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

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Experimental studies have shown that features in the vibrational spectra of H_3O^+ can be modulated not only by the type messengers, but also by the number of messengers. Recently, we compared the experimental $H_3O^+Ar_m$, 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 isotopolgues of this ionic cluster to glean into the details of the vibrational couplings manifested in the spectra region of 1500-3800 cmcm^{-1}.

[a] J-W Li, M. Morita, T. Takahashi and J-L Kuo, J. Phys. Chem. A, 119, 10887 (2015)