INVESTIGATION OF COUPLING BETWEEN OH STRETCHING AND H_2O OUT-OF-PLANE BENDING MODES IN OH-H_2O

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Hydroxyl radicals (OH) are expected to form strong hydrogen bonds with water (H_2O); such interactions are found in the gaseous environment of the atmosphere, the interface of liquid water and ice, and bulk regions of liquid water, snow, and ice. The study of binary OH-H_2O complexes will provide insight on the larger OH-H_2O complexes found in the aforementioned systems. In this study, a two-dimensional potential of both the A' and A'' binary OH-H_2O complex, taking both the OH stretching and H_2O out-of-plane bending modes into account, is constructed using density functional theory with the aug-cc-pVTZ basis. Energies and wave functions of the bound states are generated using a discrete variable representation. These two-dimensional potentials are relevant to the discussion of past experimental microwave studies and the infrared spectrum observed in this laboratory, and are significant in the directing of future experiments.