EFFECTS OF CHIRALITY IN HOMODIMERS OF 3,3,3-TRIFLUORO-1,2-EPOXYPROPANE

MARK D. MARSHALL, HELEN O. LEUNG, *Chemistry Department, Amherst College, Amherst, MA, USA*; NATHAN A. SEIFERT, YUNJIE XU, WOLFGANG JÄGER, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*.

We are investigating the suitability of 3,3,3-trifluoro-1,2-epoxypropane [2-(trifluoromethyl)-oxirane, or TFO] as a tag for chiral analysis through conversion of enantiomers into structurally distinct diastereomers via the formation of non-covalently bound heterodimers. This method can determine the absolute stereochemistry and enantiomeric composition of an analyte and shows promise for great impact in analytical chemistry. Using density functional theory, we examine the possible conformations of both homochiral (RR or SS) and heterochiral (RS or SR) homodimers of TFO to guide the search for the microwave spectra of these species. Several conformers are found for each, but the lowest energy heterochiral TFO dimer is a microwave silent one with an inversion center. However, a spectrum is observed that can be assigned to the lowest energy geometry of the homochiral TFO dimer.