

OBSERVATION OF HIGH-AMPLITUDE ZERO-POINT MOTION AND LOW-BARRIER HYDROGEN BONDS IN THE  $\text{H}_3\text{O}_2^-$  AND  $\text{H}_2\text{O}_2^-$  COMPLEXES USING ARGON PREDISSOCIATION INFRARED SPECTROSCOPY

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We used argon predissociation infrared spectroscopy in the  $600\text{-}3800\text{ cm}^{-1}$  region to investigate the quantum nature of the shared proton in the  $[\text{HO-H-OH}]^-$  and the  $[\text{O-H-OH}]^-$  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  $800\text{ cm}^{-1}$  for each complex, and are assigned to the fundamental ( $1\leftarrow 0$ ) transitions due to the shared proton excitation. Single, weak features were also recovered in the  $3650\text{-}3660\text{ cm}^{-1}$  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  $\text{H}_3\text{O}_2^-$  species are offered with the aid of diffusion Monte Carlo (DMC) calculations. In the  $\text{H}_2\text{O}_2^-$  case a preliminary analysis of the O-O stretch contribution to the zero-point energy level is proposed.