STRUCTURE DETERMINATION OF TWO STEREOISOMERS OF SEVOFLURANE DIMER BY CHIRPED PULSE FTMW SPECTROSCOPY

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Two stereoisomers of sevoflurane dimer have been detected using chirped pulse FTMW spectroscopy from 2-8 GHz. The identified complexes are distinguished by their differing helicities, and together both isomers form a diastereomeric pair, one being homochiral (RR/SS) and the other heterochiral (RS/SR). For both isomers, all 8 ^{13}C isotopologues have been assigned, and two ^{18}O isotopologues have also been detected for the homochiral isomer, for a total of 18 isotopologues. MP2/6-311++g(d,p) calculations predict the heterochiral isomer as 1.2 kJ mol^{-1} above the homochiral species, which is consistent with the observed relative intensities between the two species. A summary of these microwave results, including a comparison between the Kraitchman and ab initio structures, will be presented.