

Table S8 Kinetics of proton dissociation in the smallest intermediate complex (structure **E1-[1]**) in the S_1 state obtained from NVT-BOMD simulations over the temperature range of 250-400 K. Lifetimes (τ) and first order-rate constants (k) are in fs and ps^{-1} , respectively.

T	$\tau_{1/2}$	k	$\tau = 1/k$	ln k
250	62	11.2	89	2.42
298	54	12.8	78	2.55
320	54	12.9	78	2.55
350	52	13.4	74	2.60
400	50	13.8	73	2.62