

CHEM 3420: Physical Chemistry II — Spring 2009

Homework 7

Due in Class: Moday, March 30, 2009

1. The wavenumber of the fundamental vibrational transition of $^{35}\text{Cl}_2$ is 564.9 cm^{-1} . Calculate the force constant of the bond. (The mass of ^{35}Cl is 34.9688 amu.)
2. The force constant for the $^1\text{H}^{35}\text{Cl}$ molecule is 516 Nm^{-1} . Calculate the vibrational zero point energy of this molecule using the harmonic oscillator model. If this amount of energy were converted to translational energy, how fast would the molecule be moving? Compare this speed to the root mean square speed from the kinetic theory of gases ($v_{rms} = \sqrt{3k_bT/m}$) for $T = 300\text{ K}$.
3. Solids generally expand as the temperature increases. Such an expansion results from an increase in the bond length between adjacent atoms as the vibrational amplitude increases. Will a harmonic potential lead to thermal expansion? Will a Morse (anharmonic) potential lead to thermal expansion?
4. (a) Using the data below for $^{12}\text{C}^{16}\text{O}$ and the anharmonic oscillator model, calculate the frequency of the transition from the vibrational state $v = 1$ to $v = 0$.
(b) Also, calculate D_o for $^{12}\text{C}^{16}\text{O}$.

D_e/hc (cm^{-1})	R_e (\AA)	k (N/m)	$\bar{\nu}_e$ (cm^{-1})	$\bar{\nu}_e x_e$ (cm^{-1})
90542	1.128	1902	2169.8	13.3