The origin and strength of intra- and inter-molecular vibrational coupling is difficult to probe by direct experimental observations. However, explicitly including or not including some specific intramolecular vibrational modes to study intermolecular interaction provides a precise theoretical way to examine the effects of anharmonic coupling between modes. In this work, a full-dimension intra- and inter-molecular \textit{ab initio} potential energy surface (PES) for H$_2$O – Ar, which explicitly incorporates interdependence on the intramolecular normal-mode coordinates of the H$_2$O monomer, has been calculated. In addition, four analytic vibrational-quantum-state-specific PESs are obtained by least-squares fitting vibrationally averaged interaction energies for the $(\nu_1,\nu_2,\nu_3)=(0,0,0),(0,0,1),(1,0,0),(0,1,0)$ states of H$_2$O to the three-dimensional Morse/long-range potential function. The resulting vibrationally averaged PESs provide good representations of the experimental infrared data, with RMS discrepancies smaller than 0.02 cm$^{-1}$ for all three rotational branches of the asymmetric stretch fundamental transitions. The infrared band origin shifts associated with three fundamental bands of H$_2$O in H$_2$O – Ar complex are predicted for the first time and are found to be in good agreement with the (extrapolated) experimental values. Upon introduction of additional intramolecular degrees of freedom into the intermolecular potential energy surface, there is clear spectroscopic evidence of intra- and intermolecular vibrational couplings.\textsuperscript{a}

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