

THE CONVERSION OF STYRENE OXIDE ENANTIOMERS INTO SPECTROSCOPICALLY DISTINGUISHABLE DIASTEREOMERS THROUGH COMPLEXATION WITH 3,3,3-TRIFLUORO-1,2-EPOXYPROPANE

MARK D. MARSHALL, HELEN O. LEUNG, *Chemistry Department, Amherst College, Amherst, MA, USA*; MELANIE SCHNELL, SERGIO R DOMINGOS, ANNA KRIN, *FS-SMP, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany*.

3,3,3-Trifluoro-1,2-epoxypropane [2-(trifluoromethyl)-oxirane, or TFO] has shown promise as a tag for chiral analysis through conversion of enantiomers into spectroscopically distinguishable diastereomers via the formation of non-covalently bound heterodimers. We demonstrate the suitability of this method through characterization of the microwave rotational spectrum of complexes formed between TFO and styrene oxide (SO). Molecular dynamics calculations are used to quickly identify possible heterodimer conformations which are then optimized and evaluated using density functional theory. Using a mixture of racemic samples of both species, we observe and assign spectra for the lowest energy conformers of both homochiral (RR/SS)-TFO-SO and heterochiral (RS/SR)-TFO-SO. Had a single enantiomer of TFO been used, say (R), the spectra are sufficiently distinct and sufficiently well predicted by theory that (RR)-TFO-SO and (RS)-TFO-SO are readily identified and separately analyzed.