STRUCTURE STUDY OF FORMIC ACID CLUSTERS BY CHIRPED-PULSE FTMW SPECTROSCOPY

DANIEL P. ZALESKI, JUSTIN L. NEILL, MATT T. MUCKLE, AMANDA L. STEBER, and BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., P.O. Box 400319, Charlottesville, VA 22904*; KEVIN O. DOUGLASS, *National Institute of Standards and Technology, Optical Technology Division, Gaithersburg, MD 20899*.

The large bandwidths and high sensitivity afforded by chirped-pulse FTMW spectrometers allow for the detection of large molecules (10+ heavy atoms) and their isotopomers in natural abundance. With the isotopic information, an experimental structure can be obtained by using Kraitchmans equations. Clusters of carboxylic acids are of interest because of the different possibilities for hydrogen bonding that lead to the formation of larger clusters. The first study of formic acid clusters by microwave spectroscopy was presented by Bauder and the formic acid dimer with one water molecule complexed was identified.[a] Previously the formic acid trimer cluster was reported where the third formic acid attaches itself to the already formed formic acid dimer.[b] Here we present the full heavy atom and partial deuterium Kraitchman substitution structure of formic acid trimer. In addition we have identified two new nonplanar formic acid clusters - formic acid pentamer and the cluster of formic acid trimer with one water molecule attached. For the latter, two tunneling states with an energy splitting of 178 MHz are observed for the normal species and 13C isotopomers. Candidate structures and the difficulty of modeling these clusters by electronic structure theory will be discussed.

[a] Dominque Priem, Tae-Kyu Ha, and Alfred Bauder. *J. Chem. Phys.* 113, 1, (2000), 169-175.

[b] Conformational Studies in Formic Acid Oligimers. Richard D. Suenram, Pam L. Crum, Kevin O. Douglass, and Brooks H. Pate. *The Ohio State 59th International Symposium on Molecular Spectroscopy*.