The Morse potential is a widely used form to describe anharmonic effects in diatomic molecules. The potential energy function is given by:

$$V(r) = D_e[\, 1 - \exp(-a(r-r_e))\,]^2$$

Where D_e is the bond dissociation energy, r_e is the equilibrium bond distance and **a** is a parameter (units of 1/distance) that is related to the curvature of the bottom of the well.

We showed (last week) that $k = 2a^2 D_e$ for the Morse potential. If we know the fundamental frequency of the vibration v_e, we can write, $k = 4\pi^2 \mu v_e^2$. Equating these two, we get:

$$a = 2\pi\, v_e[2D_e/\mu]^{-1/2}$$

Consider $^1H^{35}Cl$ which has the following values for the relevant constants in SI units

$$D_e = 7.427E^{-19}\ J\ ;\ v_e = 9.004E^{13}\ Hz,\ r_e = 127.4E^{-12}\ m$$

1) Calculate a
2) Use excel or another program to create a graph of V(r) for the Morse potential. You may want to shift your energy units from SI to cm^{-1}

3) Use the following exact formula for the quantized vibration energy levels of the Morse oscillator to calculate the energies of the all the bound states in the well:

$$E_n = (n+^1/_2)hv_e - (n+^1/_2)^2 x_e h v_e \quad \text{where } x_e = hv_e/4D_e \text{ and is called the anharmonicity constant}$$

4) How do the energy levels in (3) compare with those of a pure harmonic oscillator with the same force constant?

Please hand this in or send by email by Tuesday, September 14.