VIBRATIONAL ANYLASIS ON $I(H_2O)^-$ and $I(D_2O)^-$ SPECTRA

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Hydrated halide clusters provide good systems for investigating the effect of the intramolecular hydrogen-bond on the spectrum of ions and molecules. In this work, the vibrational spectra of $I(H_2O)^-$ and $I(D_2O)^-$ were studied. We focused on the couplings between the two O-H stretch modes and the in-plane bending mode, which is the frustrated rotation of the water molecule in the plane of the complex. A reduced-dimensional analysis with these three modes was developed to investigate the effect of the couplings on the spectra. The model potential in the analysis was obtained from ab initio calculation with MP2/aug-cc-pVTZ-PP level of method and basis set. The doublet structure of the O-H stretch mode in the spectrum was attributed to the tunneling splitting from the in-plane bending mode double-well potential energy surface.