Table S6 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 500 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	500	170	497	186
E^{Tot}	-207.9592	0.0075	-207.9596	0.0076
E^{Pot}	-207.9734	0.0053	-207.9738	0.0058
E^{Kin}	0.0143	0.0049	0.0142	0.0053
E^{Ex}	0.0186	0.0274	0.0154	0.0256
$E^{Nosé}$	0.0010	0.0014	0.0010	0.0013
$R_{O\text{-}O}$	2.47	0.089	2.44	0.046
$R_{O\text{-}H}$	1.21	0.109	1.21	0.087
$R_{O..H}$	1.27	0.118	1.25	0.086

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.