

AN IMPROVED ANALYSIS OF THE SEVOFLURANE-BENZENE STRUCTURE BY CHIRPED PULSE FTMW SPECTROSCOPY

NATHAN A. SEIFERT, CRISTOBAL PEREZ, DANIEL P. ZALESKI, JUSTIN L. NEILL, BROOKS H. PATE, *Department of Chemistry, University of Virginia, McCormick Rd., Charlottesville, VA 22904-4319*; ALBERTO LESARRI, MONTSERRAT VALLEJO, *Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain*; EMILIO J. COCINERO, FERNANDO CASTANO, *Departamento de Química Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Campus de Leioa, Ap. 644, E-48080 Bilbao, Spain*; ISABELLE KLEINER, *Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), CNRS et Universités Paris Est et Paris Diderot, 61. av Général de Gaulle, 94010 Créteil, France*.

Recent improvements to the 2-8 GHz CP-FTMW spectrometer at University of Virginia have improved the structural and spectroscopic analysis of the sevoflurane-benzene cluster. Previously reported results^a, although robust, were limited to a fit of the a-type transitions of the normal species in the determination of the six-fold barrier to benzene internal rotation. Structural analysis was limited to the benzene hydrogen atom positions using benzene-d₁. The increased sensitivity of the new 2-8 GHz setup allows for a full internal rotation analysis of the a- and c-type transitions of the normal species, which was performed with BELGI. A fit value for V₆ of 32.868(11) cm⁻¹ is determined. Additionally, a full substitution structure of the benzene carbon atom positions was determined in natural abundance. Also, new measurements of a sevoflurane/benzene-d₁ mixture enabled detection of 33 of the 60 possible ²D / ¹³C double isotopologues. This abundance of isotopic data, a total of 45 isotopologues, enabled a full heavy atom least-squares r₀ structure fit for the complex, including positions for all seven fluorines in sevoflurane.

^aN. A. Seifert, D. P. Zaleski, J. L. Neill, B. H. Pate, A. Lesarri, M. Vallejo, E. J. Cocinero, F. Castaño. 67th OSU Int. Symp. On Mol. Spectrosc., Columbus, OH, 2012, MH13.