VIBRATIONAL COUPLING IN SOLVATED FORM OF EIGEN PROTON: TUNING THE COUPLING VIA ISOTOPLOGUES

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Experimental studies have shown that features in the vibrational spectra of H$_3$O$^+$ can be modulated not only by the type messengers, but also by the number of messengers. Recently, we compared the experimental H$_3$O$^+$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 ab initio methods.$^a$ In this work, we studied isotopologues of this ionic cluster to glean into the details of the vibrational couplings manifested in the spectra region of 1500-3800 cm$^{-1}$.