AN IMPROVED CHIRPED PULSE FTMW ANALYSIS OF THE STRUCTURES OF PHENOL DIMER AND TRIMER

NATHAN A. SEIFERT, CRISTÓBAL PÉREZ, AMANDA L. STEBER, DANIEL P. ZALESKI, JUSTIN L. NEILL, BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319*; ALBERTO LESARRI, *Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47001 Valladolid, Spain*.

With the recent improvements for chirped pulse FTMW (CP-FTMW) spectroscopy between 2-18 GHz, substitution structures of molecules and clusters with more than 10 heavy atoms are becoming routine. While previous CP-FTMW results for phenol dimer reported at this conference by Steber et al.[a] necessitated reduced-band measurements in order to achieve the sensitivity to detect the carbon isotopologues, the latest improvements for the 2-8 GHz arrangement have enabled full band detection of all 12 ^{13}C and 2 ^{18}O isotopologues of phenol dimer in natural abundance, with improved fits for all detected species. In addition, the added sensitivity of this new 2-8 GHz configuration has enabled a full carbon substitution structure of phenol trimer. The experimental structure of phenol trimer, in agreement with the M06-2X/6-311++g(d,p) *ab initio* structure, is a C_3 oblate symmetric top with 21 heavy atoms; however, all possible isotopic substitutions are off-symmetry axis, so the resulting detected isotopologues have been fit as c-type prolate asymmetric tops. Use of Kraitchman′s equations for structural determination of a symmetric top molecule require some assumptions from the *ab initio* structure for the complete r_s structure of the trimer. A detailed summary of these methods, as well as the microwave results for both species, will be presented.

[a] A. L. Steber, J. L. Neill, D. P. Zaleski, B. H. Pate, A. Lesarri. 67th OSU Int. Symp. On Mol. Spectrosc., Columbus, OH, 2012, MH13.