Spectroscopy

Exercises Chapter 2D

1. Calculate the fraction of H_2 and NaCl molecules in the ground vibrational state at 300 K.
   For H_2 , ω_e = 4159.2 cm^{-1} and for NaCl, ω_e = 378.0 cm^{-1}.

2. Treating the rotational quantum number *J* as a continuous parameter, show that the value of *J* in the most populated rotational state is the nearest integer to

$$J_{max} = \frac{1}{2}\left(\sqrt{\frac{2k_BT}{B}} - 1\right)$$

   Calculate J_{max} for $H^{35}Cl$ (B = 10.6 cm^{-1}) and $^{127}I^{35}Cl$ (B = 0.114 cm^{-1}) at 300 K.

3. The summation that occurs in the rotational Boltzmann distribution can be evaluated approximately by converting the summation to an integral. Show that

$$\sum_{J=0}^{\infty}(2J+1)\,e^{-\frac{BJ(J+1)}{k_BT}} \approx \int_0^{\infty} e^{-\frac{BJ(J+1)}{k_BT}}\, d\left[J(J+1)\right]$$

$$= \frac{k_BT}{B} = \frac{8\pi^2 cIk_BT}{h}$$

   This is an excellent approximation for values of B/k_BT less than 0.05 or so. Using this result, calculate and plot the fraction of $^{127}I^{35}Cl$ molecules in the J^{th} rotational state versus *J* assuming a temperature of 25°C. (*B* = 0.114 cm^{-1})