

A PEPTIDE CO SOLVENT IN A CHIRALITY INDUCTION MODEL SYSTEM: BROADBAND ROTATIONAL SPECTROSCOPY OF THE 2,2,2-TRIFLUOROETHANOL- -PROPYL ENE OXIDE ADDUCT

JAVIX THOMAS, YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada.*

Chirality induction in a model system, i.e. the 2,2,2-trifluoroethanol (TFE)- propylene oxide (PO) adduct, was investigated in detail using chirped pulse and cavity based Fourier transform microwave spectroscopy, complemented with high level ab initio calculations. Hydrogen-bonding interaction of TFE with the permanently chiral PO molecule results in eight binary TFE- -PO diastereomers. Rotational spectra of four of them were observed experimentally and unambiguously assigned and identified. Unlike the TFE dimer where an extreme case of chirality synchronization was previously reported, diastereomers due to both the g+ and g- forms of TFE were observed, indicating that the tunneling between the two isoenergetic gauche forms of TFE was quenched. Comparison to the previous studies reveals that perfluorination increases the hydrogen-bonding energy by about 70% over its ethanol counterpart. TFE- -PO serves as a prototype system for chirality induction which leads to chirality amplification rather than a system with chirality synchronization.