

HCL/DCI Constants-For credit, please understand what these equations mean.

$$B_e, B_0, B_2, \alpha_e, \omega_e, x_e, k, D, r_e, r_0, r_2 \quad (1)$$

1. B_0 and B_2 - Solve from your plots

$$\Delta\nu(m) = 2m(B_2 - B_0) + 2B_2 \quad (2)$$

2. B_e and α_e - Solve system of equations, make certain you include where these equations come from!

$$B_2 = B_e - \frac{5}{2}\alpha_e \quad B_0 = B_e - \frac{1}{2}\alpha_e \quad (3)$$

3. r , one method for getting it

$$B = \frac{h}{8\pi^2 c \mu r^2} \quad (4)$$

4. ν_0 - There are many ways to obtain this graphically or by solving equations. Once you find it, getting ω_e is rather trivial (solve the system of equations given in 6). The central equation to keep in mind is:

$$\nu(m) = \nu_0 + m^2(B_2 - B_0) + m(B_2 + B_0) \quad (5)$$

5. ω_{e^*} and ν_{0^*} - For different isotopes, a handy short-cut (you also need to use this to find ν_0 of the fundamental band for each isotope - see page 15 for a reference value) .

$$\frac{\omega_e}{\omega_{e^*}} = \sqrt{\frac{\mu^*}{\mu}} \quad (6)$$

6. x_e and ω_e - Use the Herzberg reference to get the fundamental harmonic transition frequency for $H^{35}Cl$. ΔE is in wavenumbers and can be obtained from Manual/Herzberg and your calculated ν_0 (for the 1st and 2nd transition respectively).

$$\Delta E_{0 \rightarrow 2} = 2\omega_e - 6\omega_e x_e \quad \Delta E_{0 \rightarrow 1} = \omega_e - 2\omega_e x_e \quad (7)$$

7. k , from Hooke's law

$$2\pi c \omega_e = \sqrt{\frac{k}{\mu}} \quad (8)$$

8. D - Two methods to consider here, use the one you think best.

$$\nu(m) = \nu_0 + m^2(B_2 - B_0) + m(B_2 + B_0) - 4Dm^3 \quad (9)$$

$$D = \frac{4B_e^3}{\omega_e^2} \quad (10)$$

9. Don't forget to analyze your peak heights.

$$N_J \propto (2J + 1)e^{-BJ(J+1)hc/kT} \quad (11)$$