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An Accurate Full-Dimensional H_4O Potential Energy Surface and Dynamics of Exchange Reaction $H_2 + H'_2O \rightarrow HH' + HOH'$

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Supporting Information

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Figure S1. (a) Potential energy as a function of the H-H bond length for $H_2\cdots H_2O$, which are calculated at the level of CCSD(T)-F12a/AVTZ for 0.4 Å ≤ $r_{H\text{-}H}$ ≤ 4 Å and MRCI-F12+Q_{rot}/AVTZ for $r_{H\text{-}H}$ ⩾ 2Å. (b) Potential energy as a function of an O-H bond length for $H_2\cdots H_2O$, which are calculated by CCSD(T)-F12a/AVTZ for 0.65 Å ≤ $r_{O\text{-}H}$ ≤ 4 Å and MRCI-F12+Q_{rot}/AVTZ for $r_{O\text{-}H}$ ⩾ 2Å.

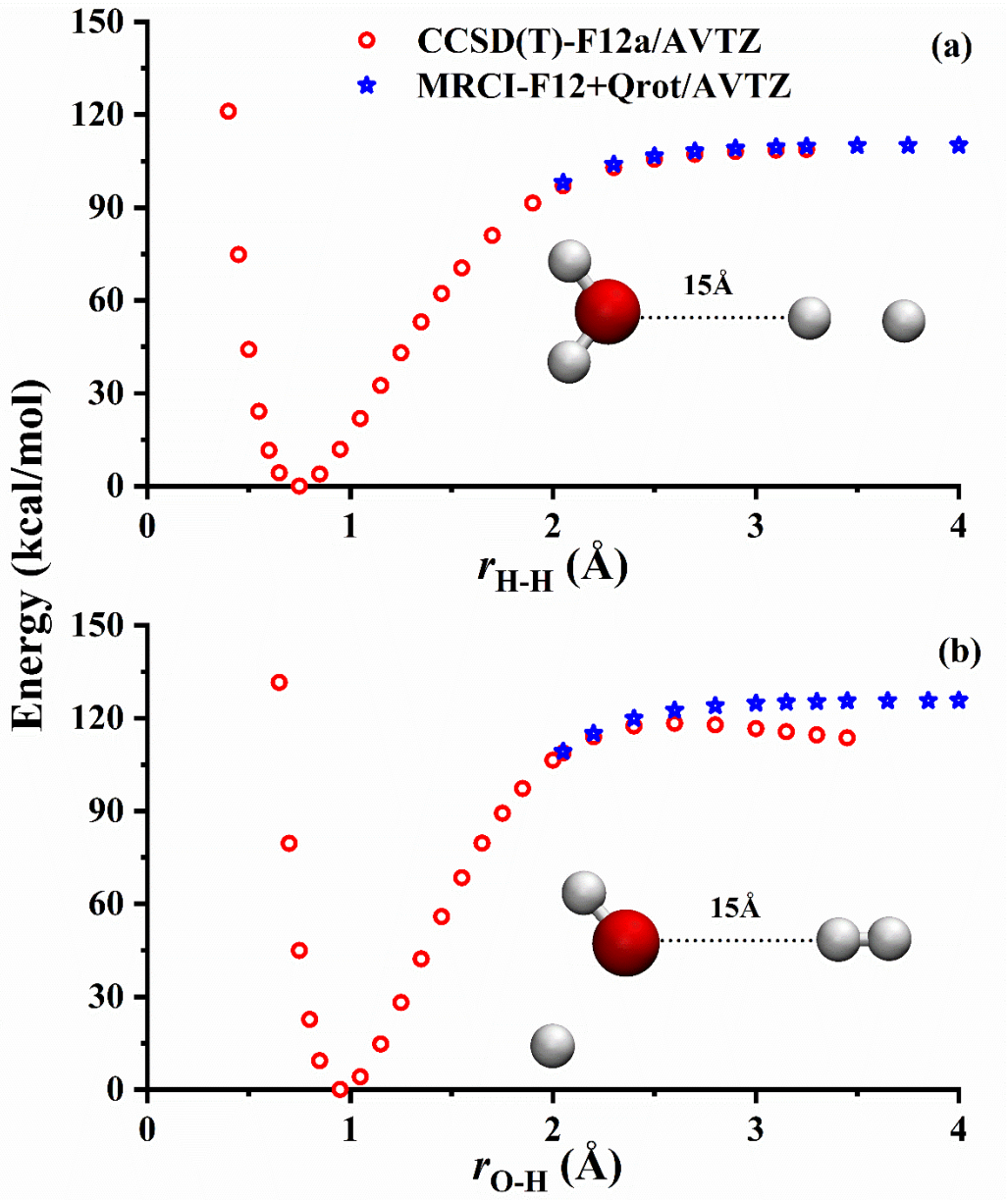

Figure S2. (a) One-dimensional cuts for nine normal coordinates of the transition state, and the points are the results by ab initio calculation. (b) The normal mode vector corresponding to each vibration mode of the transition state.