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

Table S7 Average lowest singlet-excitation ($<E^{Ex}>$) and kinetic ($<E^{Kin}>$) energies and the corresponding standard deviations ($\sigma_E{}^{Ex}$ and $\sigma_E{}^{Kin}$, respectively) of structure **E1-[1]** obtained from NVT-BOMD simulations over the temperature range of 250-500 K.

T	$<E^{Ex}>$	$\sigma_E{}^{Ex}$	$<E^{Kin}>$	$\sigma_E{}^{Kin}$	$<E^{Ex}>/<E^{Kin}>$
250	0.0185	0.0114	0.0071	0.0030	2.6145
298	0.0222	0.0147	0.0084	0.0044	2.6361
320	0.0213	0.0140	0.0091	0.0056	2.3440
350	0.0241	0.0146	0.0099	0.0048	2.4350
400	0.0254	0.0162	0.0113	0.0061	2.2393
500	0.0271	0.0172	0.0142	0.0054	1.9044

Energies and temperatures are in atomic unit (au) and K, respectively.