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Table S8Kinetics of proton dissociation in the smallest intermediate complex (structure
E1-[1]) in the S1 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.

Т	$ au_{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