

5.73

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

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

* 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.]

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

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

B. Calculate the two diagonal and one off-diagonal matrix elements of

$$\mathbf{H}^{\text{SO}} = \sum_I a(r_i) \ell_i \cdot s_i :$$

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

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

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

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

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

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

MIT OpenCourseWare
<https://ocw.mit.edu/>

5.73 Quantum Mechanics I
Fall 2018

For information about citing these materials or our Terms of Use, visit: <https://ocw.mit.edu/terms>.