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Quiz 34

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

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

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

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.]

$\left| {}^1\mathrm{D}_2\ M_J = 2 \right\rangle =$

$\left| {}^3\mathrm{P}_2\ M_J = 2 \right\rangle =$

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

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

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

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

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