OBSERVATION OF HIGH-AMPLITUDE ZERO-POINT MOTION AND LOW-BARRIER HYDROGEN BONDS IN THE $H_3O_2^-$ AND $H_2O_2^-$ COMPLEXES USING ARGON PREDISSOCIATION INFRARED SPECTROSCOPY

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We used argon predissociation infrared spectroscopy in the 600-3800 cm^{-1} region to investigate the quantum nature of the shared proton in the $[HO\text{-}H\text{-}OH]^-$ and the $[O\text{-}H\text{-}OH]^-$ complexes. High-level theoretical calculations anticipate the zero-point levels to lie above the barriers in their respective proton transfer coordinates, consequently giving rise to high-amplitude proton motion. Experimentally, very intense, sharp bands are observed below 800 cm^{-1} for each complex, and are assigned to the fundamental ($1\leftarrow0$) transitions due to the shared proton excitation. Single, weak features were also recovered in the 3650-3660 cm^{-1} region for each complex, and are assigned to "hydroxide-like" OH stretches that result from large-amplitude proton oscillation along the heavy atom axis. Assignments of the three fundamental transitions associated with the three-dimensional confinement of the shared proton in the $H_3O_2^-$ species are offered with the aid of diffusion Monte Carlo (DMC) calculations. In the $H_2O_2^-$ case a preliminary analysis of the O-O stretch contribution to the zero-point energy level is proposed.