CHEM 361 L EXPERIMENT 3

Computational Chemistry II: IR Spectrum of a Compound

(revised January, 2019)

Introduction

The frequency of the stretching vibration of the C-O bond is studied using the infrared spectrum. The force constant of the bond is slightly affected by the electron distribution on adjacent atoms, so most of the variation will be due to the reduced mass of the vibrating system. In this experiment, density function theory will be used to explore the influence of structure on the vibrational frequency.

Procedure

The Chemistry Department has Gaussview and Gaussian available on a number of departmental computers. In a previous experiment, you optimized structures of an amino acid and its zwitterionic form. The instructor provided you with a selection of reagents, all of which have the same general formula : XC-O-Y , where X and Y are substituents. You have acquired the IR spectrum for each of the reagents. Using Gaussview, build each of these molecules and optimize the geometry using the b3lyp DFT method and the 631++g(d,p) basis set. Once you have optimized the geometry for a particular molecule, perform a frequency calculation for the optimized structure. If one or more of the frequencies are negative, consult the lab instructor regarding potential subsequent steps.

Calculations

Plot the predicted frequency of the C-O stretch versus the observed value. Is there a linear relationship between the two? Can any additional variability be explained by electron density at the C or O? The report for the accompanying experiment (Assignment of an Infrared Spectral Band) should be included in the report for this experiment.

References

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