INFRARED AND RAMAN SPECTRA, CONFORMATIONAL STABILITY, AND AB INITIO CALCULATIONS OF CYCLOBUTYL TRIFLUOROSILANE

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The infrared (3500 to 40 cm^{-1}) spectra of gaseous and solid and the Raman spectrum (3500 to 30 cm^{-1}) of liquid and solid cyclobutyl trifluorosilane, c-$C_4H_7SiF_3$, have been recorded. From the Raman spectrum of the liquid qualitative depolarization values have been obtained. Both the axial and equatorial conformers have been identified in the fluid phases. Variable temperature (-55 to -150°C) studies of the infrared spectra of the sample dissolved in liquid xenon and krypton have been carried out. From these data, the enthalpy difference has been determined to be 25±10 cm^{-1}(0.30±0.12 kJ/mol), with the equatorial conformer being the more stable form. A complete vibrational assignment is proposed for both conformers based on infrared band contours, relative intensities, depolarization values and group frequencies and the assignments are supported by normal coordinate calculations utilizing ab initio force constants. Complete equilibrium geometries have been determined for both rotamers by ab initio calculations employing different basis sets at the levels of restricted Hartree-Fock (RHF) and/or Moller-Plesset (MP) to second order. The results are discussed and compared to those obtained for some similar molecules.