MW SPECTROSCOPY COUPLED WITH ULTRAFAST UV LASER VAPORIZATION: SUCCINIC ACID IN THE GAS PHASE

ESTIBALIZ MENDEZ, PATRICIA ECIJA, EMILIO J. COCINERO, FERNANDO CASTANO, FRANCISCO J. BASTERRETXEA, *Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Ap.644, E-48940, Bilbao, Spain*; PETER D. GODFREY, DON MCNAUGHTON, *School of Chemistry, Box 23 Victoria 3800 Monash University, Australia*; MICHAELA K. JAHN, K.P. RAJAPPAN NAIR, JENS-UWE GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Gottfried-Wilhelm-Leibniz-Universität, 30167 Hannover, Germany*.

Recent lab and field measurements have indicated critical roles of organic acids in enhancing new atmospheric aerosol formation. In order to understand the nucleation process, here we report an experimental and theoretical investigation of chemical structure of succinic acid. We have used the technique of Fourier Transform Microwave Spectroscopy (FTMW). Succinic acid was vaporized by UV ultrafast laser ablation to suppress thermal decomposition processes[a] and seeded into an expanding stream of Ne forming a supersonic jet. The rotational spectrum detected the presence of a single most stable conformation in the cm- mm- wave regions for which accurate rotational and centrifugal distortion parameters have been determined. The study was extended to all monosubstituted isotopic species (^{13}C, ^{18}O, $D(O)$), which were positively identified, leading to an accurate determination of the effective and substitution structures of the molecule. The experimental study was supplemented by *ab initio* (MP2) and DFT (M06-2X and B3LYP) calculations.

[a] E. J. Cocinero, A. Lesarri, P. Écija, F. J. Basterretxea, J. U. Grabow, J. A. Fernández and F. Castaño, *Angew. Chem. Int. Ed.*, 51, 3119-3124, 2012.