CONFORMATIONAL ANALYSIS OF 3,3,3-TRIFLUORO-2-(TRIFLUOROMETHYL)PROPANOIC ACID

JAVIX THOMAS, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*; MICHAEL J CARRILLO, AGAPITO SERRATO III, *Chemistry, University of Texas Rio Grande Valley, Brownsville, TX, USA*; ELIJAH G SCHNITZLER, WOLFGANG JÄGER, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*; WEI LIN, *Chemistry, University of Texas Rio Grande Valley, Brownsville, TX, USA*.

Partially fluorinated carboxylic acids exhibit rich conformational landscapes. We report the first high-resolution spectroscopic study of 3,3,3-trifluoro-2-(trifluoromethyl)propanoic acid. Its rotational spectrum was measured using both broadband chirped-pulse and narrow-band cavity-based Fourier transform microwave spectrometers. Two dominant conformers were observed, and their structures confirmed with the aid of quantum chemical calculations. Both conformers take on the Z form of the carboxylic acid group. Similarities and differences between this and other fluorinated carboxylic acids are discussed.