

SUPPORTING INFORMATION

Proton Transfer Rates in Ionized Water Clusters (H_2O)_n ($n=2-4$)

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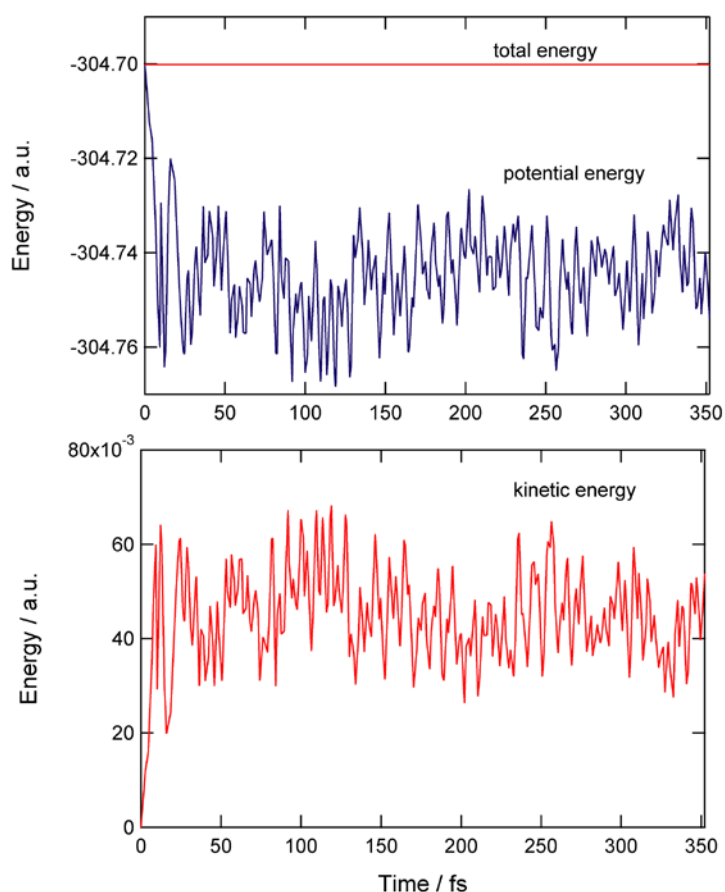


Figure S1. Results of direct AIMD calculation for ionization of water tetramer. (Upper) total and potential energies of the system, and (Lower) kinetic energy. The calculations were carried out at the MP2/6-311++G(d,p) level.

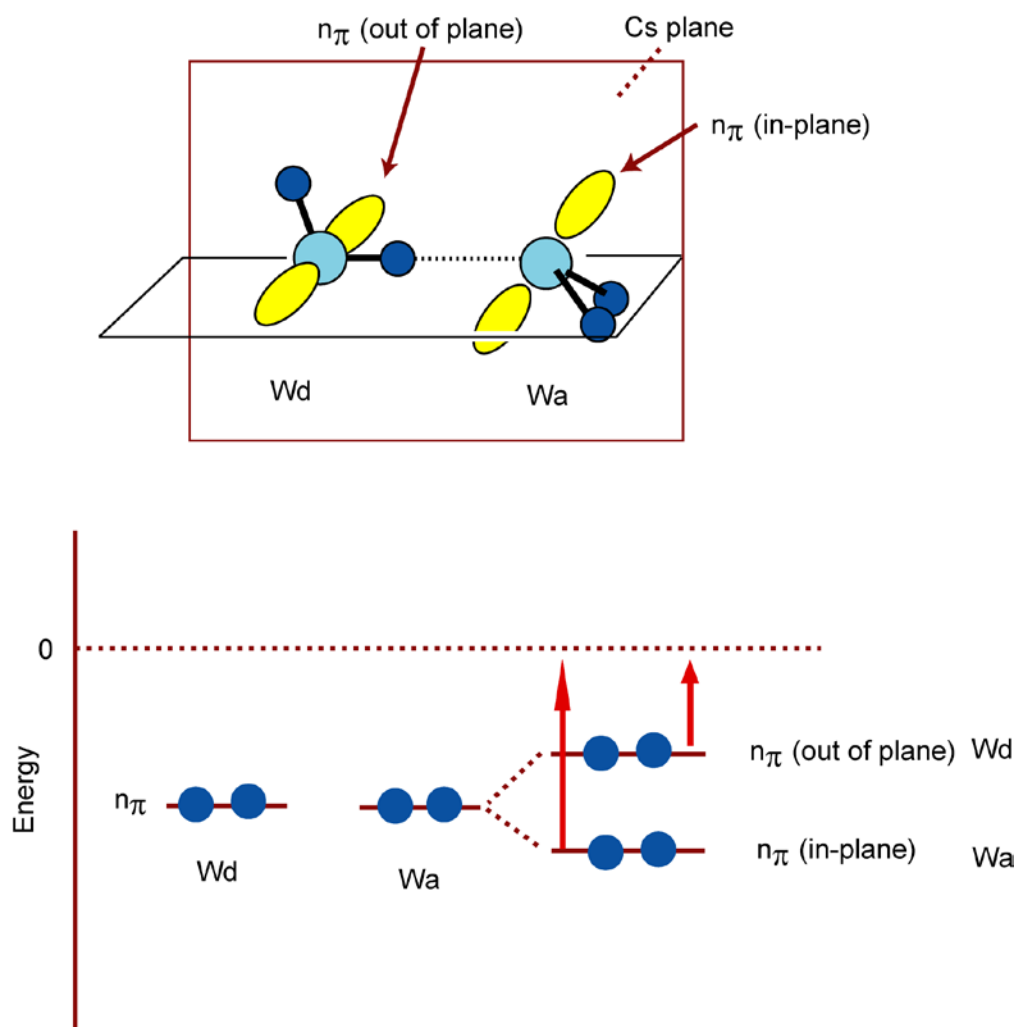


Figure S2. Schematic illustration of orbital interaction and orbital splitting in water dimer.

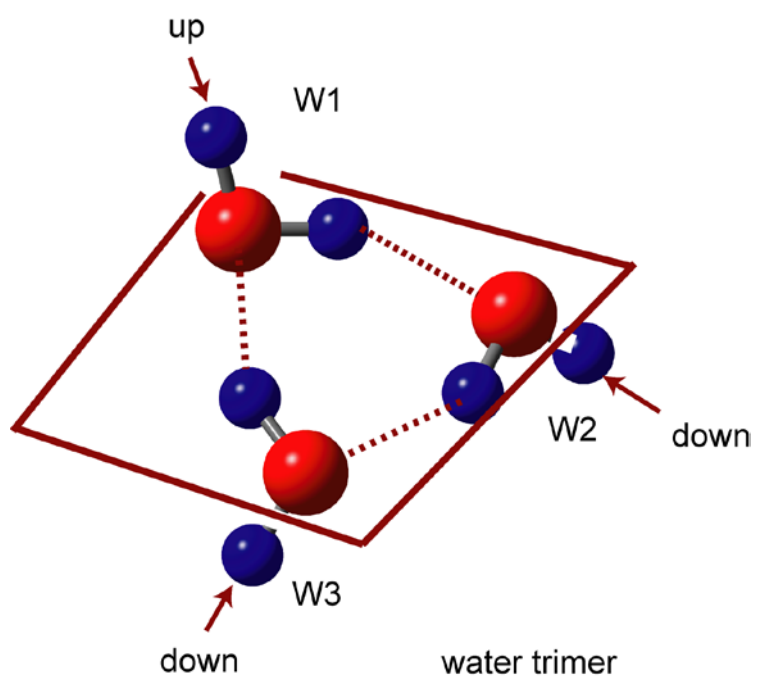


Figure S3. Schematic illustration of structure of water trimer.

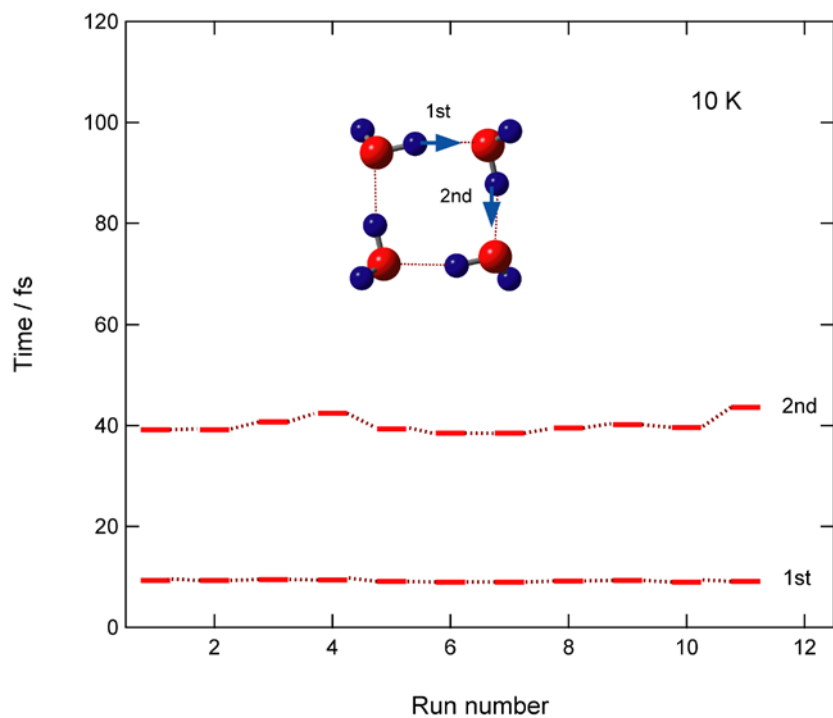


Figure S4. Temperature effects on rate of proton transfer in water tetramer cation.

Simulation temperature of $(\text{H}_2\text{O})_4$ was 10 K.