INFRARED ACTION SPECTROSCOPY OF THE OH-H₂O COMPLEX

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Hydroxyl radicals (OH) are expected to form strong hydrogen bonds with water (H₂O), 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-H₂O complex is produced in the gas phase by the association of photolytically generated OH radicals with H₂O 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-H₂O, 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.

^aY. Xie and H. F. Schaefer, J. Chem. Phys. 98, 8829 (1993).

^bM. D. Marshall and M. I. Lester, J. Phys. Chem. B. 109, 8400 (2005).