

Rough calc

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$$r_{x,y} = 0.944A$$

$$r_z = 0.545A$$

$$I_a = I_b = m_c(3\alpha r_z)^2 + m_H \left[3r_z^2(3\alpha - 1)^2 + \frac{3}{2}r_{x,y}^2 \right] = 12u \left(\frac{3}{15} 0.545A \right)^2 + u \left(3(0.545A)^2 \left(\frac{3}{15} - 1 \right)^2 + \frac{3}{2}(0.944A)^2 \right)$$

$$= (1.425 \times 10^{-1} + 6.4 \times 10^{-1} + 1.3367)uA^2 = 2.119uA^2$$

$$I_c = 3m_H[r_{x,y}^2] = 3u[0.944A] = 2.673uA^2$$

$$6.626070040 \times 10^{-34} kg \frac{m^2}{s} \times \frac{1u}{1.6605 \times 10^{-27} kg} \times \left(\frac{10^{10} A}{m} \right)^2 = 3.9904065 \times \frac{10^{-07} um^2}{s} \left(\frac{10^{10} A}{m} \right)^2 = 3.990406528 \times 10^{13} \frac{uA^2}{s} = h$$

$$h = 3.990406528 \times 10^{13} \frac{uA^2}{s}$$

$$\hbar = 6.350929239 \times 10^{12} \frac{uA^2}{s}$$

$$c = 29979245800 \frac{cm}{s}$$

$$B_e = \frac{h}{8\pi^2 I_a} = 5.05390 \times 10^{11} \times \frac{1}{2.119uA^2} = 2.3850 \times 10^{11} Hz$$

$$B'_e = \frac{h}{8\pi^2} \left(\frac{I_a - I_c}{I_a I_c} \right) = 3.990406528 \times 10^{13} \frac{uA^2}{s} \times \frac{1}{8\pi^2} \frac{(2.119uA^2 - 2.673uA^2)}{2.119uA^2 \times 2.673uA^2}$$

$$= 5.05390 \times 10^{11} \frac{-0.554}{5.664uA^2}$$

$$= -4.94325 \times 10^{10} Hz$$

$$\tilde{B}_e = \frac{B_e}{c} = 2.3850 \times 10^{11} Hz \times \frac{1}{29979245800 cm Hz} \approx 7.9555 cm^{-1}$$

$$\tilde{B}'_e = -4.94325 \times 10^{10} Hz \times \frac{1}{29979245800 cm Hz} \approx -1.648 cm^{-1}$$

$$\tilde{E} = \tilde{B}_e(J(J+1)) + \tilde{B}'_e K^2$$

$$g(J, K=0) = (2J+1)$$

$$g(J, K \neq 0) = 2(2J+1)$$

$$k_b = 1.38064852 \times 10^{-23} \frac{J}{K}$$

$$\tilde{k}_b = 1.38064852 \times 10^{-23} \frac{J}{K} \times 5.03445 \times 10^{22} \frac{cm^{-1}}{J} = 0.69508 \frac{cm^{-1}}{K}$$

Energy transitions

$$P: \Delta E_{rot}(\Delta J = 1, \Delta K) = 2h\tilde{B}_e(J'+1) + h\tilde{B}'_e(K''^2 - K'^2)$$

$$Q: \Delta E_{rot}(\Delta J = 0, \Delta K) = h\tilde{B}'_e(K''^2 - K'^2)$$

$$R: \Delta E_{rot}(\Delta J = -1, \Delta K) = -2h\tilde{B}_e J + h\tilde{B}'_e(K''^2 - K'^2)$$