GEOMETRIES AND CONFORMATIONAL CONVERSION OF THE BINARY 3,3,3-TRIFLUOROPROPANOL CONFORMERS: ROTATIONAL SPECTRA AND DFT CALCULATIONS

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Fluorinated alcohols have been widely used as co-solvents to study folding and unfolding behaviors of proteins and peptides. The detailed mechanism by which this happens is yet to be established. Recent molecular dynamics simulations suggested that clusters of the fluoroalcohol play an important role in the mechanism. In the current study, we applied jet-cooled chirped pulse Fourier transform microwave spectroscopy to probe structure and dynamics of 3,3,3-trifluoropropanol (TFP)[1] and its dimer. In comparison to 2,2,2-trifluoroethanol,[2] TFP is the smallest trifluoroalcohol molecule which exhibits folded conformations in its monomer form, thus serving as a prototype system for structural diversity associated with folding. The possible structural candidates of the TFP dimer were explored by using CREST, a recently developed conformational searching tool and nearly 70 stable binary conformers were identified. Rotational spectra of three low energy binary TFP conformers were assigned and their carriers identified. To help explain the observation of the binary conformers, a combined kinetic and thermodynamic conformational distribution model was developed to explain the non-observation of some lower energy conformations and to provide quantitatively explanation for the experimental conformational abundances. The study of the conformations of TFP and its dimer is a first and important step in understanding how TFP aggregates in bulk.

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