 1$ $S = 1/2$

$J = 3/2, 1/2$

${}^2P_{1/2}$ $\mathbf{{}^2P_{3/2}}$

Kr $(Z = 36)$ $4p^6$

↑↓	↑↓	↑↓
+1	0	−1

$M_L = 0$ $M_S = 0$

$L = 0$ $S = 0 \Rightarrow J = 0$

$\mathbf{{}^1S_0}$