Problem set 3
(Vibrational Spectroscopy)

1. Calculate the first three vibrational energy levels for $^{1}H_2$ given that ω_e = 4401.2 cm^{-1}, assuming the oscillator to be simple harmonic. Now assume that the oscillator behaves anharmonically, with an anharmonicity constant, $\omega_e x_e$ = 121.5. Plot the energy level diagram again for the first three vibrational energy levels. Discuss the difference in the two examples. What is the zero-point energy in the two cases?

2. A molecule has a vibration with a frequency of 600 cm^{-1}. You are using a spectrometer that can detect a system only if it has a population of more than 10% (relative to the population in the v=0 level). Predict if the hot band for this vibration can be detected by your spectrometer, at room temperature.

3. The fundamental and the overtone transition in $^{14}N^{16}O$ occur at 1876.1 and 3724.2 cm^{-1}. Calculate ω_e and $\omega_e x_e$. Calculate the zero point energy. Assuming a Morse potential is adequate, calculate $\mathcal{D}_e$ and $\mathcal{D}_0$.