HYDROGEN BONDING IN CHIRAL MOLECULAR COMPLEX: DIRECT DETECTION OF PROPYLENE OXIDE-WATER ADDUCT IN GAS PHASE

ZHENG SU AND YUNJIE XU, *Department of Chemistry, University of Alberta, Edmonton, AB, T6G 2G2, Canada*.

High resolution spectroscopy and *ab initio* calculations of chiral molecules and their molecular complexes promise to provide rich structural and dynamical information about this class of molecular systems. In this talk, we will report the detailed rotational spectroscopic and high level *ab initio* studies of the hydrogen bonded propylene oxide-water (C_3H_6O-H_2O) complex. Two distinct structural conformers of the 1:1 molecular adduct were detected experimentally. Rotational spectra of the four isotopomeric species, namely C_3H_6O-H_2O, C_3H_6O-DOH, C_3H_6O-HOD and C_3H_6O-D_2O were recorded for the two conformers. The effect of the methyl group on the stability of the $O_{epoxy}\cdots$H-O type hydrogen bond will be examined by comparing with the closely related ethylene-water adduct.[a]

[a] W. Caminati, P. Moreschini, I. Rossi, and P. G. Favero *J. Am. Chem. Soc.* **1998**, 120, 11144-11148.