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

Supporting Information

Unraveling Structural Dynamics in Isoenergetic Excited S_1 and Multi-excitonic ^{1}(TT) states of 9,10-bis(phenylethynyl)anthracene (BPEA) in Solution using Ultrafast Raman Loss Spectroscopy

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Transient absorption features measured at various concentrations are given in Table S1.

TA	300 μM			150 μM			75 μM		
	460 nm	575 nm	650 nm	460 nm	575 nm	650 nm	460 nm	575 nm	650 nm
τ_1 (ps)	0.7 (rise)	0.96 (rise)	11	0.51 (rise)	1.6 (rise)	11	0.6 (rise)	2.2 (rise)	12.5
τ_2 (ps)	141	47	1027	140	45	1053	145	45	1227
τ_3 (ps)	1956	2310	-	2050	3343	-	1960	2540	-

Table S1: Kinetics observed at various wavelengths (460, 575 and 650 nm) for concentrations of 75, 150 and 300 μM.

The kinetics of the 575 nm is sensitive to concentration *i.e.,* it exhibits ultrafast rise component changes from 0.96 ps to 2.20 ps as concentration changes from 300 to 75 μM.

DFT and TD-DFT methods are employed to understand the electronic structure and molecular vibrational frequencies of BPEA using Gaussian 09 package. Molecular structure with numbering of the atoms is given in Figure S1. For ground state calculation, we adapted DFT with restricted B3LYP functional and 6-311+G(d) basis set. Similarly, for excited state, TD-DFT with restricted B3LYP functional and 6-311+G(d) basis set has been adapted.

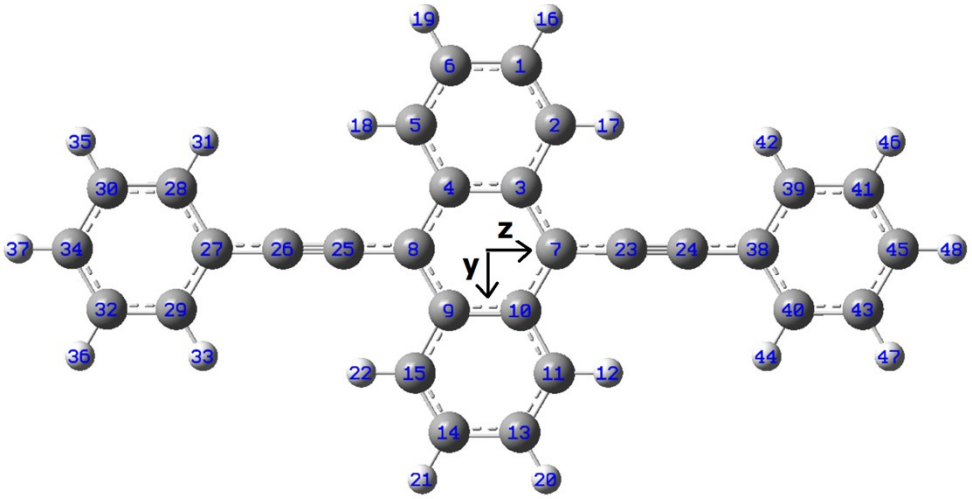

Figure S1: The molecular structure of BPEA with numbering on each atom.