CHARACTERIZING THE GAS-PHASE HETERODIMERS OF THE CHIRAL TAGGING CANDIDATES *TRANS*-1,3,3,3-TETRAFLUORO-1,2-EPOXYPROPANE AND 3,3,3-TRIFLUORO-1,2-EPOXYPROPANE BY QUANTUM CHEMISTRY AND MICROWAVE SPECTROSCOPY

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As part of our efforts in evaluating substituted oxiranes for use as potential chiral tags for the conversion of enantiomeric molecules into spectroscopically distinct diastereomeric complexes for chiral analysis, we examine the gas-phase heterodimers formed between two such species using quantum chemistry and microwave spectroscopy. The lowest energy isomers of the various diastereomers of 3,3,3-trifluoro-1,2-epoxypropane–trans-1,3,3,3-tetrafluoro-1,2-epoxypropane are predicted to share structural features with the previously characterized 3,3,3-trifluoro-1,2-epoxypropane homodimers. Like the homodimers, the diastereomeric heterodimers have significantly different rotational constants, and thus, easily distinguishable microwave spectra. The spectrum of (*S*)-3,3,3-trifluoro-1,2-epoxypropane–(1*R*, 2*S*)-trans-1,3,3,3-tetrafluoro-1,2-epoxypropane and its enantiomer has been obtained and analyzed to be consistent with the quantum chemistry predictions. Despite being predicted at a lower energy, the search for the spectrum of (*S*)-3,3,3-trifluoro-1,2-epoxypropane–(1*S*, 2*R*)-trans-1,3,3,3-tetrafluoro-1,2-epoxypropane and its enantiomer is on-going.