Excited-state Intramolecular Charge Transfer Dynamics in 4-methoxy-4'-nitrostilbene: Excitation wavelength and Solvent Dependence

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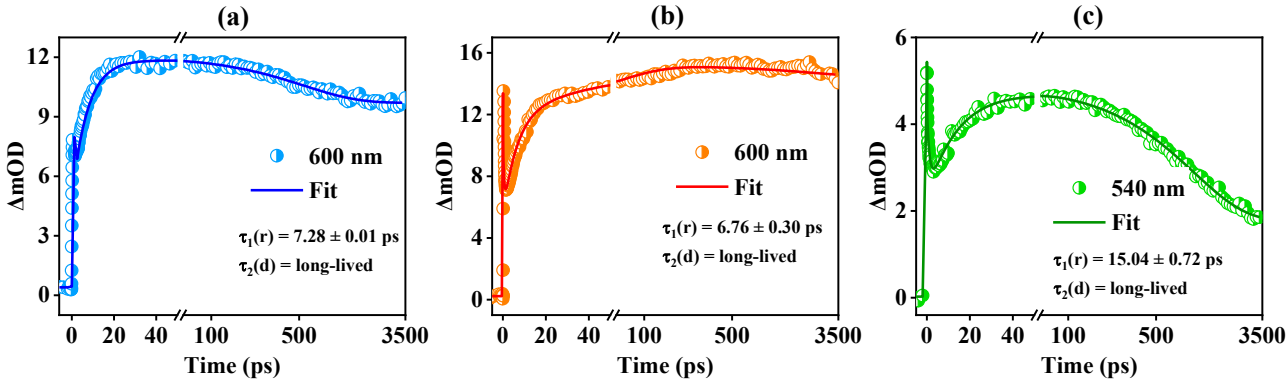


Figure S1: Single wavelength kinetics at few selective wavelengths along with the best-fit functions in TOL with excitation at (a) 310 nm, (b) 370 nm, and (c) 510nm. The lifetimes are given in the insets.

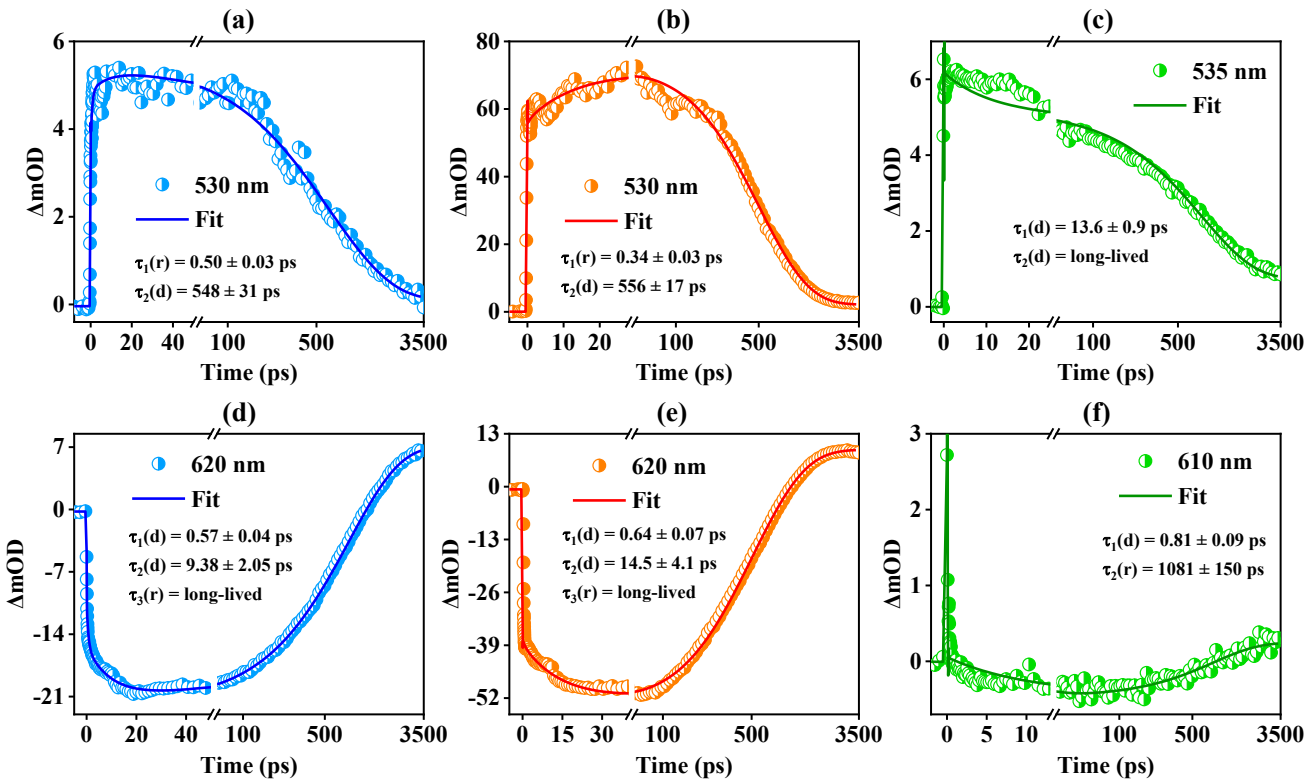


Figure S2: Single wavelength kinetics at few selective wavelengths along with the best-fit functions in MeCN with excitation at (a,d) 310 nm, (b,e) 370 nm, and (c,f) 510nm. The lifetimes are given in the insets.

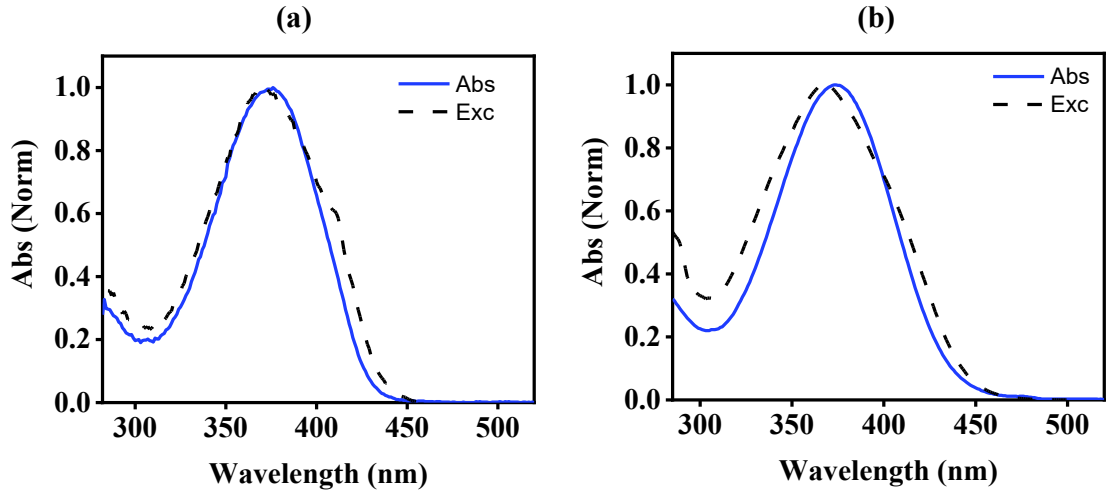


Figure S3: The steady-state absorption (solid lines) and excitation (dotted lines) spectra of MNS in (a) TOL and (b) MeCN. The emission wavelength was chosen at 470 nm for TOL and 630 nm for MeCN.

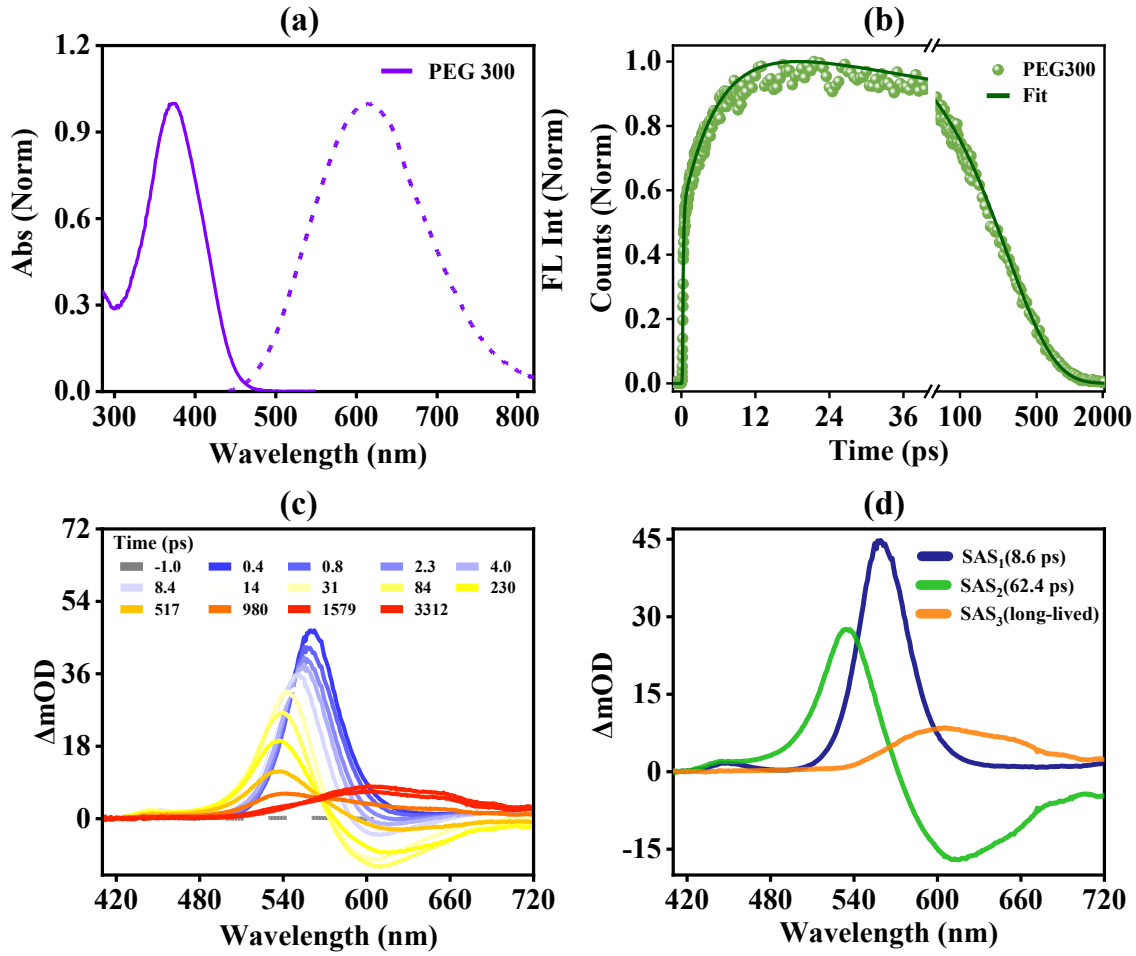


Figure S4: (a) Steady-state absorption and emission spectra, (b) fs-fluorescence up-conversion measured at 620 nm, (c) fs-TA spectra at different time delays, and (d) species-associated spectra of MNS in PEG 300.

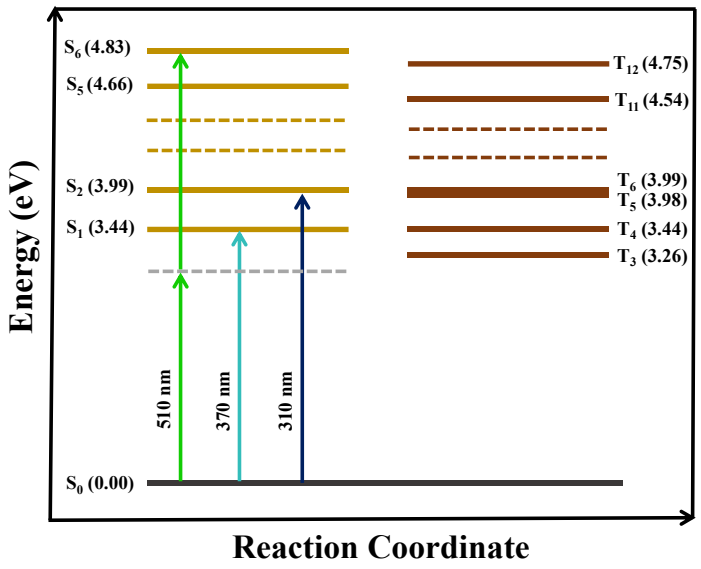
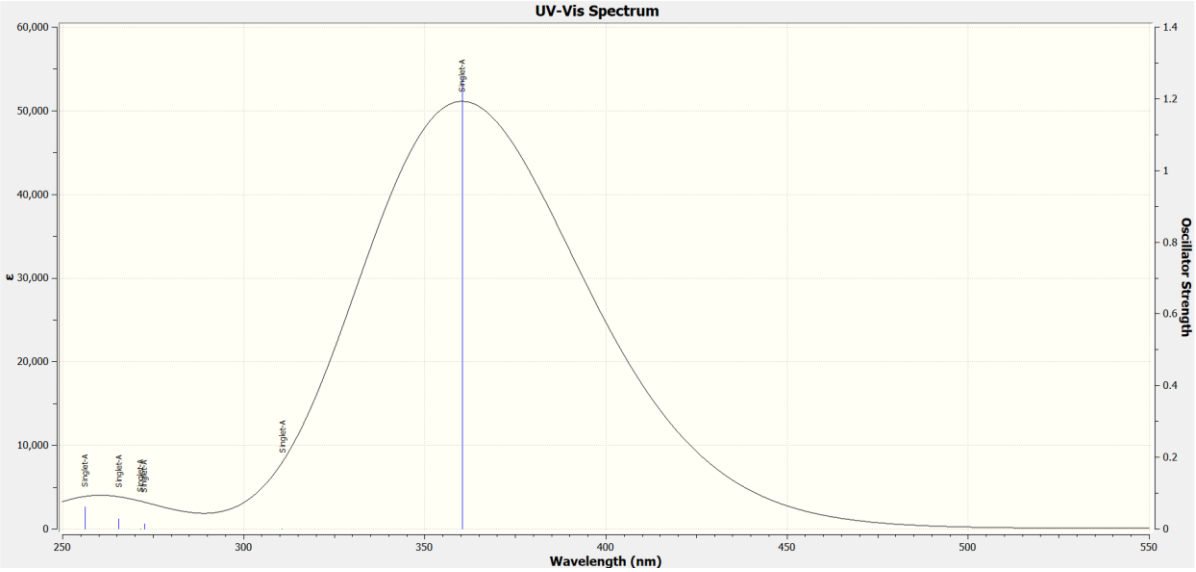


Figure S5: Simplified energy level diagram of MNS showing computed vertical excitation energies (in eV) of key singlet and triplet states in TOL.

(a)



(b)

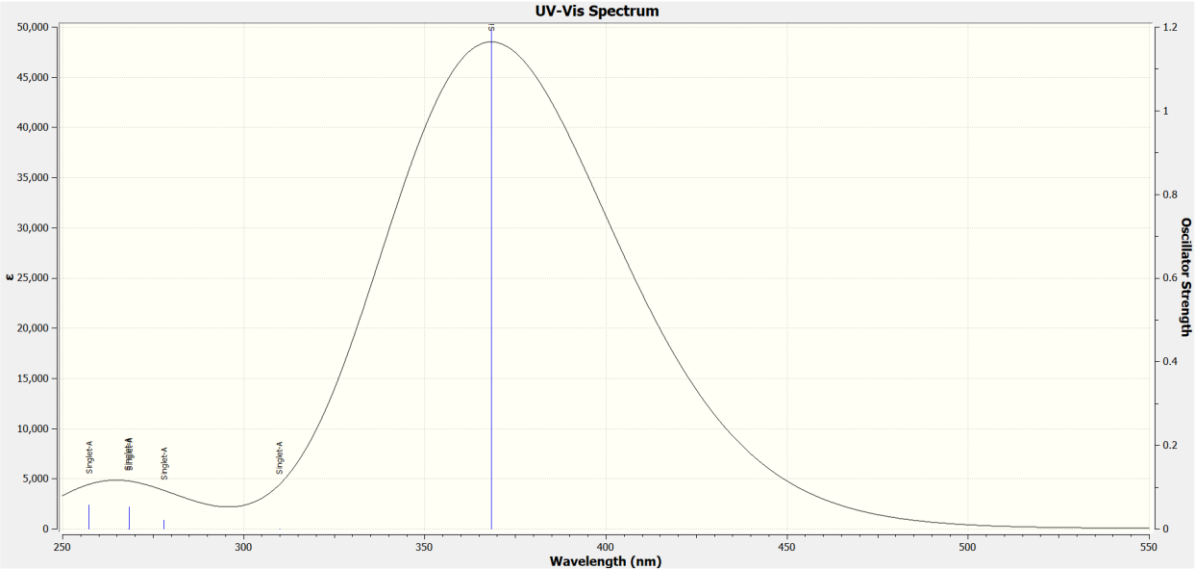


Figure S6: TD-DFT calculated UV–Vis absorption spectrum of MNS in (a) TOL and (b) MeCN. The blue sticks denote the calculated singlet excited states (S_1–S_6), with stick heights proportional to the oscillator strengths (f).

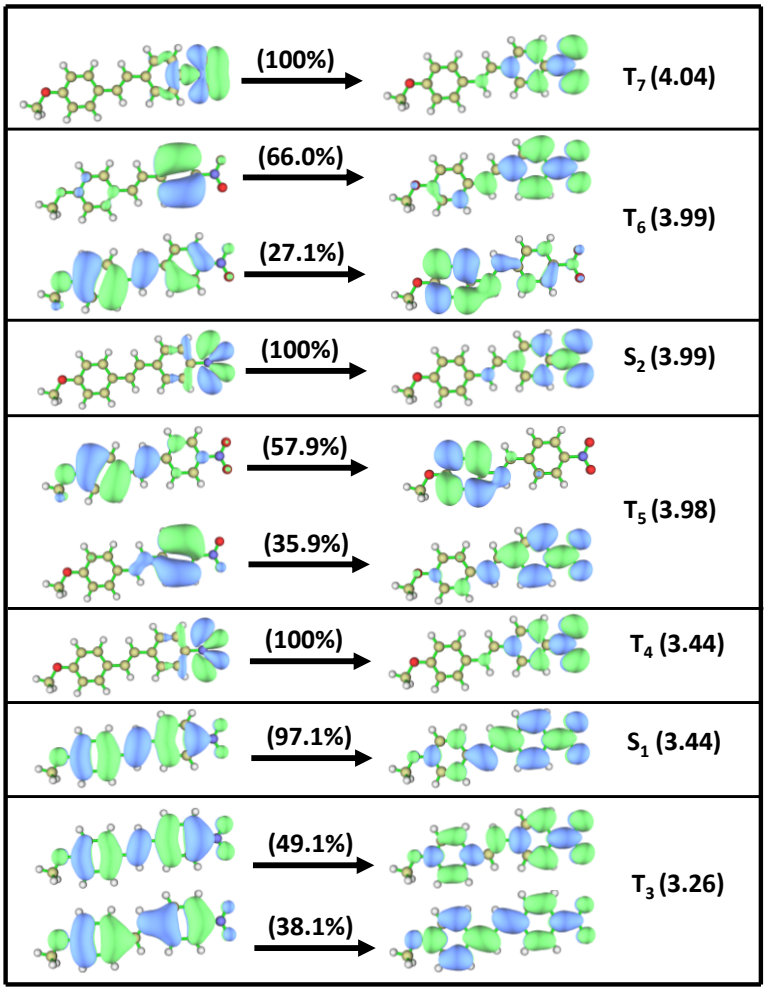


Figure S7: NTO analysis of MNS in TOL.

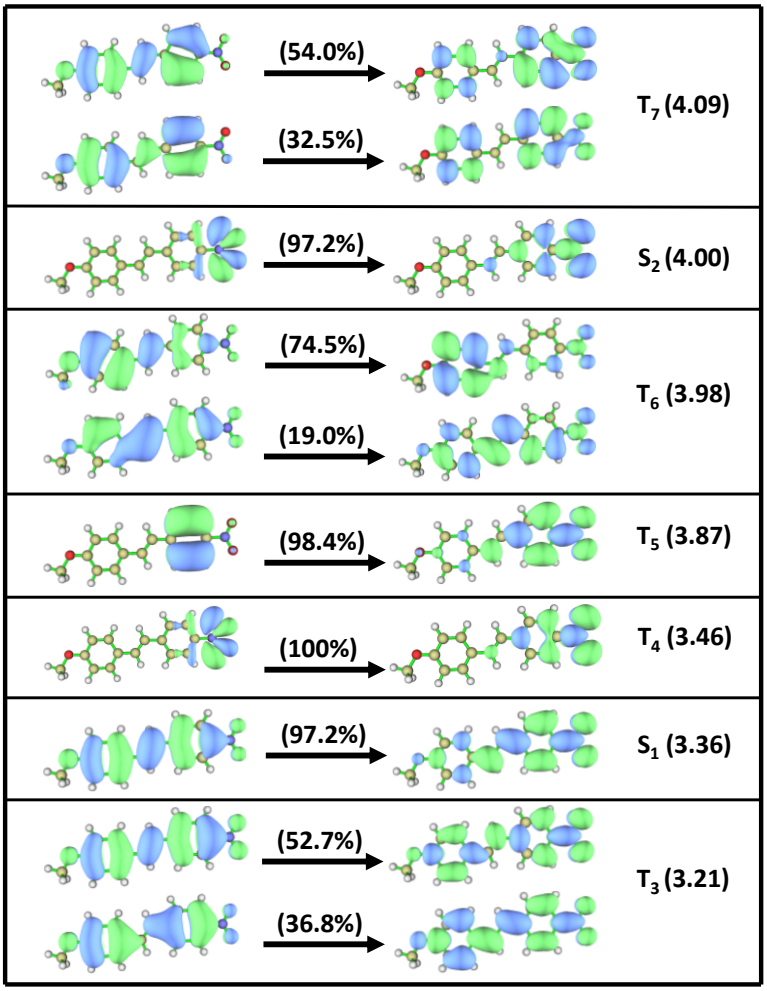


Figure S8: NTO analysis of MNS in MeCN.

Table S1. TD-DFT calculated vertical excitation energies (E), corresponding wavelengths (λ), and oscillator strengths (f) for the low-lying singlet excited states of MNS in TOL.

State	E (eV)	λ (nm)	f
S_1	3.44	360.35	1.26
S_2	3.99	310.47	0.00
S_3	4.54	272.58	0.01
S_4	4.56	271.52	0.00
S_5	4.66	265.54	0.02
S_6	4.83	256.18	0.06

Table S2. TD-DFT calculated vertical excitation energies (E), corresponding wavelengths (λ), and oscillator strengths (f) for the low-lying singlet excited states of MNS in MeCN.

State	E (eV)	λ (nm)	f
S_1	3.36	368.42	1.19
S_2	4.00	309.88	0.00
S_3	4.45	278.04	0.02
S_4	4.61	268.47	0.05
S_5	4.62	268.03	0.00
S_6	4.81	257.32	0.05

Table S3. SOC and singlet–triplet energy gaps (ΔE) between S_1/S_2 and triplet states (T_1–T_7) for MNS in TOL.

Triplet State	**T_1**	**T_2**	**T_3**	**T_4**	**T_5**
SOC (cm^{-1})	0.014	0.037	0.014	7.282	0.020
ΔE (S_1–T_n) (eV)	1.347	0.612	0.173	-0.002	-0.547

Triplet State	**T_4**	**T_5**	**T_6**	**T_7**
SOC (cm^{-1})	0.020	6.280	3.429	36.660
ΔE (S_2–T_n) (eV)	0.546	0.002	-0.003	-0.059

Table S4. Polarizability (α) and first hyperpolarizability (β) were computed in TOL and MeCN.

Property	**TOL (esu)**	**MeCN (esu)**
α	4.02×10^{-24}	4.75×10^{-24}
β	1.29×10^{-28}	2.17×10^{-28}