## **Electronic Supplementary Information**

## Solvent Effect on Electron and Proton Transfer in the Excited State of Hydrogen Bonded Phenol-Imidazole Complex

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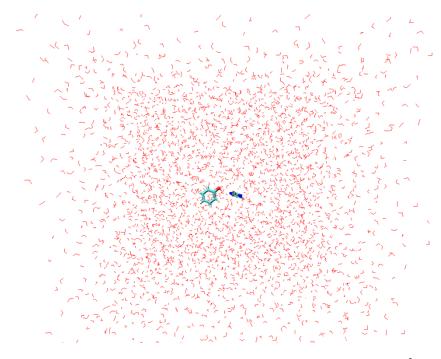
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**Fig S2.** Behaviors of  $R_{O-N}$  and  $\angle_{COH}$  both in vacuum and water.



**Fig S1.** Initial structure of PH-IM in water box with cubic length of 22 Å for QM/MM calculation

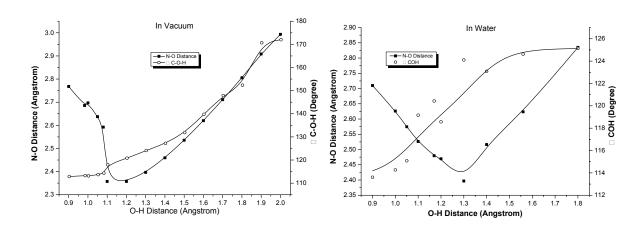


Fig S2. Behaviors of  $R_{O-N}$  and  $\angle_{COH}$  both in vacuum and water.