Name

5.73

Quiz 34

November 27, 2002

1.

* Use the standard order for np spin-orbitals on Page 30-4: $1\alpha,1\beta,0\alpha,0\beta,-1\alpha,-1\beta$

* Recall that $\langle\|a_1a_2\|\|F(i)\|\|a_1a_2\|\rangle = \sum_i \langle a_i|f|a_i\rangle$

$$\langle\|a_1b\|\|F(i)\|\|a_1a_2\|\rangle = \langle b|f|a_2\rangle$$

* The electronic states that arise from the p^2 electronic configuration are ^1D, ^3P, and ^1S.

A. Construct the two Slater determinantal wavefunctions that correspond to $M_J = M_L + M_S = +2$.
[HINT: both $|LSJM_J = 2\rangle$ coupled states are single Slater determinants.]

$\left|{}^1D_2 \;\; M_J = 2\right\rangle =$

$\left|{}^3P_2 \;\; M_J = 2\right\rangle =$

B. Calculate the two diagonal and one off-diagonal matrix elements of $\mathbf{H}^{SO} = \sum_I a(r_i)\ell_i \bullet s_i$:

(i) $\left\langle {}^1\mathrm{D}_2 \;\; \mathrm{M_J} = 2\left|\zeta_\mathrm{p}\left(\ell_{1z}\mathrm{s}_{1z} + \ell_{2z}\mathrm{s}_{2z}\right)\right|{}^1\mathrm{D}_2 \;\; \mathrm{M_J} = 2\right\rangle =$

(ii) $\left\langle {}^3\mathrm{P}_2 \;\; \mathrm{M_J} = 2\left|\zeta_\mathrm{p}\left(\ell_{1z}\mathrm{s}_{1z} + \ell_{2z}\mathrm{s}_{2z}\right)\right|{}^3\mathrm{P}_2 \;\; \mathrm{M_J} = 2\right\rangle =$

(iii) $\left\langle {}^3\mathrm{P}_2 \;\; \mathrm{M_J} = 2\left|\tfrac{1}{2}\zeta_\mathrm{p}\left(\ell_{1-}\mathrm{s}_{1+} + \ell_{2-}\mathrm{s}_{2+}\right)\right|{}^1\mathrm{D}_2 \;\; \mathrm{M_J} = 2\right\rangle =$