Tutorial 8

Name:

Harmonic Oscillator

1. For a classical harmonic oscillator, the particle cannot go beyond the points where the total energy equals the potential energy (the kinetic energy is zero at these points). These are called the "classical turning points". Identify the classical turning points for the ground state of the quantum harmonic oscillator – i.e., use the ground state energy. Write an integral giving the probability that the particle will go beyond these classically-allowed points. (You don't need to evaluate the integral.) *Useful:*

$$\psi_v(x) = N_v H_v\left(\frac{x}{\alpha}\right)\exp\left(-\frac{x^2}{2\alpha^2}\right), \quad v = 0, 1, 2, \ldots$$

where $\alpha = \dfrac{\hbar^{1/2}}{(mk)^{1/4}}$, $N_v = \dfrac{1}{\alpha^{1/2}\pi^{1/4}\left(v!2^v\right)^{1/2}}$

The H_v are called **Hermite Polynomials**:

$H_0(y) = 1$
$H_1(y) = 2\,y$
$H_2(y) = 4\,y^2 - 2$
$\ldots$

2. Under the assumption of molecular vibration as that of a harmonic oscillator. There are two strong infrared bands of phenol (C_6H_6O) that correspond to the C-O and O-H stretching. The wavenumbers are given on the IR spectrum, at 3373 cm^{-1} and 1224 cm^{-1}. In general, the force constant, k, depends on the bond strength. It values around 500 $N \cdot m^{-1}$ for single bond, 1000 $N \cdot m^{-1}$ for double bond, and 2000 $N \cdot m^{-1}$ for triple bond.

PHENOL

INFRARED SPECTRUM
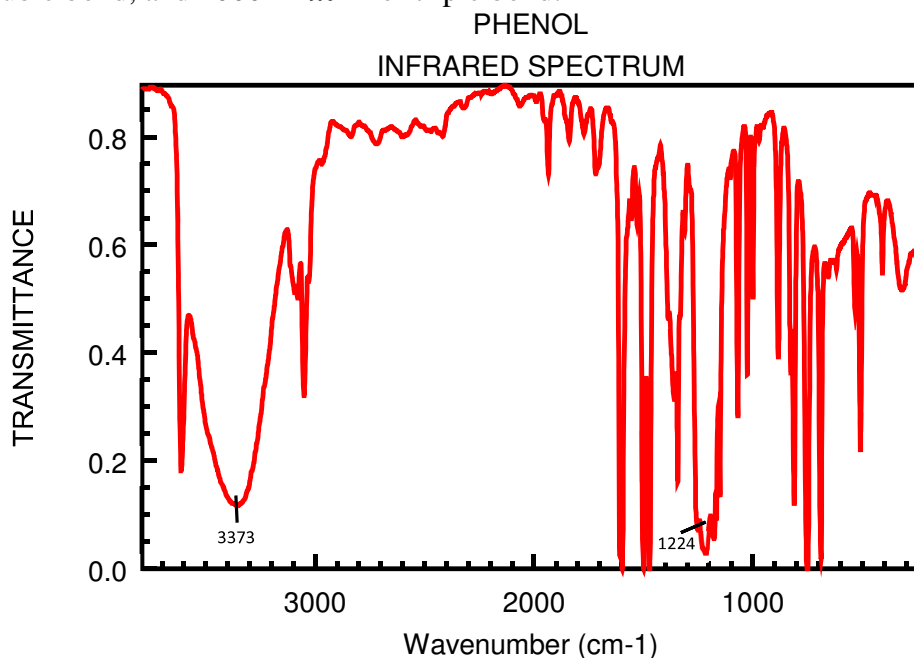
NIST Chemistry WebBook (http://webbook.nist.gov/chemistry)

Hint: Each stretching behaves like diatomic molecule within polyatomic molecule, if the associated stretching frequency is different from other vibrational frequencies within the molecule.

(a) Find the reduced mass for each stretching.

(b) Can you assign the bands based on your current chemistry knowledge and lab experience? YES! Assign them.

(c) Justify your assignment by finding the force constant for each stretching. Briefly explain the assignment and comment on the bond strength.