

THE MICROWAVE SPECTRA AND MOLECULAR STRUCTURES OF THE CHIRAL TAGGING CANDIDATE *CIS*-1,3,3,3-TETRAFLUORO-1,2-EPOXYPROPANE AND ITS GAS PHASE HETERODIMER WITH THE ARGON ATOM

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We are exploring how argon binding to substituted oxiranes, which have potential applications as chiral tags, is modulated by varying the identity of the substituents on the epoxy ring. Previously studied systems generally showed close contacts primarily to atoms contained in the ring. However, for complexes with *cis*-1,3,3,3-tetrafluoro-1,2-epoxypropane (cFTFO) multiple minima with similar energies are predicted by quantum chemistry calculations including some with significant interactions between the argon atom and substituents on the oxirane. Analysis of the rotational spectra obtained using chirped pulse Fourier transform microwave spectroscopy for four isotopologues of Ar-cFTFO reveals that the argon atom binds to the back of the ring; very different from Ar-3,3,3-trifluoro-1,2-epoxypropane (Ar-TFO) and Ar-3,3-difluoro-1,2-epoxypropane, but similar to Ar-*trans*-1,3,3,3-tetrafluoro-1,2-epoxypropane. The utility of cFTFO in chiral analysis is explored via quantum chemistry calculations on the TFO-cFTFO heterodimer and progress on the observation and analysis of the two diastereomeric forms of this species will be reported.