

THE MICROWAVE SPECTRUM AND MOLECULAR STRUCTURE OF TRIFLUOROETHYLENE-ACETYLENE

HELEN O. LEUNG, MARK D. MARSHALL, WINN T. CASHION, *Department of Chemistry, Amherst College, P.O. Box 5000, Amherst, MA 01002-5000.*

The rotational spectra of six isotopomers of the 1,1,2-trifluoroethylene-acetylene complex have been collected in the 6–21 GHz region. In addition to the most abundant isotopomer, spectra are obtained for four isotopomers containing substitution in the HCCH subunit (HCCD, $H^{13}C^{13}CH$, and $H^{13}CCH$, which forms two different isotopomers for the complex) and for one isotopomer containing a substitution in the CHF CF_2 subunit ($CHF^{13}CF_2$). The spectra of the three isotopomers with a single substitution of ^{13}C are observed in natural abundance upon pulsed jet expansion of a mixture of HCCH, CHF CF_2 , and Ar. Both *a*- and *b*-type transitions are seen, and the deuterium nuclear quadrupole hyperfine structure in HCCD-CHF CF_2 is resolved and analyzed. Both the Kraitchman substitution coordinates and the spectroscopic constants are consistent with a planar structure in which a hydrogen bond is formed between H in HCCH and the F on C-2 in CHF CF_2 with a secondary interaction between the H (geminal to the F involved in the hydrogen bond) in CHF CF_2 and the acetylenic bond.