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Quiz 34 ANSWERS

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 $\left\langle \| a_1 a_2 \| \left| F(i) \right| \| a_1 a_2 \| \right\rangle = \sum_i \left\langle a_i | f | a_i \right\rangle$

$$\left\langle \| a_1 b \| \left| F(i) \right| \| a_1 a_2 \| \right\rangle = \left\langle b | f | a_2 \right\rangle$$

* 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.]

$$\left|{}^1D_2\ M_J = 2\right\rangle = \boxed{\|1\alpha 1\beta\|}$$

$$\left|{}^3P_2\ M_J = 2\right\rangle = \boxed{\|1\alpha 0\alpha\|}$$

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

(i) $\left\langle {}^1D_2\ M_J = 2 \right| \zeta_p \left(\ell_{1z}\mathbf{s}_{1z} + \ell_{2z}\mathbf{s}_{2z}\right) \left| {}^1D_2\ M_J = 2 \right\rangle =$

$$\boxed{\hbar^2\zeta_p\left[1\cdot\frac{1}{2}+1\cdot\left(-\frac{1}{2}\right)\right]=0}$$

(ii) $\left\langle {}^3P_2\ M_J = 2 \right| \zeta_p \left(\ell_{1z}\mathbf{s}_{1z} + \ell_{2z}\mathbf{s}_{2z}\right) \left| {}^3P_2\ M_J = 2 \right\rangle =$

$$\boxed{\hbar^2\zeta_p\left[1\cdot\frac{1}{2}+0\cdot\frac{1}{2}\right]=\hbar^2\zeta_p\frac{1}{2}}$$

(iii) $\left\langle {}^3P_2\ M_J = 2 \right| \tfrac{1}{2}\zeta_p \left(\ell_{1-}\mathbf{s}_{1+} + \ell_{2-}\mathbf{s}_{2+}\right) \left| {}^1D_2\ M_J = 2 \right\rangle =$

$$\boxed{\frac{1}{2}\hbar^2\zeta_p\left[\left\langle 1\beta \right| \ell_+\mathbf{s}_- \left| 0\alpha \right\rangle\right]=\frac{1}{2}\hbar^2\zeta_p[1\cdot 2-1\cdot 0]^{1/2}=2^{-1/2}\hbar^2\zeta_p}$$