Supporting Information

High-Level Reverse Intersystem Crossing of Charge Transfer Compounds: Fluoresce or Not to Fluoresce?

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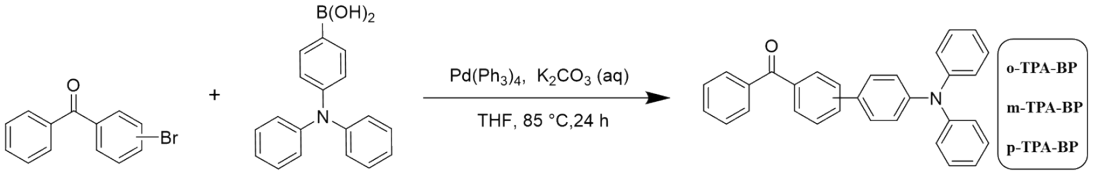
Content

A. Experimental methods

1. Synthesis method

General: All the compounds and solvents were purchased from commercial resources and were used without further purification. The synthesis of *o*, *m*, *p*-TPA-BP was based on the Suzuki- Miyaura cross-coupling reaction. ^{1}H nuclear magnetic resonance (^{1}H NMR) and ^{13}C nuclear magnetic resonance (^{13}C NMR) spectra were recorded in $CDCl_3$ by using an AV-400MHz Ultra Shield NMR (Bruker Biospin, Germany) at 400 MHz for ^{1}H NMR and 101 Hz for ^{13}C NMR. The high-resolution mass spectrometry (HRMS) was carried out by Autoflex speed MALDI TOF/TOF mass spectrometer (Bruker Biospin, Germany).



Scheme S1. The general synthesis method of *o*, *m*, *p*-TPA-BP.

2-[4-(Diphenylamino)phenyl]benzophenone (*o*-TPA-BP):

In a 50 ml sealed tube, 347 mg (1.2 mmol) of 4-(diphenylamine)phenylboronic acid, 261 mg (1.0 mmol) of *o*-bromobenzophenone was dissolved in 10 ml THF, followed by 1 ml of saturated K_2CO_3 aqueous solution. After stirring 24 hours under the N_2, the product was extracted by 5 ml dichloromethane three times, and then the organic layer was washed by 5 ml saturated NH_4Cl three times. The crude product was further purified by silica column chromatography after evaporation. The pale yellow solid was obtained in 57.2% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.62 – 7.55 (m, 2H), 7.51 – 7.43 (m, 2H), 7.29 (d, J = 7.6 Hz, 1H), 7.20 (t, J = 7.8 Hz, 2H), 7.09 (d, J = 6.3 Hz, 1H), 6.98 (t, J = 7.4 Hz, 1H), 6.87 (dd, J = 11.2, 8.2 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.27, 147.52, 147.19, 140.82, 138.85, 137.73, 134.50, 132.39, 130.63, 130.05, 129.84, 129.43, 129.20, 129.14, 127.92, 127.07, 124.02, 123.97, 122.75. HRMS(MALDI-TOF-MS): *m/z* 425.23 (M^+, calcd. 425.18).

3-[4-(Diphenylamino)phenyl]benzophenone (*m*-TPA-BP):

In a 50 ml sealed tube, 347 mg (1.2 mmol) of 4-(diphenylamine)phenylboronic acid, 261 mg (1.0 mmol) of *m*-bromobenzophenone was dissolved in 10 ml THF, followed by 1 ml of saturated K_2CO_3 aqueous solution. After stirring 24 hours under the N_2, the product was extracted by 5 ml dichloromethane three times, and then the organic layer was washed by 5 ml saturated NH_4Cl three times. The crude product was further purified by silica column chromatography after evaporation. The white solid was obtained in 68.9% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.03 (t, J = 1.7 Hz, 1H),

7.89 – 7.85 (m, 2H), 7.77 (ddt, J = 25.2, 7.7, 1.4 Hz, 2H), 7.65 – 7.59 (m, 1H), 7.57 – 7.52 (m, 2H), 7.52 – 7.48 (m, 3H), 7.29 (dd, J = 8.5, 7.2 Hz, 4H), 7.18 – 7.13 (m, 6H), 7.06 (td, J = 7.3, 1.2 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 196.85, 147.74, 147.56, 140.90, 138.18, 137.67, 133.78, 132.56, 130.56, 130.16, 129.40, 128.78, 128.48, 128.39, 128.16, 127.90, 124.64, 123.67, 123.21. HRMS(MALDI-TOF-MS): *m/z* 425.33 (M^+, calcd. 425.18).

4-[4-(Diphenylamino)phenyl]benzophenone (*p*-TPA-BP):

In a 50 ml sealed tube, 347 mg (1.2 mmol) of 4-(diphenylamine)phenylboronic acid, 261 mg (1.0 mmol) of *p*-bromobenzophenone was dissolved in 10 ml THF, followed by 1 ml of saturated K_2CO_3 aqueous solution. After stirring 24 hours under the N_2, the product was extracted by 5 ml dichloromethane three times, and then the organic layer was washed by 5 ml saturated NH_4Cl three times. The crude product was further purified by silica column chromatography after evaporation. Pale yellow solid was obtained in 81.6% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.91 – 7.85 (m, 1H), 7.85 – 7.80 (m, 1H), 7.70 – 7.65 (m, 1H), 7.63 – 7.57 (m, 1H), 7.56 – 7.47 (m, 2H), 7.32 – 7.27 (m, 2H), 7.18 – 7.13 (m, 3H), 7.09 – 7.04 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 196.35, 148.14, 147.44, 144.73, 137.90, 135.61, 133.25, 132.29, 130.85, 129.98, 129.39, 128.30, 127.96, 126.27, 124.79, 123.35, 123.33. HRMS(MALDI-TOF-MS): *m/z* 425.28 (M^+, calcd. 425.18).

2. Steady-state UV-vis spectroscopy

Three molecules were prepared into 10^{-5} M solution of cyclohexane (C-hexane), dichloromethane (DCM), ethyl acetate (EA), Dimethylformamide (DMF), and acetonitrile (ACN). The UV-vis spectra of each sample were recorded by UV-1780 UV-vis spectrophotometer (Shimadzu, Japan).

3. Steady-state photoluminescence spectroscopy

Three molecules were prepared into 10^{-4} M solution of C-hexane, DCM, EA, DMF, and ACN, or doped PMMA film**.** The photoluminescence spectra were measured by Cary Eclipse fluorescence spectrometer (Agilent, USA). The temperature-dependent photoluminescence spectrum of the doped film was measured by FLS1000 Steady State & Time-resolved Photoluminescence Spectrometer (Edinburgh, UK).

4. Transient decay spectroscopy

The transient decay spectra of the 10^{-4} M solution and doped PMMA film of three molecules were measured by FLS1000 Steady State & Time-resolved Photoluminescence Spectrometer (Edinburgh, UK).

5. Phosphorescence spectroscopy

The phosphorescence spectra of the doped PMMA film of *p*-TPA-BP were measured by LP920 transient absorption/emission spectrometer (Edinburgh, UK) with a 355 nm pump beam obtained from the third harmonic output of an Nd:YAG laser. The Phosphorescence spectrum was measured with a delayed gate.

6. Fs-TA spectroscopy

The fs-TA measurement system is constituted from a femtosecond regenerative amplified Ti:sapphire laser system (Coherent, Astrella-Tunable-F-1k) and the fs-TA spectrometer system (Ultrafast Systems, Helios Fire). With the 1-kHz repetition frequency and the 84-fs pulse width at 800 nm, the amplifier has an output power of 7.4 W. The white-light continuum probe pulse was generated a (320-700 nm) in a CaF_2 plate, using approximately 4% from the output of the amplifier. The probe beam was subsequently split into two beams by spectroscope. One probe beam directly passed through the sample, while the other acted as the reference, and was sent directly to the reference detector so that monitored the fluctuations of the probe beam. The instrument response function (IRF) value for the fs-TA system was 120 fs. At each point of the temporal delay, data were collected after averaging for 2 s. and the maximum delay was 8 ns. In this study, the 10^{-5} M solution for three molecules was excited by a 300 nm pump beam. All the sample solutions were tested in a 2 mm path-length cuvette. The spectrometric data were recorded in 3D wavelength-time-absorbance matrices, and the chirp correction was done for all the data before analysis.

The principal components were ensured by singular value decomposition (SVD), and then the global fitting was carried out with the selected principal components and exponential function using the sequential kinetics scheme based on the fs-TA spectra by *Glotaran 1.5.1*.

7. Ns-TA spectroscopy

The ns-TA measurement is based on the pump-probe ns-TA spectrometer system (Ultrafast System, EOS). The pump beam is generated from the femtosecond regenerative amplified Ti:sapphire laser system with a similar configuration to fs-TA measurement, while the probe beam is generated from a photonic crystal fiber-based sub-nanosecond pulsed probe light source. In this study, the 10^{-5} M solution for three molecules was excited by a 300 nm pump beam. All the sample solutions were tested in a 2 mm path-length cuvette. The spectrometric data were recorded in a 3D wavelength-time-absorbance matrix.

The single-wavelength kinetic was extracted from the recorded 3D matrices, and fitting was done by the *Surface Explorer V4.0* based on equation (1).

$$S(t) = e^{-\left(\frac{t - t0}{tp}\right)} \times \sum_{i} A_i e^{-\left(\frac{t - t0}{tp}\right)} \qquad (1)$$

8. DFT & TD-DFT calculation

The optimization of minimal-energy geometries for three molecules in S_0, LE, and CT states and the potential energy surface (PES) scanning were by *Gaussian 16* package based on M062X/6-311G(d,p) level. The PES scanning was conducted by calculating the energy of the geometry with fixing dihedral of the highlight two phenyl rings (Fig. 3) in different states, and the oscillator strength was calculated based on each fixed structure. The relative energy level of singlet state and triplet state, and the spin-orbital coupling matrix element (SOCME) based on the minimal-energy geometries for three molecules in LE state or CT state were calculated by *ORCA 5.0.3* on the level of M062X /6-311G(d,p). The electron-hole distribution was calculated by *Multifwn 3.8*, and the depiction was conducted by *VMD*.

B. Single Crystal Structure

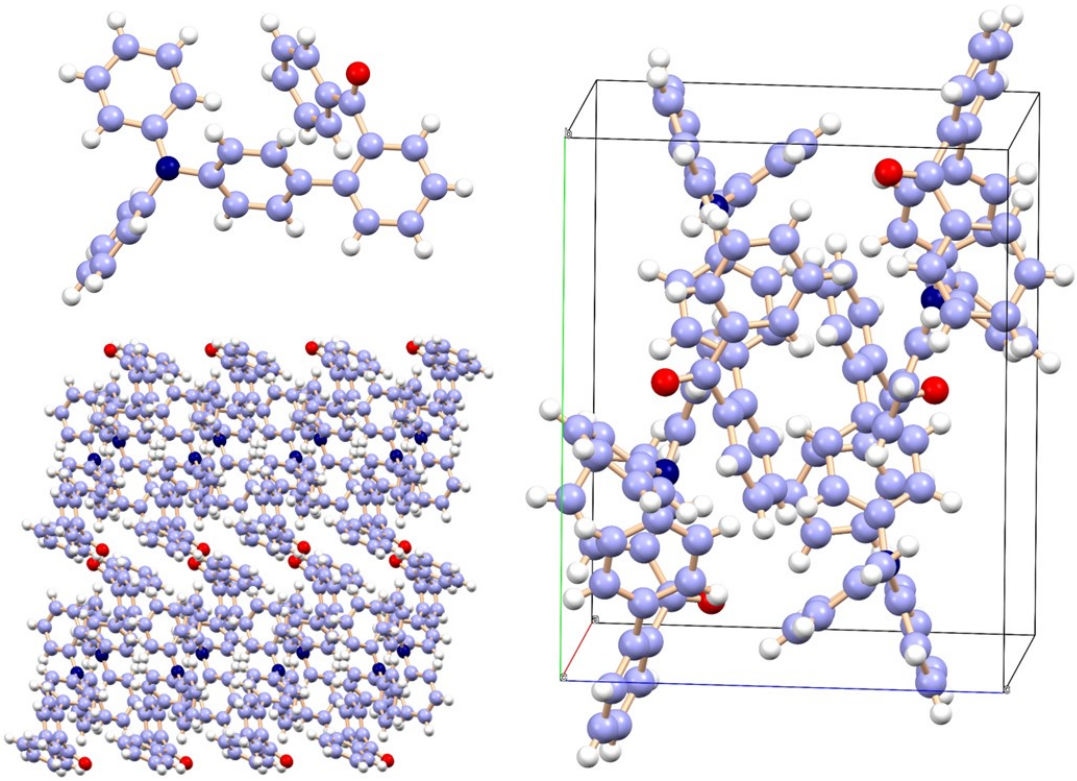


Fig. S1. Single-crystal structure of *o*-TPA-BP

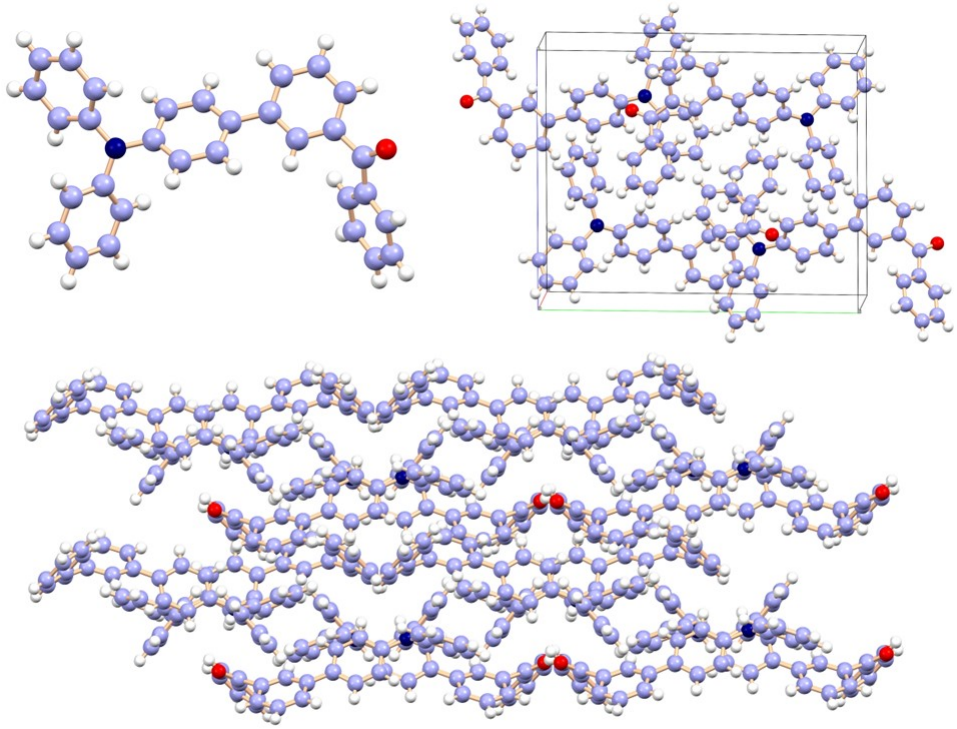


Fig. S2. Single-crystal structure of *m*-TPA-BP

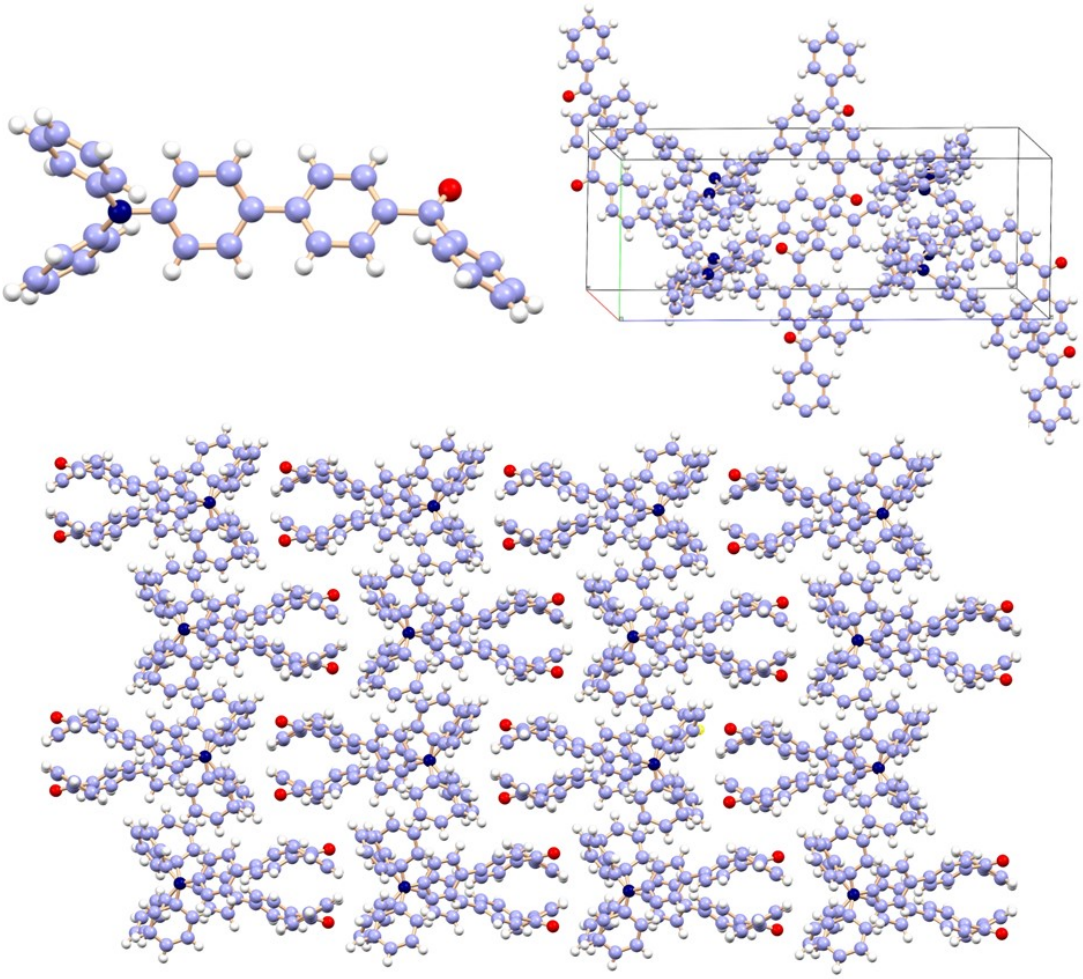


Fig. S3. Single-crystal structure of *p*-TPA-BP

C. Steady-state UV-vis absorption spectra

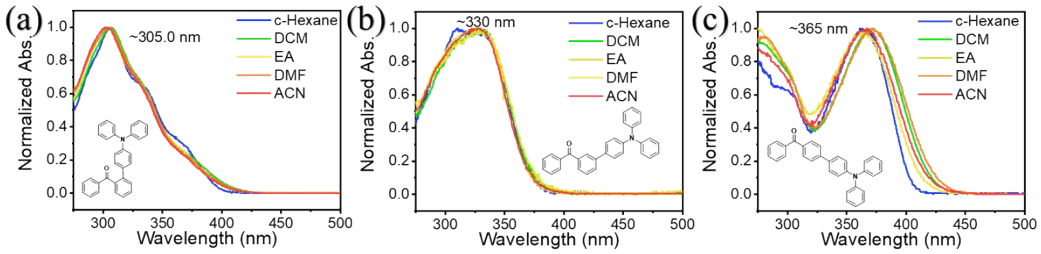


Fig. S4. Steady-state UV-vis absorption spectra of (a)*o*-TPA-BP, (b)*m*-TPA-BP, and (c)*p*-TPA-BP measured in different solvents.

D. Photoluminescence spectra and kinetics

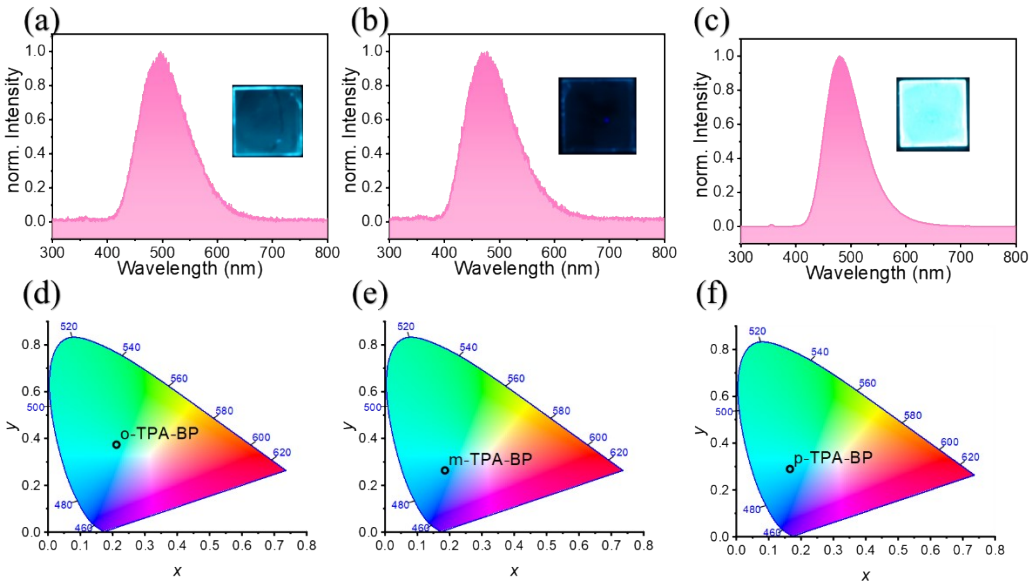


Fig. S5. Steady-state PL spectra of the film state (a) *o*-TPA-BP (Φ=0.11), (b) *m*-TPA-BP(Φ=0.02), and (c) *p*-TPA-BP(Φ=0.42) with 355-nm excitation; CIE 1931 color space of the film state (d) *o*-TPA-BP, (e) *m*-TPA-BP, and (f) *p*-TPA-BP.

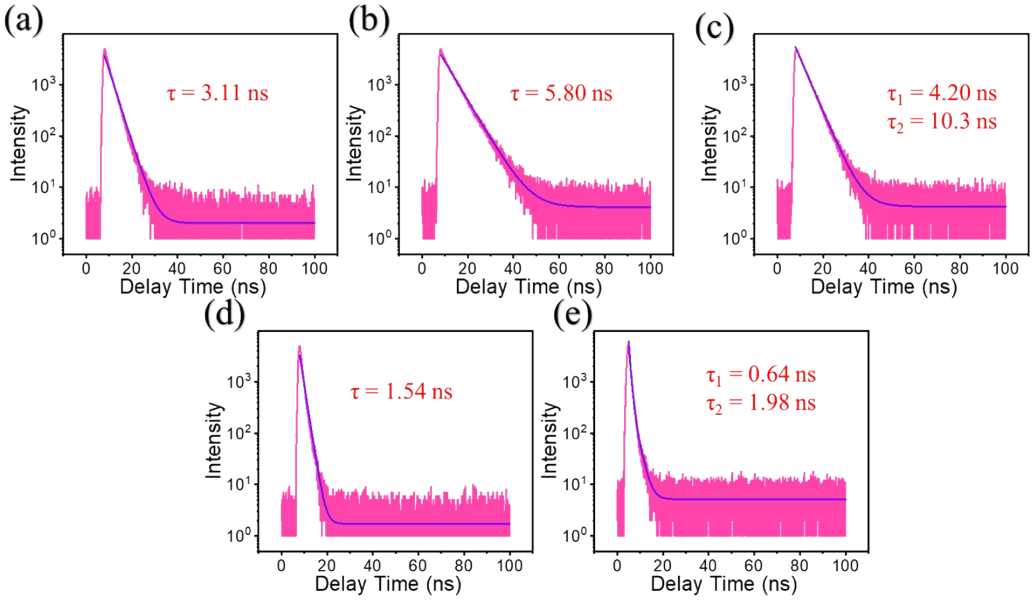


Fig. S6 Kinetic fitting for the transient PL decay curve of the for (a) *o*-TPA-BP (τ = 3.11 ns), (b) *m*-TPA-BP (τ = 5.80 ns), and (c) *p*-TPA-BP (τ_1= 4.20 ns, τ_2= 10.3 ns) measured in DCM. (a) *p*-TPA-BP measured in cyclohexane (τ= 1.54 ns), and (b) *p*-TPA-BP measured in ACN (τ_1= 0.64 ns, τ_2= 1.98 ns)

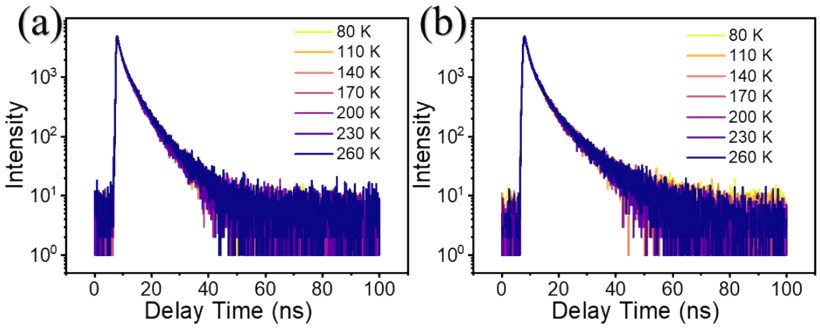


Fig. S7. The photoluminescence decay curves of (a) *o*-TPA-BP and (b) *m*-TPA-BP in different temperatures from 80 K to 260 K at the wavelength of intensity maxima.

E. Fs/ns-TA spectra and kinetic

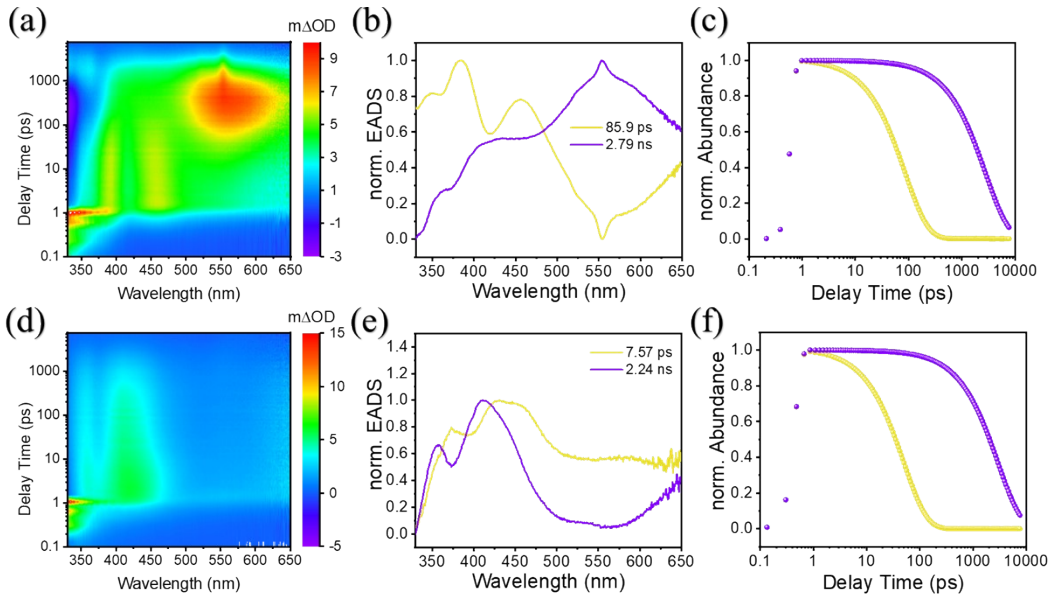


Fig. S8. (a) Fs-TA spectra, (b) normalized EADS obtained from global analysis (RMS=3.7×10^{-4}), and (c) time evolution of the state population (the color of the fitting trace is consistent with the EADS spectra represented in Fig. S8b) of the *o*-TPA-BP measured in cyclohexane; (d)Fs-TA spectra, (e) normalized EADS obtained from global analysis (RMS=2.2×10^{-4}), and (f) time evolution of the state population (the color of the fitting trace is consistent with the EADS spectra represented in Fig. S8e) of the *o*-TPA-BP measured in DCM.

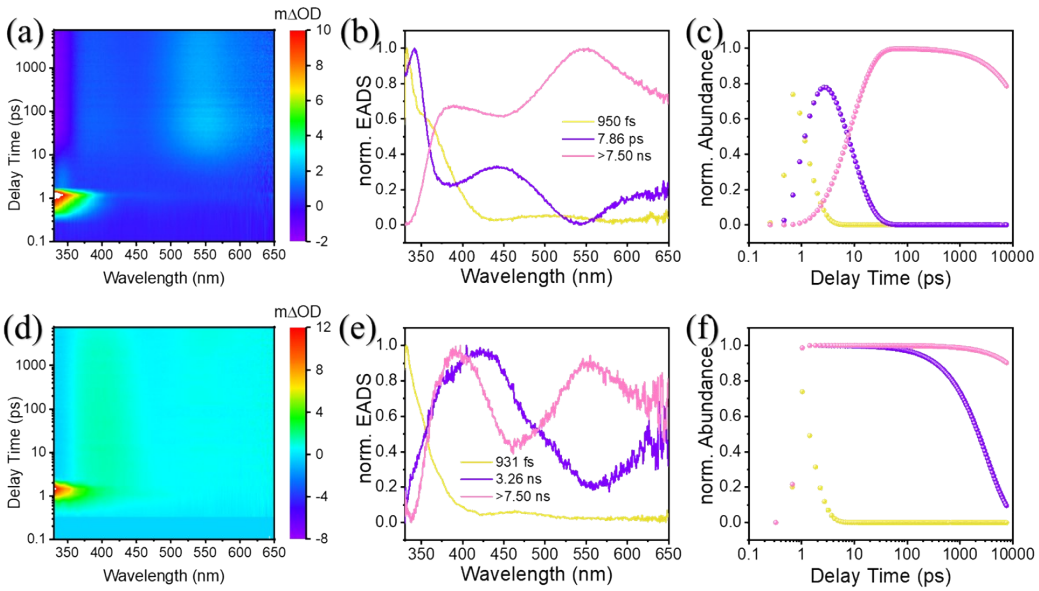


Fig. S9. (a)Fs-TA spectra, (b) normalized EADS obtained from global analysis (RMS=1.9×10^{-4}), and (c) time evolution of the state population (the color of the fitting trace is consistent with the EADS spectra represented in Fig. S9b) of the *m*-TPA-BP measured in cyclohexane; (d)Fs-TA spectra, (e) normalized EADS obtained from global analysis (RMS=1.7×10^{-4}), and (f) time evolution of the state population (the color of the fitting trace is consistent with the EADS spectra represented in Fig. S9e) of the *m*-TPA-BP measured in DCM.

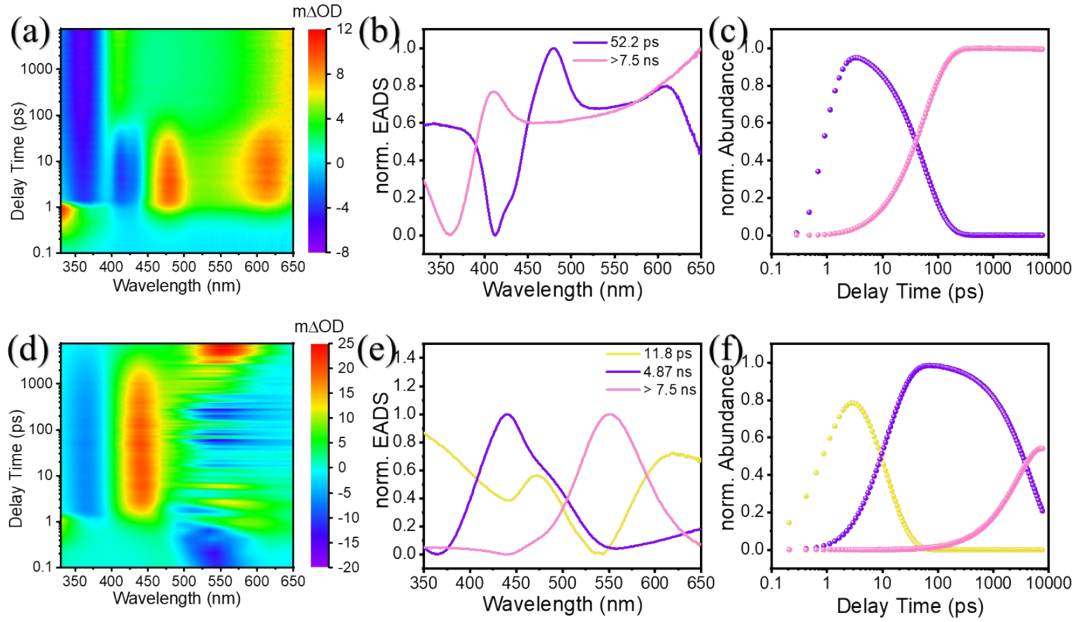


Fig. S10. (a)Fs-TA spectra, (b) normalized EADS obtained from global analysis (RMS=2.1×10^{-4}), and (c) time evolution of the state population (the color of the fitting trace is consistent with the EADS spectra represented in Fig. S10b) of the *p*-TPA-BP measured in cyclohexane; (d)Fs-TA spectra, (e) normalized EADS obtained from global analysis (RMS=2.2×10^{-3}), and (f) time evolution of the state population (the color of the fitting trace is consistent with the EADS spectra represented in Fig. S10e) of the *p*-TPA-BP measured in DCM.

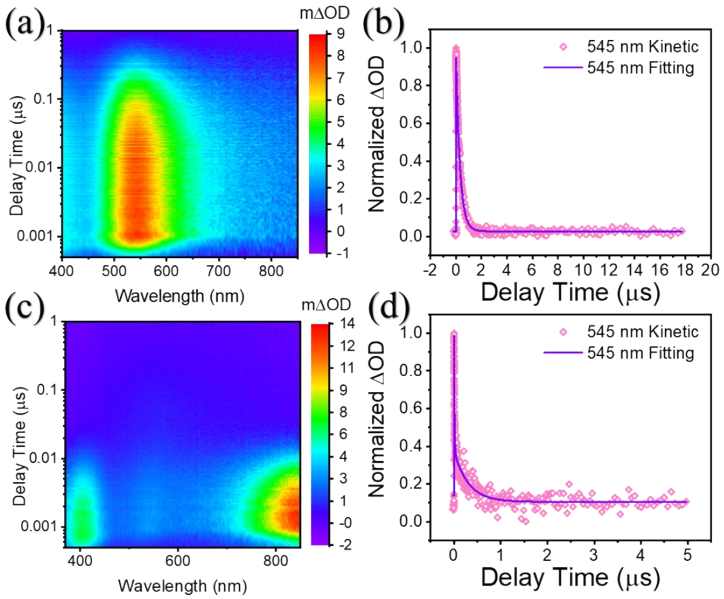


Fig. S11. (a)Ns-TA spectra, and (b) kinetic fitting at 545 nm (τ =315.6 ns) for *m*-TPA-BP measured in cyclohexane; (c) Ns-TA spectra, and (b) kinetic fitting at 545 nm (τ =303.4 ns) for *m*-TPA-BP measured in DCM.

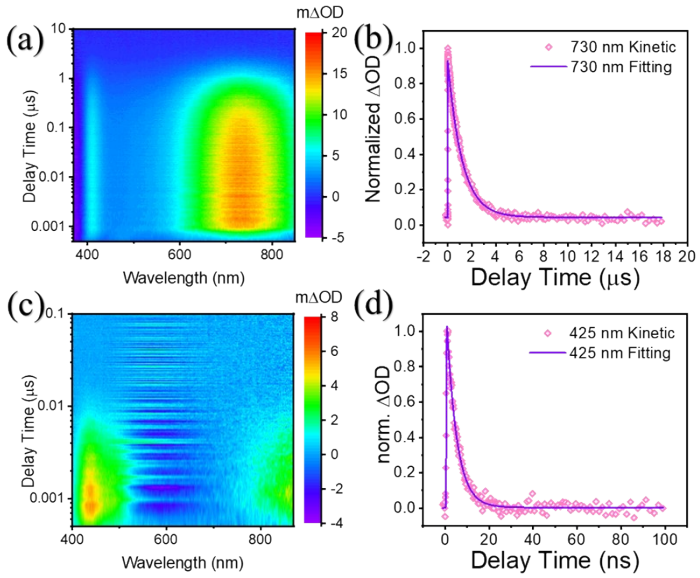


Fig. S12. (a)Ns-TA spectra, (b) kinetic fitting at 425 nm (τ =1.15 μs) for *p*-TPA-BP measured in cyclohexane; (c) Ns-TA spectra, (d) kinetic fitting at 440 nm (τ_1 =4.60 ns, τ_2 =36.2 ns) and for *p*-TPA-BP measured in DCM.

F. DFT calculations and TD-DFT calculations

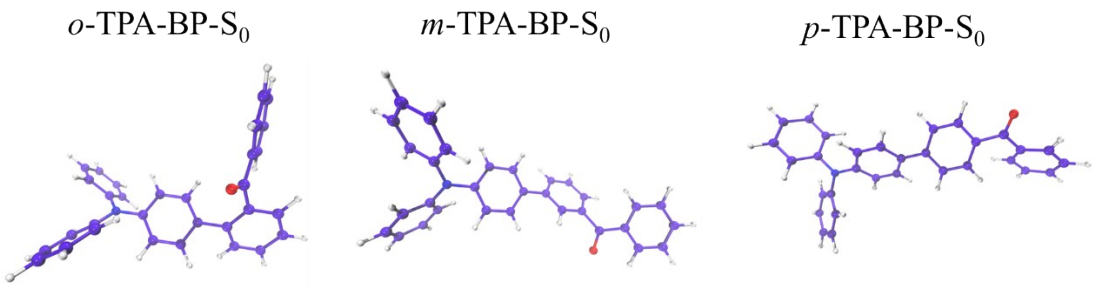


Fig. S13. Minimal-energy geometry of *o*-TPA-BP, *m*-TPA-BP, and *p*-TPA-BP in ground state.

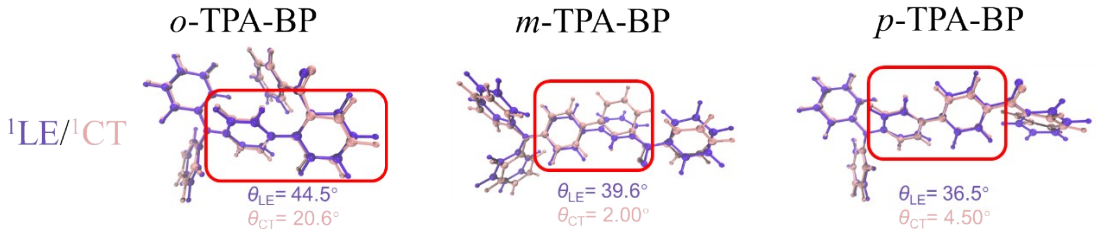


Fig. S14. Comparison of the minimal-energy geometry of *o*-TPA-BP *m*-TPA-BP, and *p*-TPA-BP in LE state and CT state.

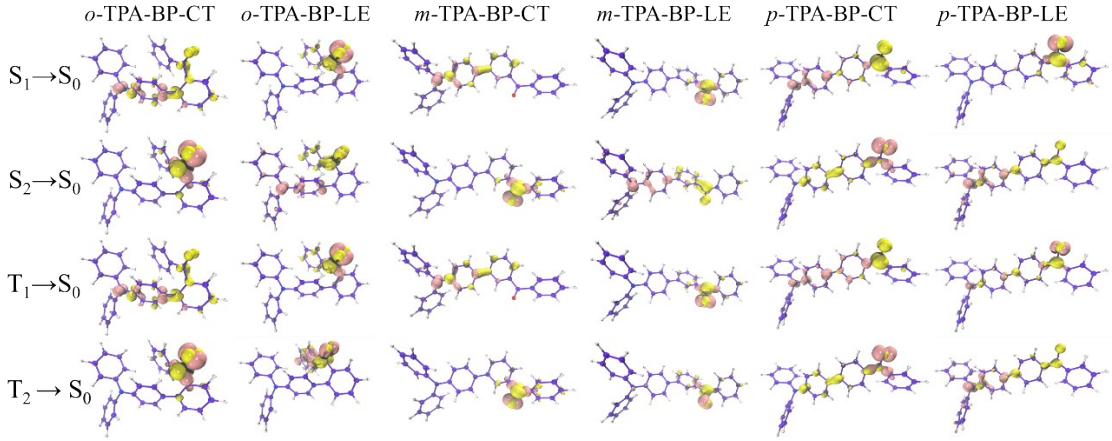


Fig. S15. Electron-hole distribution of the different transitions for *o*-TPA-BP, *m*-TPA-BP, and *p*-TPA-BP in excited state(The pink isosurface represent for electron and yellow isosurface represent for hole, isovalue = 0.005).

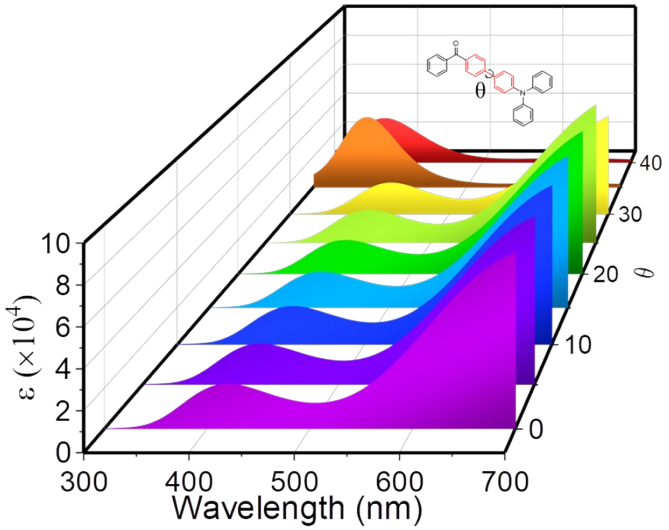


Fig. S16 . TD-DFT simulated excited-state absorption spectra of the CT state with different dihedral between two highlight phenyl rings of *p*-TPA-BP.

Table S1. Vertical absorption energy and the corresponding oscillator strength of *o*-TPA-BP, *m*-TPA-BP, and *p*-TPA-BP based on the S_0 state geometry.

S_0 geometry								
o-TPA-BP			*m*-TPA-BP			*p*-TPA-BP		
Singlet	E_{VA} (eV)	f_{osc}	Singlet	E_{VA} (eV)	f_{osc}	Singlet	E_{VA} (eV)	f_{osc}
S1	3.706	0.004	S1	3.735	0.001	S1	3.707	0.040
S2	4.003	0.334	S2	4.074	0.680	S2	3.885	0.838
S3	4.244	0.127	S3	4.247	0.025	S3	4.258	0.020
S4	4.341	0.124	S4	4.317	0.059	S4	4.456	0.225
S5	4.433	0.237	S5	4.444	0.228	S5	4.76	0.008
S6	4.916	0.053	S6	4.895	0.056	S6	4.878	0.049
S7	4.965	0.059	S7	4.976	0.066	S7	4.975	0.009
S8	5.057	0.013	S8	5.142	0.021	S8	5.013	0.028
S9	5.192	0.016	S9	5.216	0.020	S9	5.208	0.086
S10	5.262	0.055	S10	5.355	0.064	S10	5.242	0.360

Table S2. Vertical emission energy of *o*-TPA-BP, *m*-TPA-BP, and *p*-TPA-BP based on the LE state geometry.

LE geometry											
o-TPA-BP				*m*-TPA-BP				*p*-TPA-BP			
Singlet	E_{VE} (eV)	Triplet	E_{VE} (eV)	Singlet	E_{VE} (eV)	Triplet	E_{VE} (eV)	Singlet	E_{VE} (eV)	Triplet	E_{VE} (eV)
S1	2.996	T1	2.562	S1	3.166	T1	2.64	S1	3.155	T1	2.598
S2	3.499	T2	3.167	S2	3.926	T2	3.19	S2	3.721	T2	2.998
S3	4.103	T3	3.179	S3	4.114	T3	3.326	S3	4.257	T3	3.335
S4	4.318	T4	3.487	S4	4.269	T4	3.579	S4	4.46	T4	3.592
S5	4.449	T5	3.599	S5	4.447	T5	3.673	S5	4.575	T5	3.729
S6	4.715	T6	3.894	S6	4.889	T6	3.819	S6	4.822	T6	3.821
S7	4.828	T7	3.978	S7	4.908	T7	3.835	S7	4.888	T7	4.205
S8	4.911	T8	4.099	S8	4.976	T8	4.145	S8	4.93	T8	4.296
S9	4.932	T9	4.219	S9	4.985	T9	4.304	S9	4.987	T9	4.307
S10	4.973	T10	4.364	S10	5.023	T10	4.328	S10	5.001	T10	4.352

Table S3. Vertical emission energy of *o*-TPA-BP, *m*-TPA-BP, and *p*-TPA-BP based on the CT state geometry.

CT geometry											
o-TPA-BP				*m*-TPA-BP				*p*-TPA-BP			
Singlet	E_{VE} (eV)	Triplet	E_{VE} (eV)	Singlet	E_{VE} (eV)	Triplet	E_{VE} (eV)	Singlet	E_{VE} (eV)	Triplet	E_{VE} (eV)
S1	3.067	T1	2.518	S1	3.355	T1	2.230	S1	3.151	T1	2.211
S2	3.540	T2	3.135	S2	3.738	T2	3.276	S2	3.683	T2	3.198
S3	4.162	T3	3.175	S3	3.813	T3	3.361	S3	3.889	T3	3.463
S4	4.356	T4	3.547	S4	4.170	T4	3.536	S4	4.15	T4	3.544
S5	4.475	T5	3.596	S5	4.299	T5	3.689	S5	4.322	T5	3.636
S6	4.664	T6	3.759	S6	4.740	T6	3.820	S6	4.606	T6	3.777
S7	4.821	T7	3.979	S7	4.798	T7	3.949	S7	4.647	T7	3.855
S8	4.861	T8	4.121	S8	4.951	T8	4.179	S8	4.842	T8	4.132
S9	4.909	T9	4.194	S9	5.022	T9	4.245	S9	4.91	T9	4.154
S10	4.992	T10	4.316	S10	5.205	T10	4.368	S10	5.025	T10	4.333

Table S4. Energy gap between singlet state and triplet state (ΔE_{ST}) and SOCME of *o*-TPA-BP, *m*-TPA-BP, and *p*-TPA-BP based on the LE state geometry.

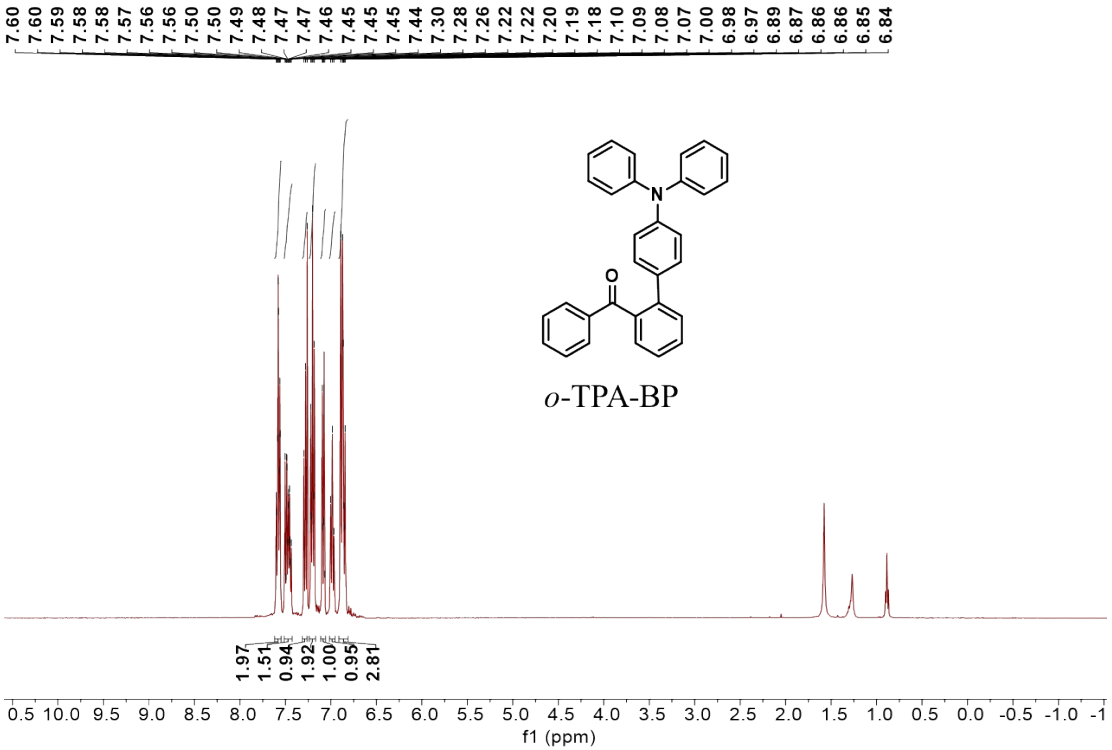
LE geometry			
	S-T	ΔE_{ST} (eV)	SOCME (cm^{-1})
o-TPA-BP	S1-T1 (^{1}LE-^{3}LE)	0.94	4.34
	S1-T2 (^{1}LE-^{3}CT)	-0.05	14.39
	S1-T3	-0.31	27.49
m-TPA-BP	S1-T1 (^{1}LE-^{3}LE)	0.53	13.86
	S1-T2 (^{1}LE-^{3}CT)	-0.02	29.42
	S1-T3	-0.16	23.27
p-TPA-BP	S1-T1 (^{1}LE-^{3}LE)	0.56	16.30
	S1-T2 (^{1}LE-^{3}CT)	0.16	19.45
	S1-T3	-0.18	30.54

Table S5. Energy gap between singlet state and triplet state (ΔE_{ST}) and SOCME of *o*-TPA-BP, *m*-TPA-BP, and *p*-TPA-BP based on the CT state geometry.

CT geometry			
	S-T	ΔE_{ST} (eV)	SOCME (cm^{-1})
o-TPA-BP	S1-T1(^{1}CT-^{3}CT)	0.55	0.25
	S1-T2 (^{1}CT-^{3}LE)	-0.07	2.48
	S1-T3	-0.11	1.99
m-TPA-BP	S1-T1(^{1}CT-^{3}CT)	1.13	0.18
	S1-T2 (^{1}CT-^{3}LE)	0.08	0.34
	S1-T3	-0.01	0.63
p-TPA-BP	S1-T1(^{1}CT-^{3}CT)	1.09	0.42
	S1-T2 (^{1}CT-^{3}LE)	0.01	5.54
	S1-T3	-0.27	3.72

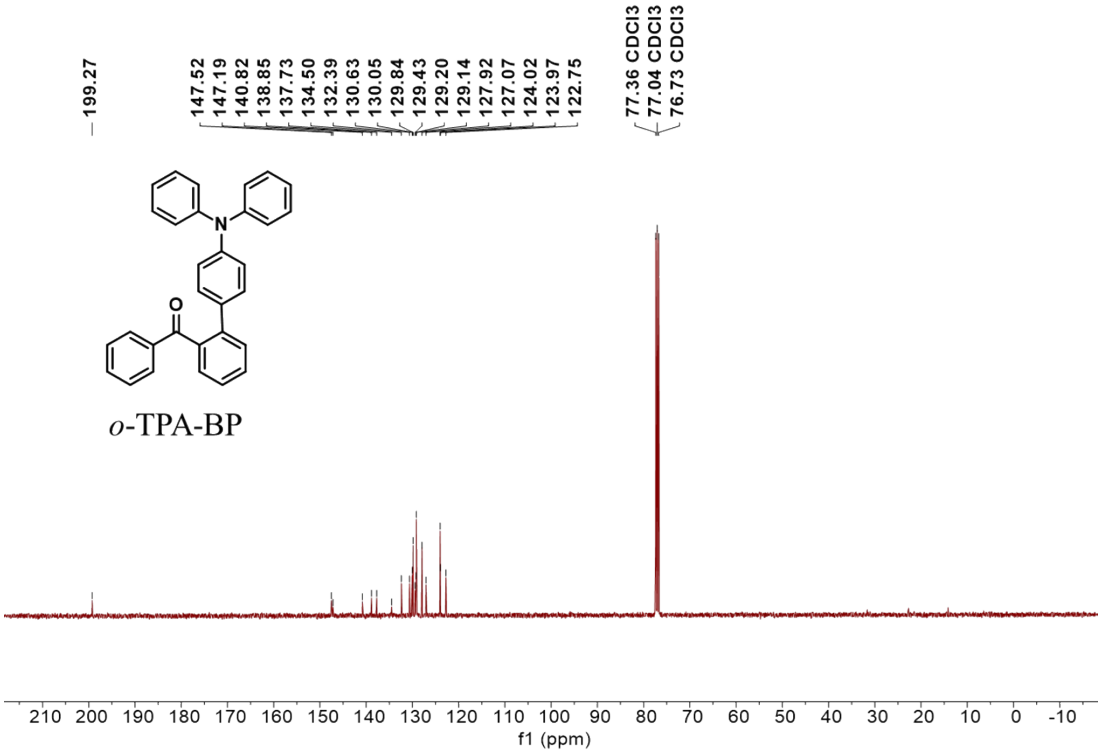
G. ^{1}H NMR and ^{13}C NMR spectra

^{1}H NMR spectra of *o*-TPA-BP:



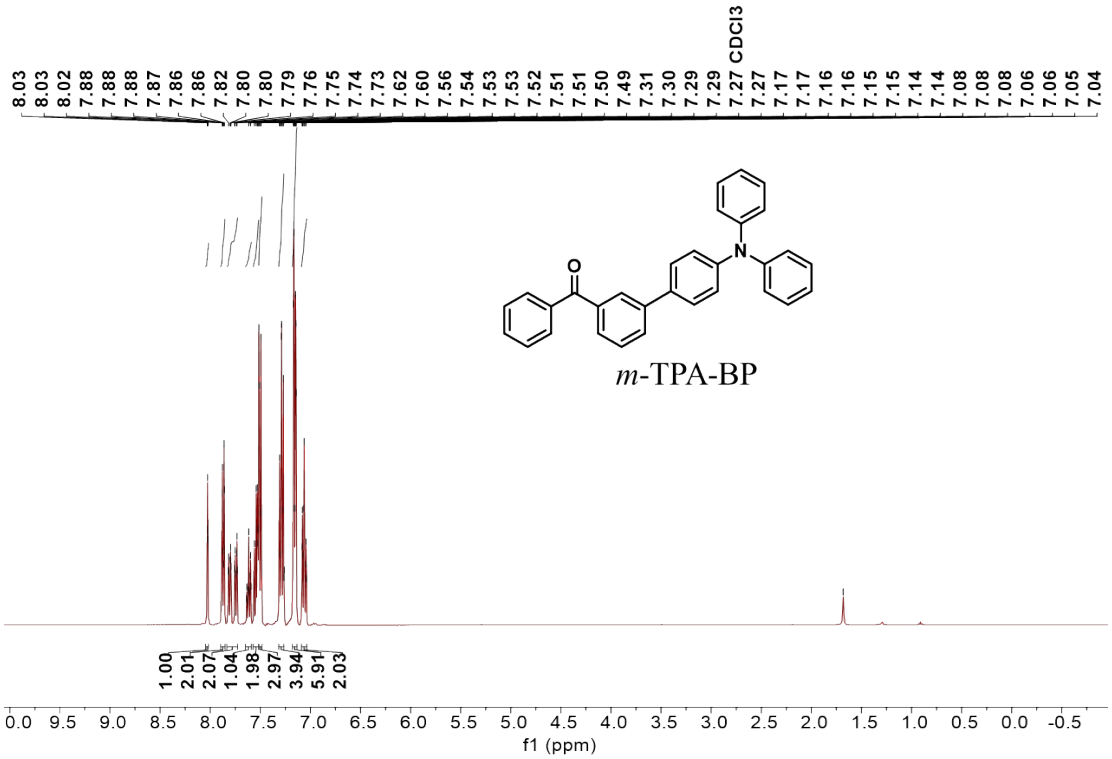
o-TPA-BP

^{13}C NMR spectra of *o*-TPA-BP:

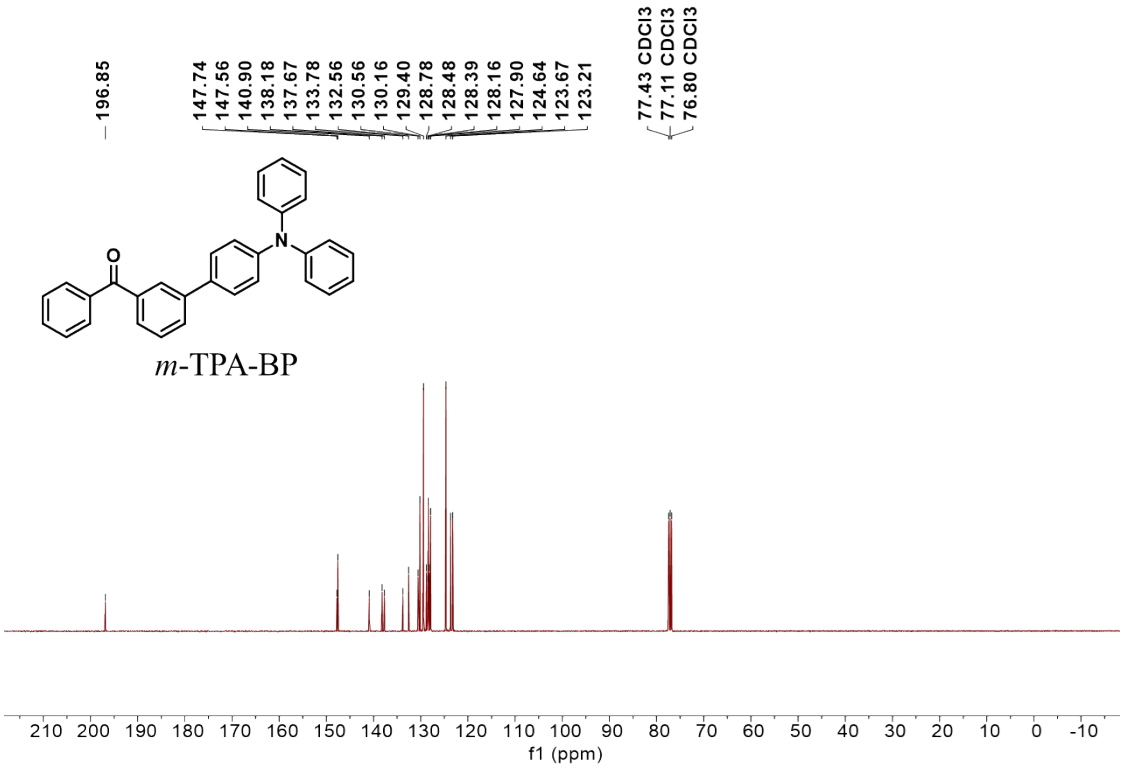


o-TPA-BP

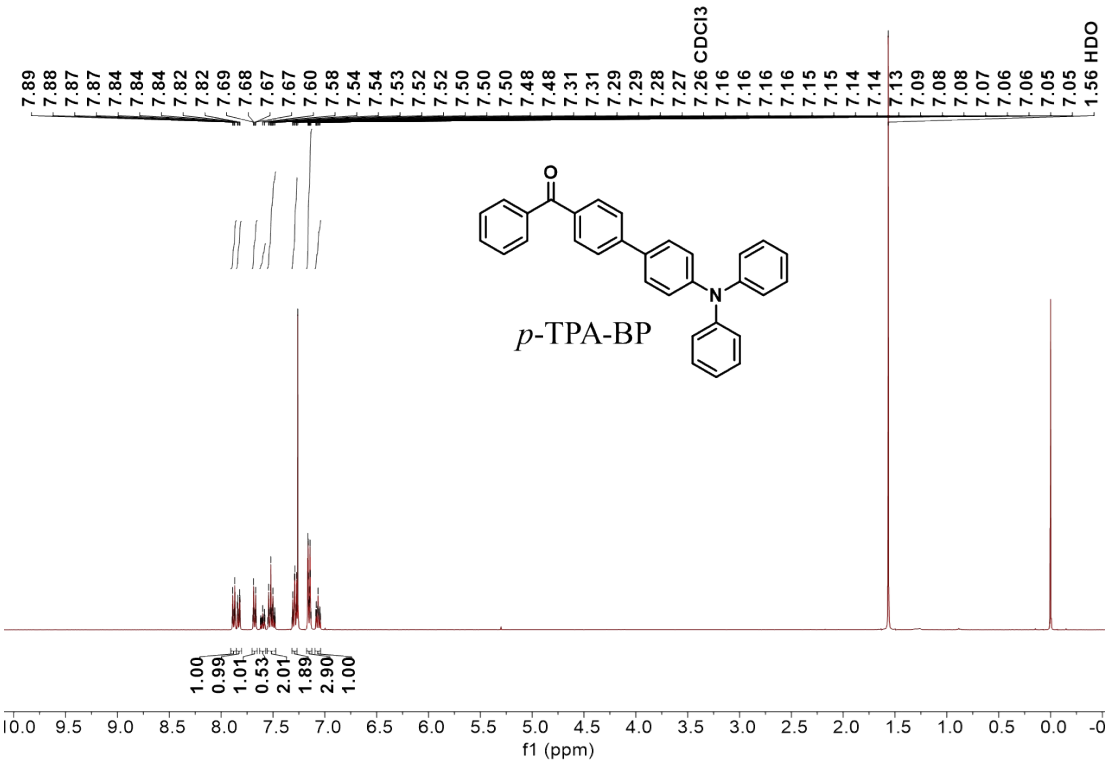
^{1}H NMR spectra of *m*-TPA-BP:



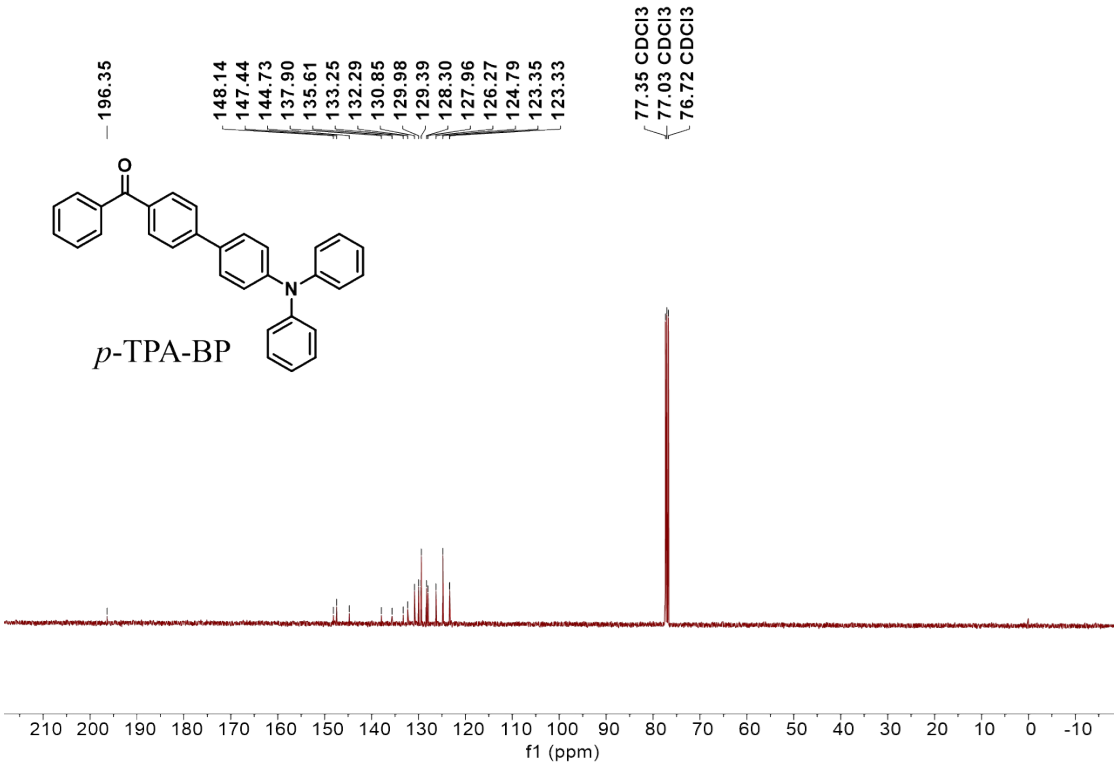
^{13}C NMR spectra of *m*-TPA-BP:



^{1}H NMR spectra of *p*-TPA-BP:



^{13}C NMR spectra of *p*-TPA-BP:



H. XYZ Coordinate

o-TPA-BP S_0:

C	4.69878100	2.81114800	2.45342100
C	4.05692800	1.59071000	2.31127700
C	4.02332900	0.95580900	1.06776900
C	4.62255700	1.56462400	-0.03617100
C	5.25562800	2.79484000	0.10607300
C	5.29907200	3.41423800	1.34974400
H	4.73026500	3.29768000	3.42077700
H	3.56884200	1.10694400	3.14866400
H	4.58507400	1.08273500	-1.00627800
H	5.71374100	3.26882000	-0.75344400
H	5.79754200	4.37004300	1.46027900
C	3.28118100	-0.34412500	0.96019200
O	2.54007900	-0.71093600	1.83941400
C	3.50701200	-1.19959300	-0.25962400
C	2.43123900	-1.69825600	-1.01092400
C	4.81115100	-1.59947200	-0.55149700
C	2.70377900	-2.60721500	-2.03657800
C	5.06264300	-2.51473400	-1.56534000
H	5.63015700	-1.20558100	0.04103200
C	4.00177300	-3.02026900	-2.30773500
H	1.88119600	-2.97461200	-2.63985500
H	6.07770600	-2.83017700	-1.77283700
H	4.18547900	-3.72701200	-3.10817100
C	1.03484300	-1.25403900	-0.77849200
C	0.71861400	0.10132200	-0.66108700
C	-0.00379300	-2.18273500	-0.70070600
C	-0.58642400	0.51770400	-0.45647800
H	1.50703000	0.84462100	-0.72736100
C	-1.31534500	-1.77630600	-0.50764500
H	0.22136800	-3.24062300	-0.77704400
C	-1.62080300	-0.41945100	-0.37621100
H	-0.81480600	1.57214500	-0.35856400
H	-2.11124000	-2.50851200	-0.44220600
N	-2.95455300	-0.00361100	-0.15748400
C	-3.44440400	1.16871700	-0.78047100
C	-3.10073300	1.46145300	-2.10349600
C	-4.27711100	2.04753700	-0.08182000
C	-3.57620700	2.61679900	-2.70877800
H	-2.45824500	0.77892300	-2.64704100
C	-4.76131000	3.19134000	-0.70212400

H	-4.54090000	1.82415400	0.94501700
C	-4.41202400	3.48647700	-2.01584200
H	-3.30072100	2.83054500	-3.73475900
H	-5.40614700	3.86293500	-0.14773800
H	-4.78648000	4.38310800	-2.49370700
C	-3.78823400	-0.74240200	0.71753300
C	-5.13475500	-0.94615000	0.40383700
C	-3.27359500	-1.27529600	1.90257400
C	-5.95086400	-1.66370400	1.26789300
H	-5.53227200	-0.53507300	-0.51658100
C	-4.09417600	-2.00653400	2.75098300
H	-2.23013600	-1.11549000	2.14765600
C	-5.43659800	-2.20196800	2.44306500
H	-6.99325900	-1.81333700	1.01249400
H	-3.68137700	-2.41491800	3.66578400
H	-6.07450000	-2.76736000	3.11090000

o-TPA-BP LE:

C	-1.28863400	3.58734200	0.88443900
C	-2.17961400	2.92473500	0.05668400
C	-2.68504900	1.65871500	0.42114700
C	-2.25399800	1.08281000	1.63411000
C	-1.35236400	1.75358500	2.44169800
C	-0.86233400	3.01004100	2.07947300
H	-0.92395000	4.56639000	0.59435700
H	-2.50063500	3.37551200	-0.87434400
H	-2.63892100	0.11595600	1.93554700
H	-1.02995800	1.29566300	3.36961400
H	-0.16118600	3.52944500	2.72119500
C	-3.60745100	0.98255900	-0.44591900
O	-4.03756400	1.48335200	-1.55140000
C	-4.08100600	-0.43195900	-0.32325700
C	-3.17382500	-1.51528900	-0.26954000
C	-5.46192000	-0.66401200	-0.28685000
C	-3.69970100	-2.79648800	-0.06467300
C	-5.95539700	-1.94500200	-0.11052100
H	-6.13161800	0.18348300	-0.36438200
C	-5.06749100	-3.01259800	0.01132800
H	-3.01595500	-3.63611900	-0.01416600
H	-7.02405900	-2.11268900	-0.06103100
H	-5.44448300	-4.01932600	0.14618100
C	-1.71658500	-1.31395000	-0.37662100
C	-1.17033400	-0.45671900	-1.34016900
C	-0.84972000	-1.93190300	0.52847900

C	0.18360200	-0.18715000	-1.36113100
H	-1.81965400	0.00595700	-2.07496200
C	0.50901000	-1.65861900	0.52295800
H	-1.25553100	-2.58633000	1.29248700
C	1.03678500	-0.75911900	-0.40725200
H	0.59624700	0.48738100	-2.10144300
H	1.16131800	-2.10819900	1.26157700
N	2.39738200	-0.39570600	-0.37918000
C	2.75091600	0.96986400	-0.53526700
C	1.93507100	1.97622000	-0.01070800
C	3.92319400	1.31550700	-1.21207800
C	2.29159000	3.30852100	-0.17031700
H	1.02169900	1.71685500	0.51349400
C	4.27671500	2.65068800	-1.35191300
H	4.55019400	0.53154400	-1.62037000
C	3.46302900	3.65484300	-0.83583300
H	1.64780500	4.07651500	0.24238300
H	5.18817200	2.90705700	-1.87875700
H	3.73918000	4.69541800	-0.95290600
C	3.37929200	-1.34128300	0.00333300
C	4.40325200	-0.99186200	0.88746300
C	3.32830900	-2.64236100	-0.50530600
C	5.36180100	-1.93020200	1.24750200
H	4.44185000	0.01520300	1.28485900
C	4.28153500	-3.57707300	-0.12605600
H	2.53718000	-2.90875700	-1.19632600
C	5.30585300	-3.22705900	0.74835900
H	6.15080000	-1.64613600	1.93368500
H	4.23057600	-4.58179000	-0.52852800
H	6.05256600	-3.95660500	1.03591400

o-TPA-BP CT:

C	-1.42386100	3.52884600	0.67361800
C	-2.29209200	2.81629000	-0.14232200
C	-2.82638500	1.60044800	0.28511100
C	-2.49879100	1.11421100	1.55130900
C	-1.63307200	1.82970900	2.37065500
C	-1.09023500	3.03471800	1.93203200
H	-1.01608400	4.47339500	0.33250300
H	-2.57996700	3.18877300	-1.11804900
H	-2.92719900	0.18208600	1.89985700
H	-1.38817500	1.45112300	3.35577800
H	-0.41578200	3.59029400	2.57436300
C	-3.79123500	0.90299200	-0.63893400

O	-4.39094300	1.55894200	-1.47121400
C	-4.05736700	-0.55134500	-0.47888200
C	-3.06441900	-1.53828700	-0.09892900
C	-5.39095500	-0.92891800	-0.61486400
C	-3.56968000	-2.80699000	0.35127700
C	-5.82684800	-2.19830700	-0.26333800
H	-6.09429400	-0.17463000	-0.94776200
C	-4.89725900	-3.12695100	0.25623800
H	-2.87422400	-3.56522900	0.68579600
H	-6.87357800	-2.46036900	-0.34792000
H	-5.23354600	-4.11006400	0.56370200
C	-1.67636700	-1.33167500	-0.24145900
C	-1.12455800	-0.34146000	-1.15380800
C	-0.69776600	-2.09885800	0.52282500
C	0.19591600	-0.05365500	-1.19189600
H	-1.78990700	0.14132900	-1.85896900
C	0.62378000	-1.79392500	0.49961000
H	-1.03916600	-2.86476400	1.20526900
C	1.12233500	-0.73194800	-0.32295900
H	0.58086900	0.66581300	-1.90484900
H	1.31457400	-2.32272800	1.14577100
N	2.44646700	-0.33237600	-0.26146500
C	2.77501300	1.04117400	-0.39051000
C	1.93034500	2.01010800	0.16114800
C	3.92799200	1.43106900	-1.07981100
C	2.24226100	3.35467000	0.01811700
H	1.03753200	1.70607700	0.69579200
C	4.23150600	2.77818600	-1.20607300
H	4.57110700	0.67542300	-1.51473900
C	3.39158800	3.74672600	-0.66070800
H	1.58213700	4.09683500	0.45113200
H	5.12372000	3.07422400	-1.74437400
H	3.63170700	4.79725800	-0.76676600
C	3.47142500	-1.27992000	-0.01394600
C	4.52354800	-0.97516900	0.85490000
C	3.41996800	-2.53280000	-0.63139900
C	5.51391400	-1.91640100	1.09387500
H	4.55177900	-0.00584900	1.33774900
C	4.41218500	-3.46914200	-0.37691600
H	2.60456700	-2.75419400	-1.30974500
C	5.46337800	-3.16662900	0.48299400
H	6.32457100	-1.67551700	1.77081200
H	4.36846100	-4.43618000	-0.86300800
H	6.23760200	-3.89861600	0.67590700

m-TPA-BP S_0:

C	-8.62187600	-0.57338000	-1.37879400
C	-7.32512800	-1.04860100	-1.25157200
C	-6.33605500	-0.24740100	-0.67808700
C	-6.65105900	1.04783100	-0.26414300
C	-7.94687700	1.52991000	-0.41182900
C	-8.93368500	0.71731800	-0.95845100
H	-9.38952600	-1.20337400	-1.81152300
H	-7.05262300	-2.03949100	-1.59416200
H	-5.87974000	1.68614200	0.15021000
H	-8.18480500	2.54037700	-0.10245300
H	-9.94504300	1.09156500	-1.06442400
C	-4.94102300	-0.79511200	-0.61463100
O	-4.57091200	-1.61276900	-1.42635800
C	-4.00636900	-0.32395600	0.46072000
C	-2.64037600	-0.34531000	0.18444500
C	-4.45303000	0.05749600	1.72645500
C	-1.70531400	0.03731400	1.14529500
H	-2.32120400	-0.65156800	-0.80518700
C	-3.52839200	0.42122900	2.69885400
H	-5.51131100	0.04533100	1.95765700
C	-2.17069200	0.41976200	2.40921100
H	-3.86739600	0.69627700	3.69029300
H	-1.45594500	0.68941900	3.17861900
C	-0.25547100	0.03314900	0.83841300
C	0.58564100	1.04051500	1.31907700
C	0.31262000	-0.97627900	0.05621900
C	1.94268400	1.04042600	1.03763600
H	0.16937800	1.84689500	1.91256700
C	1.66587000	-0.97818400	-0.24316900
H	-0.31328200	-1.77893600	-0.31725300
C	2.50032900	0.03122800	0.24681500
H	2.57928900	1.83042400	1.41759000
H	2.08789400	-1.76787500	-0.85305100
N	3.88051400	0.03535900	-0.05346100
C	4.59887300	-1.18387100	-0.11822000
C	5.55127500	-1.38931000	-1.11991500
C	4.36494800	-2.19277000	0.81990200
C	6.26061500	-2.58163800	-1.17320700
H	5.73064300	-0.60809300	-1.84899400
C	5.06691100	-3.38845400	0.74724500
H	3.62922100	-2.03196100	1.59902500
C	6.02096800	-3.58949100	-0.24503400

H	6.99647100	-2.72715700	-1.95513100
H	4.87429400	-4.16270800	1.48038700
H	6.57098200	-4.52090700	-0.29443200
C	4.54520700	1.25797700	-0.31861600
C	3.92263200	2.25175800	-1.07857600
C	5.83373800	1.48088900	0.17422100
C	4.57723200	3.45013000	-1.32959000
H	2.92574000	2.07693100	-1.46559600
C	6.48679800	2.67556700	-0.09743200
H	6.31563700	0.71041200	0.76439800
C	5.86295600	3.66868100	-0.84556300
H	4.08216100	4.21201900	-1.91994200
H	7.48613400	2.83458100	0.29003500
H	6.37303800	4.60179400	-1.04961900

m-TPA-BP LE:

C	8.59220300	0.68182800	-1.49445900
C	7.26866700	1.07310600	-1.35841700
C	6.35308200	0.25145600	-0.67847900
C	6.79485700	-0.98064200	-0.16573900
C	8.12309700	-1.35168800	-0.29927000
C	9.02993800	-0.52552000	-0.96038600
H	9.28765600	1.32866000	-2.01595200
H	6.93729000	2.02310400	-1.75837800
H	6.08958500	-1.65016300	0.30990700
H	8.45028400	-2.30374000	0.10170400
H	10.06533900	-0.82538400	-1.06345500
C	4.95494600	0.66361500	-0.56140600
O	4.51031600	1.48871200	-1.45458300
C	4.00294900	0.23793300	0.46639700
C	2.62755300	0.26017300	0.18860100
C	4.43835100	-0.15350200	1.74341300
C	1.69223600	-0.11879800	1.15093600
H	2.29180200	0.53436600	-0.80424600
C	3.50796500	-0.54432700	2.69261700
H	5.49166800	-0.12248300	1.99034000
C	2.14606000	-0.53040600	2.40753400
H	3.84734900	-0.83920100	3.67860400
H	1.42933400	-0.80673700	3.17177300
C	0.24314500	-0.09184000	0.83903000
C	-0.61035800	-1.10082600	1.29382500
C	-0.31241500	0.94235200	0.08077900
C	-1.96683500	-1.07815800	1.01038500
H	-0.20341300	-1.92491700	1.86897100

C	-1.66499200	0.96695100	-0.22142200
H	0.32334600	1.74745600	-0.27018300
C	-2.51164700	-0.04396200	0.24323400
H	-2.61326700	-1.86936000	1.37081800
H	-2.07718100	1.77616200	-0.81218400
N	-3.89183600	-0.02398600	-0.05799000
C	-4.59554500	1.20481400	-0.08987400
C	-5.54753300	1.44754000	-1.08365600
C	-4.34708100	2.18682100	0.87287300
C	-6.24170100	2.64974600	-1.10522100
H	-5.73845800	0.68730500	-1.83174300
C	-5.03385800	3.39272600	0.83196200
H	-3.61197100	1.99705300	1.64603200
C	-5.98723700	3.63089600	-0.15269300
H	-6.97735300	2.82415400	-1.88142500
H	-4.83003900	4.14560500	1.58411100
H	-6.52547900	4.57015000	-0.17731200
C	-4.57107500	-1.23167800	-0.35272600
C	-3.96012700	-2.21421400	-1.13637600
C	-5.86206800	-1.45141000	0.13510200
C	-4.62860400	-3.39859100	-1.41567700
H	-2.96105900	-2.04201700	-1.51891800
C	-6.52896300	-2.63162500	-0.16473600
H	-6.33477700	-0.68994200	0.74408800
C	-5.91675100	-3.61372900	-0.93660800
H	-4.14235900	-4.15198900	-2.02398400
H	-7.52995100	-2.78834100	0.21939400
H	-6.43756300	-4.53578900	-1.16261800

m-TPA-BP LE:

C	8.63756700	1.23107000	-0.59699800
C	7.34838300	1.50163500	-0.16238300
C	6.33829400	0.55133600	-0.32108100
C	6.62474600	-0.66064600	-0.95113400
C	7.91278600	-0.92160900	-1.40548600
C	8.92078200	0.01787800	-1.21949800
H	9.42139100	1.96606600	-0.45887900
H	7.09777700	2.44817000	0.30103200
H	5.83717700	-1.38926300	-1.10339500
H	8.12855200	-1.85796400	-1.90570300
H	9.92608900	-0.19146900	-1.56567800
C	4.95082400	0.92102800	0.11850700
O	4.60893300	2.08307700	0.11551900
C	4.00190300	-0.15652400	0.54867700

C	2.65677600	0.08587400	0.37856800
C	4.44547500	-1.34763900	1.16527800
C	1.65320900	-0.85907800	0.77654200
H	2.38699800	1.03569300	-0.06141800
C	3.48893900	-2.28022400	1.59040100
H	5.49939600	-1.51932100	1.33888900
C	2.14527300	-2.06330700	1.40258500
H	3.81533700	-3.19140300	2.07820900
H	1.45177400	-2.82058800	1.73894500
C	0.28136000	-0.62033800	0.57167900
C	-0.75052100	-1.55948000	1.01124100
C	-0.21443000	0.58202100	-0.09662600
C	-2.06945600	-1.33193200	0.80658200
H	-0.46597600	-2.45545300	1.54304000
C	-1.53416700	0.80849300	-0.29139400
H	0.48850300	1.30897300	-0.47629500
C	-2.52465200	-0.13886500	0.14766400
H	-2.80610600	-2.03839800	1.17070800
H	-1.86111100	1.69843500	-0.81598200
N	-3.87495400	0.09154100	-0.06076200
C	-4.39135500	1.41146500	-0.01623800
C	-5.36086000	1.82120800	-0.93709300
C	-3.91760600	2.31286300	0.94138400
C	-5.85095800	3.11764200	-0.89110600
H	-5.71628200	1.12080300	-1.68325300
C	-4.40902900	3.61071700	0.97022200
H	-3.17215500	1.98362900	1.65534900
C	-5.37742400	4.01926700	0.05877900
H	-6.59910200	3.42938100	-1.60983400
H	-4.03895100	4.30257100	1.71702300
H	-5.75993300	5.03185000	0.08688400
C	-4.75297700	-0.99011800	-0.32428400
C	-4.33754400	-2.03872000	-1.15019900
C	-6.02786800	-1.02092000	0.24970500
C	-5.19106500	-3.10595800	-1.39313500
H	-3.35121200	-2.00115800	-1.59695300
C	-6.87461600	-2.08845300	-0.00858400
H	-6.34046900	-0.20957100	0.89599300
C	-6.46178300	-3.13655500	-0.82744900
H	-4.86338800	-3.91249800	-2.03777300
H	-7.85960100	-2.10713000	0.44191000
H	-7.12552500	-3.96953300	-1.02240400

p-TPA-BP S_0:

C	9.04829100	0.90078200	-0.21033600
C	8.76026000	1.80214500	0.81155700
C	7.52411100	1.76384000	1.44667300
C	6.56496200	0.83939000	1.04797600
C	6.84726700	-0.06126400	0.01977400
C	8.10047800	-0.03607600	-0.59478500
C	5.88243000	-1.13066300	-0.40104700
C	4.40892100	-0.88229900	-0.29977100
C	3.56755400	-1.98664700	-0.15208300
C	2.19438700	-1.82096100	-0.09650100
C	1.61964200	-0.54925100	-0.21906000
C	2.46688400	0.54888300	-0.39767200
C	3.84509800	0.38808300	-0.42857600
O	6.29504900	-2.18906600	-0.81969900
C	-5.35166400	-3.13773600	1.20835500
C	-6.54620800	-3.23701800	0.50238600
C	-6.90721500	-2.21803700	-0.37310400
C	-6.08241100	-1.11544500	-0.55138900
C	-4.88624200	-1.01228900	0.16317400
C	-4.52871100	-2.03075400	1.05031300
N	-4.04779900	0.11785100	-0.00702900
C	-2.64739800	-0.04256000	-0.06321000
C	-4.62247200	1.41009200	-0.09377500
C	-5.69763200	1.76009600	0.72702700
C	-6.26513000	3.02365400	0.63087000
C	-5.76182300	3.95855700	-0.26766400
C	-4.68668300	3.61256100	-1.07987400
C	-4.12357700	2.34579600	-1.00381900
C	-1.79617900	0.89762100	0.52663300
C	-0.42166500	0.73441300	0.46431400
C	0.15124900	-0.37340800	-0.16768700
C	-0.70861000	-1.31097000	-0.74843000
C	-2.08368700	-1.14856300	-0.70813100
H	10.01443000	0.92584500	-0.69962400
H	9.50304900	2.52939600	1.11734000
H	7.30684800	2.45186200	2.25465200
H	5.60675400	0.80141300	1.55251100
H	8.31061700	-0.76396800	-1.36906900
H	4.01497100	-2.97020700	-0.07438600
H	1.55464600	-2.68109600	0.06358400
H	2.03869800	1.53394300	-0.54260800
H	4.48203500	1.24996700	-0.58894500
H	-5.06226000	-3.92078400	1.89908700

H	-7.18885200	-4.09860000	0.63351400
H	-7.83241200	-2.28554800	-0.93298000
H	-6.35786100	-0.32526100	-1.23982900
H	-3.60379300	-1.94732500	1.60863700
H	-6.08354200	1.03448800	1.43319200
H	-7.09911200	3.28147600	1.27277300
H	-6.20295000	4.94515100	-0.33501100
H	-4.28973200	4.32853800	-1.78972400
H	-3.29386900	2.07181700	-1.64470600
H	-2.22176000	1.75076600	1.04103800
H	0.21888500	1.46053400	0.95222900
H	-0.29265500	-2.16190100	-1.27600000
H	-2.73331700	-1.87474200	-1.18171300

p-TPA-BP LE:

C	9.15424200	0.74329000	-0.11717800
C	8.17470900	-0.15959900	-0.50239500
C	6.87617700	-0.06606100	0.02824500
C	6.59796300	0.93889600	0.97128800
C	7.58450900	1.84013100	1.33744300
C	8.86565400	1.75190400	0.79626000
H	10.14905200	0.66153000	-0.53876400
H	8.39954600	-0.93133600	-1.22780800
H	5.61978400	0.98899100	1.43241800
H	7.35586100	2.60909800	2.06592500
H	9.63163300	2.45842200	1.09066400
C	5.85826900	-1.03616400	-0.36587800
O	6.26433500	-2.17548800	-0.82677700
C	4.40845100	-0.84966600	-0.30554000
C	3.56165600	-1.96502100	-0.18732700
C	3.82734500	0.42502800	-0.42097600
C	2.18769800	-1.80262300	-0.14847000
H	3.99343700	-2.95343100	-0.09244300
C	2.45343600	0.57198300	-0.36917800
H	4.45664100	1.29088500	-0.58404800
C	1.60282500	-0.53406500	-0.22926300
H	1.55556500	-2.67317600	-0.01572300
H	2.02427300	1.56102200	-0.48420200
C	0.13650100	-0.36341300	-0.17516800
C	-0.72335000	-1.29649000	-0.76546900
C	-0.44078600	0.73587800	0.46966100
C	-2.09863900	-1.13920600	-0.72045400
H	-0.30640000	-2.13942700	-1.30490400
C	-1.81562800	0.89502500	0.53409300

H	0.19723400	1.45775700	0.96699400
C	-2.66477600	-0.04148500	-0.06380200
H	-2.74716800	-1.86221100	-1.20057900
H	-2.24327000	1.74177800	1.05746200
N	-4.06648400	0.11417600	-0.00447100
C	-4.89882500	-1.01884900	0.17165400
C	-4.52912700	-2.03749100	1.05385800
C	-6.10066700	-1.12694100	-0.53306100
C	-5.34572500	-3.14836300	1.21722700
H	-3.59976600	-1.95084400	1.60420100
C	-6.91870100	-2.23360300	-0.34951200
H	-6.38563800	-0.33738700	-1.21830500
C	-6.54582400	-3.25226600	0.52142900
H	-5.04673300	-3.93105000	1.90429900
H	-7.84815700	-2.30457700	-0.90188700
H	-7.18339400	-4.11697000	0.65669700
C	-4.64454000	1.40419800	-0.09349500
C	-5.72394700	1.75203000	0.72301100
C	-4.14362000	2.34183800	-1.00069900
C	-6.29363300	3.01438900	0.62489400
H	-6.11117400	1.02578700	1.42776000
C	-4.70923800	3.60730200	-1.07868900
H	-3.31019200	2.07023900	-1.63771100
C	-5.78869500	3.95082000	-0.27115600
H	-7.13067700	3.27018800	1.26364400
H	-4.31047200	4.32444500	-1.78636000
H	-6.23157200	4.93652900	-0.33992900

p-TPA-BP CT:

C	9.00981600	1.01485700	-0.00908400
C	8.77469700	1.55268400	1.25365300
C	7.58455000	1.27234100	1.91565600
C	6.62075000	0.47461300	1.30874000
C	6.84517100	-0.05548900	0.03697300
C	8.05585600	0.20370000	-0.60724600
C	5.87414700	-0.98540500	-0.63284900
C	4.43376900	-0.76933900	-0.50030200
C	3.55730200	-1.82968700	-0.88356000
C	2.20663800	-1.69708800	-0.81269600
C	1.57949600	-0.46951100	-0.36572500
C	2.48776900	0.61256000	-0.04269300
C	3.84106300	0.46610200	-0.10796800
O	6.30742500	-1.91934200	-1.30030500
C	-5.28733700	-3.08699300	1.45991200

C	-6.48829400	-3.24105900	0.77468400
C	-6.87741500	-2.28133400	-0.15569300
C	-6.07362900	-1.17883300	-0.40739100
C	-4.86950200	-1.02547400	0.28433500
C	-4.47978500	-1.98265100	1.22427200
N	-4.04250800	0.10135100	0.03323400
C	-2.66669200	-0.04064500	-0.06011700
C	-4.64762400	1.37686700	-0.12090000
C	-5.68941400	1.76527600	0.72503800
C	-6.27628600	3.01257800	0.56770600
C	-5.82824900	3.88382600	-0.42125700
C	-4.78893800	3.49515300	-1.26045700
C	-4.20094700	2.24559700	-1.11947100
C	-1.78887700	1.00580500	0.35509500
C	-0.44008400	0.87028600	0.26318800
C	0.18799800	-0.33051200	-0.26297500
C	-0.73423900	-1.37698100	-0.67145300
C	-2.08210600	-1.23848200	-0.57360000
H	9.94156100	1.22238700	-0.52172700
H	9.52238900	2.17998800	1.72450000
H	7.40871400	1.66928900	2.90840100
H	5.70217400	0.24079200	1.83492500
H	8.23096100	-0.24907200	-1.57574000
H	4.01011000	-2.75216200	-1.22439400
H	1.59419700	-2.54353500	-1.09023900
H	2.09303700	1.58102600	0.23077300
H	4.47613600	1.31610200	0.10848800
H	-4.98045900	-3.82409800	2.19191900
H	-7.11717600	-4.10178700	0.96461100
H	-7.80825000	-2.39639100	-0.69760800
H	-6.36672500	-0.43388100	-1.13750000
H	-3.54933700	-1.84875800	1.76324900
H	-6.02736500	1.08689500	1.49931500
H	-7.08130300	3.30945500	1.22889500
H	-6.28700700	4.85771300	-0.53750600
H	-4.43975900	4.16277000	-2.03871500
H	-3.40001800	1.93009200	-1.77757300
H	-2.21445300	1.90775500	0.77837200
H	0.17572900	1.67719300	0.63207700
H	-0.34895500	-2.29003600	-1.10070500
H	-2.73368100	-2.03304400	-0.91690000