ROTATIONAL SPECTRA OF 4,4,4-TRIFLUOROBUTYRIC ACID AND THE 4,4,4-TRIFLUOROBUTYRIC ACID-FORMIC ACID COMPLEX

YOON JEONG CHOI, Department of Chemistry, Wesleyan University, Middletown, CT, USA; ALEX TREVIÑO, Department of Chemistry, University of Texas Rio Grande Valley, Brownsville, TX, USA; <u>SUSANNA L. STEPHENS</u>, Department of Chemistry, Wesleyan University, Middletown, CT, USA; S. A. COOKE, Natural and Social Science, Purchase College SUNY, Purchase, NY, USA; STEWART E. NOVICK, Department of Chemistry, Wesleyan University, Middletown, CT, USA; WEI LIN, Department of Chemistry, University of Texas Rio Grande Valley, Brownsville, TX, USA.

The pure rotational spectra of 4,4,4-trifluorobutyric acid, $CF_3CH_2CH_2COOH$, and its complex with formic acid, were studied by a pulsed nozzle, chirped-pulse Fourier transform microwave spectrometer in the frequency range of 8-12 GHz. The rotational constants and centrifugal distortion constants were determined for the first time. Quantum chemical calculations were carried out exploring possible conformations of 4,4,4-trifluorobutyric and the structure of the 4,4,4-trifluorobutyric acid-formic acid complex using B3LYP/aug-cc-pVTZ and MP2/aug-cc-pVTZ calculations. The experimental spectroscopic constants are compared to those obtained from *ab initio* calculations.