CHEM 361 L

EXPERIMENT 2

Assignment of an Infrared Spectral Band

(last update: January 2014)

Introduction

The frequency of the stretching vibration of the carbon-oxygen single bond will be determined using the infrared spectra of a variety of compounds containing this moiety. The vibrational frequency is given by:

$$\nu = (1/2\pi c)(k/\mu)^{1/2}$$

where ν is the frequency (cm^{-1}), k is the force constant, μ is the reduced mass, and c is the speed of light.

In order to identify the peak corresponding to this vibration, the student will determine the rough location expected for the peak from the frequencies of other C-X singly bonded species (X = N,F,Cl, etc.). The intensity of the C-O stretching peak should also be large, given the electronegativity difference across the bond.

Procedure

The instructor will provide you with a selection of reagents, all of which have the same general formula: X-C-O-Y, where X and Y are the substituents. Place some of each sample on a disposable IR sample card and acquire the infrared spectrum of each. Also acquire spectra of acetone and hexane to ensure that they do not exhibit the C-O band.

Calculations

Look up the stretching frequencies for a number of C-X compounds (three such frequencies are C-N : 1100 cm^{-1}; C-F: 1000 cm^{-1}; C-Cl: 750 cm^{-1}). Plot the observed frequency versus $(1/\mu)^{1/2}$, assuming that this bond vibrates independently of the remainder of the molecule. From the least-squares fit of the plotted data, interpolate the predicted frequency of C-O.

Determine the mean value of the C-O stretching frequency, including the standard deviation of this quantity. Discuss agreement with the predicted value, the relative

intensity of this peak from compound to compound, and any structural characteristics that may influence the location or intensity of this peak.