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

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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-d_1. 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 V_6 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-d_1 mixture enabled detection of 33 of the 60 possible ^2D / ^{13}C double isotopologues. This abundance of isotopic data, a total of 45 isotopologues, enabled a full heavy atom least-squares r_0 structure fit for the complex, including positions for all seven fluorines in sevoflurane.

[a]N. 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.