

VIBRATIONAL COUPLING IN SOLVATED FORM OF EIGEN PROTON

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The most simple solvated proton, the hydronium ion H_3O^+ has been studied experimentally in its bare case as well as with the messenger techniques. Recent studies have shown that features in the vibrational spectra can be modulated not only by the different messengers, but also by the number of messengers. Theoretical molecular dynamics simulations have shed some light on the $\text{H}_3\text{O}^+(\text{H}_2)_n$ clusters, but understanding on the effect of microsolvation by the messengers toward the spectra is still far from complete. We compare the experimental $\text{H}_3\text{O}^+\text{Ar}_m$ $m=1-3$ spectra with accurate theoretical simulations and obtain the peak position and absorption intensity by solving the quantum vibrational Schrodinger equation using the potential and dipole moment obtained from DFT methods. One of the main goals of the study is to glean into the vibrational couplings induced by the microsolvation by the argon on the spectra region of $1500-3800\text{ cm}^{-1}$, and to provide assignment on the peaks observed in these regions.