RAMAN AND INFRARED SPECTRA, CONFORMATIONAL STABILITY, AB INITIO CALCULATIONS AND VIBRATIONAL ASSIGNMENTS FOR ETHYL FLUOROSILANE

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The infrared (3500 to 30 cm^{-1}) spectra of gaseous and solid and the Raman (3500 to 10 cm^{-1}) spectra of the liquid with quantitative depolarization ratios and solid ethyl fluorosilane, $FSiH_2CH_2CH_3$, have been recorded. These data indicate that two conformers are present in the fluid states but only one conformer is present in the annealed crystalline state. The mid-infrared spectra of the sample dissolved in liquefied xenon as a function of temperature (-100 to -55°C) have been recorded. Utilizing conformer pairs at 1022 (gauche), 1010 (trans), 719 (gauche), 727 (trans), and 693 (trans) cm^{-1} the enthalpy difference has been determined to be 101±18 cm^{-1} (1.21±0.22 kJ/mol) with the gauche conformer the more stable species and the one remaining in the solid. The optimized geometries, conformational stabilities, harmonic force fields, infrared intensities, Raman activities, depolarization ratios, and vibrational frequencies will be reported for both conformers from MP2/6-31G* ab initio calculations. The gauche conformer is predicted to be the more stable rotamer from ab initio calculations in agreement with the experimental results.