# Problem Set 3

1. From the equation the value of B is 20.56 $cm^{-1}$.
   Use this value to plot the energy levels in question 1a, which will be located at 0, 2B, 6B, 12 B and 20B.
   The spectral lines occur at 2B, 4B, 6B and 8B which is required to plot the spectrum in 1b.
   Use this value of B and the reduced mass of HF to get the value of the bond length, ***r*,** in 1c. Calculations of this type were done in earlier assignments.
   Equation 2, gives you the value of B to be 20.56 $cm^{-1}$ and the centrifugal distortion constant D to be 2.13 x $10^{-3}$ $cm^{-1}$.
   Use this equation to plot the energy levels and spectrum in 1d and 1e.

   To calculate the vibrational frequency in problem 1d, use the equation

   $$\begin{aligned} \omega_e^2 &= 4B^3/D \\ &= 4 \times (20.56)^3/( 2.13 \times 10^{-3}) \\ &= 1.632 \times 10^7 \\ \omega_e &= 4039.9\ cm^{-1} \end{aligned}$$

2. The energy level equation for the harmonic oscillator is

   $$G(v) = \omega_e\ (v+ ½) \text{ and}$$

   For the anharmonic oscillator the energy level equation is

   $$G(v) = \omega_e\ (v+ ½) + \omega_e x_e\ (v+ ½)^2$$

   Use these equations to plot the energy levels and the spectra for problems 2 and 3..

   Use the selection rules $\Delta v = \pm 1$ for the harmonic oscillator.

   For the anharmonic oscillator, in addition to the $\Delta v = \pm 1$, other overtone transitions involving $\Delta v = \pm 2$, $\Delta v = \pm 3$,… are also possible, though with progressively weaker intensities. The fundamental with the $\Delta v = \pm 1$, from v=0 to v=1, will be the strongest.

   Hot bands involve transitions, from higher vibrational levels, such as from v=1, v=2 etc. These also have weak intensities due to the smaller populations in these levels relative to the population in v=0.