Supporting Information for

Quintet-Triplet Mixing Determines the Fate of the Multiexciton State Produced by Singlet Fission in a Terrylenediimide Dimer at Room Temperature

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Additional Experimental Methods

Sample Preparation of TDI_2 in 5CB

Transient Optical Spectroscopy: A 200 μm demountable cuvette face and a glass slide were placed in piranha solution. After immersion in piranha solution overnight, the glassware was dried in an oven. The demountable cuvette was then immersed in a dilute solution of trichlorooctadecylsilane in toluene. After two hours of immersion, the demountable cuvette was rinsed with dry toluene. In a glovebox, **TDI_2** was dissolved in 5CB and the resulting solution was placed between the silylated cuvette face and the glass slide.

Electron Paramagnetic Resonance Spectroscopy: Sample solutions for X-band were loaded into quartz tubes (2.40 mm o.d. × 2.00 mm i.d.), subjected to three freeze–pump–thaw degassing cycles on a vacuum line (10^{-4} Torr), and sealed under vacuum using an oxy-hydrogen torch.

Magnetic Field Effect Setup

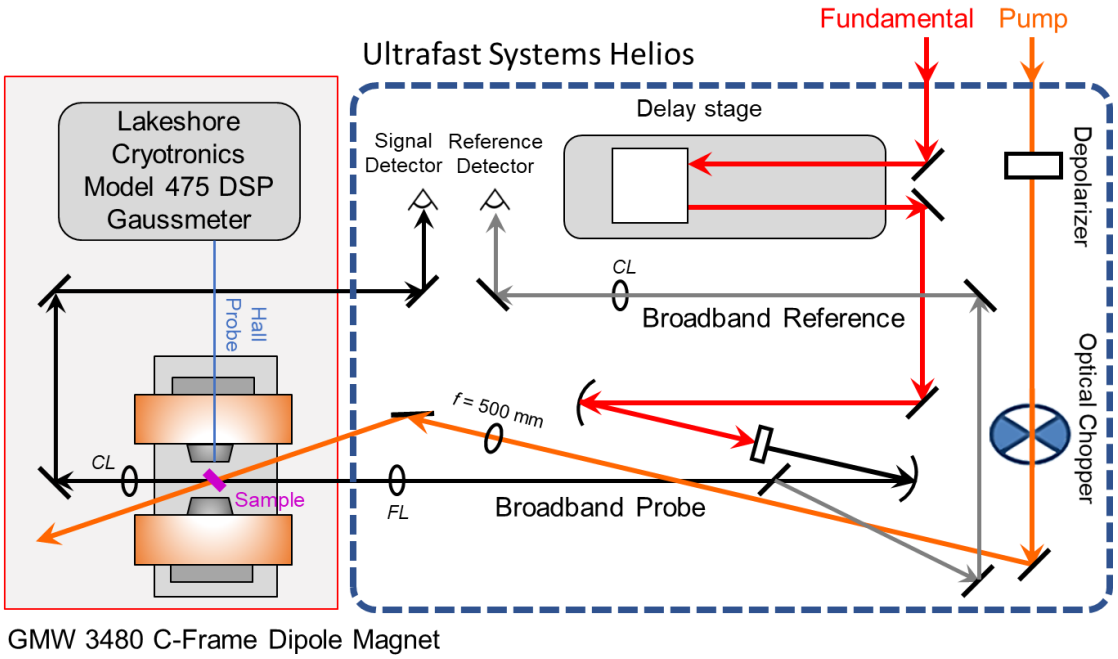


Fig. S1. Schematic of the transient absorption apparatus equipped with the dipole electromagnet.

For the liquid crystal sample, the cell was oriented at 45° relative to the field (and to the direction of the probe) to maximize alignment of the liquid crystal in the short direction of the silylated cell while still allowing transmission of the probe. The depolarized pump was crossed with the probe at an angle of approximately 20° to minimize pump scatter from the liquid crystal.

Q-Band Setup

The mw frequency was controlled with a Keysight M8190A and upconverted to Q-band frequencies using the Millitech bridge; the signal, detected in quadrature, was digitized using an Agilent U1082A Acqiris card; a GMW model 3474-140 magnet was used and it was controlled with a Lakeshore 475 DSP Gaussmeter; all of the timing was synchronized using a Stanford Research Systems Model DG645 Digital Delay Generator; and all of the hardware was controlled using SpecMan (1).

Data Processing Description

Transient Optical Spectroscopy: The fsTA and nsTA data were all scatter-subtracted and chirp-corrected, and the visible and NIR data sets were spectrally merged using SurfaceXplorer 4 (Ultrafast Systems, LLC). Kinetic analysis was performed using home written programs in MATLAB and was based on a global fit to selected single-wavelength kinetics. Sequential first-order kinetic models were used to fit the transient data and each model used the minimum number of components necessary.

Electron Paramagnetic Resonance Spectroscopy: The EPR spectra were processed in MATLAB. The time evolution and off-resonance background were fit in the same fashion as the nsTA and spectral simulations were performed using EasySpin (2).

Magnetic Field Effect: To determine the triplet yield as a function of magnetic field, each spectrum was averaged from 620 to 640 nm and from 2 to 20 μs. The resulting averaged signals

were then corrected for changes in the zero-field amplitude during runtime, and then normalized to the value at 0 mT to generate the resulting MFE plot. Data were scatter-subtracted but not chirp-corrected (due to the lower number of sampled time points near excitation) prior to data analysis; the <1 ns chirp of the probe will not affect the spectra at the delays where the triplet yield is determined. A similar process was used to determine the relative stimulated emission and excited-state absorption intensities; however, before the spectra were averaged, their amplitudes were normalized to the value at 0 mT.

Synthesis

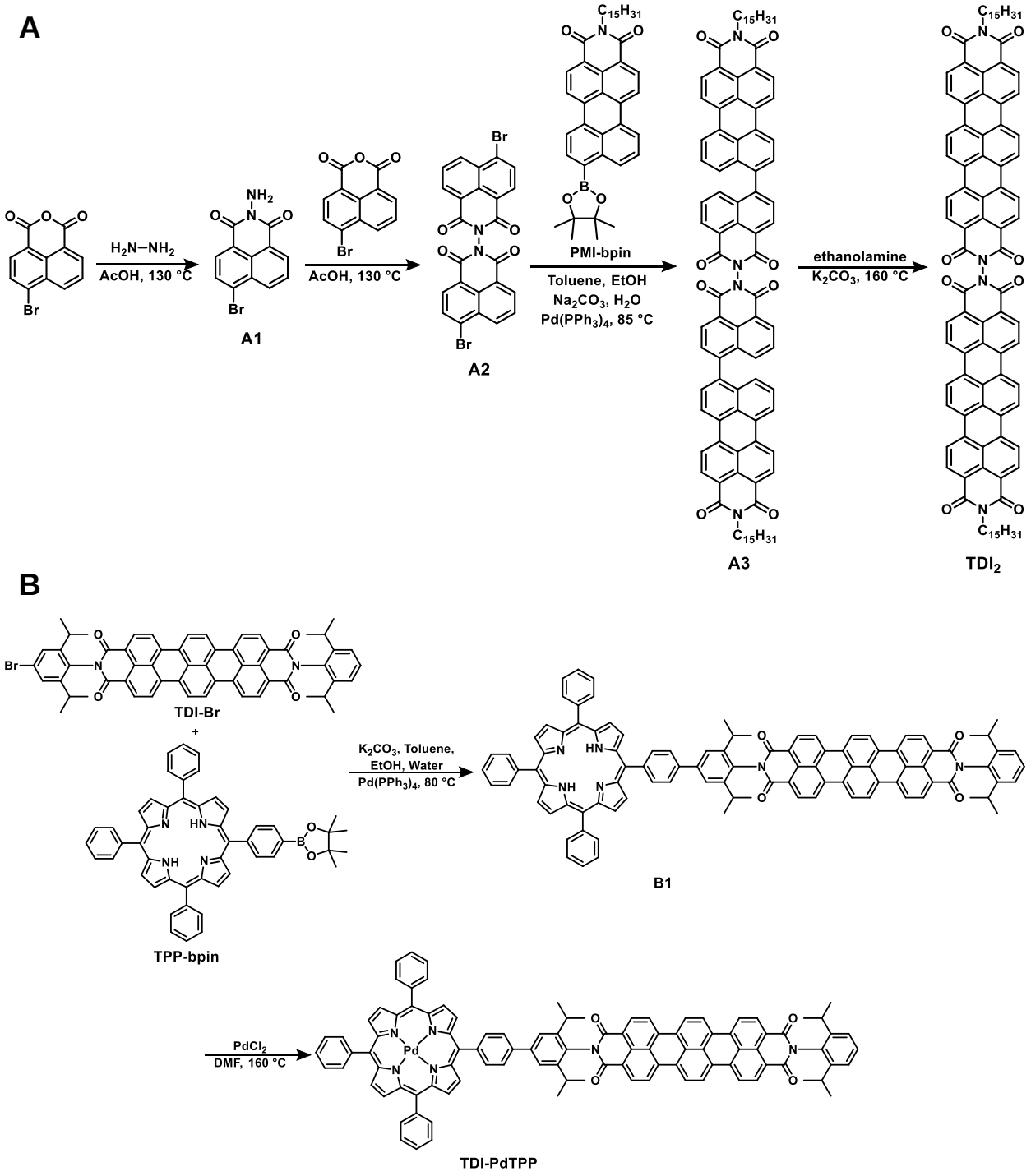
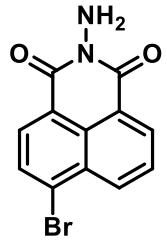


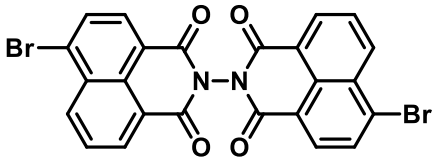
Fig. S2. Synthetic scheme of (A) **TDI_2** and (B) **TDI-PdTPP**.

^{1}H NMR were collected at ambient temperature and at 100 °C at 500 MHz; ^{13}C NMR spectra were collected at ambient temperature at 126 MHz. Chemical shifts are reported in ppm relative to chloroform and *o*-dichlorobenzene. Mass spectrometry was performed on an Agilent 6210 LC-TOF to generate high-resolution HR-ESI-MS or HR-APPI-MS spectra at the Integrated Molecular Structure Education and Research Center (IMSERC) at Northwestern University. All solvents and reagents were obtained from commercial supplies and used without further purification. Column chromatography was performed using silica gel from Sorbent Technologies (Atlanta, GA) and HPLC was performed on a Shimadzu HPLC. Synthesis of N-(1-heptyloctly)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-perylene-3,4-dicarboximide (**PMI-bpin**), *N*-(4-bromo-2,6-diisopropylphenyl)-*N'*-(2,6-diisopropylphenyl)-terrylene-3,4:11,12-tetracarboxdiimide (**TDI-Br**), and 5,10,15-triphenyl-20-[4-(4,4,5,5-tetramethyl-[1,3,2]dioxaborolan-2-yl)-phenyl]-porphyrin (**TPP-bpin**) have been previously reported (3-5).

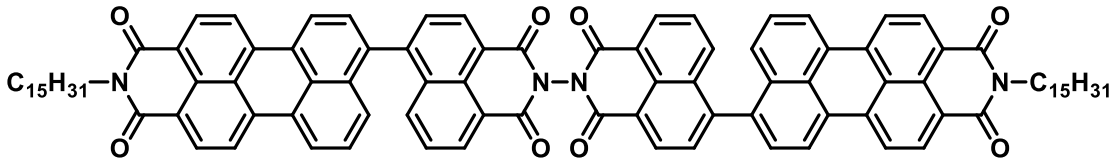


4-bromo-*N*-amino-1,8-naphthalimide (A1). 4-bromo-1,8-naphthalic anhydride (2.77 g, 10 mmol), hydrazine hydrate (0.80 mL), and acetic acid (31 mL) were combined in an 100 mL two neck round bottom flask. The flask was purged with N_2 for 15 minutes and was then heated at reflux (130 °C) for 2.5 h. The reaction mixture was cooled to room temperature and yellow crystals precipitated out of solution. The suspension was filtered and resulted in the product as a yellow solid (1.97 g, 68%). ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.70 (d, J = 7.3 Hz, 1H; CH), 8.62 (d, J

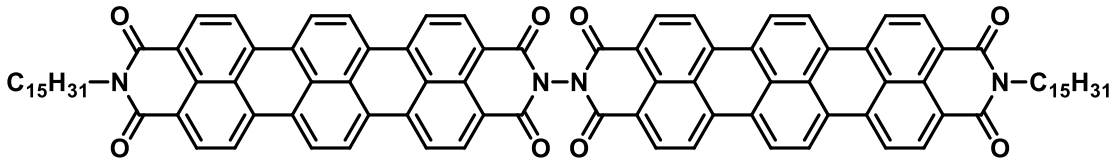
= 8.6, 1H; CH), 8.46 (d, *J* = 7.9 Hz, 1H; CH), 8.07 (d, *J* = 7.9 Hz, 1H; CH), 7.88 (t, *J* = 7.9 Hz, 1H; CH), 5.53 (br s, 2H; NH_2). ^{13}C NMR (126 MHz, $CDCl_3$, 25 °C) δ 160.39 (C=O) 133.86 132.29 131.53 131.27 130.97 130.72 128.21 127.72 122.33 121.46. MS (ESI) *m/z* calcd for $C_{12}H_8{}^{79}BrN_2O_2^+$ ($[M+H]^+$) 290.9764, found: 290.9768.



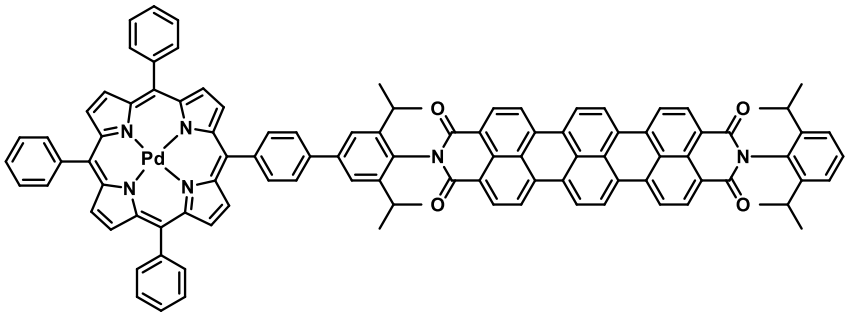
Compound A2. A1 (500 mg, 1.7 mmol), 4-bromo-1,8-naphthalic anhydride (725 mg, 2.6 mmol), and acetic acid (5 mL) were combined into a 25 mL two neck round bottom flask. The flask was purged with N_2 for 15 minutes and was then heated at reflux (130 °C) for 48 h. Acetic acid was removed under reduced pressure and the resulting solid was redissovled in $CHCl_3$. The suspension was filtered through basic alumina to remove excess 4-bromo-1,8-naphthalic anhydride. The resulting filtrate was evaporated under reduced pressure. Purification by column chromatography on SiO_2 with 3:2 hexanes:$CHCl_3$ as the eluent resulted in the product as a white solid (179 mg, 20%). ^1H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.75 (d, *J* = 6.9 Hz, 1H; CH), 8.71 (d, *J* = 8.7, 1H; CH), 8.51 (d, *J* = 7.7 Hz, 1H; CH), 8.12 (d, *J* = 7.8 Hz, 1H; CH), 7.92 (t, *J* = 7.9 Hz, 1H; CH). ^{13}C NMR (12,6 MHz, $CDCl_3$, 25 °C) δ 160.44 (C=O), 134.52, 133.22, 132.27, 131.17, 131.35, 131.09, 129.49, 128.27, 122.65, 121.77. MS (ESI) *m/z* calcd for $C_{24}H_{11}{}^{79}Br_2N_2O_4^+$ ($[M+H]^+$) 548.9080, found: 548.9085.



Compound A3. A2 (179 mg, 0.3 mmol), **PMI-bpin** (209 mg, 0.7 mmol), sodium carbonate (197 mg), toluene (30 mL), ethanol (1.9 mL), and water (1.9 mL) were combined into a 100 mL two neck round bottom flask. The flask was purged with N_2 for 15 minutes and $Pd(PPh_3)_4$ (33 mg) was added. The flask was pruged with N_2 for an additional 15 minutes and the resulting reaction mixture was heated to 85 °C overnight. After cooling, the reaction mixture was extracted with CH_2Cl_2 and water. The organic layers were combined, dried over sodium sulfate, and evaporated under reduced pressure. The material was purifed by column chromatography on SiO_2 (CH_2Cl_2) resulting in a red solid (358 mg, 78%). ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.90 (d, J = 3.5 Hz, 1H), 8.88 (d, J = 3.5 Hz, 1H), 8.81-8.75 (m, 2H), 8.72-8.60 (m, 6H), 8.57 (d, J = 8.0 Hz, 2H), 8.55-8.49 (m, 4H), 8.00 (d, J = 8.4 Hz, 2H), 7.93 (d, J = 7.5 Hz, 2H), 7.75-7.68 (m, 4H), 7.56 (t, J = 7.8 Hz, 2H), 7.43 (d, J = 8.5 Hz, 2H), 5.27-5.18 (m, 2H; NCH), 2.33-2.22 (m, 4H), 1.93-1.82 (m, 4H), 1.42-1.16 (m, 40H), 0.87-0.80 (m, 12H). ^{13}C NMR (126 MHz, $CDCl_3$, 25 °C) δ 161.07 (C=O), 161.04 (C=O), 160.93 (C=O), 160.89 (C=O), 145.70, 138.67, 133.78, 133.42, 133.70, 131.95, 131.62, 130.30, 129.98, 129.83, 129.07, 128.71, 128.31, 127.77, 127.44, 126.68, 123.93, 122.91, 122.65, 122.32, 120.79, 120.67, 54.53, 32.43, 31.83, 29.57, 29.25, 27.02, 22.63, 14.08. MS (APPI): *m/z* calcd for $C_{98}H_{91}N_4O_8^+$, $[M+H]^+$ 1451.6831, found: 1451.6813.



TDI$_2$. A3 (358 mg, 0.25 mmol), ethanolamine (2.3 mL), and potassium carbonate (1.6 g) were combined into a 10 mL round bottom flask. The flask was purged with N_2 for 15 minutes and was then heated at 160 °C overnight. The reaction mixture was cooled to room temperature and methanol was added. The blue precipitate was filtered and rinsed with water to removed excess potassium carbonate. The material was purifed by column chromatography on SiO_2 (CH_2Cl_2/methanol) followed by size exclusion chromatography (Bio-Rad Bio-Beads, S-X1, THF). The product was further purified by HPLC (100% CH_2Cl_2 to 96% CH_2Cl_2/4% methanol gradient at 21 mL/min) to afford a dark blue solid (10 mg, 3%). ^{1}H NMR (500 MHz, *o*-$C_6D_4Cl_2$, 100 °C) δ 8.61-8.34 (m, 8H; TDI CH), 8.30-7.90 (m, 16H; TDI CH), 5.40-5.28 (m, 2H; NCH), 2.50-2.34 (m, 4H), 2.07-1.94 (m, 4H), 1.57-1.08 (m, 40H), 0.85-0.70 (m, 12H). ^{13}C NMR was not obtained. MS (APPI) *m/z* calcd for $C_{98}H_{87}N_4O_8^+$ ([*M*+H]$^+$) 1447.6518, found: 1447.6507.



TDI-PdTPP. TDI-Br (27 mg, 0.03 mmol), **TPP-bpin** (110 mg, 0.15 mmol), potassium carbonate (16 mg), toluene (2.5 mL), ethanol (0.25 mL), and water (0.25 mL) were combined into a 10 mL two neck round bottom flask. The flask was purged with N_2 for 15 minutes and $Pd(PPh_3)_4$ (14 mg) was added. The flask was pruged with N_2 for an additional 15 minutes and the resulting reaction mixture was heated to 80 °C overnight. After cooling, the reaction mixture was extracted with

$CHCl_3$ and water. The organic layers were combined, dried over sodium sulfate, and evaporated under reduced pressure. The material was purifed by column chromatography on SiO_2 (CH_2Cl_2 with 1% triethylamine) followed by size exclusion chromatography (Bio-Rad Bio-Beads, S-X1, CH_2Cl_2) leading to a blue-green solid, **B1**, which was used without further purification. (2) **B1** (9 mg, 0.006 mmol) and $PdCl_2$ (43 mg) were combined in 3 mL of DMF. The reaction mixture was heated at 160 °C for 3 h. After cooling to room temperature, the DMF was evaporated under reduced pressure. The product was further purified by preparative scale TLC on SiO_2 with 1:9 hexanes:$CHCl_3$ to afford a blue-green solid (8 mg, 17%). ^{1}H NMR (500 MHz, $CDCl_3$, 25 °C) δ 8.97 (d, J = 4.9 Hz, 2H), 8.89-8.81 (m, 7H), 8.79 (d, J = 7.9 Hz, 2H), 8.77-8.72 (m, 4H), 8.69 (d, J = 8.2 Hz, 2H), 8.67 (d, J = 8.1 Hz, 2H), 8.30 (d, J = 7.8 Hz, 2H), 8.20 (t, J = 7.0 Hz, 6H), 8.08 (d, J = 8.0 Hz, 2H), 7.89 (br s, 2H), 7.83-7.71 (m, 9H), 7.52 (t, J = 7.8 Hz, 1H), 7.38 (m, J = 7.9 Hz, 2H), 7.31-7.29 (m, 1H), 2.96 (h, J = 6.8 Hz, 2H), 2.80 (h, J = 7.0 Hz, 2H), 1.22 (d, J = 2.1 Hz, 12H), 1.21 (d, J = 2.2 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$, 25 °C) δ 162.89 (C=O), 162.75 (C=O), 145.34, 144.67, 140.77, 140.60, 140.57, 135.24, 135.12, 133.51, 133.12, 131.15, 131.05, 130.21, 130.15, 130.11, 130.07, 129.98, 128.99, 128.71, 127.77, 126.75, 125.71, 124.74, 123.66, 123.62, 123.06, 122.43, 120.89, 120.87, 120.77, 120.61, 28.34 (*i*Pr, CH), 28.19 (*i*Pr, CH), 23.18 (*i*Pr, CH_3), 23.01 (*i*Pr, CH_3). MS (APPI): *m/z* calcd for $C_{102}H_{73}N_6O_4Pd^+$ ([*M*+H]$^+$) 1551.4722, found 1551.4778.

UV-Vis Spectra of TDI_2 and TDI-PdTPP

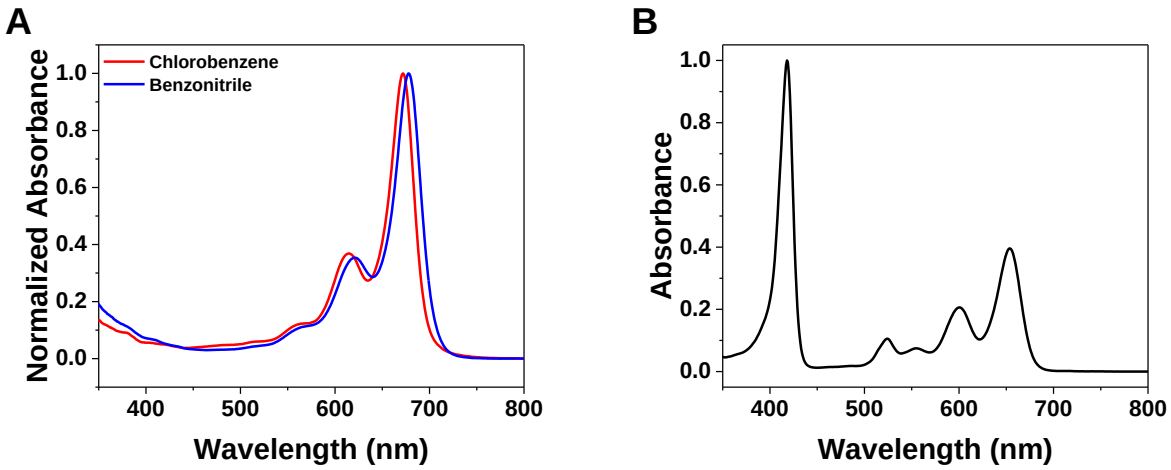


Fig. S3. UV-Vis spectra of (A) **TDI_2** in chlorobenzene (red) and benzonitrile (blue) and (B) **TDI-PdTPP** in toluene.

Global Fit of the fsTA Data of TDI_2 in 5CB at 345 mT

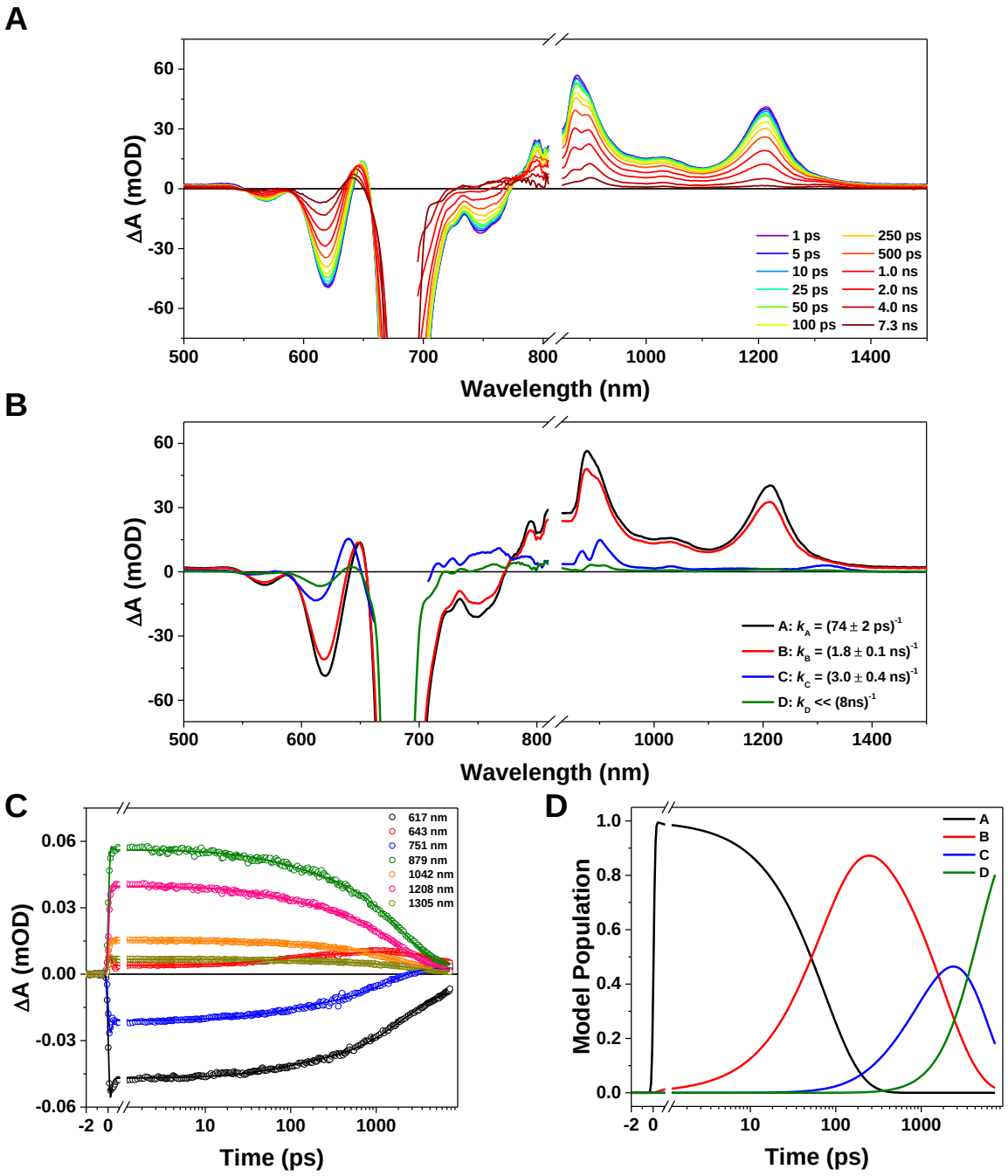


Fig. S4. (A) FsTA spectra at selected time delays, (B) evolution-associated spectra, (C) single-wavelength kinetics at 617 (black), 643 (red), 751 (blue), 879 (green), 1042 (orange), 1208 nm (pink), and 1305 nm (dark yellow), and (D) population dynamics obtained by global analysis with an A → B → C → D model of **TDI_2** in 5CB at 345 mT, λ_{ex} = 685 nm.

Global Fit of the fsTA Data of TDI_2 in 5CB at 0 mT

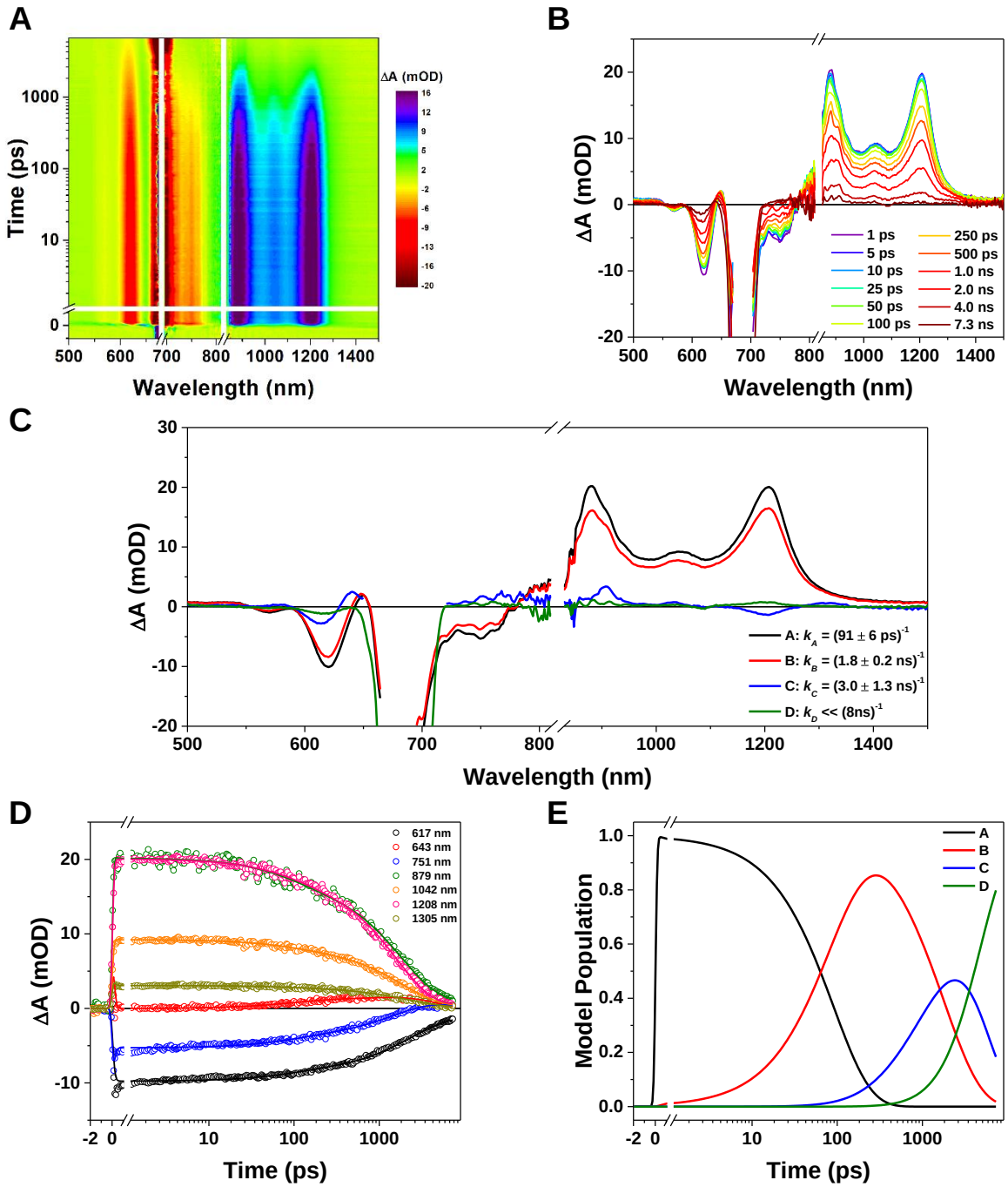


Fig. S5. (A) Contour plot of the fsTA data, (B) fsTA spectra at selected time delays, (C) evolution-associated spectra, (D) single-wavelength kinetics at 617 (black), 643 (red), 751 (blue), 879 (green), 1042 (orange), 1208 nm (pink), and 1305 nm (dark yellow), and (e) population dynamics obtained by global analysis with an A → B → C → D model of **TDI_2** in 5CB at 0 mT, λ_{ex} = 685 nm.

Global Fit of the fsTA Data of TDI_2 in Chlorobenzene at 0 mT

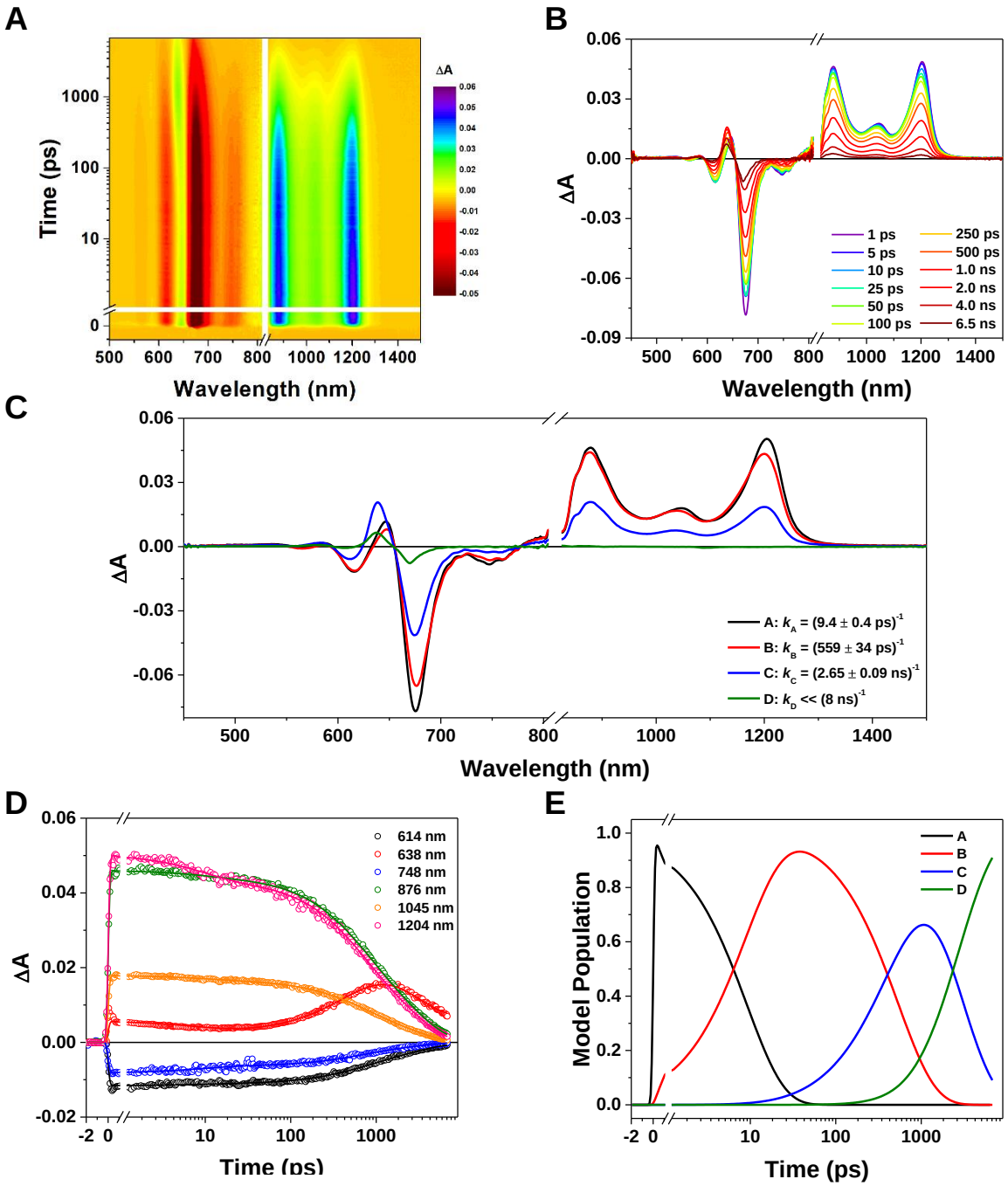


Fig. S6. (A) Contour plot of the fsTA data, (B) fsTA spectra at selected time delays, (C) evolution-associated spectra, (D) single-wavelength kinetics at 614 (black), 638 (red), 748 (blue), 876 (green), 1045 (orange), and 1204 nm (pink), and (E) population dynamics obtained by global analysis with an A → B → C → D model of **TDI_2** in chlorobenzene at 0 mT, λ_{ex} = 675 nm.

Global Fit of the fsTA Data of TDI_2 in Chlorobenzene at 345 mT

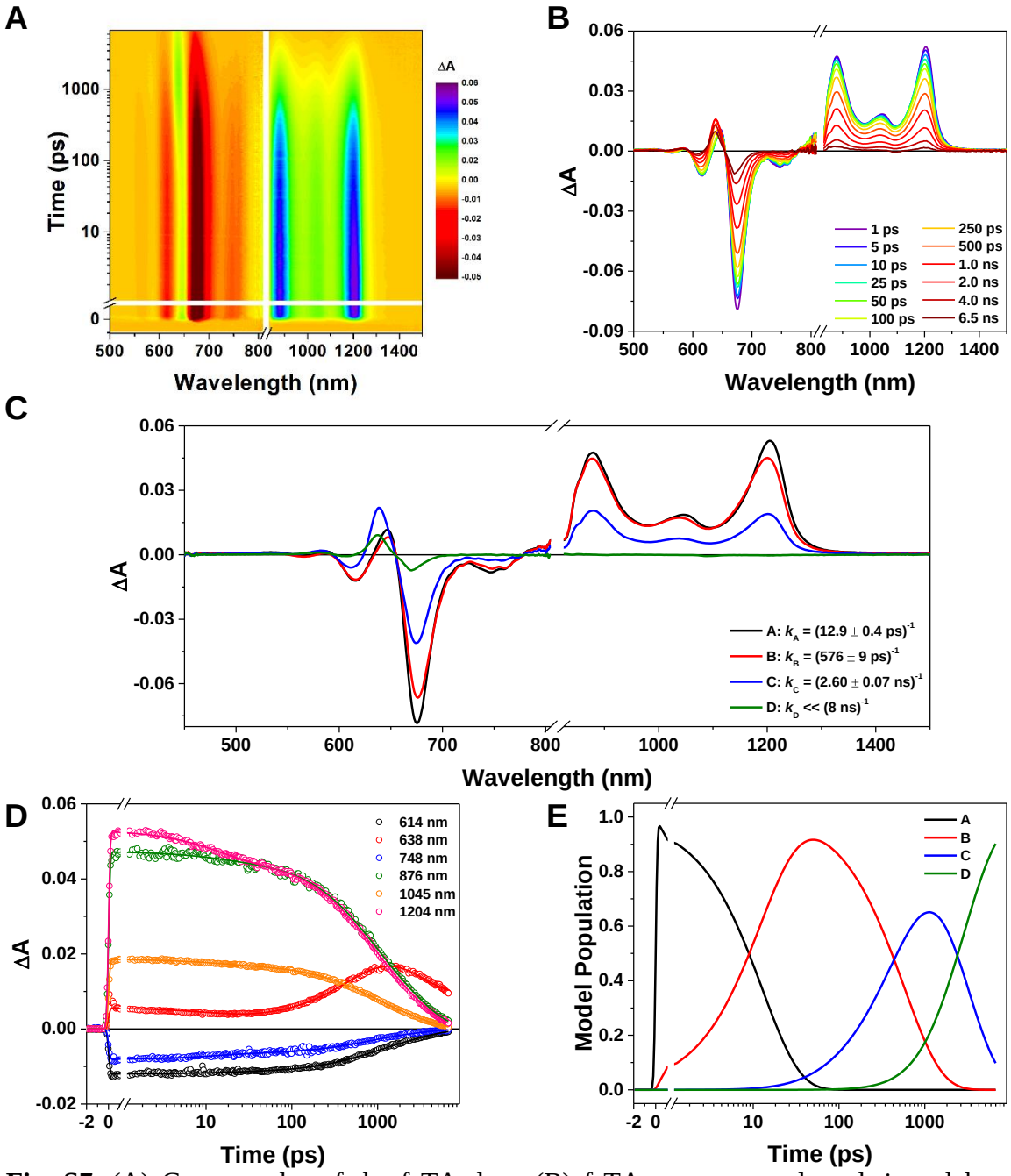


Fig. S7. (A) Contour plot of the fsTA data, (B) fsTA spectra at selected time delays, (C) evolution-associated spectra, (D) single-wavelength kinetics at 614 (black), 638 (red), 748 (blue), 876 (green), 1045 (orange), and 1204 nm (pink), and (E) population dynamics obtained by global analysis with an A → B → C → D model of **TDI_2** in chlorobenzene at 345 mT, λ_{ex} = 675 nm.

Global Fit of the fsTA Data of TDI_2 in Benzonitrile at 0 mT

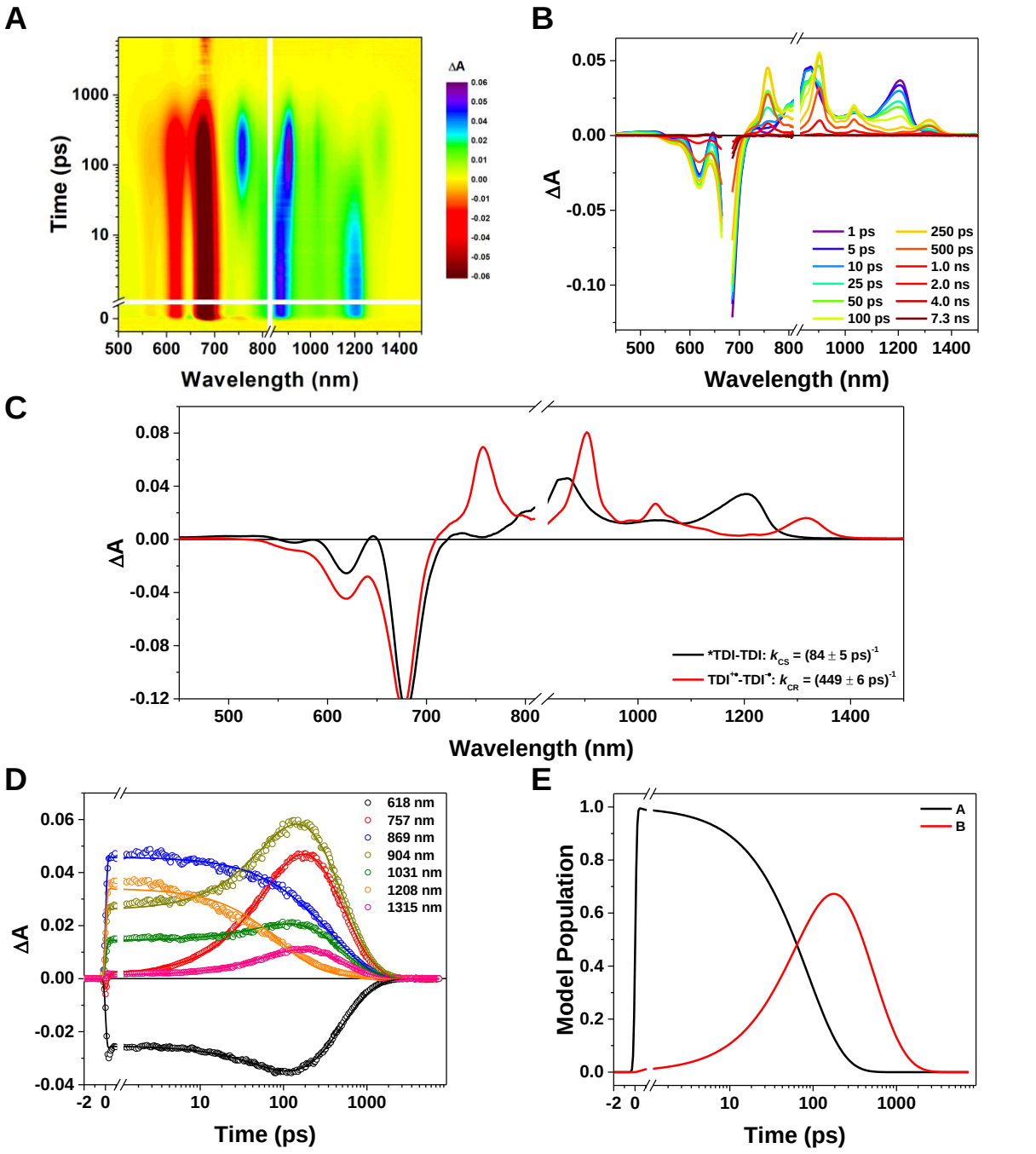


Fig. S8. (A) Contour plot of the fsTA data, (B) fsTA spectra at selected time delays, (C) evolution-associated spectra, (D) single-wavelength kinetics at 618 (black), 757 (red), 869 (blue), 904 (dark yellow), 1031 (green), 1208 (orange), and 1315 nm (pink), and (E) population dynamics obtained by global analysis with a *TDI-TDI → $TDI^{+\bullet}$-$TDI^{-\bullet}$ → ground model of **TDI_2** in benzonitrile at 0 mT, λ_{ex} = 675 nm.

NsTA of TDI_2 in 5CB

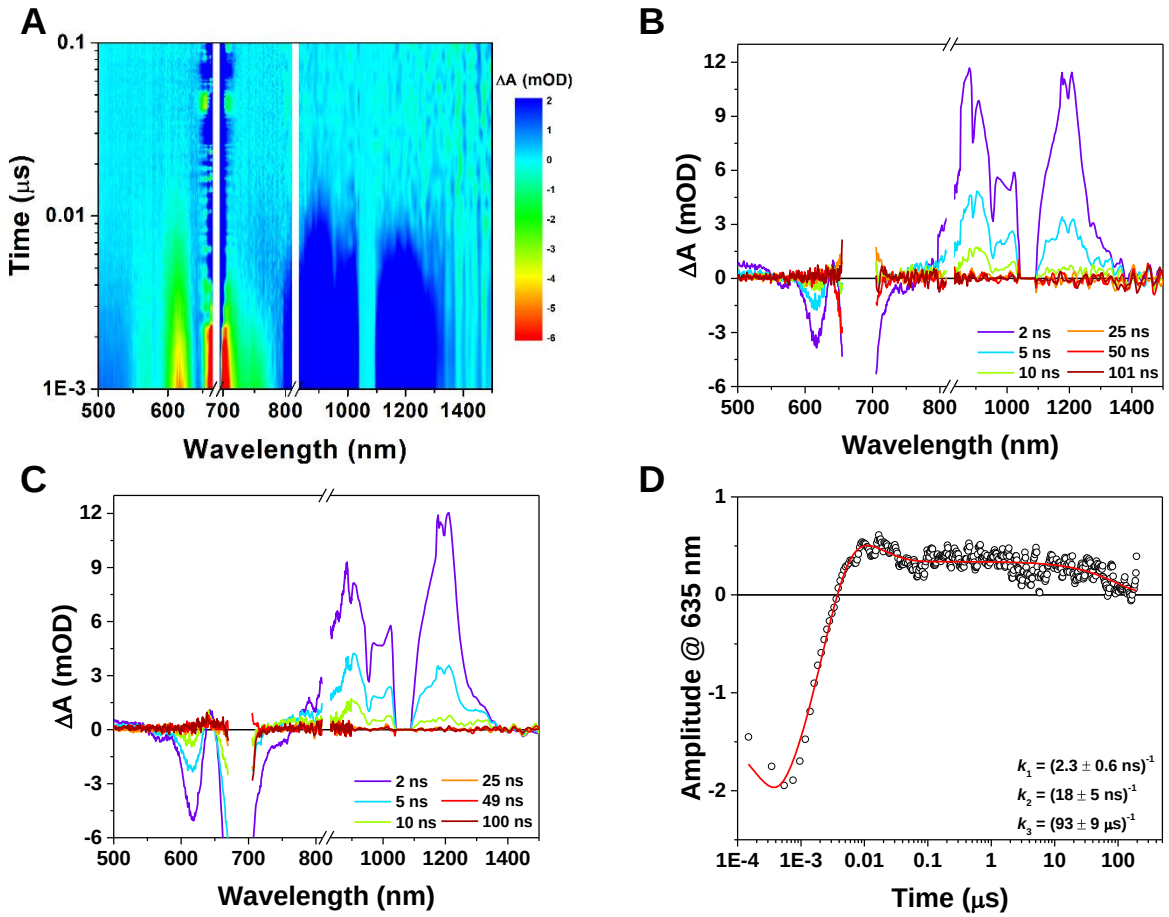


Fig. S9. (A) Contour plot of the nsTA data and (B) nsTA spectra at selected time delays of **TDI_2** in 5CB at 0 mT, λ_{ex} = 685 nm. (C) nsTA spectra at selected time delays of **TDI_2** in 5CB at 345 mT and (D) its single-wavelength kinetic fit (smoothed) at 635 nm. The T_1 state lives ~93 μs.

TDI-PdTPP Sensitization Experiment (fsTA and nsTA)

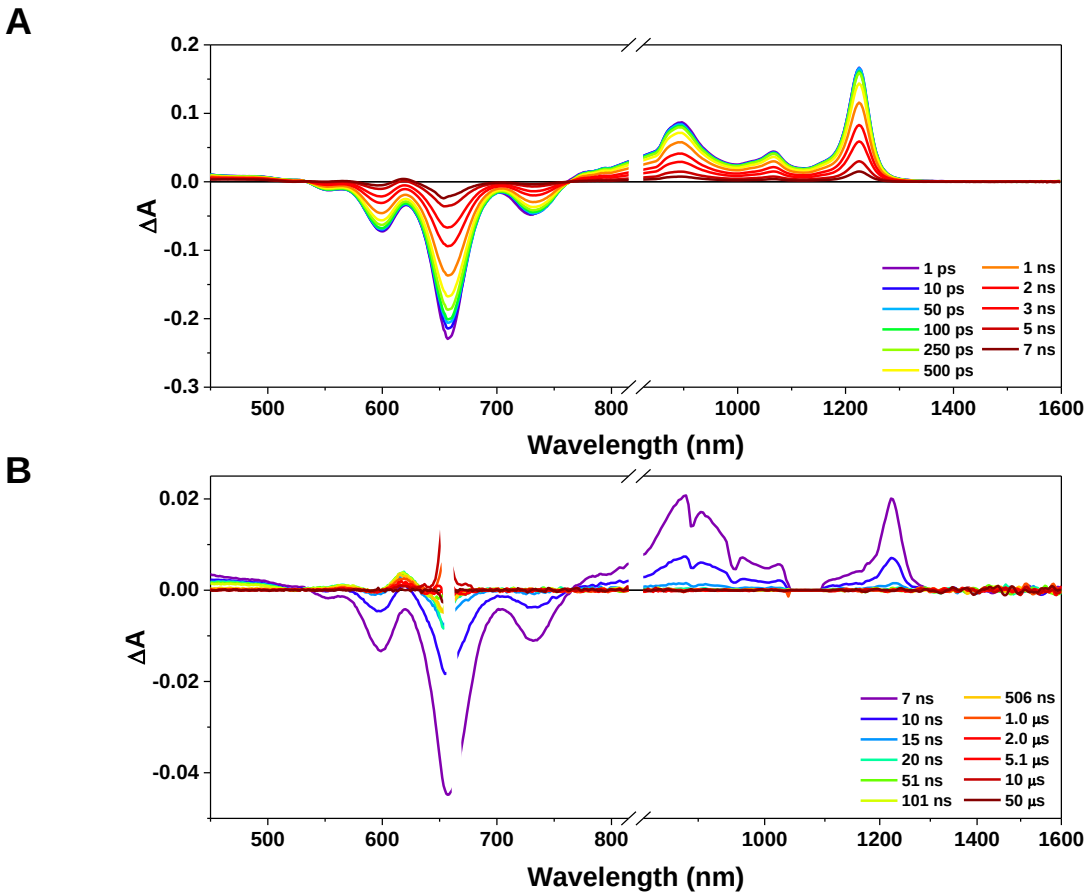


Fig. S10. (A) FsTA and (B) nsTA spectra at selected time delays of **TDI-PdTPP** in toluene, λ_{ex} = 655 nm.

TREPR Fitting Description

The TREPR spectra of the triplet species, Fig. 4B and Fig. S12D, were fit utilizing the *pepper* function in EasySpin and the fit parameters are given in Table S1. The polarization of the **TDI-PdTPP** triplet was generated utilizing the built-in functionality for the intersystem crossing mechanism, where the zero-field eigenstates are selectively populated. The spin-polarized T_1 state in **TDI$_2$** was fit through linear regression to selectively populate the high-field eigenstates. The lineshape of the triplet in Fig. S12D differs significantly from that observed in Fig. 4B; this is partially due to the mechanism through which the triplet sublevels are populated, but mostly due to the ordering induced on **TDI$_2$** by the 5CB. The liquid crystal partially aligns **TDI$_2$** such that the molecular long axis is perpendicular to the magnetic field. Interestingly, only the D_{yy} component of the zero-field splitting tensor contributes significantly to the TREPR spectrum.

The TREPR spectrum of the **TDI$_2$** quintet was fit using the *pepper* function in EasySpin using a modified version of *resfields* that emulated the method described Tayebjee et al (6). The intensity of each resonant transition was weighted by the probability that the responsible numerically solved eigenvectors had singlet character. The dominant transitions present in the fit are labeled in Figure S12E; other transitions such as $^3(T_1T_1)$, $m_s = +1 \rightarrow {}^3(T_1T_1)$, $m_s = 0$ are present but have small contributions to the overall spectrum. The fit parameters for the quintet are provided in Table S2. As with the triplet in **TDI$_2$**, the quintet EPR spectrum shows partial ordering due to the liquid crystal, which restricts the molecular orientations that contribute to the spectrum.

Table S1. Triplet Fit Parameters

Molecule	Zero-Field Splitting (MHz)	Population	Peak-Peak Linewidth (mT)
TDI-PdTPP	$\|D\|$ = 848 E/D = 0.133	$\|T_x\rangle$ = 0 $\|T_y\rangle$ = 0 $\|T_z\rangle$ = 1	1.05
TDI_2	$\|D\|$ = 861 E/D = 0.133	$\|T_{+1}\rangle$ = 0.7626 $\|T_0\rangle$ = 0.2374 $\|T_{-1}\rangle$ = 0	0.85

Table S2. Quintet Fit Parameters

Parameter	Value
J (GHz)	5.325
Triplet-Triplet Coupling Tensor (MHz)	[12 12 24]
ZFS Tensors (MHz)	[574 -156 -418] [-156 574 -418]
Peak-Peak Linewidth (mT)	1.9

*The tensors are written such that the triplet-triplet coupling defines the molecular frame where the z-component is along the length of the molecule.

Orientation of TDI-PdTPP

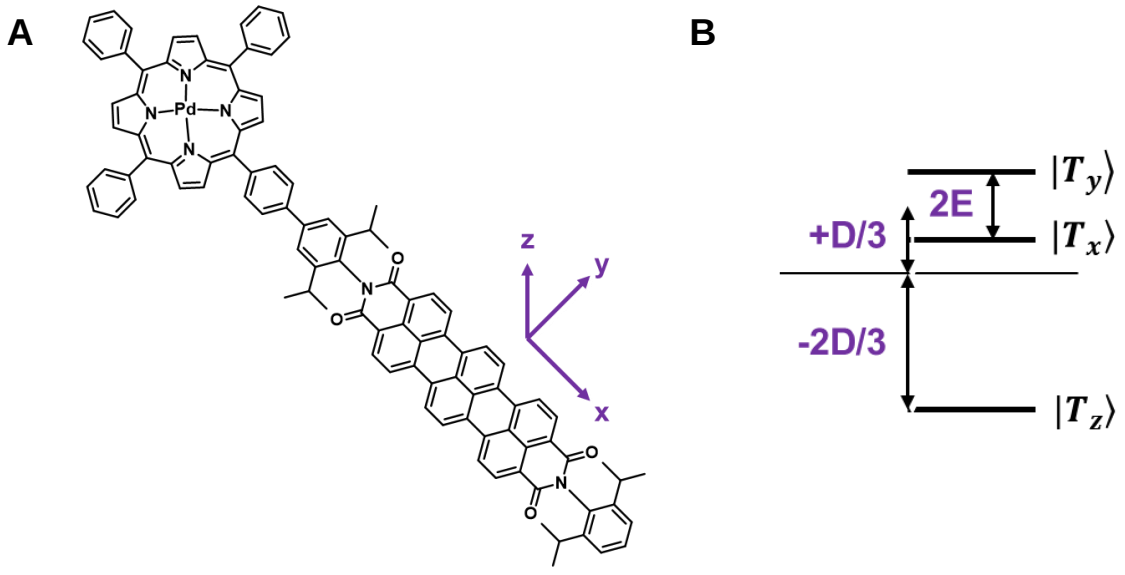


Fig. S11. (A) Molecular axes of **TDI-PdTPP**. (B) Zero-field splitting convention used with respect to the molecular axis.

TDI_2 X-Band TREPR Fits and Kinetics

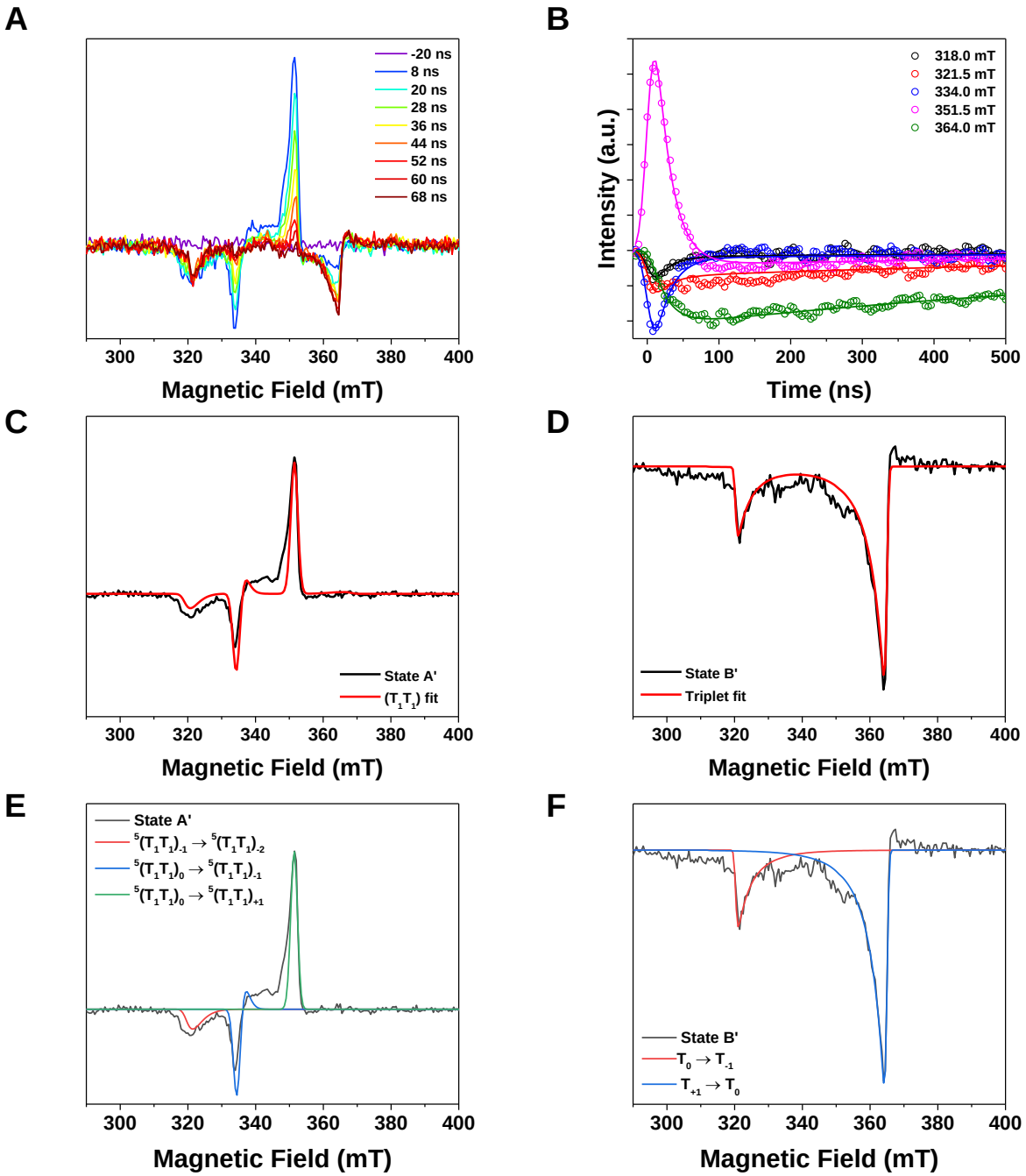


Fig. S12. (A) TREPR spectra (9.628 GHz) at selected time delays and (B) single-wavelength kinetics at 318.0 (black), 321.5 (red), 334.0 (blue), 351.5 (magenta), and 364.0 mT (green) of **TDI_2** in 5CB at room temperature, λ_{ex} = 660 nm. Fits of (C) state A' and (D) state B' to the (T_1T_1) pair and triplet, respectively. The dominant transitions between the (E) $^5(T_1T_1)$ and (F) T_1 sublevels that are present in the (T_1T_1) fit of state A' and T_1 fit of state B', respectively.

Global Fit of the nsTA Data of TDI_2 in Chlorobenzene at 0 mT

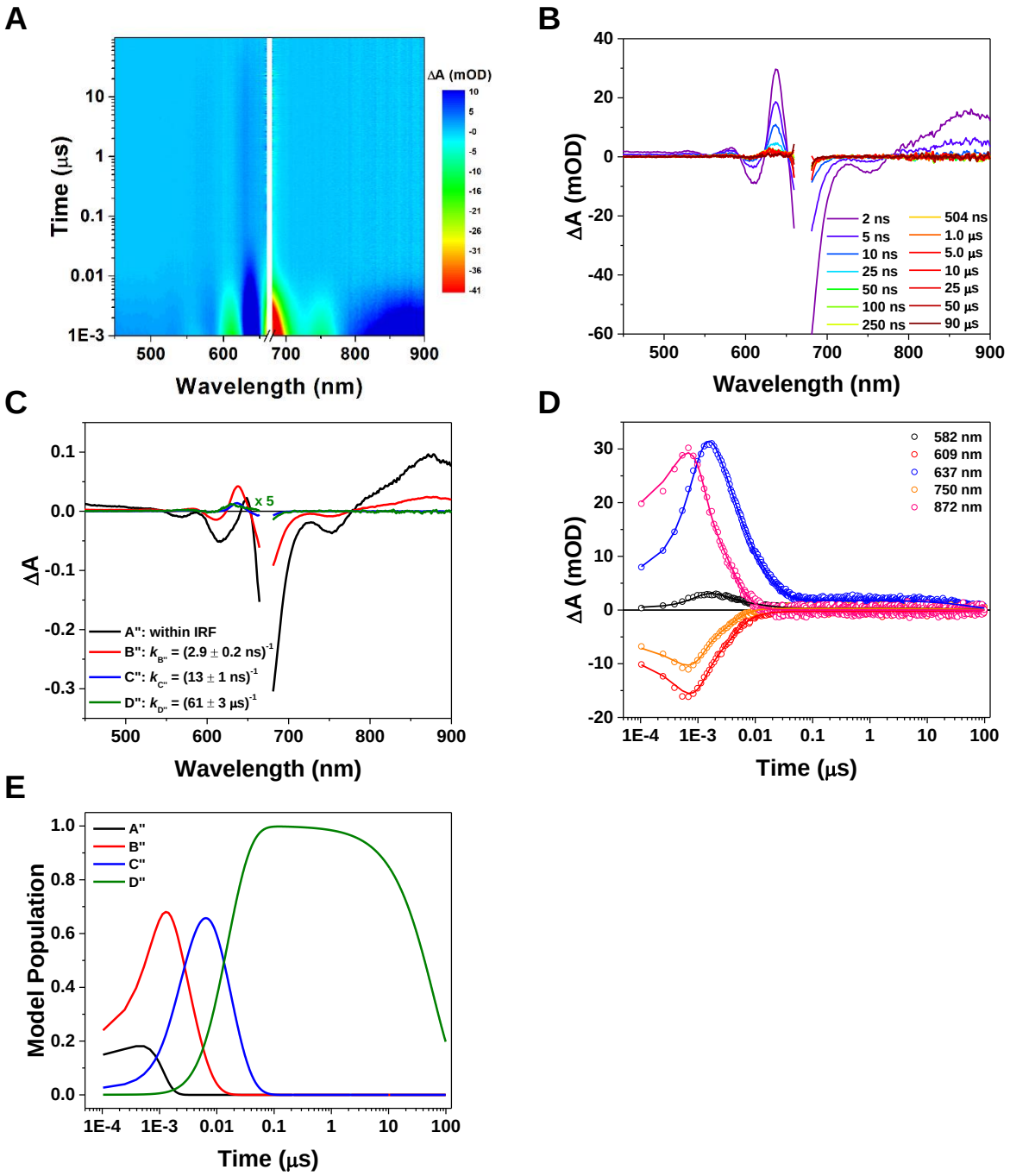


Fig. S13. (A) Contour plot of the nsTA data, (B) nsTA spectra at selected time delays, (C) evolution-associated spectra, (D) single-wavelength kinetics at 582 (black), 609 (red), 637 (blue), 750 (orange), and 872 nm (pink), and (E) population dynamics obtained by global analysis with an A" → B" → C" → D" → ground model of **TDI_2** in chlorobenzene at 0 mT, λ_{ex} = 675 nm.

Global Fit of the nsTA Data of TDI_2 in Chlorobenzene at 345 mT

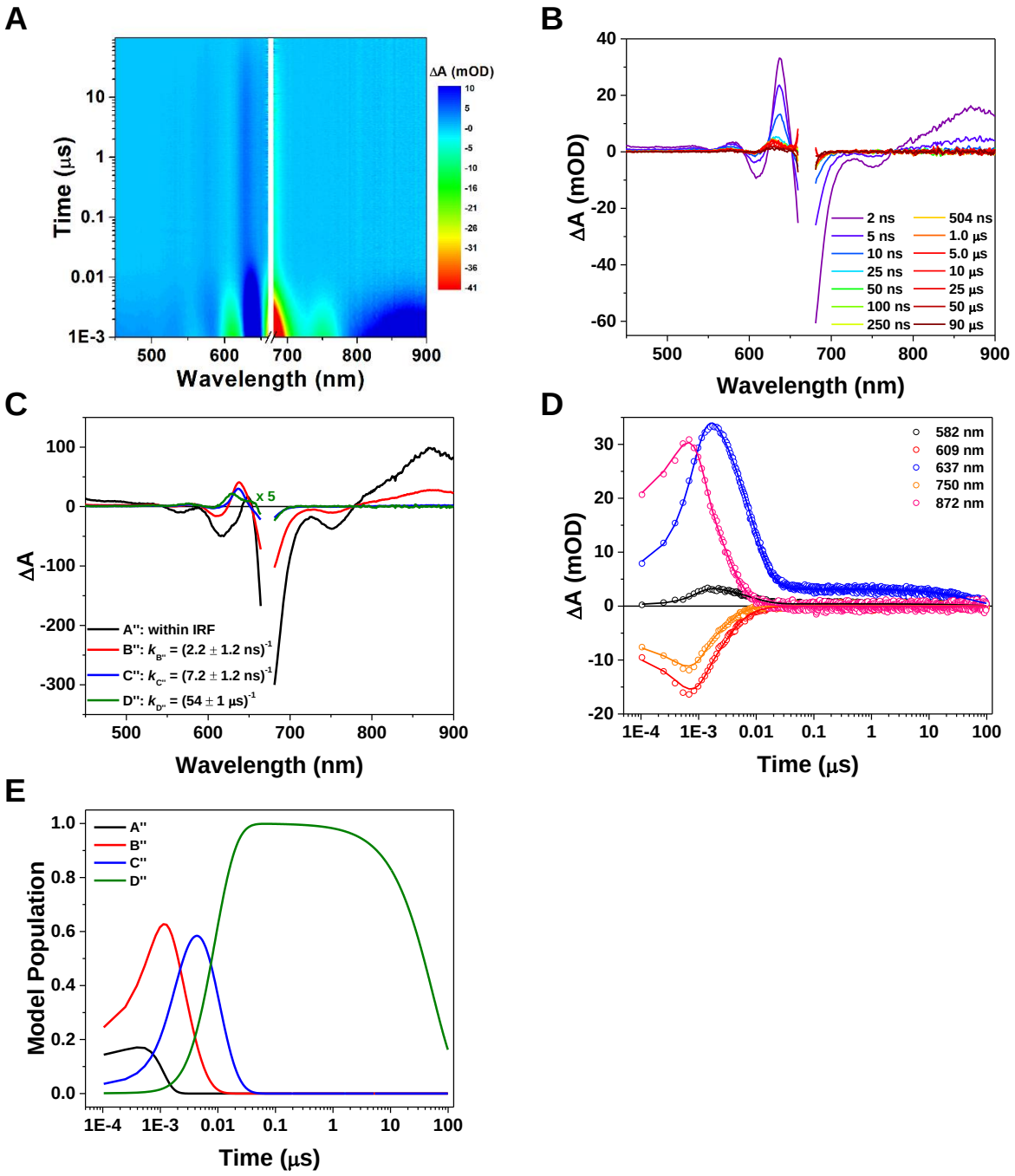


Fig. S14. (A) Contour plot of the nsTA data, (B) nsTA spectra at selected time delays, (C) evolution-associated spectra, (D) single-wavelength kinetics at 582 (black), 609 (red), 637 (blue), 750 (orange), and 872 nm (pink), and (E) population dynamics obtained by global analysis with an A'' → B'' → C'' → D'' → ground model of **TDI_2** in chlorobenzene at 345 mT, λ_{ex} = 675 nm.

Triplet Sensitization of TDI_2

Triplet sensitization of **TDI_2** was performed in chlorobenzene by photoexcitation of anthracene (in large excess) at 355 nm. Rapid intersystem crossing populates the anthracene T_1 state (1.85 eV); the anthracene T_1 state triplet energy transfers to the lower energy TDI T_1, which allows for optical characterization of the TDI T_1 state by nanosecond transient absorption spectroscopy. The sample was deoxygenated by four freeze-pump-thaw cycles.

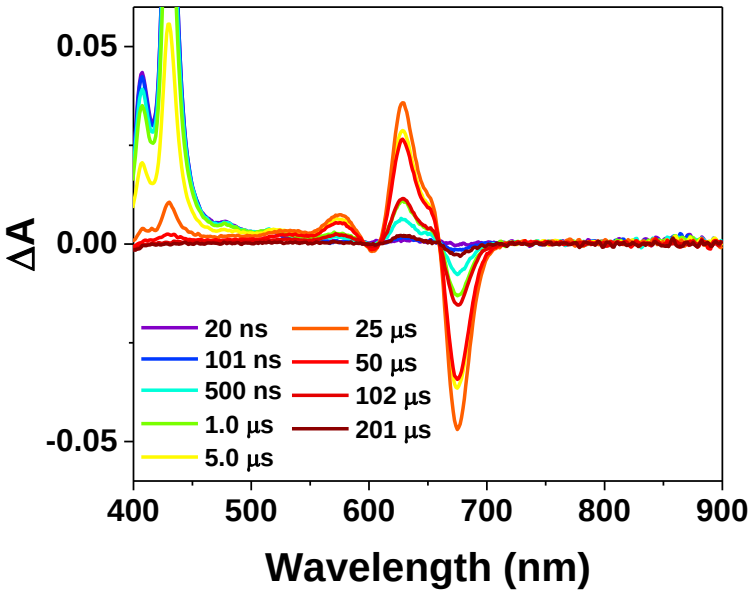


Fig. S15. NsTA spectra of anthracene-sensitized **TDI_2** (orange to red, Δt >5 μs) in chlorobenzene, λ_{ex} = 355 nm.

Steady-State and Time-Resolved Fluorescence of TDI_2

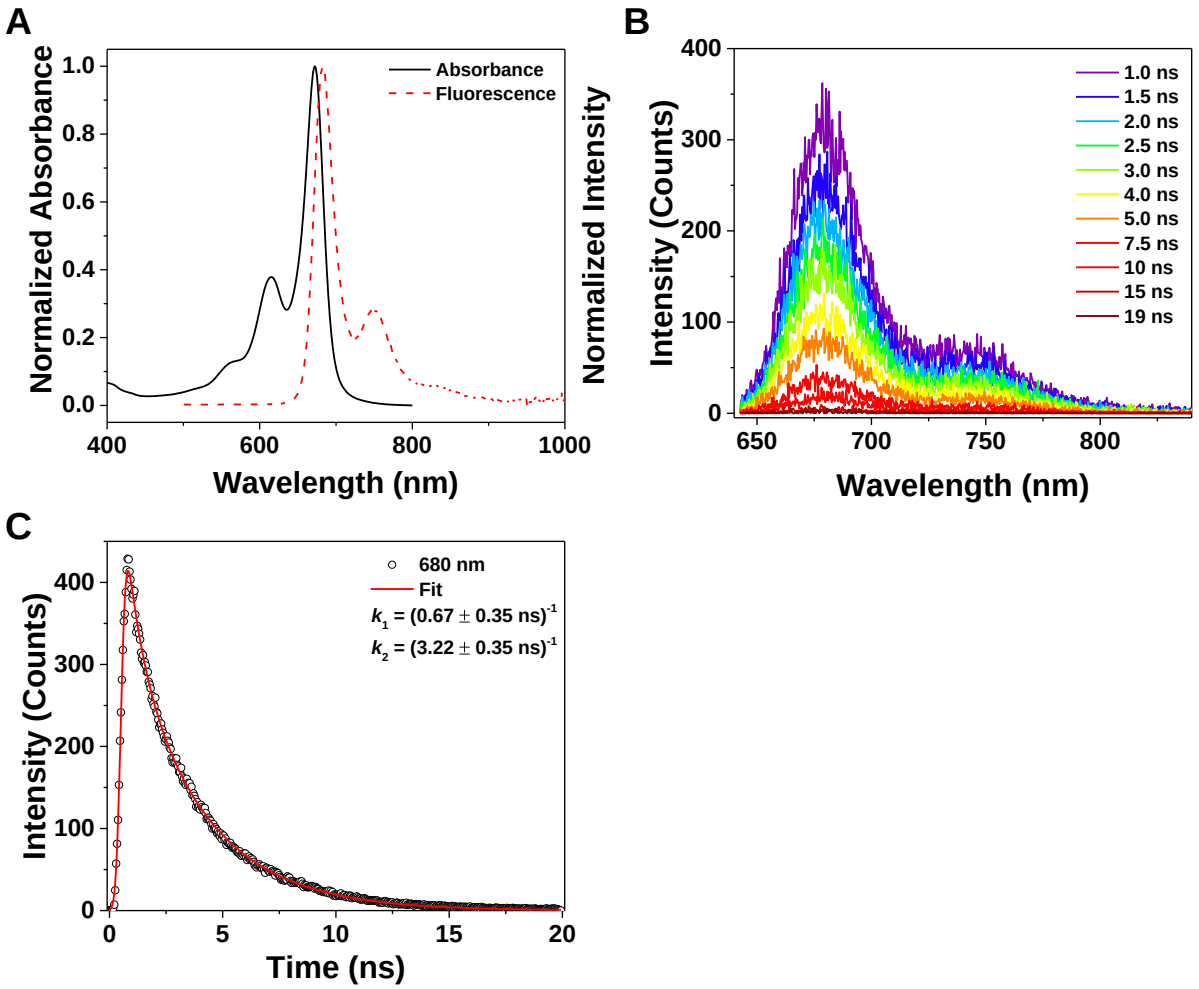


Fig. S16. (A) Steady-state absorption (solid) and fluorescence (dashed) spectra of **TDI_2** in chlorobenzene. (B) TRF spectra at selected time delays and (C) single-wavelength kinetic fit at 680 nm of **TDI_2** in chlorobenzene collected with the 20 ns window.

TDI_2 Q-Band TREPR Spectrum and Fit

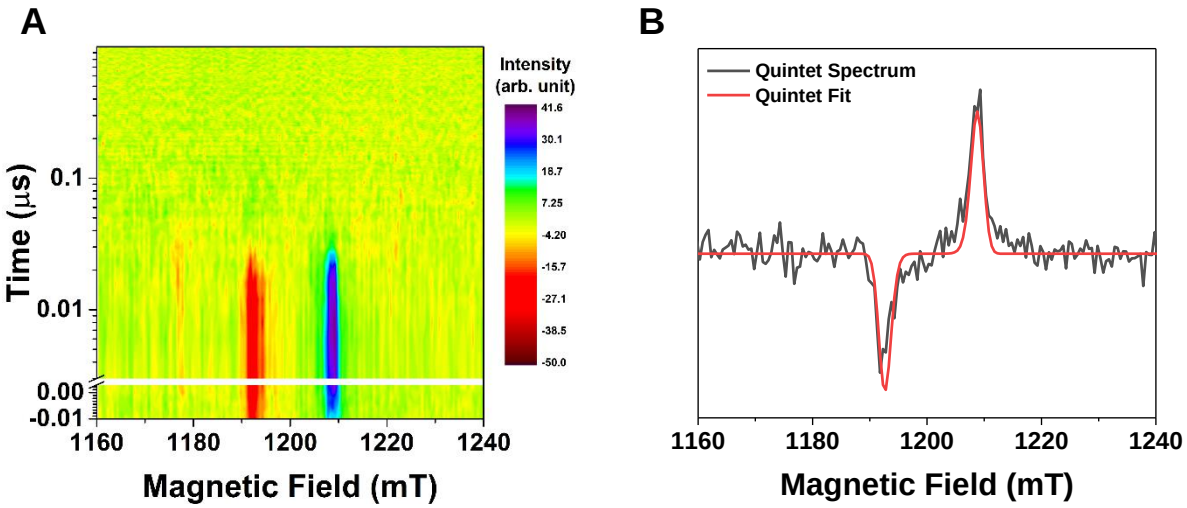


Fig. S17. (A) Contour plot of the TREPR spectra (Q-band) of **TDI_2** in 5CB collected at room temperature, λ_{ex} = 660 nm and (B) its corresponding quintet spectrum fit.

MFE on the (T_1T_1) Decay Rate

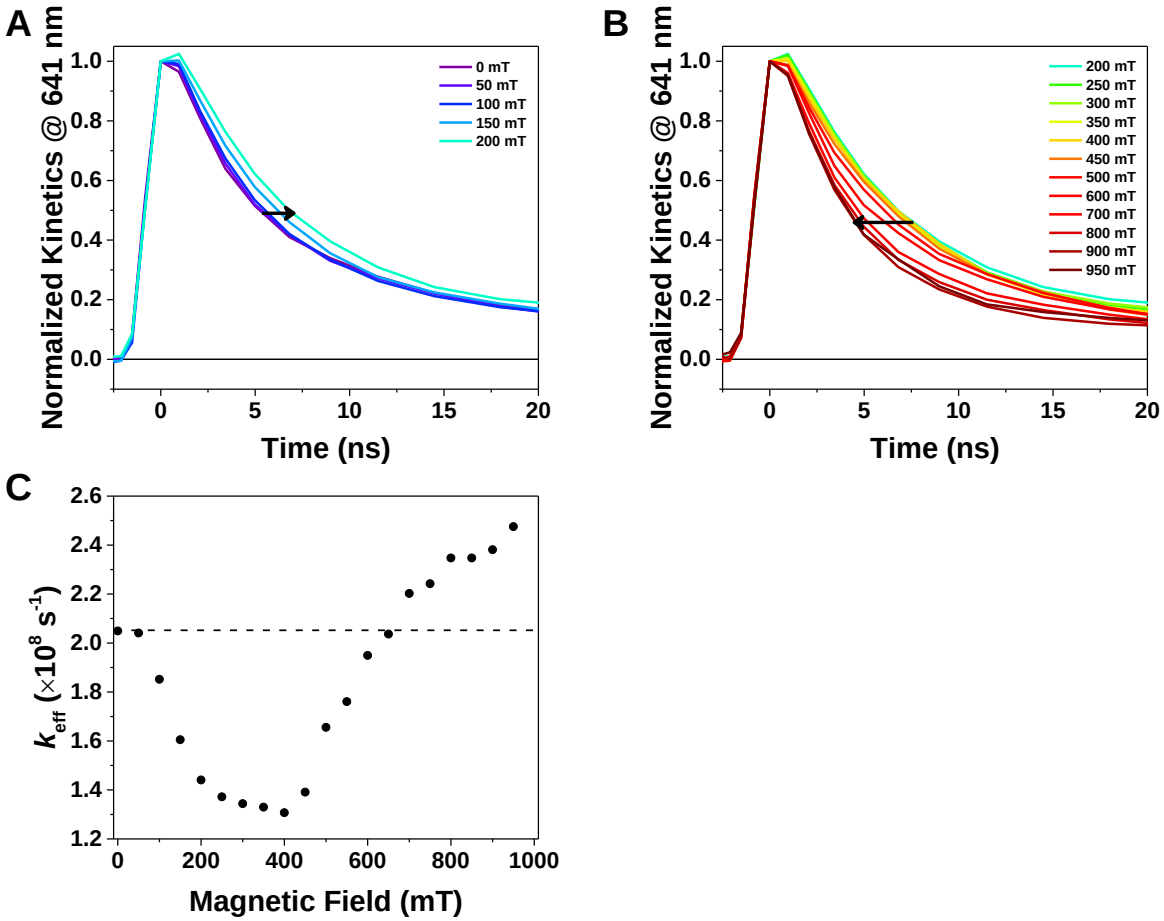


Fig. S18. Normalized single-wavelength kinetics at 641 nm as a function of magnetic field from (A) 0 to 200 mT and (B) 200 to 950 mT. (C) Effective (T_1T_1) decay rate (k_{eff}) as a function of magnetic field. k_{eff} accounts for singlet channel annihilation, triplet channel annihilation, and dissociation into two uncorrelated triplets. The effective rate was determined by fitting each kinetic trace from 0 to 15 ns to a single exponential with a long-time offset.

MFE on the Stimulated Emission and Singlet Excited-State Absorption Features

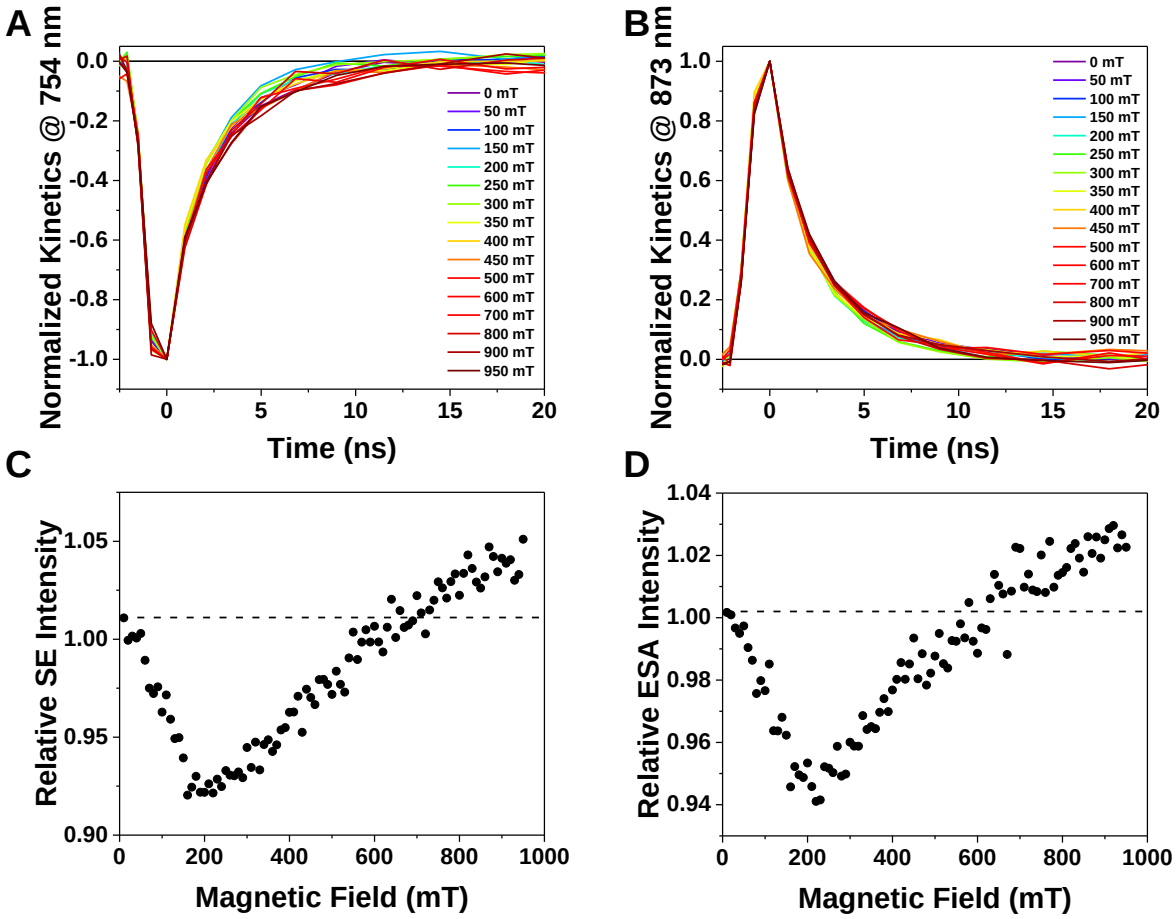


Fig. S19. Normalized single-wavelength kinetics at (A) 754 nm and (B) 873 nm as a function of magnetic field. (C) Stimulated emission (SE) and (D) excited-state absorption (ESA) intensity relative to that at 0 mT of **TDI$_2$** as a function of magnetic field. Spectra collected in chlorobenzene were averaged from 735 to 770 nm and 800 to 900 nm, respectively, and integrated from 0 to 10 ns.

Computational Data

Table S3. TDI_2 Geometry Across Different States

State	Angle Between the Two TDI Units	N-N Bond Length (Å)
Singlet Ground State	89.99°	1.369
Singlet Excited State	89.97°	1.369
Triplet State	89.98°	1.369
Quintet State	90.00°	1.369

Table S4. Computed TDI Ground and Excited-State Energies

State	*N,N*-Dimethyl TDI	Simplified TDI_2
Singlet Excited State	1.95 eV	1.73 eV
Triplet State	0.85 eV	0.85 eV
Quintet State	3.87 eV	1.71 eV

*The spin density of the quintet state of the simplified **TDI_2** is delocalized across both TDI subunits as shown in Fig. S19.

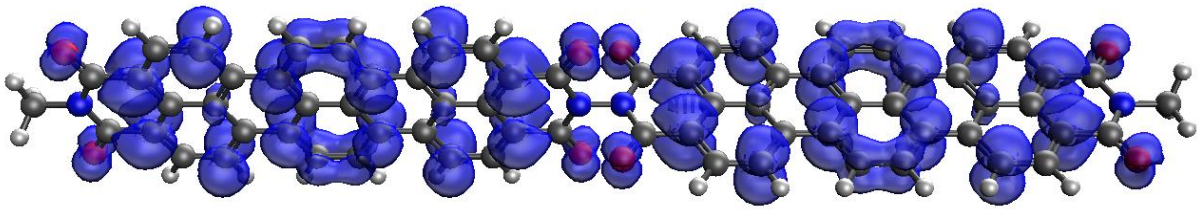


Fig. S20. Spin density visualization of the quintet state of simplified **TDI_2** (isovalue = 0.01)

TDI_2: Singlet Ground State

C	15.7006104185	-0.8858796644	0.8697571008	H	11.6368023955	2.4130548759	-2.3730737984
C	15.6971959068	0.8798464175	-0.8655769926	C	9.9287033076	-0.8802939557	0.8680129150
C	14.2237677996	-0.8684757601	0.8540118098	C	9.9284584941	0.8807584652	-0.8669369789
O	16.3334666332	-1.6297548742	1.6004795911	C	9.2164612129	0.0001221516	0.0005516421
C	14.2219726467	0.8690125608	-0.8546573229	C	9.1940577845	-1.7199692524	1.6961868999
O	16.3471943641	1.6164030961	-1.5888844117	C	9.1933822232	1.7202980875	-1.6948826606
C	13.5122193838	0.0001229652	0.0000039455	C	7.7837399481	-0.0001219270	0.0006148854
C	13.5298734514	-1.7195251835	1.6915291963	C	7.8061710646	-1.7199400491	1.6961035845
C	13.5291073726	1.7206570578	-1.6919179490	H	9.6959673009	-2.4040134288	2.3709593493
C	12.0891703663	0.0002523256	0.0002833687	H	9.6949338604	2.4046039247	-2.3696541914
H	14.0937235288	-2.3811898299	2.3417978739	C	7.8054956702	1.7198223626	-1.6946725238
C	12.1352516863	-1.7252815856	1.6981100812	C	7.0714195698	-0.8802722689	0.8678270820
H	14.0933860830	2.3821753576	-2.3421264605	C	7.0710540901	0.8797918407	-0.8665048060
C	12.1344008369	1.7264000288	-1.6977504372	H	7.3047039664	-2.4041123623	2.3709704193
C	11.3910288514	-0.8845323253	0.8712931644	H	7.3037599252	2.4039408421	-2.3694007122
C	11.3908451810	0.8852721765	-0.8706075973	C	5.6089713561	-0.8847988671	0.8714417961
H	11.6382692679	-2.4119270147	2.3738982893	C	5.6086362866	0.8837370668	-0.8701465397

C	4.9082775475	-0.0006822942	0.0006314291	C	-7.8061951599	-1.6948996297	-1.7199471719
C	4.8689677466	-1.7269892993	1.7002072820	C	-7.8054718996	1.6951574001	1.7205240131
C	4.8683315275	1.7256470457	-1.6989150076	C	-9.2164613259	0.0005088868	0.0001371261
C	3.4839636439	-0.0009557163	0.0006174243	C	-9.1940868837	-1.6945772240	-1.7203784831
C	3.4752878559	-1.7232667142	1.6959691482	H	-7.3047519508	-2.3696917490	-2.4042153665
H	5.3681620967	-2.4125123831	2.3752113332	H	-7.3037122405	2.3696765654	2.4048263763
C	3.4746606967	1.7213719826	-1.6947153738	C	-9.1933533448	1.6957091544	1.7206607519
H	5.3672893100	2.4113923852	-2.3738734839	C	-9.9288288188	-0.8664951856	-0.8806724802
C	2.7790033551	0.8713279713	-0.8581420011	C	-9.9283330884	0.8680304647	0.8807978107
C	2.7793158350	-0.8734854932	0.8593875711	H	-9.6959154271	-2.3690192072	-2.4048043329
H	2.9131121728	-2.3853451972	2.3473150878	H	-9.6949859708	2.3704880027	2.4049035341
H	2.9122424420	2.3832759033	-2.3460305601	C	-11.3912262173	-0.8694706584	-0.8852439630
C	1.3065693440	0.8957698714	-0.8823276026	C	-11.3906476934	0.8719518579	0.8850310648
C	1.3068675319	-0.8983770134	0.8836296169	C	-12.0891701963	0.0015687098	-0.0000610726
O	0.6475385298	1.6211477501	-1.5965283757	C	-12.1351635021	-1.6960222767	-1.7266176768
N	0.6846111540	-0.0014602883	0.0005968203	C	-12.1344889804	1.6988621564	1.7260239030
O	0.6480923757	-1.6242465857	1.5975720959	C	-13.5122190879	0.0021194609	-0.0001130075
N	-0.6846115376	-0.0014828920	0.0006954360	C	-13.5298686950	-1.6893827268	-1.7210448922
C	-1.3068445583	-0.8842230793	-0.8965388269	H	-11.6378795556	-2.3714688381	-2.4133787484
C	-1.3065930318	0.8814806934	0.8978574484	C	-13.5291120651	1.6930446274	1.7201392883
C	-2.7792868049	-0.8598197430	-0.8718504552	H	-11.6371920708	2.3741395251	2.4129445537
O	-0.6480361527	-1.5985922670	-1.6219572444	C	-14.2233818802	0.8562623274	0.8686750527
C	-2.7790330646	0.8575131565	0.8731565889	C	-14.2223581752	-0.8518610014	-0.8693496579
O	-0.6475955751	1.5953727897	1.6235704144	H	-14.0944410831	-2.3391182288	-2.3827779445
C	-3.4839640032	-0.0010268979	0.0006334031	H	-14.0926690094	2.3433803742	2.3819870091
C	-3.4752481458	-1.6961486622	-1.7218931702	C	-15.7002179528	0.8729647859	0.8857949005
C	-3.4747011267	1.6941256585	1.7231492576	C	-15.6975851624	-0.8617619599	-0.8805290778
C	-4.9082778706	-0.0007218748	0.0005574108	O	-16.3327404363	1.6037139235	1.6299277409
H	-2.9130597041	-2.3474873882	-2.3839686615	N	-16.3413569923	0.0043365490	0.0007918611
C	-4.8689282507	-1.7000273700	-1.7260081279	O	-16.3479097474	-1.5848315536	-1.6170312874
H	-2.9122958035	2.3452767975	2.3852248094	C	-17.7962571180	-0.0187476701	-0.0230976663
C	-4.8683717586	1.6986210289	1.7270946696	H	-18.1543452300	0.2391605578	-1.0226130044
C	-5.6089599012	-0.8712000992	-0.8839026530	H	-18.1549432162	-1.0215892453	0.2209229002
C	-5.6086483757	0.8701179669	0.8848993952	H	-18.1499037874	0.7038867514	0.7096945335
H	-5.3681124173	-2.3747673740	-2.4118006640	N	16.3413563915	-0.0019395130	-0.0002424662
H	-5.3673396940	2.3736410494	2.4127699187	C	17.7962459608	0.0210336668	-0.0249042466
C	-7.0713942206	-0.8671328604	-0.8798278769	H	18.1559273822	1.0181335947	0.2402767885
C	-7.0710799249	0.8668637407	0.8805665982	H	18.1502075024	-0.7173524767	0.6918603374
C	-7.7837401573	0.0000607012	0.0002976881	H	18.1530152472	-0.2155135359	-1.0301546006

TDI$_2$: Singlet Excited State

C	15.6607596319	-0.8916980196	0.8756659543	C	12.1112186596	1.7337171860	-1.7034332065
C	15.6590442304	0.8809685732	-0.8655130665	C	11.3579866365	-0.8849836090	0.8717391144
C	14.1968043335	-0.8717704049	0.8574660429	C	11.3592182432	0.8845854948	-0.8688346871
O	16.3086778346	-1.6347015414	1.6045617406	H	11.6077881079	-2.4194169928	2.3804551738
C	14.1962216197	0.8690149710	-0.8535511991	H	11.6100222165	2.4191871233	-2.3771833538
O	16.3259555186	1.6146255775	-1.5867344507	C	9.9121781891	-0.8797823234	0.8671645523
C	13.4884825016	-0.0012139953	0.0019868308	C	9.9132452570	0.8801278039	-0.8651183183
C	13.4926953690	-1.7271402643	1.6987498091	C	9.1997911519	0.0003232693	0.0007049672
C	13.4946390626	1.7254566008	-1.6951617069	C	9.1667563454	-1.7289036080	1.7036350130
C	12.0602421771	-0.0005678822	0.0017019705	C	9.1687354831	1.7296167673	-1.7019940577
H	14.0597651311	-2.3876940041	2.3475907655	C	7.7618478733	0.0005493002	0.0001203334
C	12.1094232053	-1.7343296856	1.7066410526	C	7.7935527589	-1.7285813657	1.7029549367
H	14.0632043987	2.3854121409	-2.3434833937	H	9.6739998376	-2.4112874268	2.3762642183

H	9.6767259853	2.4119319733	-2.3741375818	H	-5.3482672104	2.3791142276	2.4121656400
C	7.7954873475	1.7297890717	-1.7024533096	C	-7.0537655346	-0.8649994972	-0.8805760440
C	7.0479163705	-0.8783968968	0.8650494599	C	-7.0532771380	0.8675786091	0.8780928817
C	7.0488416381	0.8797051701	-0.8653602695	C	-7.7668570930	0.0012092221	-0.0009538527
H	7.2873460467	-2.4113867936	2.3757875640	C	-7.7955744018	-1.7025636508	-1.7300771921
H	7.2901127802	2.4129251506	-2.3755978087	C	-7.7944664676	1.7049189756	1.7282905378
C	5.6060736134	-0.8833150415	0.8686991762	C	-9.1992534434	0.0009951540	-0.0002991235
C	5.6069384158	0.8848587084	-0.8702894214	C	-9.1706028071	-1.7018791135	-1.7287611142
C	4.8988818717	0.0007937945	-0.0011232101	H	-7.2908258929	-2.3751548704	-2.4126687909
C	4.8595530850	-1.7396335840	1.7099927392	H	-7.2892596398	2.3775555855	2.4104887099
C	4.8611994945	1.7413213189	-1.7121481361	C	-9.1694900838	1.7038230510	1.7282154084
C	3.4658744510	0.0008497619	-0.0017305824	C	-9.9116737344	-0.8650064192	-0.8791809245
C	3.4843456585	-1.7357487120	1.7052916561	C	-9.9109528206	0.8667336134	0.8792950492
H	5.3672527204	-2.4220696229	2.3809812297	H	-9.6752367615	-2.3749613433	-2.4113590173
C	3.4859524848	1.7375404420	-1.7085987327	H	-9.6738017085	2.3766357786	2.4113142152
H	5.3695247649	2.4237934894	-2.3826500182	C	-11.3604525282	-0.8689167569	-0.8827147689
C	2.7708775770	0.8803941834	-0.8664794047	C	-11.3597138666	0.8700619888	0.8843150217
C	2.7700814197	-0.8786010695	0.8624910004	C	-12.0562641408	0.0005223589	0.0012840367
H	2.9218902056	-2.3984268619	2.3561139996	C	-12.1107056326	-1.7006736182	-1.7278504553
H	2.9240818093	2.4003393854	-2.3598105974	C	-12.1096517874	1.7012434821	1.7300250013
C	1.3264592904	0.9128669811	-0.8988804596	C	-13.4768780565	0.0002744359	0.0021707627
C	1.3256732849	-0.9109320570	0.8937450558	C	-13.5018890990	-1.6942955604	-1.7208021700
O	0.6156925386	1.6227761514	-1.5962698912	H	-11.6154242593	-2.3764210611	-2.4150513609
N	0.7150676533	0.0010541317	-0.0027443182	C	-13.5008298185	1.6941257704	1.7244549075
O	0.6142756732	-1.6205222038	1.5908140582	H	-11.6142213740	2.3773115250	2.4168000663
N	-0.6536607382	0.0013705734	-0.0028377634	C	-14.1895787684	0.8519621743	0.8688523889
C	-1.2841723617	-0.8678403689	-0.8854274874	C	-14.1887851364	-0.8521410970	-0.8640773943
C	-1.2837897135	0.8705582198	0.8800525606	H	-14.0695743060	-2.3429203465	-2.3802575703
C	-2.7787714529	-0.8500536439	-0.8670592283	H	-14.0673677460	2.3426638320	2.3848291088
O	-0.6794673855	-1.6005797424	-1.6301032617	C	-15.6745788144	0.8663101329	0.8855114962
C	-2.7783774413	0.8530416429	0.8620799015	C	-15.6718885479	-0.8618174632	-0.8732805400
O	-0.6787506539	1.6036533131	1.6241054107	O	-16.2905125399	1.6011245043	1.6336248115
C	-3.4918716312	0.0015056958	-0.0023384751	N	-16.3174839356	0.0009144265	0.0046224613
C	-3.4626663292	-1.6931366664	-1.7229963652	O	-16.3050651051	-1.5900722463	-1.6137078037
C	-3.4618672401	1.6961452356	1.7183089611	C	-17.7758861946	-0.0228629943	-0.0186186264
C	-4.9116287861	0.0014723551	-0.0019835137	H	-18.1316168849	0.2346981411	-1.0184301891
H	-2.8911682957	-2.3401820946	-2.3803173426	H	-18.1313081997	-1.0253355870	0.2291341030
C	-4.8546745321	-1.6994363438	-1.7288551682	H	-18.1315276039	0.7002803539	0.7122806293
H	-2.8900937034	2.3431417009	2.3754348645	N	16.3004801370	-0.0045113801	0.0026678460
C	-4.8538595247	1.7023497168	1.7248749992	C	17.7519060356	0.0173720153	-0.0217598146
C	-5.6058182254	-0.8677864986	-0.8841997421	H	18.1150261243	1.0141169482	0.2425685981
C	-5.6053533406	0.8706305464	0.8806556759	H	18.1028125139	-0.7227329464	0.6952220684
H	-5.3493668391	-2.3763193116	-2.4158254283	H	18.1112123516	-0.2166103245	-1.0273420539

TDI$_2$: Triplet State

C	15.6572741508	-0.8862073108	0.8749406780	C	12.0485132844	-0.0001573080	0.0033176496
C	15.6557940638	0.8783459744	-0.8582113953	H	14.0570490536	-2.3886758799	2.3522585642
C	14.1843719435	-0.8684636420	0.8579057435	C	12.1072961248	-1.7385776241	1.7130148398
O	16.2883046549	-1.6327325471	1.6076395633	H	14.0620192185	2.3879721215	-2.3429314218
C	14.1844535926	0.8674315519	-0.8485420905	C	12.1102948687	1.7387827801	-1.7066729464
O	16.3053389761	1.6160037593	-1.5839174821	C	11.3480707777	-0.8829365095	0.8712447344
C	13.4745223488	-0.0005256422	0.0043836520	C	11.3498455250	0.8830458564	-0.8658962000
C	13.4862970361	-1.7303533457	1.7051398693	H	11.6067176781	-2.4238360901	2.3867089983
C	13.4893436185	1.7300440808	-1.6969347788	H	11.6106250936	2.4241942011	-2.3808763357

C	9.9180177853	-0.8783178630	0.8659933938	C	-4.8521641000	1.7012942882	1.7218700271
C	9.9197308721	0.8786156099	-0.8630485032	C	-5.5943363181	-0.8693477526	-0.8879037716
C	9.2063847753	0.0001430796	0.0007958951	C	-5.5929362394	0.8724346768	0.8804647204
C	9.1647271936	-1.7400959180	1.7139502598	H	-5.3544796436	-2.3733923128	-2.4154956270
C	9.1678964703	1.7405099621	-1.7122396252	H	-5.3507039655	2.3763350371	2.4078331111
C	7.7677697398	0.0000902166	-0.0005714540	C	-7.0567741243	-0.8657520350	-0.8824664452
C	7.8054931975	-1.7399672353	1.7126262510	C	-7.0553857734	0.8686881567	0.8775137131
H	9.6751549097	-2.4207459631	2.3847950730	C	-7.7685759828	0.0013974135	-0.0018511421
H	9.6794608204	2.4213454834	-2.3820207005	C	-7.7920638971	-1.6940759098	-1.7215921385
C	7.8086584279	1.7403118900	-1.7134822625	C	-7.7892576443	1.6968118500	1.7180836783
C	7.0540798802	-0.8779791922	0.8630471152	C	-9.2012890121	0.0011759300	-0.0004836490
C	7.0556283733	0.8781071834	-0.8655303830	C	-9.1799680138	-1.6944105686	-1.7205417014
H	7.2940653104	-2.4206205250	2.3825682914	H	-7.2910473324	-2.3688724347	-2.4061721519
H	7.2984947997	2.4211052595	-2.3842417672	H	-7.2871060026	2.3716322347	2.4018008559
C	5.6236901979	-0.8824403863	0.8657633864	C	-9.1771513791	1.6967497135	1.7196732614
C	5.6252217281	0.8823155527	-0.8710626260	C	-9.9141818457	-0.8664688990	-0.8802510389
C	4.9227671099	-0.0001620104	-0.0033633478	C	-9.9126267685	0.8685647546	0.8807555068
C	4.8671152624	-1.7390130484	1.7079384794	H	-9.6821997641	-2.3693136586	-2.4042187760
C	4.8700788780	1.7388770423	-1.7145597089	H	-9.6783509166	2.3713895340	2.4043693864
C	3.4955702499	-0.0002918537	-0.0047271279	C	-11.3765953676	-0.8702891407	-0.8831058897
C	3.4886991444	-1.7324294627	1.6999995936	C	-11.3749592602	0.8717268792	0.8866069131
H	5.3683800184	-2.4232664486	2.3818716505	C	-12.0740007572	0.0006515263	0.0026025519
C	3.4916372981	1.7321085384	-1.7091875916	C	-12.1210160147	-1.6976055264	-1.7232780681
H	5.3724945340	2.4233249172	-2.3874336172	C	-12.1182931259	1.6984855041	1.7281823166
C	2.7921770251	0.8712669954	-0.8630753333	C	-13.4970451379	0.0003508752	0.0042362895
C	2.7907188240	-0.8718612919	0.8524028361	C	-13.5157306703	-1.6917844289	-1.7160765013
H	2.9182992262	-2.3909496058	2.3472827308	H	-11.6241444848	-2.3730410282	-2.4103522220
H	2.9223556415	2.3906593402	-2.3574219367	C	-13.5129329668	1.6918558185	1.7239336440
C	1.3233518339	0.8957461603	-0.8886268935	H	-11.6206007568	2.3742690087	2.4143188671
C	1.3218911368	-0.8964580378	0.8753629561	C	-14.2077036017	0.8543434648	0.8735990044
O	0.6664277274	1.6243113926	-1.6044966088	C	-14.2077056926	-0.8543538461	-0.8638769088
N	0.6995867901	-0.0000560334	-0.0068382099	H	-14.0806878021	-2.3421097160	-2.3769010400
O	0.6637595548	-1.6233480788	1.5918198166	H	-14.0760879778	2.3420559051	2.3862528767
N	-0.6695332955	0.0008548155	-0.0068305290	C	-15.6845618655	0.8700474808	0.8925412516
C	-1.2922790255	-0.8821077076	-0.9035858601	C	-15.6829597742	-0.8650597078	-0.8733788594
C	-1.2909248436	0.8842287576	0.8904326847	O	-16.3167479608	1.6010572727	1.6366894965
C	-2.7646748059	-0.8575608906	-0.8780537094	N	-16.3262116026	0.0010447656	0.0083237457
O	-0.6338064292	-1.5964442757	-1.6293283253	O	-16.3337070323	-1.5887526289	-1.6088893464
C	-2.7633441357	0.8602700787	0.8665712284	C	-17.7811243977	-0.0225442030	-0.0140804731
O	-0.6313594601	1.5980769476	1.6156677473	H	-18.1402393442	0.2338557379	-1.0136060146
C	-3.4687836304	0.0014586805	-0.0053008347	H	-18.1393273000	-1.0251326602	0.2317160340
C	-3.4611816176	-1.6941963531	-1.7273604799	H	-18.1342608625	0.7009710524	0.7180988314
C	-3.4584998852	1.6970135928	1.7168674075	N	16.2998292358	-0.0032416599	0.0063283332
C	-4.8931012845	0.0015536144	-0.0042829774	C	17.7546117053	0.0187462519	-0.0174424840
H	-2.8994334208	-2.3457437963	-2.3896057458	H	18.1149040676	1.0153545016	0.2488175457
C	-4.8548610180	-1.6982885208	-1.7303770871	H	18.1075425338	-0.7204978137	0.6990004750
H	-2.8957095992	2.3483456384	2.3784388525	H	18.1118824819	-0.2172694627	-1.0226494588

TDI$_2$: Quintet State

C	15.6431169031	-0.8869539712	0.8665630253	O	16.2883404928	1.6151470191	-1.5931111318
C	15.6396234985	0.8767624625	-0.8674203460	C	13.4593558740	-0.0011656003	-0.0013252372
C	14.1702027167	-0.8689862759	0.8514759438	C	13.4731420028	-1.7304349854	1.6999633536
O	16.2749602270	-1.6328506343	1.5991899921	C	13.4722191780	1.7290341351	-1.7030242051
C	14.1682942176	0.8663833506	-0.8554948038	C	12.0333570018	-0.0004598294	-0.0003747287

H	14.0446442853	-2.3886557502	2.3465270933	C	-4.9075843079	0.0002195871	0.0016395121
C	12.0941490334	-1.7384030281	1.7097192747	H	-2.9045526160	-2.3525112415	-2.3883105885
H	14.0441353788	2.3866389196	-2.3500210815	C	-4.8529663287	-1.7112937060	-1.7370337805
C	12.0931608550	1.7381072085	-1.7108069187	H	-2.9058296033	2.3529893150	2.3926100807
C	11.3339275135	-0.8828657160	0.8687554180	C	-4.8538911070	1.7117726166	1.7402865134
C	11.3336967891	0.8827212037	-0.8687998645	C	-5.6090405125	-0.8683080644	-0.8808175609
H	11.5944020160	-2.4233634634	2.3843244126	C	-5.6095090768	0.8688033127	0.8836595537
H	11.5927308122	2.4234866015	-2.3844704897	H	-5.3545995680	-2.3847796094	-2.4214434117
C	9.9038382138	-0.8779592805	0.8654467123	H	-5.3558886795	2.3853330319	2.4243555158
C	9.9035739880	0.8786164022	-0.8639718752	C	-7.0394670788	-0.8640998997	-0.8769501706
C	9.1912209332	0.0004659213	0.0010257836	C	-7.0399375442	0.8647479621	0.8788879616
C	9.1515046811	-1.7394125281	1.7145591267	C	-7.7526178607	0.0003706275	0.0007301723
C	9.1507964026	1.7404829134	-1.7123166300	C	-7.7914723447	-1.7129058530	-1.7391776491
C	7.7526174575	0.0006840789	0.0015649002	C	-7.7923613791	1.7136865611	1.7406069428
C	7.7922666142	-1.7390588912	1.7150133766	C	-9.1912211551	0.0004920901	0.0002204975
H	9.6626542628	-2.4200502112	2.3848586727	C	-9.1507042950	-1.7128208773	-1.7398176758
H	9.6615733562	2.4210856938	-2.3829288479	H	-7.2805511394	-2.3834007443	-2.4196554324
C	7.7915666490	1.7405398710	-1.7117672878	H	-7.2817812581	2.3841021347	2.4214186115
C	7.0398816232	-0.8771153217	0.8662648314	C	-9.1515975752	1.7138304031	1.7402992624
C	7.0395222771	0.8786471404	-0.8626595708	C	-9.9035319714	-0.8640752098	-0.8783864038
H	7.2816553122	-2.4195351813	2.3857444586	C	-9.9038809094	0.8652128270	0.8783181477
H	7.2806766954	2.4212819059	-2.3820188818	H	-9.6614422910	-2.3831966031	-2.4206819192
C	5.6094442556	-0.8813832483	0.8707307041	H	-9.6627861621	2.3842739612	2.4207664716
C	5.6091041702	0.8830533693	-0.8664216593	C	-11.3336586361	-0.8679892502	-0.8834557807
C	4.9075838049	0.0008420979	0.0023025907	C	-11.3339664083	0.8694009686	0.8822938715
C	4.8537482776	-1.7378007936	1.7138487001	C	-12.0333575789	0.0008863086	-0.0007442902
C	4.8531077132	1.7394698289	-1.7092678526	C	-12.0930940031	-1.7094266832	-1.7394285942
C	3.4803872597	0.0008266520	0.0025508053	C	-12.0942166007	1.7107478073	1.7374280227
C	3.4753201515	-1.7311858648	1.7074191396	C	-13.4593566440	0.0011090543	-0.0012457168
H	5.3556845005	-2.4220416739	2.3872786104	C	-13.4721534024	-1.7005486670	-1.7314834843
C	3.4746874319	1.7327987077	-1.7023792851	H	-11.5926423674	-2.3834813077	-2.4244072956
H	5.3548023371	2.4236883456	-2.3829038271	C	-13.4732094022	1.7020610221	1.7283571629
C	2.7761376886	0.8722515589	-0.8552474853	H	-11.5944908317	2.3848300630	2.4229188026
C	2.7764401812	-0.8706526625	0.8605429103	C	-14.1702366430	0.8543837997	0.8660850419
H	2.9056301390	-2.3896508097	2.3553815331	C	-14.1682624521	-0.8523786430	-0.8694892242
H	2.9047501070	2.3912198872	-2.3501690681	H	-14.0440438432	-2.3470966781	-2.3895523637
C	1.3073504546	0.8968024842	-0.8792912809	H	-14.0447382957	2.3489342915	2.3862499772
C	1.3076596643	-0.8953218456	0.8849803139	C	-15.6431527940	0.8708827332	0.8826082208
O	0.6495441460	1.6240549965	-1.5956598379	C	-15.6395909794	-0.8629284576	-0.8812770937
N	0.6845131644	0.0005788986	0.0027775575	O	-16.2750236796	1.6035269150	1.6284644204
O	0.6500866247	-1.6231465771	1.6009844423	N	-16.2846616625	0.0026545006	-0.0014997001
N	-0.6845139792	0.0003083204	0.0026697688	O	-16.2882793794	-1.5885889391	-1.6197164242
C	-1.3072649361	-0.8818608991	-0.8935196267	C	-17.7394179365	-0.0205760258	-0.0257973421
C	-1.3077468141	0.8823454389	0.8986686244	H	-18.0971213830	0.2348441958	-1.0260859205
C	-2.7760602727	-0.8576794138	-0.8692440190	H	-18.0983100851	-1.0227715461	0.2206778081
O	-0.6493884554	-1.5980420403	-1.6208948072	H	-18.0932436840	0.7038711468	0.7051643980
C	-2.7765188955	0.8580919856	0.8736790682	N	16.2846583430	-0.0042779640	-0.0030965488
O	-0.6502439773	1.5986668537	1.6262432143	C	17.7394146685	0.0179721457	-0.0283476433
C	-3.4803879986	0.0001978193	0.0020420022	H	18.0998300573	1.0146569693	0.2374736006
C	-3.4745434675	-1.7046625961	-1.7299938473	H	18.0932007611	-0.7211457051	0.6877983943
C	-3.4754654907	1.7051035178	1.7340227873	H	18.0956364186	-0.2180562576	-1.0339188268

***N,N*-Dimethyl TDI**: Singlet Ground State

C	-0.6938725205	-2.4150884939	-0.0023441218	C	-1.4282753033	-1.2353683477	-0.0018410235

C	-0.7164156006	0.0011733836	-0.0012957202	C	2.8902021830	1.2435683310	-0.0002142853
C	0.7164502763	0.0012144783	-0.0013057056	C	5.0116287135	0.0023105541	-0.0011534930
C	1.4283774993	-1.2352872972	-0.0020490523	C	5.0291593399	-2.4116221100	-0.0036546137
C	0.6940427588	-2.4150489268	-0.0024634414	H	3.1361215561	-3.3826978236	-0.0046809271
H	-1.1968096706	-3.3752286390	-0.0026442154	C	3.6332822092	2.4235129094	0.0011497937
C	-1.4279879678	1.2378174609	-0.0007409561	C	5.7218541268	1.2214051662	0.0000718509
C	1.4279544323	1.2378989493	-0.0006126688	C	5.7214616655	-1.2166778984	-0.0023240827
H	1.1970382792	-3.3751589699	-0.0028679485	H	5.5936457151	-3.3390942534	-0.0047003139
C	0.6938404416	2.4177465185	-0.0003279369	C	5.0277302830	2.4156036214	0.0012726509
C	-0.6939428018	2.4177067414	-0.0003683504	H	3.1346254942	3.3858146697	0.0021985149
H	1.1968736901	3.3778172029	-0.0000942461	H	5.5911730217	3.3435694135	0.0023428108
H	-1.1970334601	3.3777478070	-0.0000886738	C	-7.1983389543	1.2449108078	0.0001026955
C	-2.8907437479	-1.2406974803	-0.0018290443	C	-7.1965420969	-1.2314142476	-0.0016441580
C	-3.5883486761	0.0016205414	-0.0010919135	N	-7.8394729522	0.0047365128	0.0002219725
C	-3.6343312500	-2.4204306799	-0.0025181257	O	-7.8315148366	2.2874299701	-0.0006402784
C	-2.8902338056	1.2434076122	-0.0005804440	O	-7.8477809906	-2.2628001846	-0.0020489053
C	-5.0115965205	0.0020363001	-0.0009341324	C	7.1983061434	1.2452993293	0.0001644821
C	-5.0289968352	-2.4118997936	-0.0023989483	C	7.1966454290	-1.2310206147	-0.0023005740
H	-3.1359087628	-3.3828724506	-0.0032544327	N	7.8395121542	0.0051593486	-0.0008329443
C	-3.6333738236	2.4233144542	0.0000743172	O	7.8479412286	-2.2623684194	-0.0038725700
C	-5.7218829048	1.2210916726	-0.0001828881	O	7.8314350472	2.2878476640	0.0013886237
C	-5.7213637844	-1.2169941108	-0.0015621166	C	9.2949913097	-0.0260756124	-0.0006150387
H	-5.5934339094	-3.3394024587	-0.0030000421	H	9.6535174875	-0.5632909455	0.8805790659
C	-5.0278217482	2.4153276739	0.0002277347	H	9.6549276910	-0.5481398733	-0.8904916969
H	-3.1347685693	3.3856441901	0.0005165021	H	9.6460815441	1.0039111045	0.0077638817
H	-5.5913160402	3.3432634861	0.0007190022	C	-9.2949635946	-0.0265732720	0.0003700012
C	2.8908435061	-1.2405370930	-0.0023442209	H	-9.6545719005	-0.5519043764	-0.8876366597
C	3.5883811858	0.0018181494	-0.0012526477	H	-9.6537176265	-0.5606173572	0.8834672084
C	3.6344938423	-2.4202293622	-0.0036271004	H	-9.6461115727	1.0034105083	0.0054004313

***N,N*-Dimethyl TDI**: Singlet Excited State

C	-0.6857116870	-2.4344461203	-0.0005529646	C	-5.7040509392	-1.2180803115	-0.0000800264
C	-1.4292903513	-1.2344730145	-0.0004504281	H	-5.5786249930	-3.3469508584	-0.0004633099
C	-0.7166376729	0.0002474988	-0.0003504576	C	-5.0082931107	2.4236745643	0.0002952058
C	0.7166438823	0.0002406755	-0.0003316976	H	-3.1224354896	3.3951966470	0.0002369280
C	1.4292876659	-1.2344761019	-0.0004198353	H	-5.5770774240	3.3482193015	0.0004679092
C	0.6857064404	-2.4344415442	-0.0005281564	C	2.8722785057	-1.2398061975	-0.0003029999
H	-1.1955660779	-3.3903769770	-0.0006124542	C	3.5712486746	0.0005837792	-0.0000879933
C	-1.4290712580	1.2350172628	-0.0002350238	C	3.6241056385	-2.4337532338	-0.0004227855
C	1.4290827416	1.2350045058	-0.0002140863	C	2.8718673782	1.2405407255	-0.0000347572
H	1.1955634053	-3.3903679052	-0.0005669617	C	4.9954650222	0.0008524888	0.0000828661
C	0.6856932169	2.4349997420	-0.0002089815	C	5.0089850279	-2.4228029517	-0.0002521252
C	-0.6856699415	2.4350083134	-0.0002236581	H	3.1228729425	-3.3945348048	-0.0006513609
H	1.1956455533	3.3908702919	-0.0002007924	C	3.6235758664	2.4343760072	0.0001615869
H	-1.1956068413	3.3908885177	-0.0002209691	C	5.7049574096	1.2195562125	0.0002743866
C	-2.8722834886	-1.2397974865	-0.0003714606	C	5.7040539736	-1.2180934059	0.0000391194
C	-3.5712490051	0.0005980639	-0.0001567420	H	5.5786136845	-3.3469717391	-0.0003529019
C	-3.6241006456	-2.4337416108	-0.0004969494	C	5.0082842850	2.4236653397	0.0002915094
C	-2.8718663169	1.2405582304	-0.0000823402	H	3.1224229553	3.3951799139	0.0002422516
C	-4.9954688809	0.0008655248	0.0000006553	H	5.5770660387	3.3482111184	0.0004119162
C	-5.0089848293	-2.4227893885	-0.0003500167	C	-7.1776971351	1.2433174139	0.0003797691
H	-3.1228675229	-3.3945277495	-0.0007153763	C	-7.1756495147	-1.2329471165	0.0000073038
C	-3.6235784560	2.4343854824	0.0001419607	N	-7.8183769098	0.0029786119	0.0005534062
C	-5.7049660022	1.2195660041	0.0002392145	O	-7.8113878257	2.2879590639	0.0004449596

O	-7.8269357750	-2.2667461879	-0.0000929506	H	9.6324829392	-0.5629440135	0.8837775294
C	7.1776914006	1.2433192732	0.0003217579	H	9.6334621459	-0.5540721721	-0.8870496860
C	7.1756614054	-1.2329561769	0.0001582831	H	9.6248229251	1.0015572609	0.0058111710
N	7.8183827127	0.0029811302	0.0006736553	C	-9.2737142358	-0.0284880827	0.0008257557
O	7.8269498139	-2.2667489094	-0.0002042391	H	-9.6333639774	-0.5555571262	-0.8862501236
O	7.8113607574	2.2879680632	0.0002290474	H	-9.6325522048	-0.5615312323	0.8845876961
C	9.2737183329	-0.0284629076	0.0008726030	H	-9.6248392157	1.0015307438	0.0041928032

***N,N*-Dimethyl TDI**: Triplet State

C	-0.6796257050	-2.4431718593	-0.0000009548	C	3.6213802271	-2.4391366881	-0.0001972538
C	-1.4315748601	-1.2329660219	-0.0000195098	C	2.8614850400	1.2390889963	0.0000626398
C	-0.7192994912	-0.0000303055	0.0000074534	C	4.9870758413	0.0007528446	0.0000137430
C	0.7192996000	-0.0000299925	0.0000014229	C	5.0004900057	-2.4269317006	-0.0002004362
C	1.4315751917	-1.2329654871	-0.0000313047	H	3.1200972674	-3.3994545939	-0.0003290406
C	0.6796266820	-2.4431715877	-0.0000050409	C	3.6205479739	2.4394849050	0.0001478327
H	-1.1919781370	-3.3975705627	0.0000471693	C	5.6966989945	1.2183878130	0.0000624691
C	-1.4312586025	1.2330156087	0.0000387051	C	5.6960561357	-1.2169775761	-0.0000572599
C	1.4312584769	1.2330161706	0.0000248574	H	5.5724228221	-3.3494851832	-0.0003195464
H	1.1919797753	-3.3975700153	0.0000462530	C	4.9994778391	2.4277209336	0.0001218697
C	0.6795805860	2.4433037439	-0.0000053263	H	3.1192079662	3.3997545183	0.0002500141
C	-0.6795813731	2.4433034861	0.0000043563	H	5.5704886621	3.3507015029	0.0001644649
H	1.1920259798	3.3976332792	-0.0000724520	C	-7.1693033425	1.2421712657	0.0000820327
H	-1.1920274404	3.3976327519	-0.0000466942	C	-7.1674048884	-1.2317752801	-0.0000074906
C	-2.8619742697	-1.2387760151	-0.0000451833	N	-7.8112150260	0.0031210669	0.0003327277
C	-3.5609470030	0.0003990846	0.0000292094	O	-7.8015431911	2.2873688198	0.0000584601
C	-3.6213806421	-2.4391371508	-0.0001439357	O	-7.8174963929	-2.2660258441	-0.0002222332
C	-2.8614847898	1.2390883539	0.0000836351	C	7.1693033804	1.2421704337	0.0000264307
C	-4.9870757712	0.0007527643	0.0000507189	C	7.1674045551	-1.2317756849	-0.0000978888
C	-5.0004903561	-2.4269318915	-0.0001343020	N	7.8112147394	0.0031204286	0.0002670492
H	-3.1200981378	-3.3994552246	-0.0002522323	O	7.8174958653	-2.2660260131	-0.0004281695
C	-3.6205471917	2.4394845255	0.0001736579	O	7.8015446400	2.2873666906	-0.0001508621
C	-5.6966986498	1.2183880528	0.0001153490	C	9.2665280907	-0.0281067731	0.0003240583
C	-5.6960563433	-1.2169776318	-0.0000081265	H	9.6255005706	-0.5620476857	0.8833947623
H	-5.5724233485	-3.3494852646	-0.0002265022	H	9.6262550422	-0.5536048840	-0.8875867795
C	-4.9994769692	2.4277209822	0.0001732847	H	9.6175675904	1.0019086588	0.0050054437
H	-3.1192066135	3.3997539245	0.0002515312	C	-9.2665287354	-0.0281082567	0.0004456284
H	-5.5704874151	3.3507017737	0.0002184401	H	-9.6261524195	-0.5553078439	-0.8864781721
C	2.8619743336	-1.2387754020	-0.0000744185	H	-9.6256013964	-0.5603574694	0.8845157504
C	3.5609471214	0.0003995864	-0.0000001290	H	-9.6175687815	1.0019136136	0.0032652981

***N,N*-Dimethyl TDI**: Quintet State

C	-0.6958685072	-2.4256368768	0.0000443033	H	1.1998490746	3.3849941605	-0.0000993440
C	-1.4301122129	-1.2368009302	-0.0000202319	H	-1.1998496294	3.3849939627	-0.0001081030
C	-0.7162055056	0.0001928613	-0.0000059197	C	-2.8820101634	-1.2347502786	-0.0000910543
C	0.7162055341	0.0001929593	-0.0000007098	C	-3.5735055599	0.0005571863	-0.0000143265
C	1.4301123383	-1.2368007441	-0.0000255792	C	-3.6451157464	-2.4522080770	-0.0002102050
C	0.6958688395	-2.4256367862	0.0000370503	C	-2.8815459951	1.2354383108	0.0000640915
H	-1.1998212374	-3.3845700834	0.0001083058	C	-5.0054014350	0.0008147962	-0.0000066670
C	-1.4298370251	1.2372281672	0.0000046751	C	-5.0079342293	-2.4497259948	-0.0000788692
C	1.4298369364	1.2372283646	0.0000271882	H	-3.1320457670	-3.4065588036	-0.0003086288
H	1.1998217810	-3.3845699042	0.0001044441	C	-3.6443269180	2.4527006121	0.0001717572
C	0.6957766870	2.4261399891	-0.0000358915	C	-5.7142757592	1.2155777431	-0.0000963336
C	-0.6957769984	2.4261398904	-0.0000485696	C	-5.7136040627	-1.2142520038	0.0000926064

H	-5.5853613134	-3.3677692439	0.0000052285	C	-7.1781834941	1.2394418767	-0.0007187715
C	-5.0070451755	2.4505390426	0.0000383604	C	-7.1763904190	-1.2299621682	0.0006297956
H	-3.1313372545	3.4070798023	0.0002429657	N	-7.8213350400	0.0026633041	0.0002157785
H	-5.5836149876	3.3689684503	-0.0000907903	O	-7.8078045491	2.2918246854	0.0003521405
C	2.8820101866	-1.2347500348	-0.0001089678	O	-7.8236002927	-2.2715401062	-0.0003414828
C	3.5735055567	0.0005574588	0.0000103811	C	7.1781835837	1.2394418038	0.0003450044
C	3.6451156741	-2.4522078563	-0.0003301947	C	7.1763905314	-1.2299621203	-0.0003919646
C	2.8815460130	1.2354385664	0.0001177741	N	7.8213352946	0.0026630955	0.0002451065
C	5.0054014256	0.0008149935	0.0000267781	O	7.8236003153	-2.2715404892	-0.0004465579
C	5.0079341435	-2.4497258172	-0.0003790427	O	7.8078055175	2.2918244775	0.0000160008
H	3.1320455746	-3.4065585143	-0.0005578808	C	9.2764183623	-0.0281276631	0.0002854885
C	3.6443270253	2.4527008583	0.0003129997	H	9.6355160213	-0.5619847603	0.8833809685
C	5.7142757784	1.2155779345	0.0002099633	H	9.6362008775	-0.5536659886	-0.8875967464
C	5.7136040659	-1.2142518283	-0.0001610302	H	9.6269683517	1.0021388225	0.0049116831
H	5.5853611816	-3.3677690512	-0.0006392297	C	-9.2764183492	-0.0281285612	0.0005221647
C	5.0070453108	2.4505392342	0.0003500144	H	-9.6362224556	-0.5560162283	-0.8859380121
H	3.1313374483	3.4070800536	0.0005069920	H	-9.6354926752	-0.5596467522	0.8850551409
H	5.5836152007	3.3689685854	0.0005486740	H	-9.6269681605	1.0021463077	0.0025327524

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