Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Unraveling the interaction between singlet state atomic oxygen O(^{1}D) and water: toward the formation of oxywater and hydrogen peroxide

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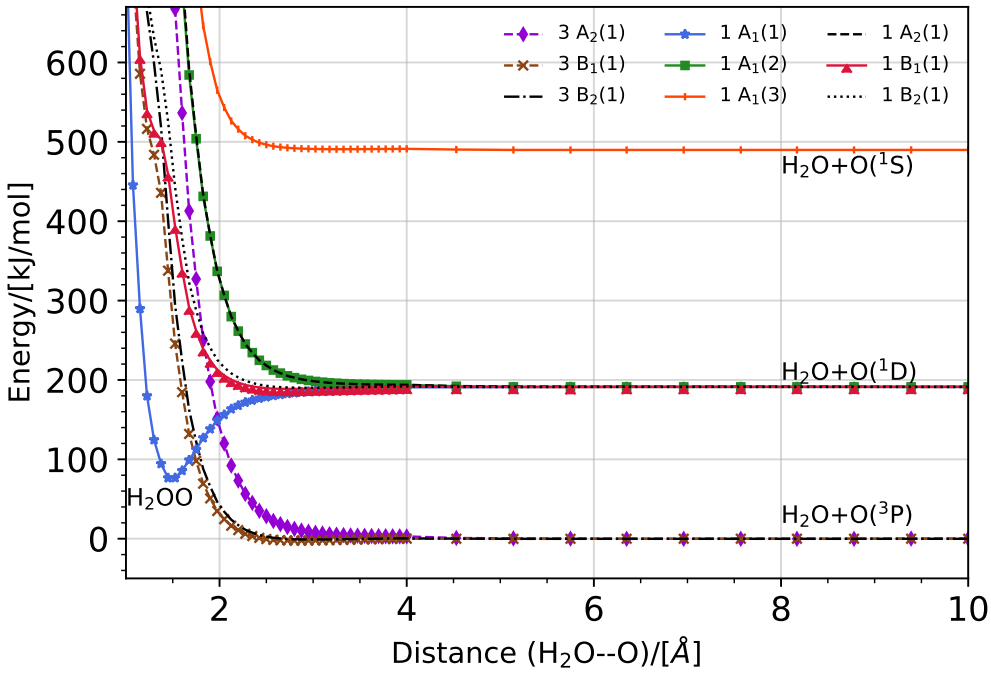

Figure S1: Potential energy curve for O.OH2 complex along the oxygen−oxygen coordinate, from 1 Å to 10 Å, at the (10,8)CASSCF-SC-NEVPT2/cc-pVTZ level of theory. The lowest lying states on the triplet energy surface, ^{3}P, on the singlet energy surface, ^{1}D, and on the second excited energy surface, ^{1}S, are shown. The energies are plotted with respect to the energy of a H_2O molecule and an O(^{3}P) atom at oxygen−oxygen distance of 10 Å. The geometry of H_2O at each distance point is held fixed.

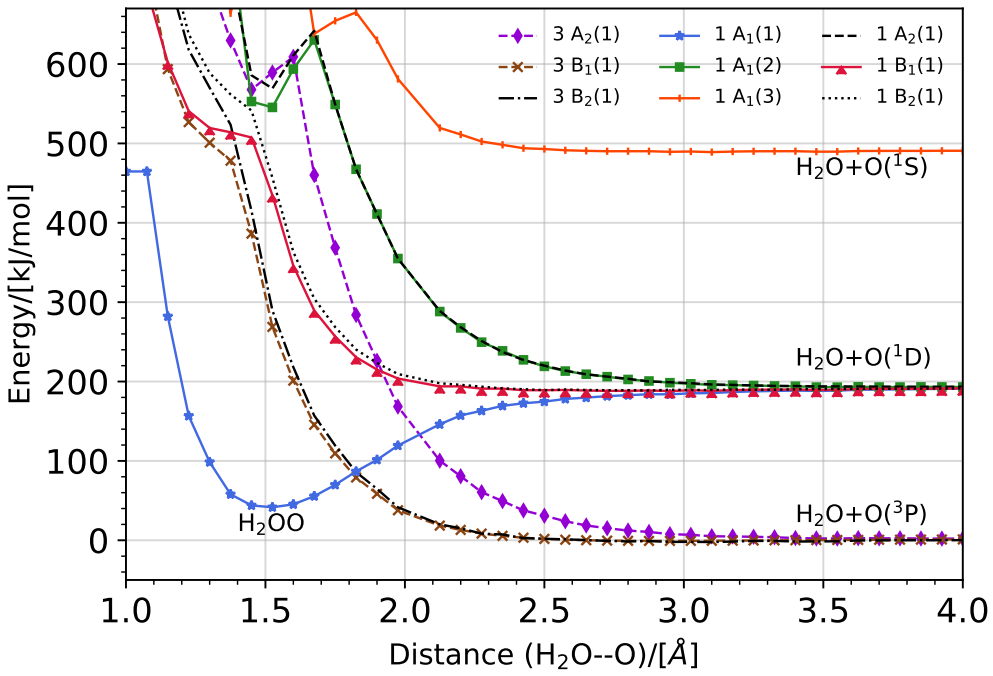

Figure S2: Potential energy curve for O.OH2 complex along the oxygen−oxygen coordinate at the (10,8)CASSCF-SC-NEVPT2/cc-pVTZ level of theory. The lowest lying states on the triplet energy surface, ^{3}P, on the singlet energy surface, ^{1}D, and on the second excited energy surface, ^{1}S, are shown. The energies are plotted with respect to the energy of a H_2O molecule and an O(^{3}P) atom at oxygen−oxygen distance of 10 Å (see Figure S1). The geometry of H_2O at each distance point is allowed to be optimized.

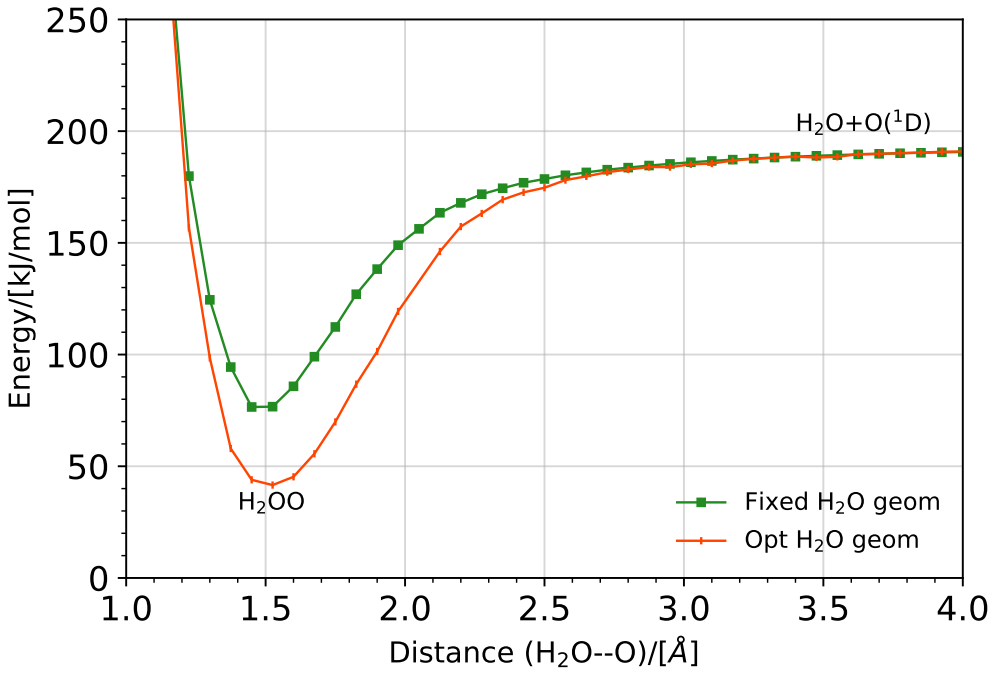

Figure S3: Potential energy curve for O.OH2 complex along the oxygen−oxygen coordinate at the (10,8)CASSCF-SC-NEVPT2/cc-pVTZ level of theory. The lowest lying state on the singlet energy surface, $1A_1(1)$, is shown for the calculations in which the geometry of H_2O at each distance point is optimized versus the calculations that the geometry of H_2O is fixed. The energies are plotted with respect to the energy of a H_2O molecule and an $O(^3P)$ atom at oxygen−oxygen distance of 10 Å (see Figure S1).