

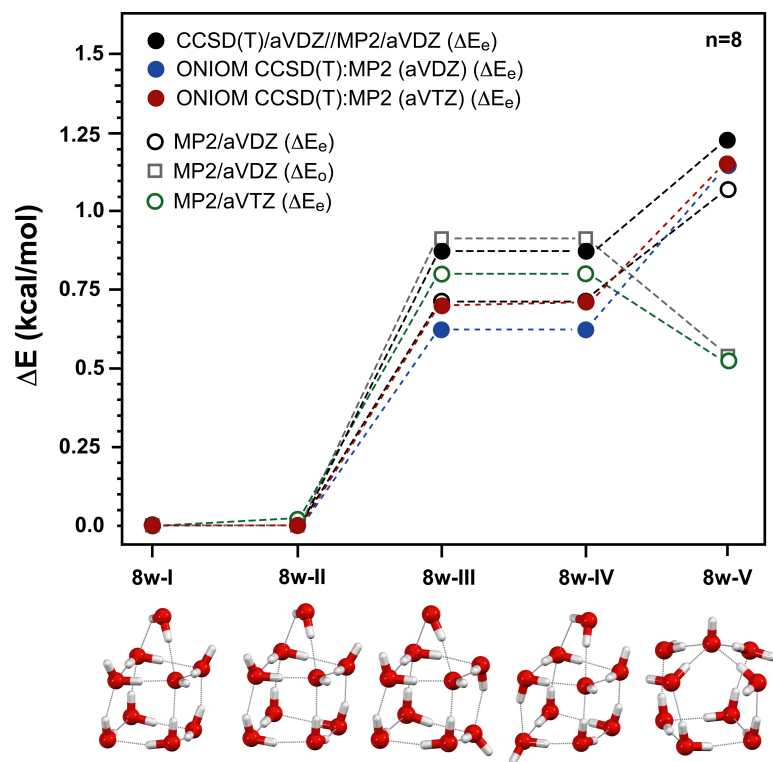
## **Supporting Information II**

relative energies,  $\text{OH}^-(\text{H}_2\text{O})_{8-26}$

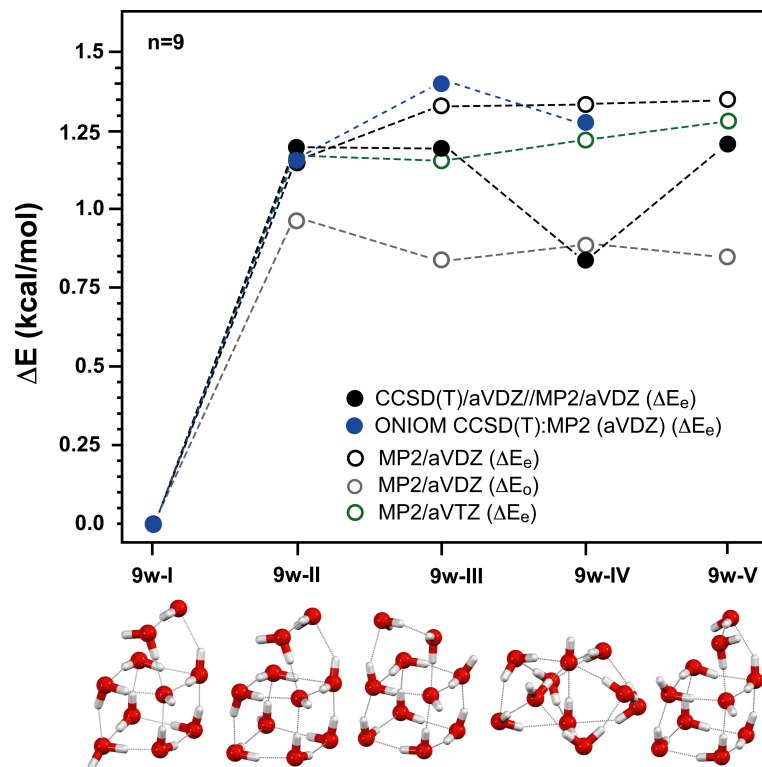
### **Structure and Solvation Dynamics of the Hydroxide Ion in Ice-like Water Clusters: a CCSD(T) and Car-Parrinello Molecular Dynamics Study**

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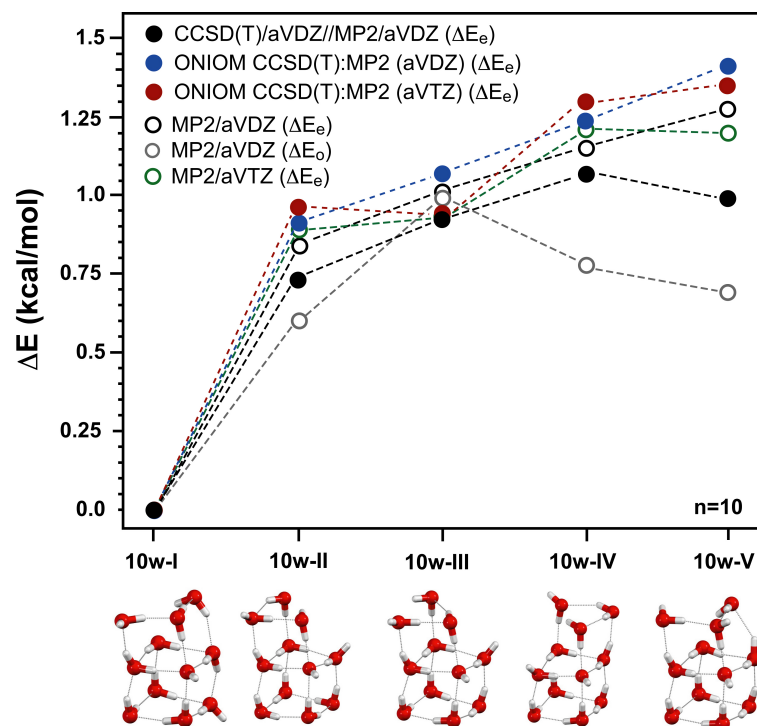
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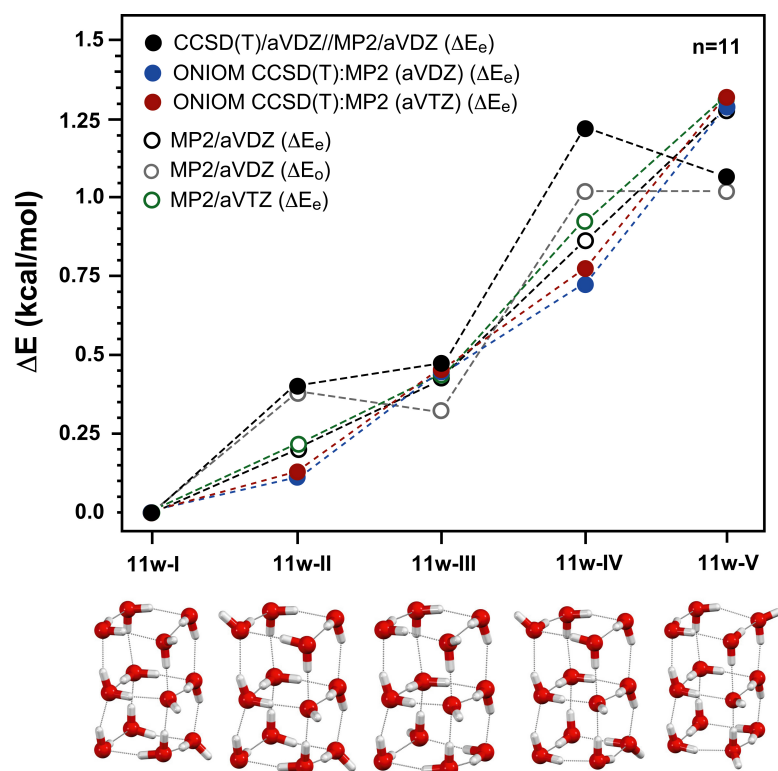
**Fig. S1)** MP2/aVDZ structures, CCSD(T)/aVDZ and CCSD(T)/aVDZ:MP2/aVDZ relative energies ( $\Delta E_e$ ) of five lowest energy  $\text{OH}^-(\text{H}_2\text{O})_8$  conformers.



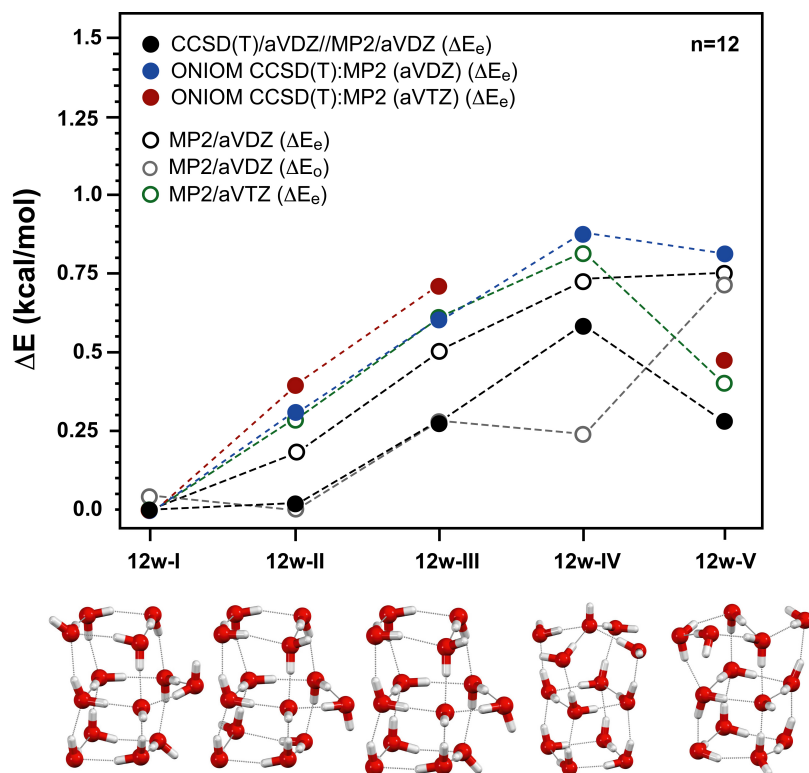
**Fig. S2)** MP2/aVDZ structures, CCSD(T)/aVDZ//MP2/aVDZ and CCSD(T)/aVDZ:MP2/aVDZ relative energies ( $\Delta E_e$ ) of five lowest energy OH(H<sub>2</sub>O)<sub>9</sub> conformers.



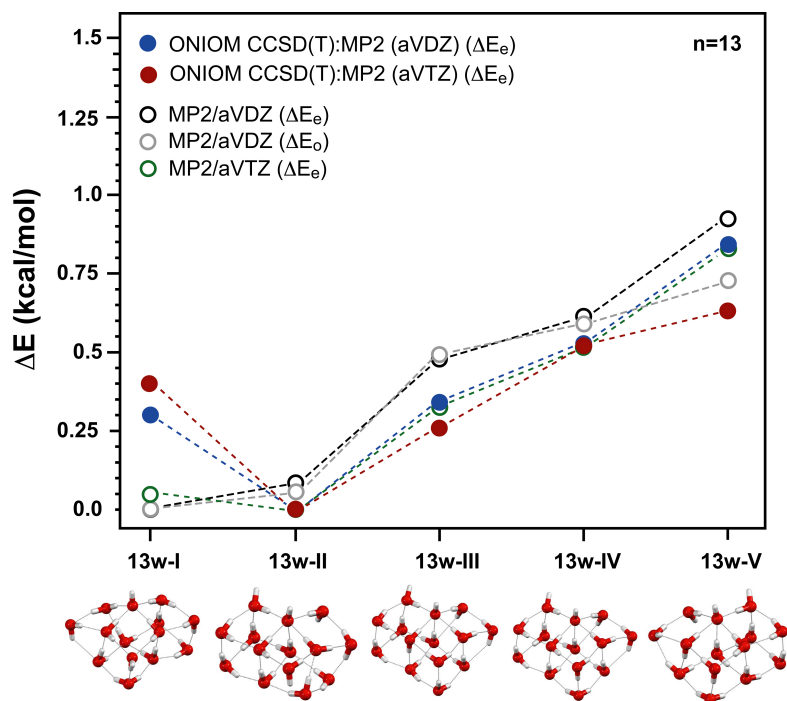
**Fig. S3)** MP2/aVDZ structures, MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), CCSD(T)/aVDZ//MP2/aVDZ and ONIOM CCSD(T)/aV(D,T)Z: MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of the five lowest energy OH<sup>+</sup>(H<sub>2</sub>O)<sub>10</sub> conformers.



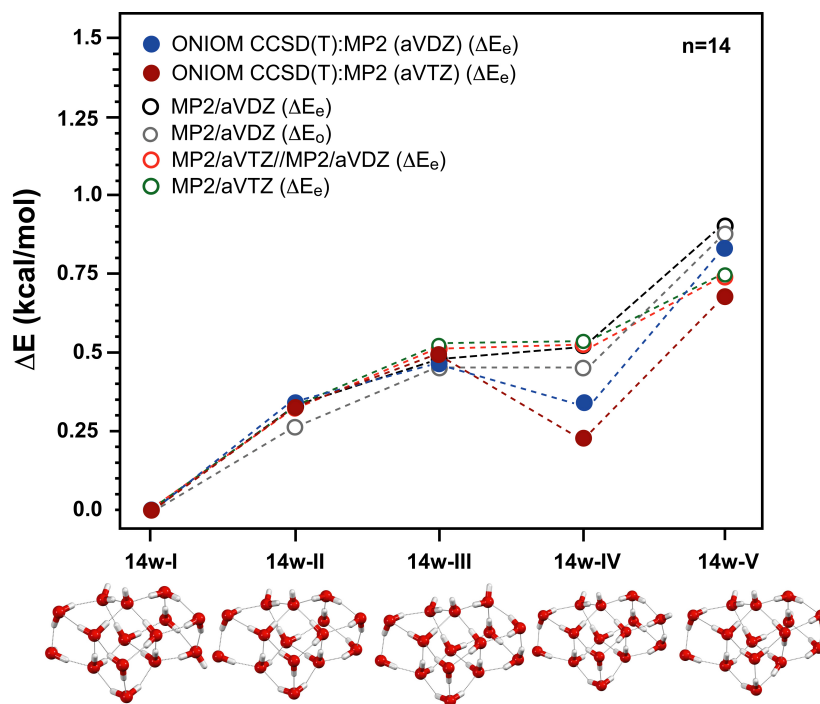
**Fig. S4)** MP2/aVDZ structures, MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), CCSD(T)/aVDZ//MP2/aVDZ and ONIOM CCSD(T)/aV(D,T)Z:MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of five lowest energy  $\text{OH}^-(\text{H}_2\text{O})_{11}$  conformers.



**Fig. S5)** MP2/aVDZ structures, MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), CCSD(T)/aVDZ//MP2/aVDZ and ONIOM CCSD(T)/aV(D,T)Z:MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of the five lowest energy  $\text{OH}(\text{H}_2\text{O})_{12}$  conformers.

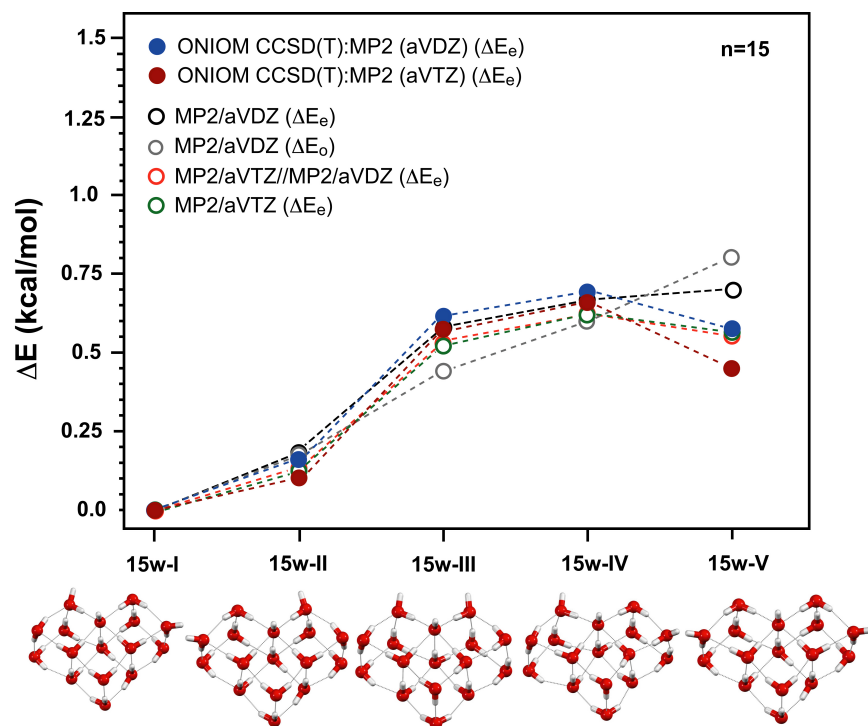


**Fig. S6)** MP2/aVDZ structures, MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), and ONIOM CCSD(T)/aV(D,T)Z:MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of the five lowest energy OH(H<sub>2</sub>O)<sub>13</sub> conformers.

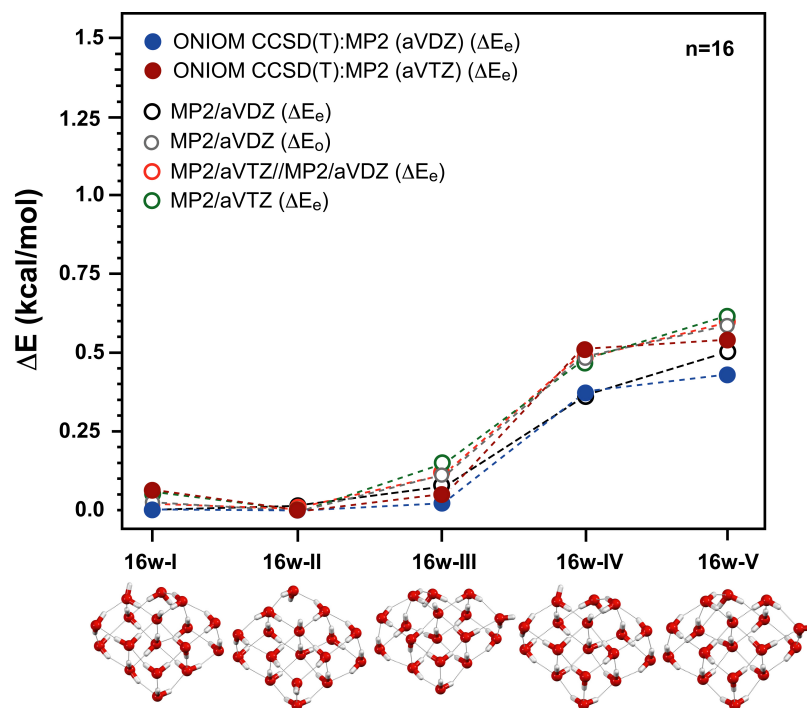


**Fig. S7)** MP2/aVDZ structures, MP2/aVTZ relative energies ( $\Delta E_e$ ), MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), and ONIOM CCSD(T)/aV(D,T)Z:MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of the five lowest energy OH(H<sub>2</sub>O)<sub>14</sub> conformers.

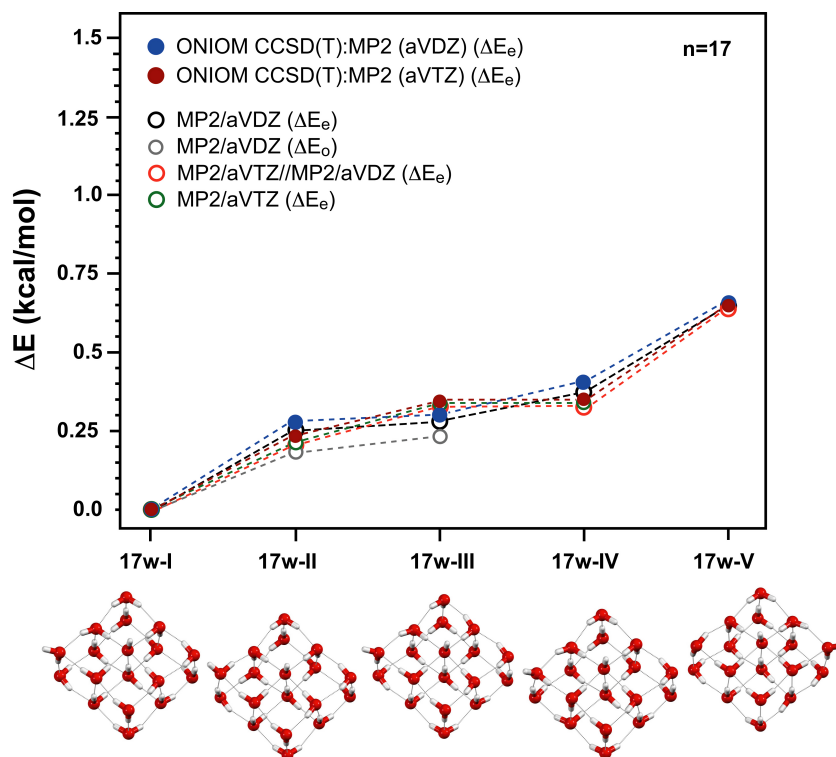




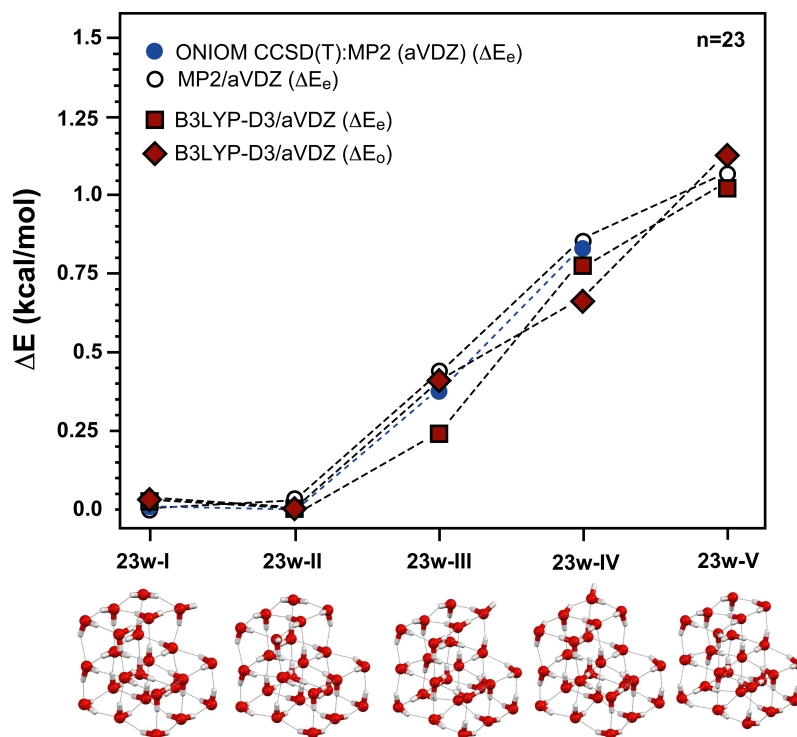
**Fig. S8)** MP2/aVDZ structures, MP2/aVTZ relative energies ( $\Delta E_e$ ), MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), and ONIOM CCSD(T)/aV(D,T)Z:MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of the five lowest energy OH(H<sub>2</sub>O)<sub>15</sub> conformers.



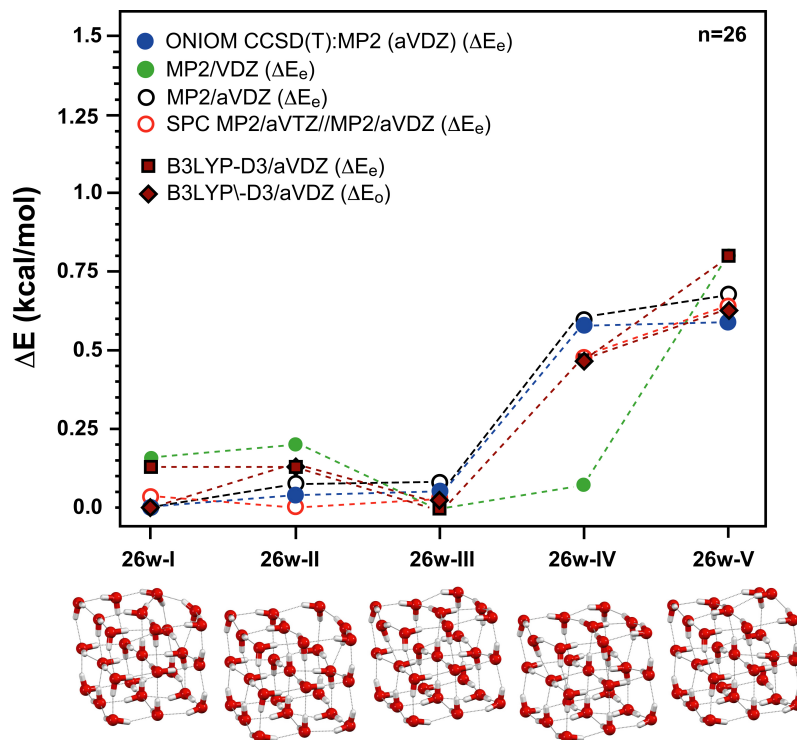
**Fig. S9)** MP2/aVDZ structures, MP2/aVTZ relative energies ( $\Delta E_e$ ), MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), and ONIOM CCSD(T)/aV(D,T)Z:MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of the five lowest energy OH(H<sub>2</sub>O)<sub>16</sub> conformers.



**Fig. S10)** MP2/aVDZ structures, MP2/aVTZ relative energies ( $\Delta E_e$ ), MP2/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), and ONIOM CCSD(T)/aV(D,T)Z:MP2/aV(D,T)Z relative energies ( $\Delta E_e$ ) of the five lowest energy OH(H<sub>2</sub>O)<sub>17</sub> conformers.



**Fig. S11)** MP2/aVDZ structures and relative energies ( $\Delta E_e$ ), B3LYP-D3/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), and ONIOM CCSD(T)/aVDZ:MP2/aVDZ relative energies ( $\Delta E_e$ ) of the five lowest energy OH(H<sub>2</sub>O)<sub>23</sub> conformers.



**Fig. S12)** MP2/aVDZ structures and relative energies ( $\Delta E_e$ ), MP2/aVTZ//MP2/aVDZ relative energies ( $\Delta E_e$ ), B3LYP-D3/aVDZ ZPE-corrected relative energies ( $\Delta E_o$ ), and ONIOM CCSD(T)/aVDZ:MP2/aVDZ relative energies ( $\Delta E_e$ ) of the five lowest energy  $\text{OH}^-(\text{H}_2\text{O})_{26}$  conformers.