THE PURE MICROWAVE AND HIGH-RESOLUTION INFRARED SPECTRA OF 4-FLUOROBUT-1-YNE

JOHN C. KESKE, FRANCES S. REES and BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22901*.

The pure rotational spectrum of the two conformers of 4-fluorobut-1-yne ($trans$ and $gauche$, and the high resolution (5MHz) infrared spectrum of the acetylenic C-H stretch of the $trans$ conformer have been assigned in an electric resonance optothermal spectrometer (EROS). There is no evidence of the $gauche$ conformer in the vibrational spectrum. The microwave-infrared double-resonance capabilities of the EROS permit rapid and accurate assignment of the congested infrared spectrum. The high-resolution infrared spectrum indicates intramolecular energy redistribution occurs as is evidenced by the fragmentation of the rovibrational spectrum. The eigenstate resolved spectra have been recorded for J=0-8, Ka 0-3. The Ka = 1-3 spectra all have similar spectra with a distribution of intensity over the many lines while the Ka = 0 spectra appear to be resilient to IVR and are dominated by a few strong transitions. From the analysis of these spectra the average decay time of the survival probability of the acetylenic C-H stretch has been determined to be 1.4 ns. The relationship between these IVR rates and conformational isomerization will also be discussed.