INVESTIGATION OF COUPLING BETWEEN OH STRETCHING AND H$_2$O OUT-OF-PLANE BENDING MODES IN OH-H$_2$O

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Hydroxyl radicals (OH) are expected to form strong hydrogen bonds with water (H$_2$O); 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$_2$O complexes will provide insight on the larger OH-H$_2$O complexes found in the aforementioned systems. In this study, a two-dimensional potential of both the $\Lambda'$ and $\Lambda''$ binary OH-H$_2$O complex, taking both the OH stretching and H$_2$O 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.