ANALYSIS OF MICROWAVE SPECTRUM, INTERNAL ROTATION AND C–H···F INTERACTIONS OF THE $CHF_3 \cdots C_2H_3F$ WEAKLY BOUND COMPLEX

LENA F. ELMUTI, DANIEL A. OBENCHAIN, REBECCA A. PEEBLES, SEAN A. PEEBLES, *Department of Chemistry, Eastern Illinois University, 600 Lincoln Ave., Charleston, IL 61920.*

C–H···X hydrogen bonds with systematic variation of halogens (X = F, Cl, Br) have been examined using Fourier-Transform Microwave (FTMW) spectroscopy. Rotational constants for trifluoromethane–vinyl fluoride (TFM···VF) were consistent with a C_S symmetry structure that exhibited both bifurcated and single C–H···F interactions between the TFM and VF. This near prolate asymmetric top exhibited three-fold internal rotation of the CF_3 group causing characteristic doubling in its spectra.

Initial assignments were completed using chirped-pulse FTMW spectroscopy with additional measurements made using a resonant-cavity FTMW spectrometer. Rotational constants from ab initio calculations at the MP2/6-311++G(2d,2p) level were in agreement with preliminary experimental values ($A = 4828$ MHz, $B = 1049$ MHz, $C = 1018$ MHz). XIAM[a] was used to provide the barrier to internal rotation ($25(5)$ cm^{-1}) and other spectral information. Spectroscopic parameters for the normal isotopic species as well as preliminary structural results on the C–H···F interactions in this complex will be presented.

[a] H. Hartwig and H. Dreizler, *Z. Naturforsch*, **51a**, (1996), 923-932.