INFRARED ACTION SPECTROSCOPY OF THE OH-H_2O COMPLEX

BRIDGET A. O'DONNELL, CRAIG MURRAY, and MARSHA I. LESTER, *Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323*.

Hydroxyl radicals (OH) are expected to form strong hydrogen bonds with water (H_2O), making complexes of OH with water important for a variety of systems, such as the gaseous environment of the atmosphere, the interface of water and/or ice, and the bulk regions of liquid water, snow, and ice. The study of binary OH-water complexes will shed new light on the intermolecular interaction between the OH radical and water molecule in these environments. In this study, the OH-H_2O complex is produced in the gas phase by the association of photolytically generated OH radicals with H_2O in the collisional region of a supersonic expansion. Infrared spectroscopy is used to identify a band at 3491 cm^{-1}, displaying a shift of –79 cm^{-1} from its hydroxyl monomer, which is consistent with *ab initio* predictions of the fundamental OH radical stretch of the complex.[a] The rotationally structured band profile is modeled using a simulation based on an a-type transition for an open-shell complex with partially quenched orbital angular momentum.[b] Following infrared excitation of OH-H_2O, the OH products of vibrational predissociation are detected by laser-induced fluorescence on the OH $A\,^2\Sigma^+$–$X\,^2\Pi$ (1,0) transition. By utilizing information from the OH product state distribution, an upper limit to the binding energy of the complex will be determined.

[a] Y. Xie and H. F. Schaefer, J. Chem. Phys. 98, 8829 (1993).
[b] M. D. Marshall and M. I. Lester, J. Phys. Chem. B. 109, 8400 (2005).