STRUCTURE OF THE SEVOFLURANE-BENZENE COMPLEX AS DETERMINED BY CHIRPED-PULSE FTMW SPECTROSCOPY

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Following previous microwave studies on sevoflurane monomer by Suenram *et al.*[a] and Vega-Toribio *et al.*[b] we report the broadband rotational spectrum of sevoflurane clustered with benzene. The structure assigned is consistent with a C-H$\cdots\pi$ interaction between the benzene ring and the $(CF_3)_2$C-H hydrogen on sevoflurane. The spectrum of this species is complicated by the six-fold internal rotation of the benzene ring over the C_1 framework of sevoflurane. The six-fold tunneling falls into a high effective barrier case where there are several bound torsional levels. The tunneling spectrum has been successfully analyzed using the BELGI internal rotation program and a barrier to internal rotation of the benzene against sevoflurane of 32.5 cm^{-1} has been determined. Structural information about the complex has been obtained by studying the complex of sevoflurane with benzene-d_1. For this complex, six unique isomers are observed making it possible to determine the positions of the benzene H-atoms in the complex. Combination of these hydrogen r_s positions with the sevoflurane monomer r_s coordinates reported by Lesarri *et al.*[c] results in a substitution structure in excellent agreement with the ab initio results. Finally, initial microwave results on two sevoflurane dimer species will also be presented.

[a] R. D. Suenram, D. J. Brugh, F. J. Lovas and C. Chu, 51st OSU Int. Symp. On Mol. Spectrosc., Columbus, OH, 1999, RB07.
[b] A. Vega-Toribio, A. Lesarri, R.D. Suenram, J. Grabow, 64th OSU Int. Symp. On Mol. Spectrosc., Columbus, OH, 2009, MH07.
[c] A. Lesarri, A. Vega-Toribio, R. D. Suenram, D. J. Brugh, J.-U. Grabow, Phys. Chem. Chem. Phys., 12, 9624-9631 (2010).