CONFORMATIONAL AND STRUCTURAL STUDIES OF ISOPROPYLAMINE FROM TEMPERATURE DEPENDENT RAMAN SPECTRA OF XENON SOLUTIONS AND *AB INITIO* CALCULATIONS

JOSHUA J. KLAASSEN, IKHLAS D. DARKHALIL, JAMES R. DURIG, *Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110, USA.*

The Raman and infrared spectra (4000 to 50 cm^{-1}) of the gas, liquid or solution, and solid have been recorded of isopropylamine, $(CH_3)_2CHNH_2$. Variable temperature (-50 to -100^oC) studies of the Raman spectra (3500 to 100 cm^{-1}) dissolved in liquid xenon have been carried out. From these data, both the *trans* and *gauche* conformers have been identified and their relative stability obtained. The enthalpy difference has been determined from 20 band pairs at 6 temperatures to be 113 +/- 11 cm^{-1} (1.35 +/- 0.13 kJ mol^{-1}) with the *trans* conformer the more stable form. The percentage of the *gauche* conformer is estimated to be 54 +/- 1 percent at ambient temperature. The conformational stabilities have been predicted from *ab initio* calculations utilizing several different basis sets up to aug-cc-pVTZ from both MP2(full) and density functional theory calculations by the B3LYP method. By utilizing previously reported microwave rotational constants along with *ab initio* MP2(full)/6-311+G(d,p) predicted structural values, adjusted r_0 parameters have been obtained for the *trans* conformer. The determined heavy atom and NH_2 distances in angstroms are C-C = 1.530(3), C-N = 1.465(3), N-H = 1.019(3) and angles in degrees NCC = 108.9(5), CCC = 111.0(5), HNC = 110.3(5). The structural parameters for the *gauche* conformer were estimated by using the same adjustment differences to the *gauche* form as those obtained for the corresponding *trans* parameters. Vibrational assignments have been provided for the observed bands for both conformers which are supported by MP2(full)/6-31G(d) *ab initio* calculations to predict harmonic force constants, wavenumbers, infrared intensities, Raman activities and depolarization ratios for both conformers. The results are discussed and compared to the corresponding properties of some related molecules.