RAMAN AND INFRARED SPECTRA, CONFORMATIONAL STABILITY, BARRIERS TO INTERNAL ROTATION, AB INITIO CALCULATIONS AND r_o STRUCTURE FOR VINYL SILYL FLUORIDE

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The Raman (3250 to 10 cm^{-1}) and infrared (3250 to 40 cm^{-1}) spectra of the gaseous and solid vinyl silyl fluoride (CH_2CHSiH_2F), have been recorded. From the far infrared spectrum of the gas, the fundamental asymmetric torsions for both the cis and gauche conformers have been observed at 102.34 and 86.56 cm^{-1}, respectively, with each having several excited state transitions falling to lower frequencies. From these transitions, the potential function to internal rotation has been determined with the following values: V_1, V_2, V_3, V_4 and V_6, with the gauche conformer thermodynamically preferred by 82 ± 20 cm^{-1}. The cis to gauche, gauche to gauche, and gauche to cis barriers are 702 (8.40 kJ/mol), 588 (7.04 kJ/mol) and 620 cm^{-1} (7.42 kJ/mol), respectively. Variable temperature (-105 to -150°C) studies of the infrared spectra of the sample dissolved in liquid krypton have been carried out. From these data, the enthalpy difference has been determined to be 76 cm^{-1} (0.91 kJ/mol). Additionally, ab initio calculations have been carried out utilizing the 6-31G(d) basis sets to obtain the conformational stability, barriers to internal rotation and optimized structural parameters.