PHY 3107, Spring 2018, Homework #8

due Tuesday, Apr. 10

1.) The energy differences in molecular excitation spectra are given in terms of the wave number, meaning weird units of $\frac{1}{\lambda}$, where the photon wavelength (λ) is for the emitted photon when the molecule transitions from a higher to a lower energy level. I.e., for HCl, the **rotational** transition from $\ell = 1$ to $\ell = 0$ results in a photon with $\frac{1}{\lambda} = 21.148\ cm^{-1}$. Assuming that chlorine has a mass of 35 times that of hydrogen: a) calculate the energy difference ΔE between the first excited and the ground rotational states, and b) calculate the rotational moment of inertia of the molecule about the center of mass, and c) calculate the bond length of the molecule.

2.) Energy differences in molecular excitation spectra often use weird units of $\frac{1}{\lambda}$, where the photon wavelength (λ) is for the emitted photon when the molecule transitions from a higher to a lower energy level. I.e., for HCl, the **vibrational** transition from $v = 1$ to $v = 0$ results in a photon with $\frac{1}{\lambda} = 2885.9\ cm^{-1}$. The vibrational energies are significantly larger than the rotational energies, which means that the levels are spaced further apart. Assuming that chlorine has a mass of 35 times that of hydrogen: a) calculate the energy difference ΔE between the first excited and the ground vibrational states, b) treating the molecule like a small spring, calculate the effective force constant for this molecule, and c) what is the classical vibrational amplitude for this HCl molecule in the $v = 0$ state?

3.) Let's look again at NaCl. The separation between the two nuclei Na(*A=23*) and Cl(*A=35.5*) is 2.4×10^{-10}m. A) Calculate the energy of the photon needed to excite the first rotational band above the ground state, in units of eV. B) What is the wavelength of the photon emitted in the transition from $\ell = 1$ to $\ell = 0$?

4.) Find the ratio of the rotational splitting in the hydrogen molecule H_2 to that of HBr. The bromine atom has approximately 80 times the mass of the hydrogen atom.

5.) Classically, there are two degrees of freedom associated with a one-dimensional oscillator (and our vibrating diatomic molecules are exactly that!). One of the degrees of freedom is associated with the kinetic energy, and one is associated with the potential energy. Therefore we can write $\Delta E = \hbar\omega = 2 \times \left(\frac{kT}{2}\right) = kT$. a) Find the classical temperature associated with the transitional $1 \rightarrow 0$ difference in vibrational energy levels in HCl given that the frequency is 8.66×10^{13} Hz. b) Based on this temperature, are vibrational levels thermally excited at normal room temperatures? c) Can you find the classical temperature associated with rotational energy levels?