POSSIBLE SIGNATURES OF CONFORMATIONAL ISOMERIZATION IN THE HIGH RESOLUTION INFRARED SPECTRUM OF 2-FLUOROETHANOL

BROOKS H. PATE, DAVID GREEN, SARAH HAMMOND and JOHN KESKE, *Department of Chemistry, University of Virginia, Charlottesville, VA 22901*.

We have measured the high resolution (5 MHz) infrared spectrum of the asymmetric -CH_2(F) stretch of 2-fluoroethanol (HO-CH_2-CH_2F) near 2980 cm^{-1} using an electric-resonance optothermal molecular beam spectrometer. The infrared spectrum has been assigned using microwave-infrared double-resonance spectroscopy techniques. The infrared spectrum originates in rotational levels of the most stable conformer, denoted Gg', where both internal rotors (C-C and C-O) are in a gauche conformation. The barrier to conformational isomerization is approximately 1000 cm^{-1}. Above this energy two new conformations are accessible, Tt and Tg. Two features of the infrared spectrum may indicate conformational isomerization following excitation of the C-H stretch: 1) The degeneracy of the two Gg' enantiomers is lifted in the infrared spectrum. For 2-fluoroethanol, the degeneracy is lifted only when highly torsionally excited states, or states from the Tt conformation, are involved in the dynamics. 2) There is a strong correlation between rotational states assigned to separate levels of near-degenerate K_a-asymmetry doublets indicating energy flow between these states. These properties of the single-photon infrared spectrum are discussed in the context of subsequent infrared-microwave double-resonance spectroscopy measurements which unambiguously demonstrate conformational isomerization following C-H stretch excitation.