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

Table S5 Averages of properties (<A>) and the corresponding standard deviations (σ_A) obtained from NVT-BOMD simulations on structure **E1-[1]** in the S_1 state at 298 K. **P1** and **P2** are for the large- and small-amplitude O-O vibrations, respectively.

Property A	**P1**		**P2**	
	<A>	**σ_A**	**<A>**	**σ_A**
T	298	135	302	151
E^{Tot}	-207.9721	0.0043	-207.9712	0.0052
E^{Pot}	-207.9806	0.0030	-207.9798	0.0042
E^{Kin}	0.0085	0.0038	0.0086	0.0043
E^{Ex}	0.0188	0.0113	0.0280	0.0185
$E^{Nosé}$	0.0007	0.0010	0.0011	0.0014
$R_{O\text{-}O}$	2.43	0.043	2.45	0.018
$R_{O\text{-}H}$	1.18	0.058	1.23	0.089
$R_{O..H}$	1.27	0.063	1.23	0.091

T = temperature; E^{Tot} = total energy; E^{Pot} = potential energy; E^{Kin} = kinetic energy; E^{Ex} = excitation energy; $E^{Nosé}$ = kinetic energy of the Nosé-Hoover thermostat bath; $R_{O\text{-}O}$ and $R_{O\text{-}H}$ = H-bond distances. Energies and temperatures are in au and K, respectively, and H-bond distances are in Å.