Abstract Submitted
for the DAMOP07 Meeting of
The American Physical Society

***Ab initio* and Rotational Spectroscopic Study of Propylene Oxide – (Water)$_{N=2/3}$ Complexes** ZHENG SU, YUNJIE XU, University of Alberta — Water is the principal constituent of the environment for all living organisms. Nearly all biological molecules required for life are chiral. Therefore the studies of the solvation of chiral molecules in water are of fundamental importance to life science. In this work, we report *ab initio* and rotational spectroscopic studies of the hydrogen bonded propylene oxide (PO) – $(H_2O)_{N=2/3}$ clusters, which is a continuing study from our success on PO with one water molecule in the gas phase. The sequential complexation of PO with a few water molecules is a significant step towards understanding the solvation process for this simplest cyclic ether chiral molecule. Complete geometry optimizations for the PO-water complexes are carried out at the MP2 level of theory with the 6-311++G(d,p) basis set using the GAUSSIAN03 software package. The calculated rotational constants and dipole moment components are used to aid the initial spectroscopic investigations. By systematically increasing the pressure, attachment of more water molecules to PO can be formed and distinguished from only one. Both experimental and theoretical results are used to extract structural and dynamic information about the complexes. The experimental analysis will in turn be used to judge the quality of the theoretical predictions and then determine the appropriate model for further calculations.

Zheng Su
University of Alberta

Date submitted: 02 Feb 2007 Electronic form version 1.4