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

Table S9 Kinetics of proton dissociation in the smallest intermediate complex (structure **E1-[1]**) in the S_1 state obtained from BOMD simulations over the temperature range of 250-500 K. **P1** and **P2** are the dynamics for the large- and small-amplitude O-O vibrations, respectively. Lifetimes (τ) and first order-rate constants (k) are in fs and ps^{-1}, respectively.

T	P1			P2		
	$\tau_{1/2}$	k	$\tau = 1/k$	$\tau_{1/2}$	k	$\tau=1/k$
250	51	13.64	73	35	19.72	51
320	86	8.08	124	48	14.43	69
350	106	6.56	152	35	19.85	50
400	79	8.80	114	50	13.86	72
500	68	10.26	97	108	6.40	156