

# Supporting Information

## Theoretical investigations on hydrogen peroxide decomposition in aquo

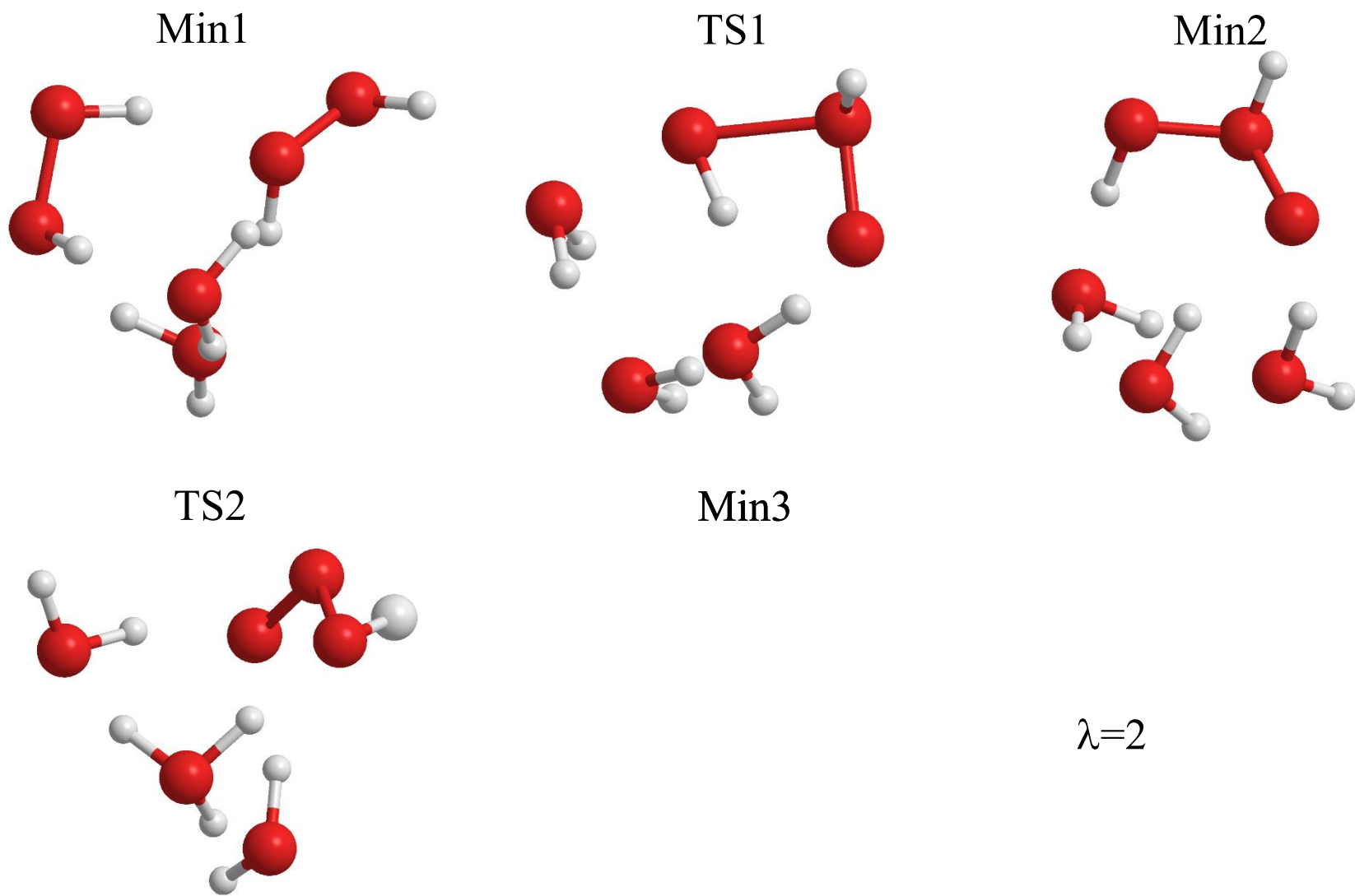
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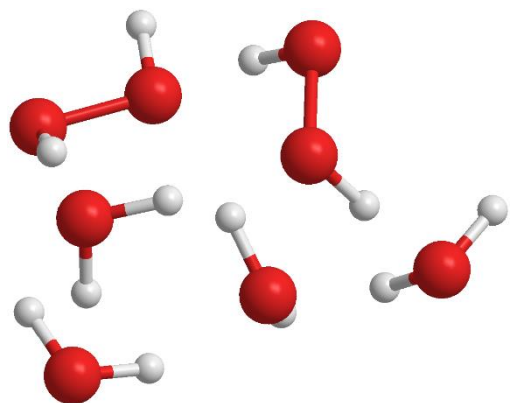
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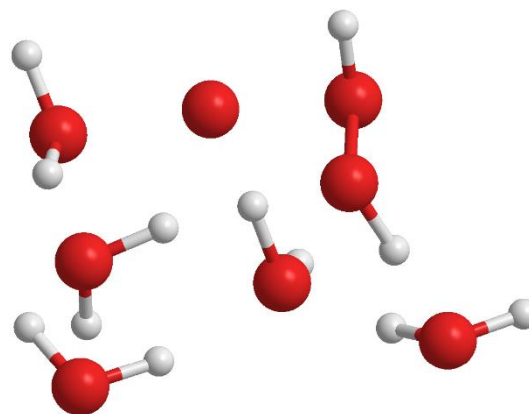
Fig. S1. Molecular structures of  $\text{H}_2\text{O}_2$  decomposition reaction at each step for the explicit hydration numbers of  $\lambda=2, 4, 6$  and  $8$ . LC-BLYP/ cc-pVDZ calculations.



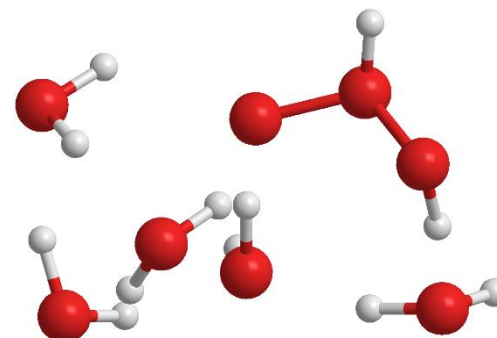
Min1



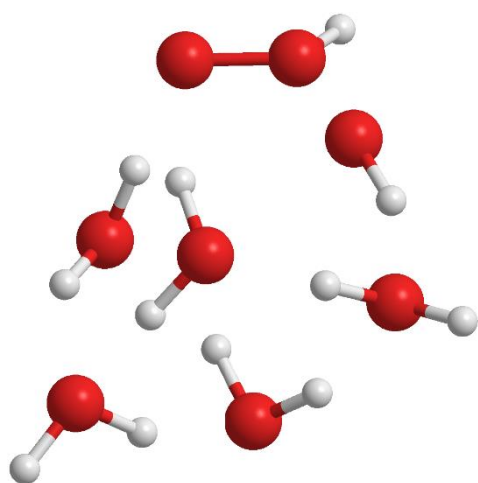
TS1



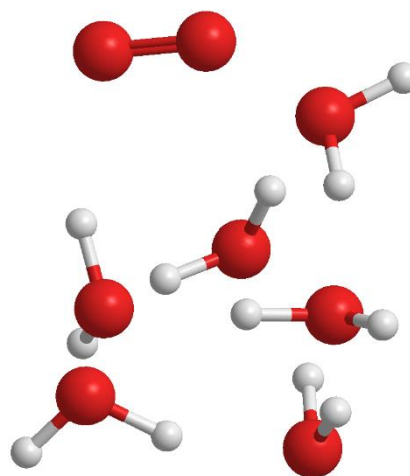
Min2



TS2

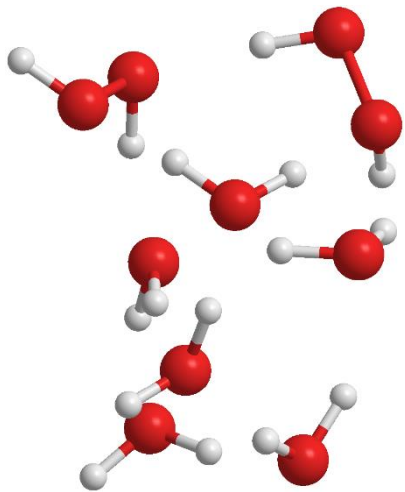


Min3

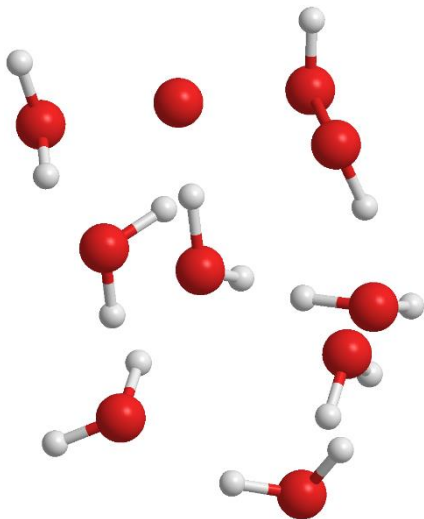


$\lambda=4$

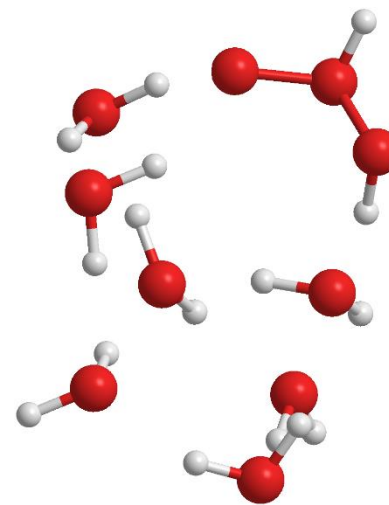
Min1



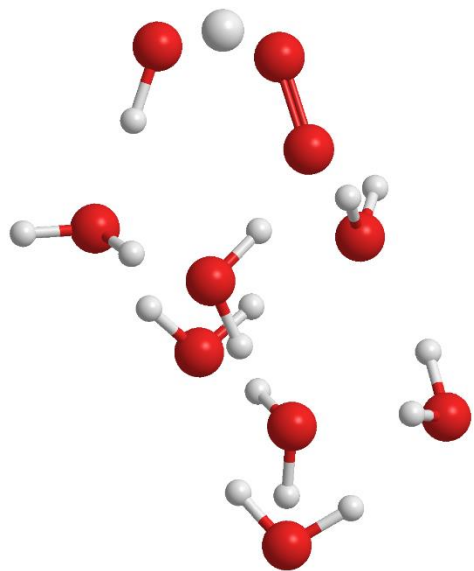
TS1



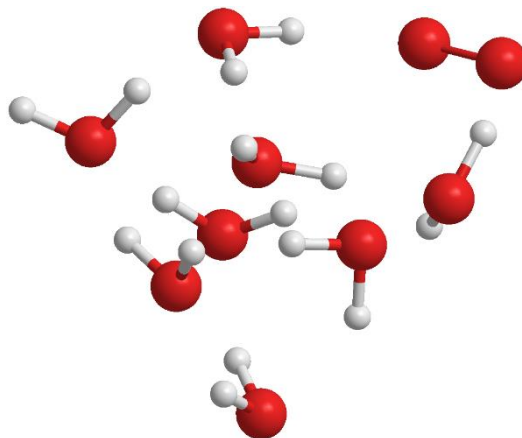
Min2



TS2

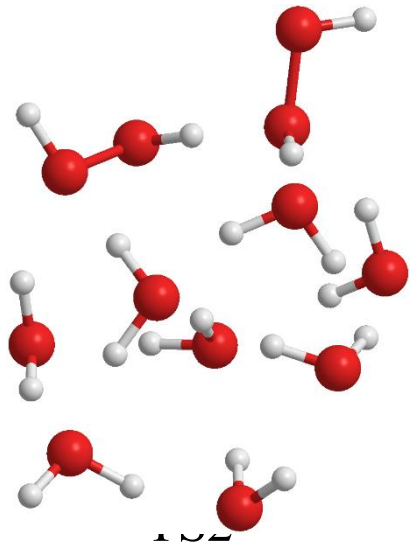


Min3

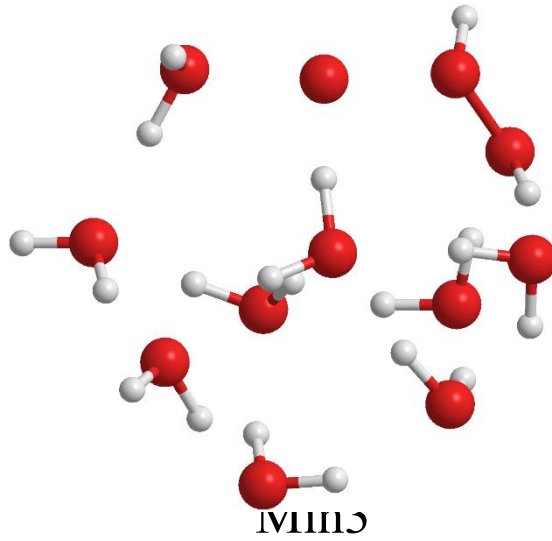


$\lambda=6$

Min1



TS1



Min2

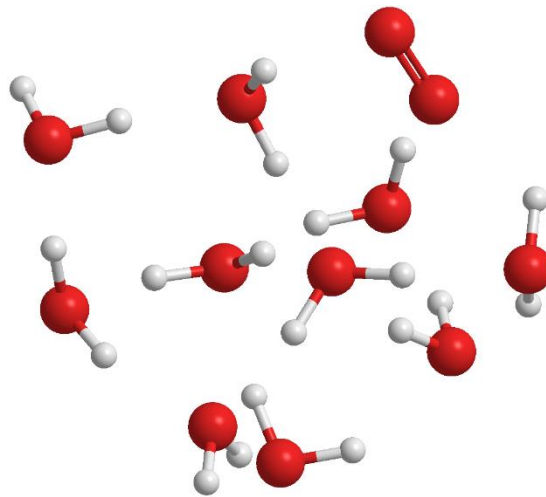
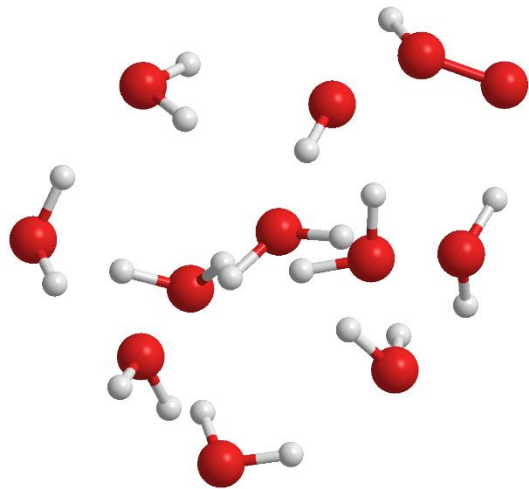
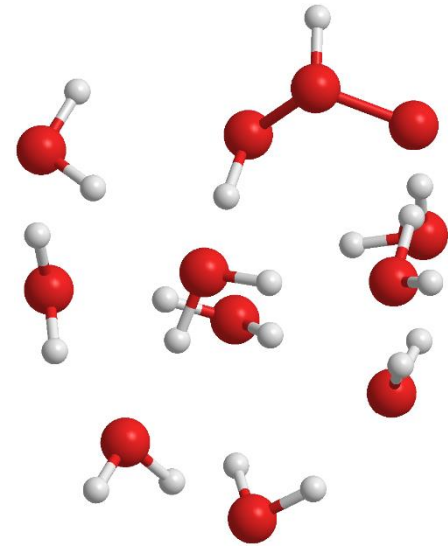


Fig. S2. Calculated vibrational spectra of OHOHO and HOOOH radicals, which are coordinated by two H<sub>2</sub>O molecules. LC-BLYP/ cc-pVDZ calculations.

