COMPLEXES OF SMALL CHIRAL MOLECULES: PROPYLENE OXIDE AND 3-BUTYN-2OL

LUCA EVANGELISTI, *Dipartimento di Chimica G. Ciamician, Università di Bologna, Bologna, Italy*; CHANNING WEST, ELLIE COLES, BROOKS PATE, *Department of Chemistry, The University of Virginia, Charlottesville, VA, USA*.

Complexes of propylene oxide with 3-butyn-2-ol were observed in the molecular rotational spectra, and isotopologue analysis allowed for structural determination of the complexes. Using a gas mixture of 0.1% propylene oxide and 0.1% 3-butyn-2-ol in neon, the broadband rotational spectrum was measured in the 2-8 GHz frequency range using a chirped-pulse Fourier transform microwave spectrometer. Four isomers of each diastereomer pair, formed by a hydrogen bond between the two monomers, are identified in quantum chemistry study of the complex using B3LYP-D3BJ with the def2TZVP basis set. The initial measurement used racemic samples of both molecules in order to obtain all possible isomers of the complex in the pulsed jet expansion. A total of six distinct spectra were assigned in the racemic measurement - three for both the homochiral and heterochiral complex. Substitution structures for the most intense homochiral and heterochiral complexes were obtained. These complexes use the two lowest energy conformations of butynol despite conformational cooling of the monomer, resulting in a single identified isomer. This result shows that a wide range monomer conformational geometries need to be examined when performing searches for the lowest energy geometry. Analysis of the diastereomer spectra was used to develop a method for determining the enantiomeric excess of 3-butyn-2-ol and propylene oxide for use as a chiral tag, which could be used in subsequent measurements to determine enantiomeric excess. The sensitivity limits for enantiomeric excess determination and the linearity of the rotational spectroscopy signals as a function of sample enantiomeric excess will be presented.