Electronic Supplementary Information

Elevating the upconversion performance of a multiple resonance thermally activated delayed fluorescence emitter *via* an embedded azepine approach

Yi-Kuan Chen,[a‡] Jian Lei,[a,b‡] and Tien-Lin Wu*[a,c]

E-mail: tlwu@mx.nthu.edu.tw

[a]Department of Chemistry, National Tsing Hua University, No. 101, Sec. 2, Kuang-Fu Rd., Hsinchu 300044, Taiwan.

[b]Institute of Atomic and Molecular Sciences, Academia Sinica, No. 1, Sec. 4, Roosevelt Rd., Taipei, 106319, Taiwan.

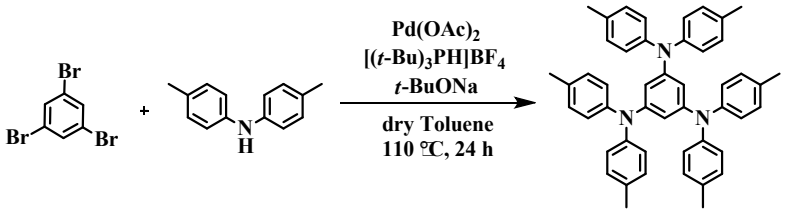
[c]College of Semiconductor Research, National Tsing Hua University, No. 101, Sec. 2, Kuang-Fu Rd., Hsinchu 300044, Taiwan.

Contents

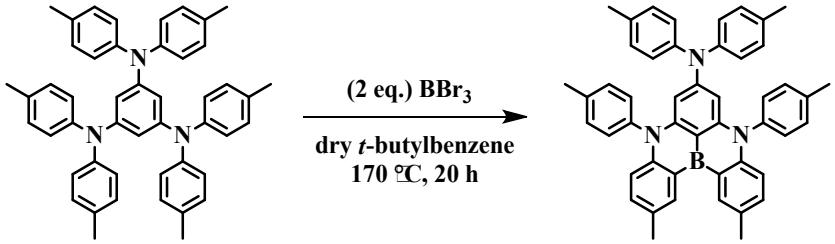
1. General Information

All chemicals and reagents were purchased from commercial providers without further purification. ^{1}H NMR, ^{13}C NMR and ^{11}B NMR spectra were measured on Varian INOVA-500 and JEOL ECZ500R/S1 NMR spectrometers. Mass spectra were performed on JMS-T200GC AccuTOF GCx HRMS. Elemental analyses were performed using an analyzer (Vario EL III CHN-OS Rapid, Elementar). UV-vis absorption spectra were recorded on a Hitachi U-3300 spectrophotometer. Fluorescence was recorded on a Hitachi F-7000 fluorescence spectrophotometer. Thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC) were performed on a thermal analyzer (2-HT, Mettler-Toledo and Q10) at a heating rate of 10 ℃/min. from 30 ℃ to 800 ℃ under nitrogen. Transient PL decay curves and phosphorescence spectra were obtained using an Edinburgh FLS980 instrument. The delayed time for the phosphorescence spectra was 6.25 milliseconds. The excitation light source for the delayed decay curves was 60 W, pulsed xenon microsecond flashlamp. The pulse widths of the nanosecond and microsecond flash lamp were within 1 ns and 1-2 μs, with the repetition rates (frequency) of 40 kHz and 100 Hz, respectively. Excitation and detection wavelengths were 340 and 470 nm, respectively. The channels applied for the prompt (100 ns) and the delayed (400 μs) decay curve were 4096 and 8000, respectively. The prompt and delayed lifetimes were fitted by FLS980 software. The HOMO levels of compounds were determined with an electrochemical analyzer (CHI600, CH Instruments). The absolute photoluminescence quantum yields (PLQYs) of the thin films were determined using an integrating sphere system (LQ-100X-PL) under a N_2 atmosphere. The PLQYs in degassed solution were obtained using 9,10-diphenylanthracene as standard. The X-ray diffraction was carried out on an X-ray diffractometer (Rigaku XtaLAB Synergy DW). The chiral separation of MR emitter, TAzBN, was completed in Daicel Chiral Technologies (China) Co., Ltd. by HPLC using Chiralpak IE column. The ee% of both enantiomers were over 98%. Circular Dichroism spectra (CD) were obtained on a JASCO J-1500 spectrometer, whereas Circular polarized luminescence (CPL) spectra were recorded on a JASCO CPL-300 spectrometer. Permanent magnets (JASCO PM-491) with various magnetic field strengths were used with a scattering angle of 0°. The device performance was measured by a spectroradiometer, CS-2000A instrument.

2. Synthetic procedure and characterization

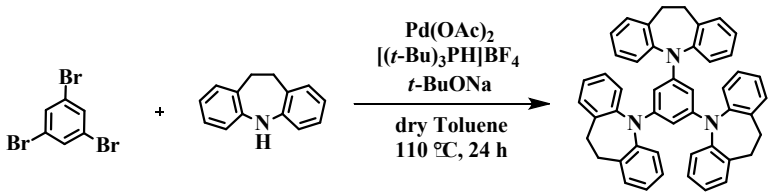


Synthesis of ***N*¹, *N*¹, *N*³, *N*³, *N*⁵, *N*⁵-hexa-*p*-tolylbenzene-1,3,5-triamine (TTA)**: 1,3,5-tribromobenzene (1.000 g, 4.80 mmol), di-*p*-tolylamine (1.880 g, 9.53 mmol), palladium acetate (0.107 g, 0.48 mmol), tri-*tert*-butylphosphonium tetrafluoroborate (0.140 g, 0.48 mmol), and sodium *tert*-butoxide (1.832 g, 19.06 mmol) were added to the pressure tube. The dry toluene (16 mL) was added to the mixture and degassed. Then, the solution was refluxed for 24 hours. After, the mixtures were cooled down, filtered through the celite, and washed with dichloromethane. The solution was evaporated, and the crude was purified by column chromatography (eluent: dichloromethane/hexane = 1/5) to obtain the white solid (1.810 g, yield: 85.8%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.92 (d, *J* = 8.5 Hz, 12H), 6.87 (d, *J* = 8.5 Hz, 12H), 6.25 (s, 3H), 2.22 (s, 18H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 148.99, 145.00, 131.67, 129.49, 123.88, 112.79, 20.70. FD-MS calcd for $C_{48}H_{45}N_3$: 663.36080. Found: 663.36017.

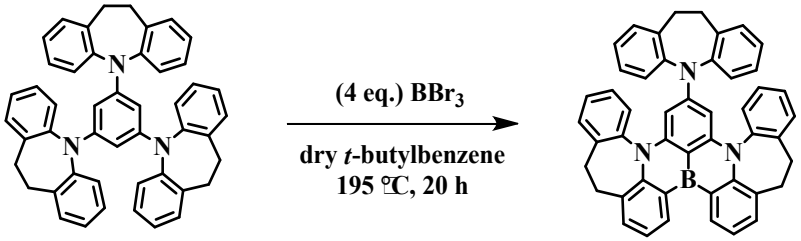


Synthesis of **TTA-BN**: *N*¹,*N*¹,*N*³,*N*³,*N*⁵,*N*⁵-hexa-*p*-tolylbenzene-1,3,5-triamine (**TTA**) (0.500 g, 0.75 mmol) and dry *tert*-butyl benzene (7.5 mL) were added to the pressure tube. The boron tribromide (0.377 g, 1.51 mmol) was slowly added in glovebox, and the solution was stirred at 170 °C for 20 hours. After, the mixtures were cooled down to room temperature, and *N*, *N*-diisopropylethylamine (0.389 g, 3.01 mmol) was added slowly in ice bath for 0.5 hour. The solution was extracted with dichloromethane and water three times, then the solvent was evaporated. The crude was purified by column chromatography (eluent: dichloromethane/hexane = 1/3) to obtain the yellow powder (0.344 g, yield: 67.9%), and the solid was further purified by gradient sublimation. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (s, 2H), 7.24 (d, *J* = 7.5 Hz, 6H), 7.15 (dd, *J* = 9.0, 2.0 Hz, 2H), 7.05 (d, *J* = 8.5 Hz, 4H), 6.87 (d, *J* = 8.0 Hz, 4H), 6.81 (d, *J* = 8.0 Hz, 4H), 6.66 (d, *J* = 8.5 Hz, 2H), 2.49 (s, 6H), 2.37 (s, 6H), 2.25 (s, 6H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 151.04,

147.99, 145.92, 143.90, 139.80, 137.58, 134.61, 133.02, 131.33, 129.94, 129.30, 128.20, 125.95, 116.70, 96.49, 21.11, 21.06, 20.78. ^{11}B NMR (160 MHz, $CDCl_3$) δ 37.6. FD-MS calcd for $C_{48}H_{42}BN_3$: 671.34773. Found: 671.34804. Anal. cal for $C_{48}H_{42}BN_3$: N 6.26, C 85.83, H 6.30. Found N 6.30, C 86.03, H 6.31.



Synthesis of **1,3,5-tris(10,11-dihydro-5*H*-dibenzo[*b*,*f*]azepin-5-yl)benzene (TAz)**: 1,3,5-tribromobenzene (0.500 g, 1.60 mmol), 10,11-dihydro-5*H*-dibenzo[*b*,*f*]azepine (0.931 g, 4.80 mmol), palladium acetate (0.053 g, 0.24 mmol), tri-*tert*-butylphosphonium tetrafluoroborate (0.069 g, 0.24 mmol), and sodium *tert*-butoxide (0.920 g, 9.60 mmol) were added to the two-neck flask, then the system was degassed. The dry toluene (8 mL) was added to the mixture, then the solution was refluxed under nitrogen for 24 hours. After, the mixtures were cooled down, diluted with dichloromethane, and filtered through the celite. The solution was evaporated, and the crude was purified by column chromatography (eluent: dichloromethane/hexane = 1/3) to obtain the white solid (0.870 g, yield: 83.3%). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.13 (d, J = 7.0 Hz, 6H), 7.04 (d, J = 7.0 Hz, 6H), 6.96 (td, J = 7.0, 1.0 Hz, 6H), 6.90 (t, J = 7.0, 1.0 Hz, 6H), 5.22 (s, 3H), 2.88 (s, 12H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 149.98, 143.54, 137.86, 130.06, 129.75, 126.11, 126.07, 89.85, 30.99. FD-MS calcd for $C_{48}H_{39}N_3$: 657.31385. Found: 657.31489.



Synthesis of **TAzBN**: 1,3,5-tris(10,11-dihydro-5*H*-dibenzo[*b*,*f*]azepin-5-yl)benzene (**TAz**) (1.000 g, 1.52 mmol) and dry *tert*-butyl benzene (10 mL) were added to the pressure tube. The boron tribromide (1.523 g, 6.08 mmol) was added slowly in the glovebox, and the solution was stirred at 195 °C for 20 hours. After, the mixtures were cooled down to room temperature, and *N*, *N*-diisopropylethylamine (1.572 g, 12.16 mmol) was added slowly in ice bath for 0.5 hour. The solution was extracted with dichloromethane and water three times, then the solvent was evaporated. The crude was purified by column chromatography (eluent: dichloromethane/hexane

= 1/4) to obtain the yellow powder (0.234 g, yield: 23.1%), and the solid was further purified by gradient sublimation. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.0 Hz, 2H), 7.27 (d, *J* = 7.5 Hz, 2H), 7.16 (t, *J* = 7.5 Hz, 2H), 7.13 (d, *J* = 7.5 Hz, 2H), 7.04 – 6.98 (m, 8H), 6.93 (t, *J* = 7.5 Hz, 2H), 6.88 (t, *J* = 7.5 Hz, 2H), 6.76 (d, *J* = 8.0 Hz, 2H), 5.46 (s, 2H), 3.62 (t, *J* = 13.5 Hz, 2H), 3.36 (d, *J* = 17.0 Hz, 2H), 3.21 (t, *J* = 14.5 Hz, 2H), 2.85 – 2.76 (m, 4H), 2.71 (d, *J* = 13.0 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.05, 150.61, 147.46, 146.63, 142.71, 140.94, 137.64, 134.06, 132.82, 130.33, 129.21, 129.13, 128.75, 126.79, 126.75, 126.73, 126.41, 121.30, 96.52, 37.50, 30.64, 30.52. ^{11}B NMR (160 MHz, $CDCl_3$) δ 40.9. FD-MS calcd for $C_{48}H_{36}BN_3$: 665.30078. Found: 665.30148. Anal. cal for $C_{48}H_{36}BN_3$: N 6.31, C 86.61, H 5.45. Found N 6.28, C 86.64, H 5.47.

3. Thermal and electrochemical properties

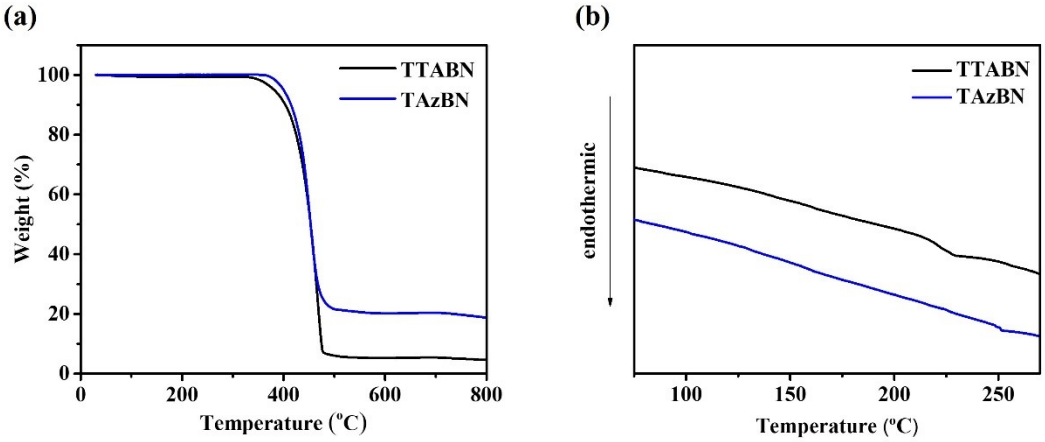


Fig. S1 (a) Thermal gravimetric analysis (TGA) and (b) differential scanning calorimetry (DSC) analysis of TTABN and TAzBN.

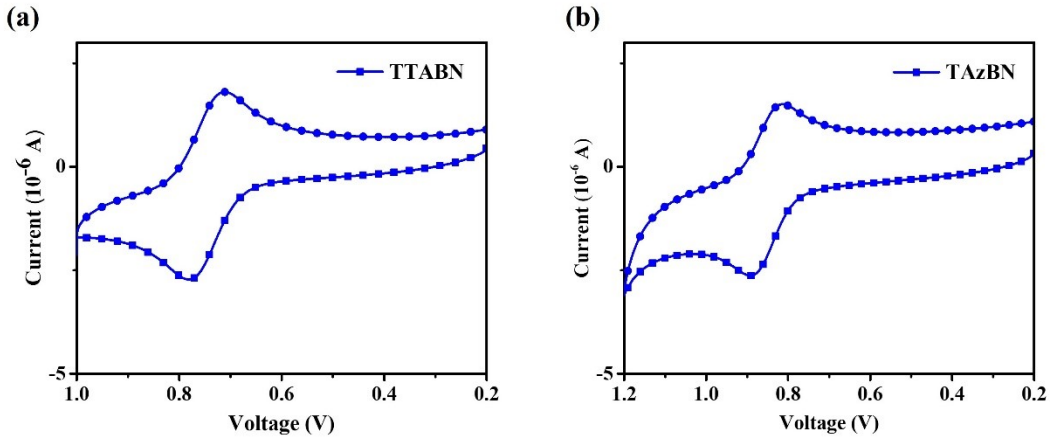


Fig. S2 Cyclic voltammograms of (a) TTABN, and (b) TAzBN in dichloromethane.

4. Single-crystal X-ray diffraction

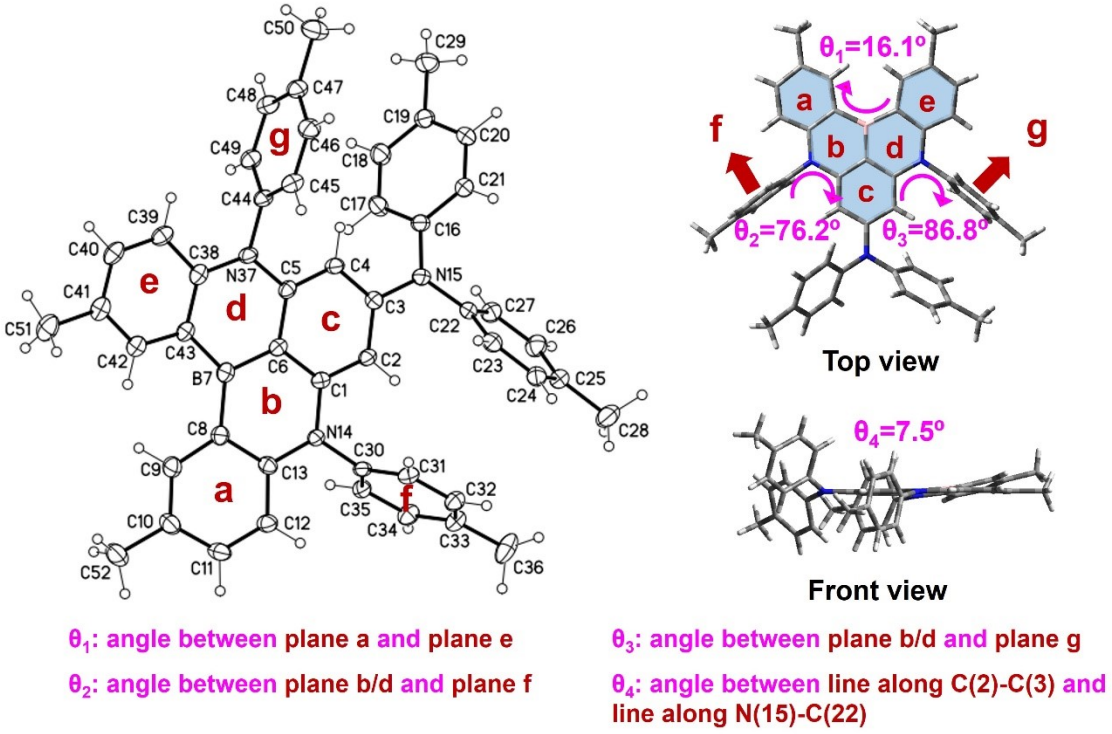


Fig. S3 Single crystal structure of TTABN and related dihedral angles.

Table S1 Crystal data and structure refinement for TTABN.

Empirical formula	$C_{96}H_{84}B_2N_6$
Formula weight	1343.31
Temperature/K	99.98(12)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.7232(2)
b/Å	9.88890(10)
c/Å	51.6585(6)
α/°	90
β/°	94.7230(10)
γ/°	90
Volume/Å^3	7495.75(15)
Z	4
ρ_{calc}g/cm^3	1.190
μ/mm^{-1}	0.523
F(000)	2848.0
Crystal size/mm^3	0.08 × 0.06 × 0.03
Radiation	Cu Kα (λ = 1.54184)

2Θ range for data collection/°	6.024 to 134.15
Index ranges	$-15 \le h \le 17$, $-11 \le k \le 11$, $-61 \le l \le 61$
Reflections collected	54420
Independent reflections	13332 [R_{int} = 0.0282, R_{sigma} = 0.0264]
Data/restraints/parameters	13332/0/950
Goodness-of-fit on F^2	1.118
Final R indexes [I>=2σ (I)]	R_1 = 0.0539, wR_2 = 0.1342
Final R indexes [all data]	R_1 = 0.0629, wR_2 = 0.1385
Largest diff. peak/hole / e $Å^{-3}$	0.36/-0.28

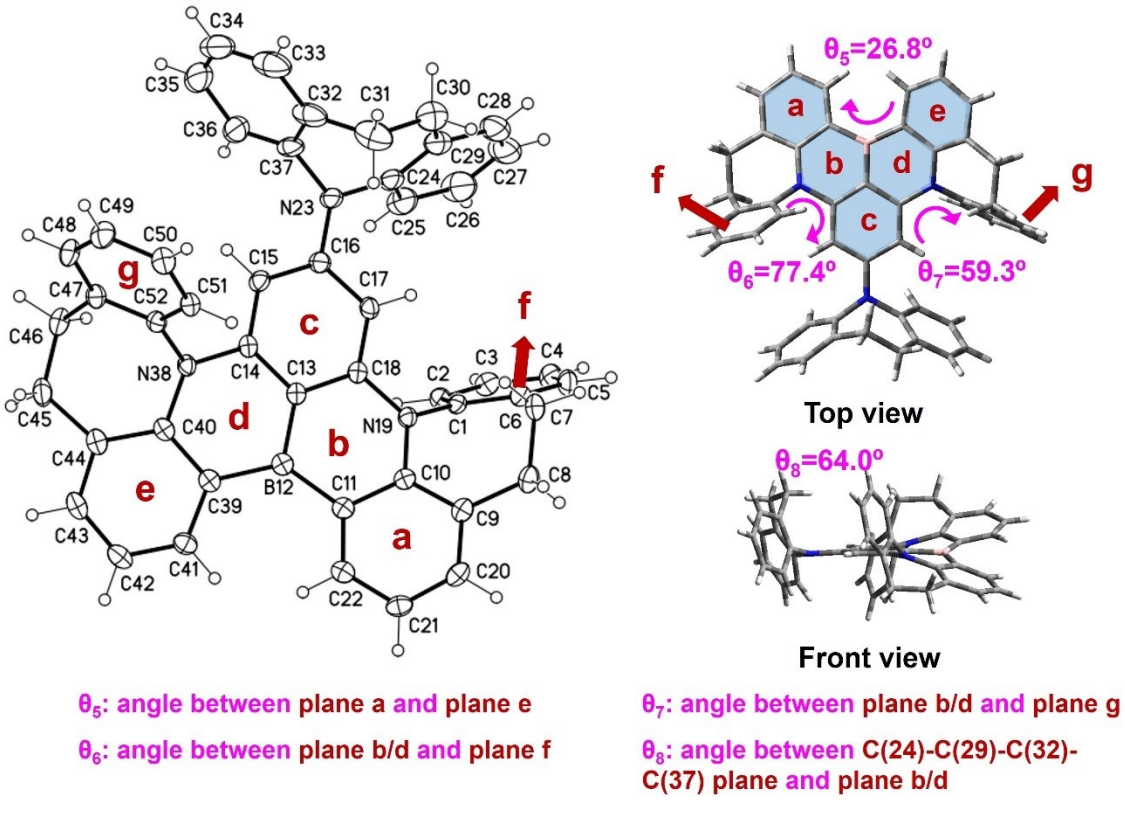


Fig. S4 Single crystal structure of TAzBN and related dihedral angles.

Table S2 Crystal data and structure refinement for TAzBN.

Empirical formula	$C_{48}H_{36}BN_3$
Formula weight	665.61
Temperature/K	100.00(10)
Crystal system	orthorhombic
Space group	Pbca
a/Å	20.72780(13)
b/Å	13.75053(9)
c/Å	25.09061(16)

α/°	90
β/°	90
γ/°	90
Volume/Å^3	7151.28(8)
Z	8
ρ_{calc}g/cm^3	1.236
μ/mm^{-1}	0.548
F(000)	2800.0
Crystal size/mm^3	0.17 × 0.14 × 0.04
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.046 to 134.156
Index ranges	-23 ≤ h ≤ 24, -16 ≤ k ≤ 15, -28 ≤ l ≤ 29
Reflections collected	42604
Independent reflections	6377 [R_{int} = 0.0236, R_{sigma} = 0.0160]
Data/restraints/parameters	6377/0/470
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0408, wR_2 = 0.1091
Final R indexes [all data]	R_1 = 0.0454, wR_2 = 0.1125
Largest diff. peak/hole / e Å^{-3}	0.49/-0.25

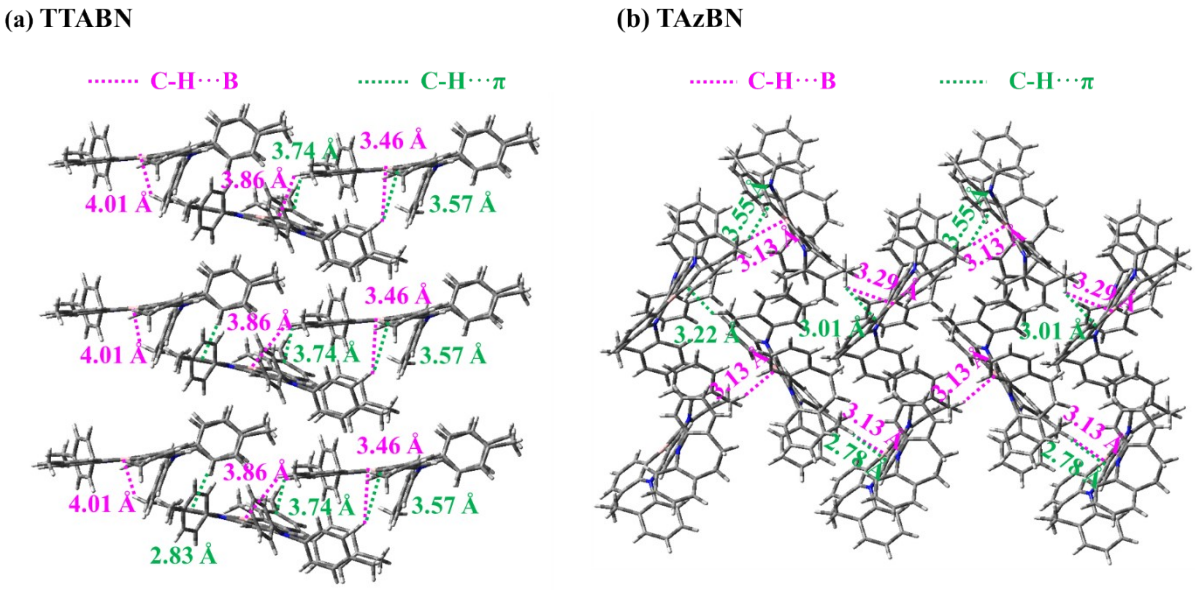


Fig. S5 Molecular packing pattern of (a) TTABN and (b) TAzBN.

5. Computational methods

In this work, the electronic structures of two emitters were calculated with Gaussian 16[1] unless specified otherwise. The ground state (S_0) geometries were optimized using the density functional theory (DFT). The time-dependent density functional theory (TD-DFT) and Tamm-Dancoff approximated density functional theory (TDA-DFT) were used to optimize the geometries of the first excited singlet state (S_1) and the triplet excited states (T_1, T_2, and T_3).[2] We utilized the polarizable continuum model (PCM)[3] and the two-layer ONIOM model[4] of the quantum mechanics/molecular mechanics (QM/MM) method, respectively, to simulate basic photophysical data in toluene and the solid phase. As shown **Figure S6b**, the innermost molecule was found to be the higher layer by the accurate high-level QM method, and the outermost molecules were treated as the lower layer using the efficient universal force field (UFF) method.[5] In the QM/MM geometry optimization process, only the atoms in the QM part can move and others in the MM part were frozen. The initial geometries of TTABN and TAzBN in the solid phase were based on the measured crystalline structures. Several functionals with different percentages of Hartree-Fock exchange (HF%), including B3LYP (20%), PBE0 (25%), BMK (42%), M06-2X (54%), CAM-B3LYP (19% HF at short range and 65% HF at long range), and ωB97XD (22.2% HF at short range and 100% HF at long range) are tested.[2, 6, 7]. It should be noted that most of the experimental ΔE_{ST} values are deduced from fluorescence and phosphorescence spectra as shown in **Figure S7a**.[2] The computational results of the vertical absorption energy (ΔE_{VA}), vertical emission energy (ΔE_{VE}), adiabatic energy (ΔE_{AD}), and the energy gap (ΔE_{ST}) were calculated as shown in **Figure S7b**. We carried out calculations of the adiabatic $\Delta E_{ST\text{-}AD}$ values, which are defined as the energy differences between the minima potential energies of the S_1 and T_1/T_2/T_3 states. The absorption and emission wavelengths (λ_{abs} and λ_{em}) were calculated using the TD-B3LYP/6-31G(d) method based on optimized the ground and excited states, respectively. Absorption and emission spectra were simulated by TD-DFT based on vertical energies at the stable geometry structures. It was found that the emission wavelength changes significantly when functionals were different, and the best approach for calculating the absorption peak ($\lambda_{abs}(S_1)$), emission peak ($\lambda_{em}(S_1)$), and the first adiabatic singlet excited energy ($\Delta E_{AD}(S_1)$) was B3LYP/6-31G (d) (**Table S3)**. The adoption of the TDA-DFT with B3LYP is appropriate for calculations of the adiabatic excited state energies and the corresponding singlet-triplet gap. Vibrational frequency analyses were carried out to confirm the local minima which showed no imaginary frequency. Consequently, the B3LYP functional and the 6-31G(d) basis set are adopted to calculate excited states in our calculations. The spin-orbit coupling (SOC) matrix between S_1 and T_n (n=1-3) states were calculated with the optimized geometries of S_1, T_1, T_2, and T_3 by the ORCA program, respectively.[8]

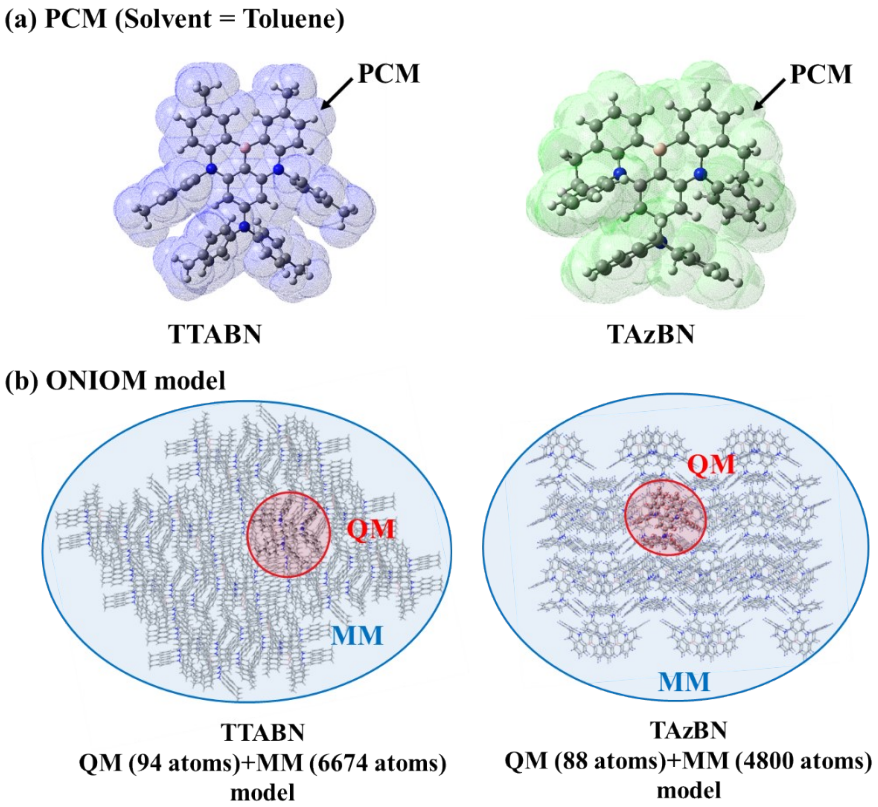


Fig. S6 (a) PCM model: (solvent = toluene) of TTABN and TAzBN. (b) ONIOM model: single TTABN or TAzBN molecule is treated as the high layer (QM), respectively, and surrounding molecules are regarded as the low layer (MM).

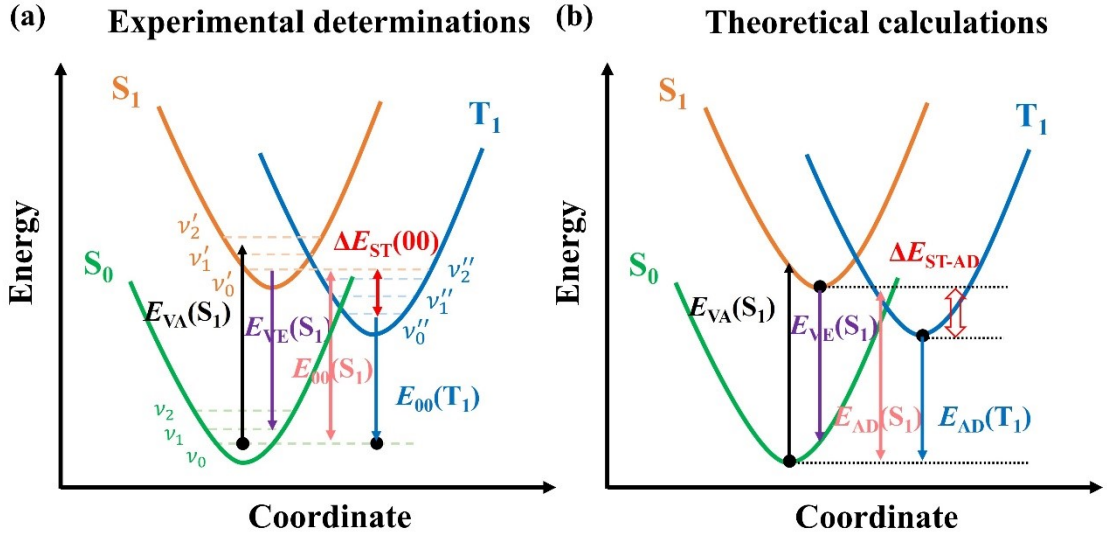


Fig. S7 Schematic potential energy surfaces of the photophysical processes for (a) experimental determinations and (b) theoretical calculations. S_0 is the singlet ground state; S_1 is the lowest singlet excited state; T_1 is the lowest triplet excited state; VA: vertical absorption; VE: vertical emission; AD: adiabatic; $\Delta E_{ST\text{-}AD}$ is the adiabatic energy gap between S_1 and T_1.

Table S3 Calculated excited-state characteristics of TTABN and TAzBN in toluene and the solid phase.

Method	$\Delta E_{VA}(S_1)$[a] [eV]	$\Delta E_{VE}(S_1)$[b] [eV]	$\Delta E_{AD}(S_1)$[c] [eV]	$\lambda_{abs}(S_1)$[d] [nm]	$\lambda_{em}(S_1)$[e] [nm]	$\Delta\lambda$[f] [nm]	HOMO[g] [eV]	LUMO[g] [eV]
TTABN (Toluene)								
B3LYP	3.06	2.87	2.97	405	432	27	-4.71	-1.25
PBE0	3.17	2.98	3.08	391	416	25	-4.96	-1.18
BMK	3.36	3.19	3.28	369	388	19	-5.41	-0.71
CAM-B3LYP	3.57	3.40	3.48	348	365	17	-5.93	-0.14
M06-2X	3.51	3.34	3.43	353	371	18	-5.90	-0.51
ωB97X-D	3.62	3.45	3.54	343	359	17	-6.49	-0.29
TAzBN (Toluene)								
B3LYP	3.03	2.74	2.89	410	452	43	-4.82	-1.38
PBE0	2.90	2.50	2.70	428	495	68	-5.17	-1.44
BMK	3.36	3.11	3.24	369	399	30	-5.54	-0.82
CAM-B3LYP	3.58	3.37	3.47	347	368	22	-6.09	-0.08
M06-2X	3.54	3.31	3.43	351	374	24	-6.09	-0.50
ωB97X-D	3.62	3.42	3.52	343	363	20	-6.70	-0.29
TTABN (Solid)								
B3LYP	3.05	2.86	2.97	406	433	27	-4.51	-0.92
PBE0	3.16	2.98	3.09	392	416	24	-4.68	-0.97
BMK	3.37	3.21	3.30	368	387	18	-5.12	-0.48
CAM-B3LYP	3.58	3.44	3.52	347	360	14	-5.67	0.05
M06-2X	3.52	3.37	3.45	353	368	15	-5.64	-0.34
ωB97X-D	3.61	3.49	3.56	343	356	13	-6.25	0.60
TAzBN (Solid)								
B3LYP	3.03	2.74	2.91	409	453	44	-4.70	-1.10
PBE0	3.15	2.87	3.04	393	432	39	-4.94	-1.01
BMK	3.37	3.13	3.28	368	396	29	-5.39	-0.53
CAM-B3LYP	3.59	3.39	3.51	345	366	21	-5.98	0.02
M06-2X	3.54	3.32	3.46	350	373	23	-5.94	-0.37
ωB97X-D	3.63	3.44	3.56	341	360	19	-6.55	0.57

[a]The vertical absorption energy. [b]The vertical emission energy. [c]The adiabatic energy. [d]The absorption wavelength. [e]The emission wavelength. [f]Stokes shift $\Delta\lambda = \lambda_{em}(S_1) - \lambda_{abs}(S_1)$ [g]The energy level of HOMO and LUMO.

Table S4 Calculated adiabatic energies of TTABN and TAzBN in toluene and the solid phase at B3LYP/6-31G(d).

Molecule	Method[a]	$\Delta E_{AD}(S_1)$[b] [eV]	$\Delta E_{AD}(T_1)$[c] [eV]	$\Delta E_{AD}(T_2)$[d] [eV]	$\Delta E_{AD}(T_3)$[e] [eV]	ΔE_{S1T1}[f] [eV]	ΔE_{S1T2}[f] [eV]	ΔE_{S1T3}[f] [eV]
Toluene								
TTABN	TD	2.97	2.54	2.78	3.04	0.43	0.19	-0.07
	TDA	2.97	2.56	2.88	3.12	0.41	0.09	-0.15
TAzBN	TD	2.93	2.56	2.83	3.10	0.37	0.10	-0.16
	TDA	2.95	2.58	2.93	3.05	0.37	0.02	-0.10
Solid								
TTABN	TD	2.97	2.56	2.87	3.08	0.42	0.11	-0.11
	TDA	3.04	2.58	2.94	3.15	0.46	0.10	-0.11
TAzBN	TD	2.91	2.56	2.82	3.14	0.36	0.09	-0.23
	TDA	2.91	2.58	2.90	3.21	0.33	0.01	-0.30

[a]The time-dependent density functional theory (TD-DFT) and Tamm-Dancoff approximated density functional theory (TDA-DFT). [b]The adiabatic energy of S_1. [c]The adiabatic energy of T_1. [d]The adiabatic energy of T_2. [e]The adiabatic energy of T_3. [f]The energy gap between S_1 and $T_1/T_2/T_3$.

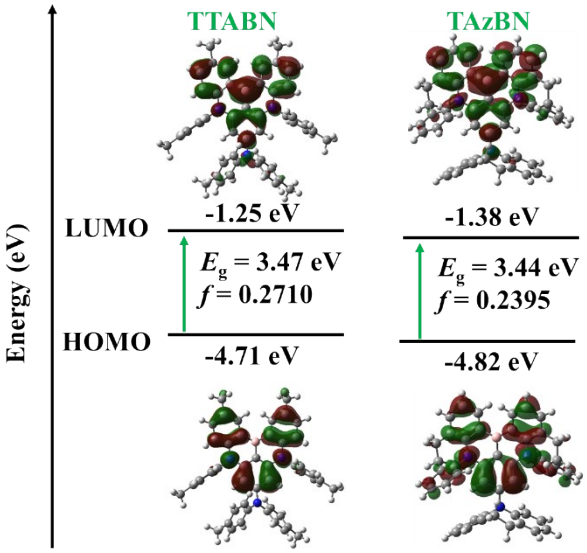


Fig. S8 Calculated HOMO and LUMO distributions, energy level gaps (E_g), oscillator strengths (f) of TTABN and TAzBN by TD-DFT at B3LYP/6-31G(d) in toluene.

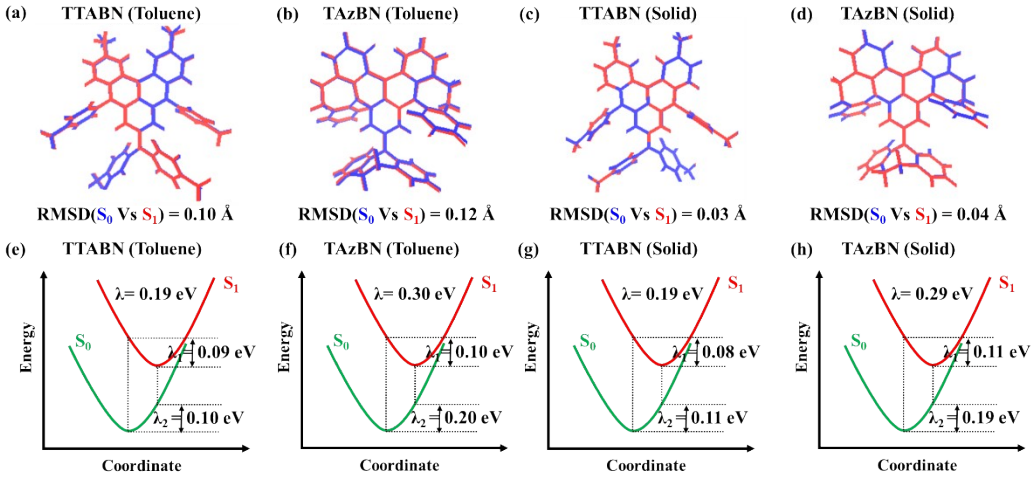


Fig. S9 Geometric root-mean-square deviation (RMSD) between optimized S_0 (blue) and S_1 (red) states of (a)TTABN and (b)TAzBN in toluene, (c)TTABN and (d)TAzBN in the solid phase, respectively. Reorganization energies with optimized S_0 and S_1 geometries of (e)TTABN and (f)TAzBN in toluene, (g)TTABN and (h)TAzBN in the solid phase, respectively, by TD-DFT.

Table S5 Calculated spin-orbit coupling (SOC) matrix elements of TTABN and TAzBN in toluene.

Molecule / Geometry[a]	TTABN			TAzBN		
	SOC(S_1T_1)	SOC(S_1T_2)	SOC(S_1T_3)	SOC(S_1T_1)	SOC(S_1T_2)	SOC(S_1T_3)
S_1	0.03	0.14	0.01	0.08	1.33	0.10
T_1	0.03	0.13	0.00	0.10	1.28	0.07
T_2	0.04	0.25	0.03	0.14	1.02	0.07
T_3	0.04	0.18	0.03	0.13	1.02	0.30

[a]At the position of the optimized $S_1/T_1/T_2/T_3$ geometries by TDA-DFT at B3LYP/6-31G(d), respectively.

6. Photophysical properties

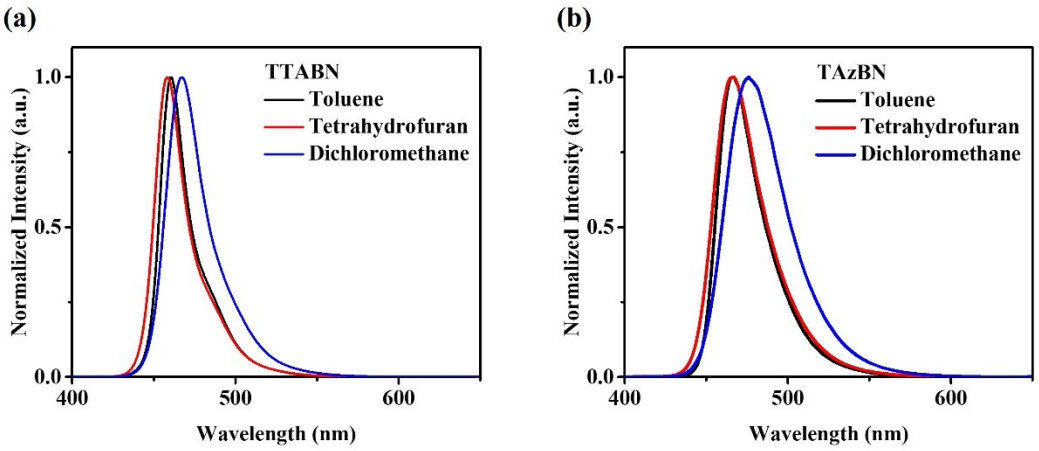


Fig. S10 Fluorescence spectra of (a) TTABN and (b) TAzBN at 300 K measured in various solvents.

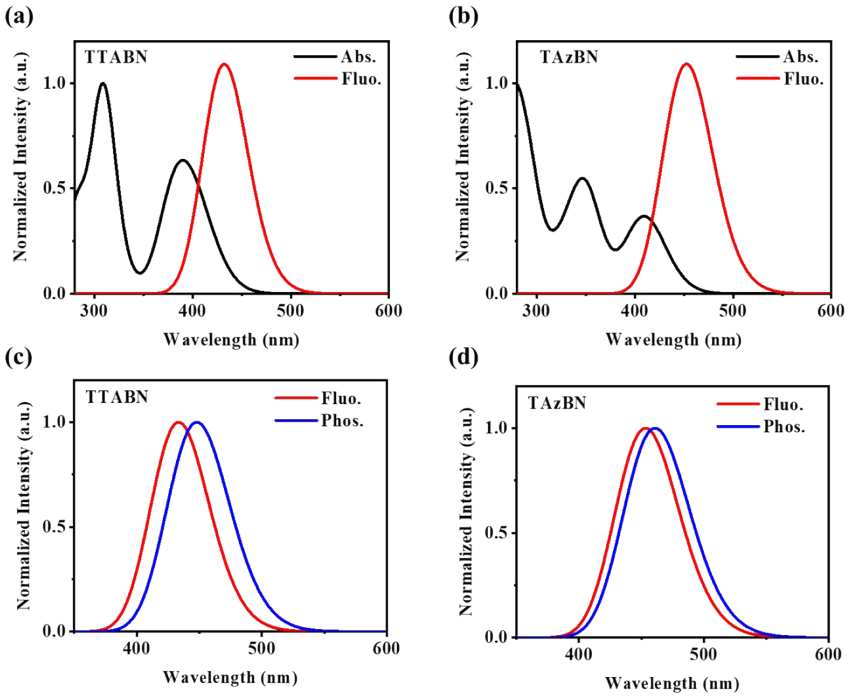


Fig. S11 Calculated absorption and fluorescence spectra of (a) TTABN and (b) TAzBN at B3LYP/6-31G(d) in toluene. Fluorescence and phosphorescence spectra of (c) TTABN and (d) TAzBN by TD-DFT at B3LYP/6-31G(d) in the solid phase.

7. Transient PL measurement

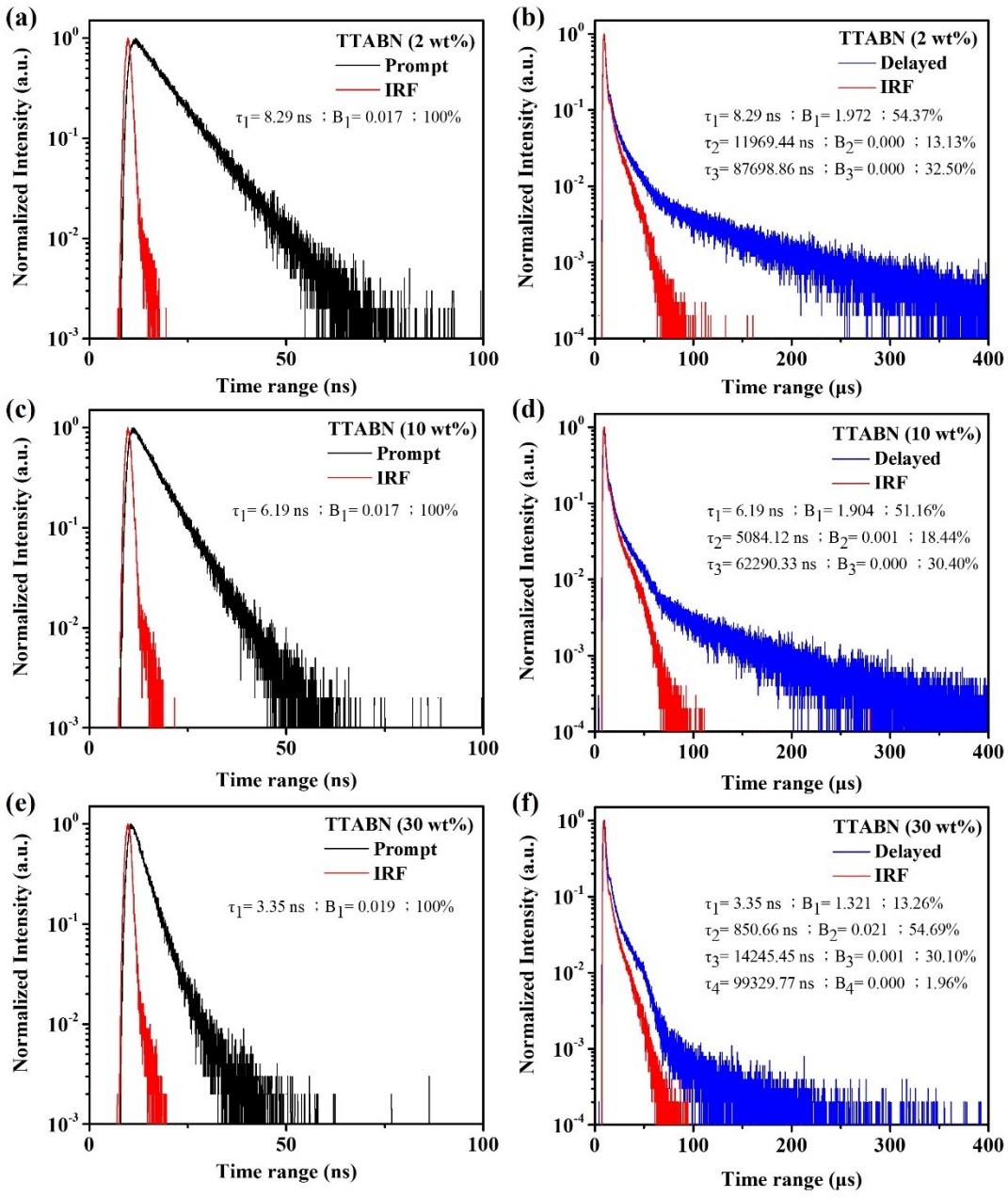


Fig. S12 Prompt (in 100 ns) and delayed curves (in 400 μs) of TTABN doped in the mCPCN film of (a)(b) 2 wt%, (c)(d) 10 wt%, and (e)(f) 30 wt%, respectively. The red curves are Instrument Response Function (IRF). The excitation and detection wavelengths are 340 and 470 nm, respectively. The insets are the prompt and delayed lifetimes which were fitted by FLS980 software.

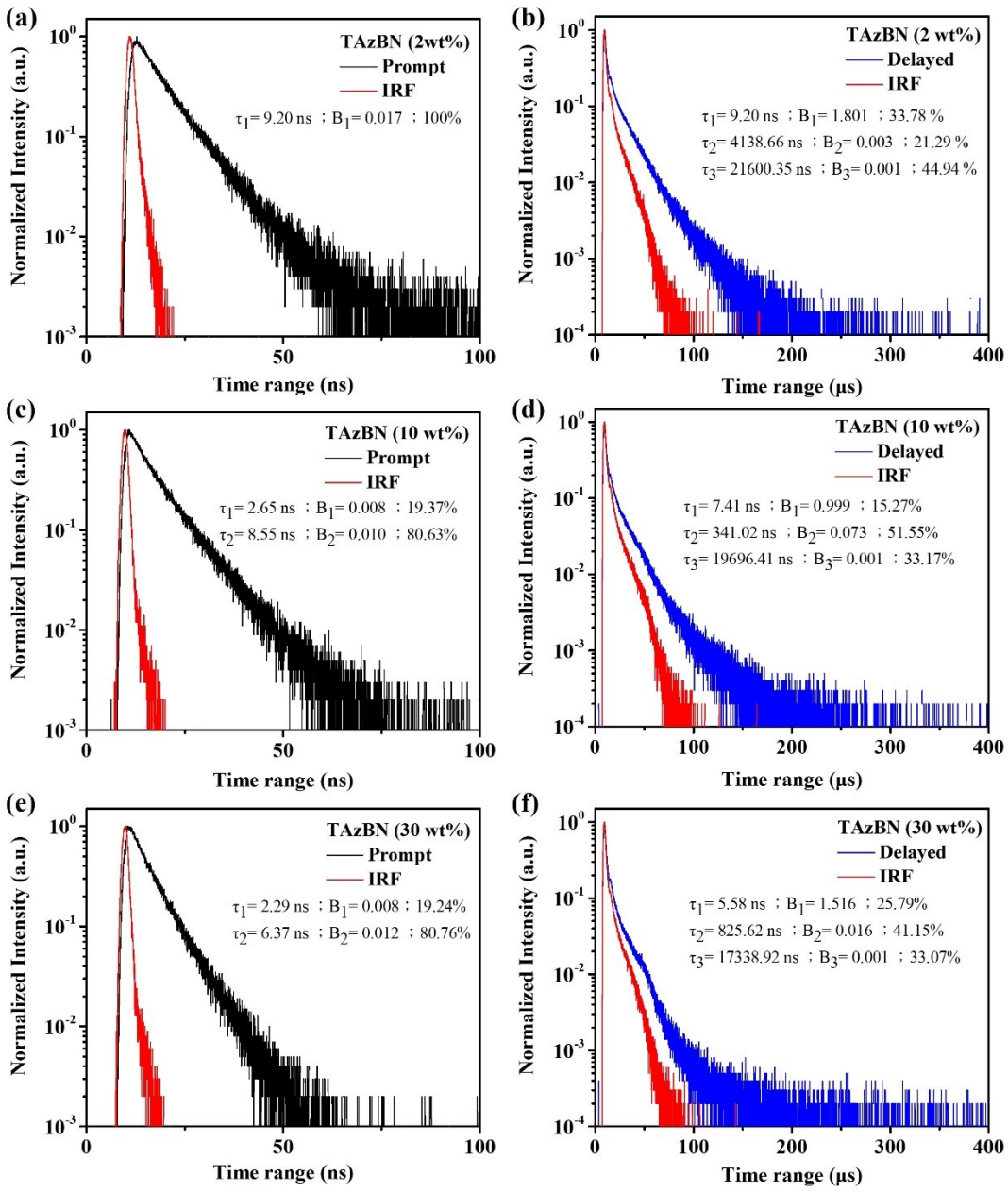


Fig. S13 Prompt (in 100 ns) and delayed curves (in 400 μs) of TAzBN doped in the mCPCN film of (a)(b) 2 wt%, (c)(d) 10 wt%, and (e)(f) 30 wt%, respectively. The red curves are Instrument Response Function (IRF). The excitation and detection wavelengths are 340 and 470 nm, respectively. The insets are the prompt and delayed lifetimes which were fitted by FLS980 software.

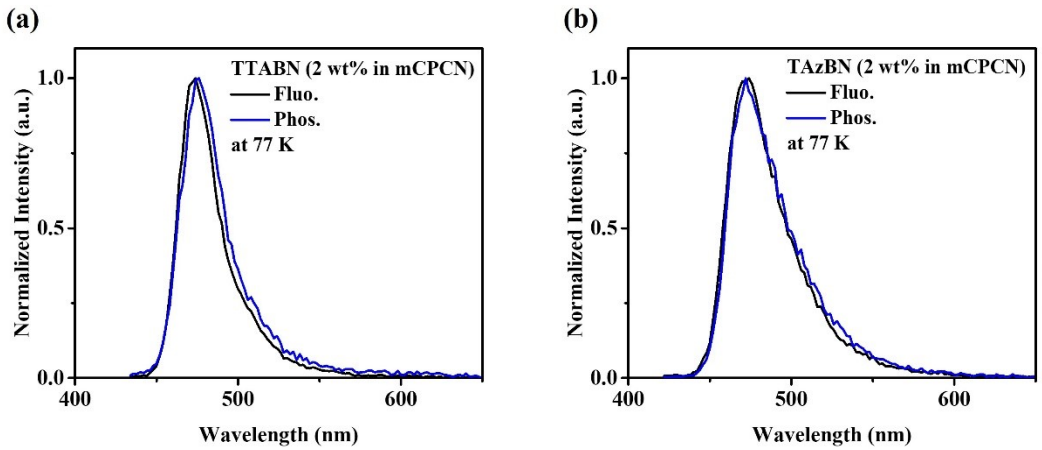


Fig. S14 Fluorescence and phosphorescence (delayed time: 6.25 ms) spectra of (a) TTABN and (b) TAzBN doped films (2 wt% in mCPCN) measured at 77 K.

The relative rate constants could be estimated using the following equations:[9]

$$k_p = 1/\tau_p \quad \text{(S1)}$$

$$k_d = 1/\tau_d \quad \text{(S2)}$$

$$k_{r,S} = \Phi_p k_p \quad \text{(S3)}$$

$$\Phi_{ISC} = \frac{k_{ISC}}{k_{r,S} + k_{nr,S} + k_{ISC}} \quad \text{(S4)}$$

Assuming (i) $k_T = k_{r,T} + k_{nr,T} \ll k_{RISC}$

$$\Phi_{RISC} = \frac{k_{RISC}}{k_{r,T} + k_{nr,T} + k_{RISC}} \approx 1 \quad \text{(S5)}$$

$$k_{nr,S} = \frac{1 - \Phi_{PL}}{\Phi_{PL}} k_r \quad \text{(S6)}$$

$$k_{RISC} = \frac{k_p k_d \Phi_{PL}}{k_{r,S}} \quad \text{(S7)}$$

$$k_{ISC} = \frac{k_p k_d \Phi_d}{k_{RISC} \Phi_p} \quad \text{(S8)}$$

Assuming (ii) $k_{nr,S} \ll k_{r,S}, k_{ISC}$

$$\Phi_{ISC} = 1 - \Phi_p \quad \text{(S9)}$$

$$k_{ISC} = k_p(1 - \Phi_p) \tag{S10}$$

$$k_{RISC} = \frac{k_p k_d \Phi_d}{k_{ISC} \Phi_p} \tag{S11}$$

$$k_T = k_{r,T} + k_{nr,T} = \frac{k_d \Phi_{PL}}{\Phi_p} - k_{RISC} \tag{S12}$$

Where $k_{r,S}$, $k_{nr,S}$, k_{ISC}, k_{RISC}, $k_{r,T}$, and $k_{nr,T}$ represent the radiative decay rate of the S_1 state, the nonradiative decay rate of the S_1 state, intersystem crossing (ISC) rate, reverse intersystem crossing (RISC) rate, the radiative decay rate of the T_1 state, the nonradiative decay rate of the T_1 state. Moreover, k_p and k_d represent the decay rate constants for prompt and delayed fluorescence, respectively, which are in reciprocal relationship with the decay time constants (τ_p and τ_d) experimentally determined from transient PL characteristics. Φ_p and Φ_d indicate prompt and delayed fluorescence components and can be distinguished from the total Φ_{PL} by comparing the integrated intensities of prompt and delayed components in the transient PL spectra. Since the results of decay curves are multi-exponential, the intensity average lifetimes are calculated according to the equation in **Table 1** and equation S13-15. The fitting results are given by following equation:[10]

$$I(t) = \sum_{i=1}^{n} B_i e^{(-t/\tau_i)} \tag{S13}$$

To calculate the average prompt or delayed lifetime, we adopted the following equation:

$$\tau_p = \frac{\sum_i B_i \tau_i^2}{\sum_i B_i \tau_i} \tag{S14}$$

$$\tau_d = \frac{\sum_i B_i \tau_i^2}{\sum_i B_i \tau_i} \tag{S15}$$

, where B_1 and τ_1 are not included

Table S6 Summary of the photophysical properties of TTABN and TAzBN.

x[a] wt%	τ_p[b] (ns)	τ_d[b] (μs)	Φ_{PL}[c] (%)	Φ_p[c] (%)	Φ_d[c] (%)	k_p[d] (10^8 s^{-1})	k_d[d] (10^5 s^{-1})	$k_{r,S}$[c] (10^7 s^{-1})	$k_{nr,S}$[d] (10^7 s^{-1})	k_{ISC}[e] (10^7 s^{-1})	k_{RISC}[f] (10^6 s^{-1})	k_T[g] (10^4 s^{-1})
							TTABN					
2	8.3	65.5	92	50	42	1.20	0.15	6.02	0.52	5.50	0.03	0.24
10	6.2	41.1	65	33	32	1.61	0.24	5.32	2.87	7.94	0.05	1.27
30	3.4	7.8	39	5	34	2.94	1.28	1.47	2.30	25.6	1.00	8.23
							TAzBN					
2	9.2	15.8	91	31	60	1.09	0.63	3.37	0.33	7.17	0.19	0.82

10	7.4	7.9	94	14	80	1.35	1.27	1.89	0.12	11.5	0.85	0.88
30	5.6	8.1	90	23	67	1.79	1.23	4.11	0.46	13.3	0.48	1.60

[a]Different concentrations of two compound doped in mCPCN films. [b]Lifetime of the prompt component (τ_p) and delayed component (τ_d). [c]Absolute PLQY (Φ_{PL}) measured in doped films, the promote (Φ_p) and delayed (Φ_d) fluorescent component of PLQY. [d]The rate constant of prompt (k_p) and delayed (k_d) component according to equations (S1) and (S2). [c]The rate constant of the radiative singlet decay ($k_{r,S}$) according to equation (S3). [d]The rate constant of the non-radiative singlet decay ($k_{nr,S}$) according to equation (S6). [e]The rate constant of intersystem crossing (k_{ISC}) according to equation (S8). [f]The rate constant of reverse intersystem crossing (k_{RISC}) according to equation (S7). [g]The sum of the rate constants of the radiative and nonradiative decay rate from the triplet state, $k_T = k_{r,T} + k_{nr,T}$, according to equation (S12).

8. Circularly polarized properties

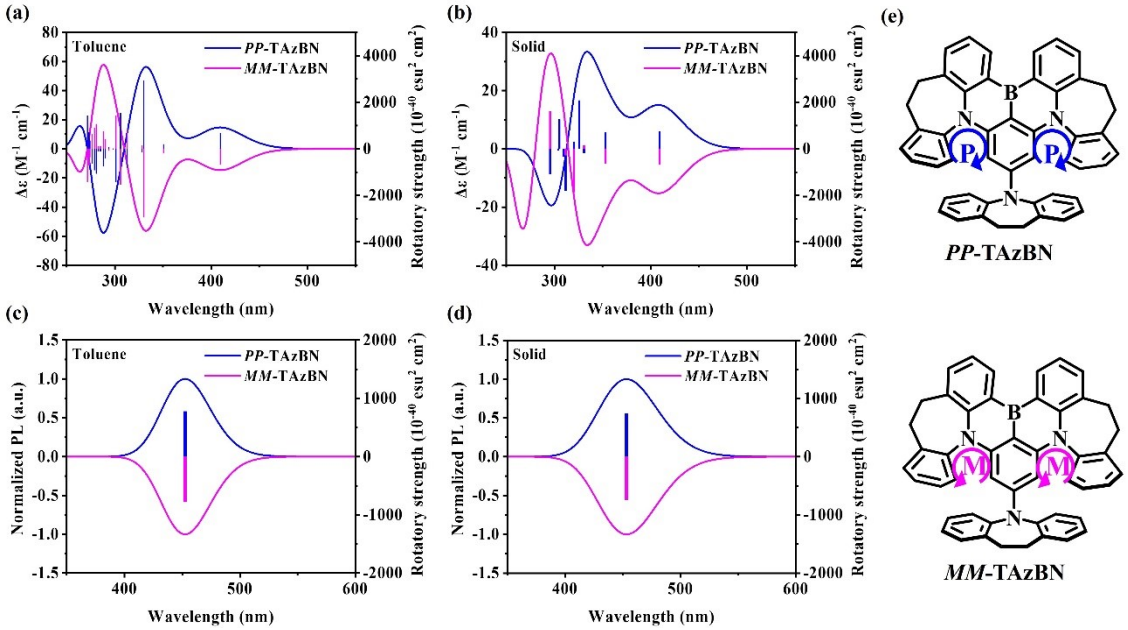


Fig. S15 Simulated circular dichroism (CD) spectra of TAzBN in (a) toluene and (b) the solid phase. Circularly polarized luminescence (CPL) spectra of TAzBN in (c) toluene and (d) the solid phase by TD-DFT at B3LYP/6-31G(d). (e) Molecular structures of *PP*-TAzBN and *MM*-TAzBN. Rotatory strength, $R = |\boldsymbol{\mu}||\boldsymbol{m}|\cos\theta_{\mu,m}$. $\boldsymbol{\mu}$ is the transition electric dipole moment, $\boldsymbol{m}$ is the transition magnetic dipole moment, and $\cos\theta_{\boldsymbol{\mu},\boldsymbol{m}}$ represents the angle of $\boldsymbol{\mu}$ and $\boldsymbol{m}$.

Transition Moment Density Analysis

The transition electric dipole moment density (TEDM) of each axis component corresponding to the one electron transition from φ_i to φ_f was calculated as follows:[11]

$$\begin{cases} \rho_x^{\mu} = \varphi_i \hat{x} \varphi_f \\ \rho_y^{\mu} = \varphi_i \hat{y} \varphi_f \\ \rho_z^{\mu} = \varphi_i \hat{z} \varphi_f \end{cases} \quad \text{(S16)}$$

where φ_i and φ_f are the molecular orbitals involved in the electronic transition, and $\hat{x}$, $\hat{y}$, and $\hat{z}$ are the position operators corresponding to each axis component. The TEDM density of the first singlet excited state (S_1) was calculated as the sum of multiple one-electron excitations as follows,

$$\begin{cases} \rho_x^{\mu}(S_1) = \sum_j w_j \rho_x^{\mu} \\ \rho_y^{\mu}(S_1) = \sum_j w_j \rho_y^{\mu} \\ \rho_z^{\mu}(S_1) = \sum_j w_j \rho_z^{\mu} \end{cases} \quad \text{(S17)}$$

where w_j is the weight of one-electron transitions for S_1. For restricted closed-shell calculations, w_j was calculated as follows, $w_j = 2c_j^2 \frac{c_j}{|c_j|}$ where c_j is the CI coefficients printed by Gaussian after TD-DFT calculations. The total TEDM density of S_1 was generated as a linear combination of each axis component as follows

$$\rho_{total}^{\mu}(S_1) = \frac{\mu_x}{|\mu|}\rho_x^{\mu}(S_1) + \frac{\mu_y}{|\mu|}\rho_y^{\mu}(S_1) + \frac{\mu_x}{|\mu|}\rho_y^{\mu}(S_1) \quad \text{(S18)}$$

where μ_x, μ_y, and μ_z are each axis component of TEDM and $|\boldsymbol{\mu}|$ is the magnitude of TEDM (i.e., $|\mu| = \sqrt{\mu_x^2 + \mu_y^2 + \mu_z^2}$ for S_1. In the similar manner, the averaged transition magnetic dipole moment (TMDE) densities of each axis component are expressed as follows,

$$\begin{cases} \rho_x^{m,ave} = \frac{1}{2}\left\{\varphi_f\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)\varphi_i - \varphi_i\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right)\varphi_f\right\} \\ \rho_y^{m,ave} = \frac{1}{2}\left\{\varphi_f\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right)\varphi_i - \varphi_i\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right)\varphi_f\right\} \\ \rho_z^{m,ave} = \frac{1}{2}\left\{\varphi_f\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)\varphi_i - \varphi_i\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)\varphi_f\right\} \end{cases} \quad \text{(S19)}$$

The TEDM density of S_1 was calculated as the sum of multiple one-electron excitations as follows,

$$\begin{cases} \rho_x^{m}(S_1) = \sum_j w_j \rho_x^{m,ave} \\ \rho_y^{m}(S_1) = \sum_j w_j \rho_y^{m,ave} \\ \rho_z^{m}(S_1) = \sum_j w_j \rho_z^{m,ave} \end{cases} \quad \text{(S20)}$$

The total TMDM density for S_1 was generated as a linear combination of each axis component as follows,

$$\rho_{total}^{m}(S_1) = \frac{m_x}{|m|}\rho_x^{m}(S_1) + \frac{m_y}{|m|}\rho_y^{m}(S_1) + \frac{m_x}{|m|}\rho_y^{m}(S_1) \quad \text{(S21)}$$

where m_x, m_y, and m_z are each axis component of TEDM and $|\boldsymbol{m}|$ is the magnitude of TEDM (i.e., $|m| = \sqrt{m_x^2 + m_y^2 + m_z^2}$ for S_1.

Table S7 Calculated Electronic Transition Properties of *PP*-TAzBN and *MM*-TAzBN.

Molecule[a]	Phase	$\|\boldsymbol{\mu}\|$[b] [10^{-18} esu·cm]	$\|\boldsymbol{m}\|$[c] [10^{-22} erg·G^{-1}]	cos$\theta_{\boldsymbol{\mu},\boldsymbol{m}}$[d]	D[e] [10^{-35} esu^2·cm^2]	G[f] [10^{-40} erg^2·G^{-2}]	R[g] [10^{-40} esu·cm·erg·G^{-1}]	$g_{abs/PL}$[h] [10^{-3}]
				Absorption[i]				
PP-TAzBN	Toluene	4.57	1.13	0.10	2.09	1.28	53.4	1.02
MM-TAzBN	Toluene	4.57	1.13	-0.10	2.09	1.28	-53.4	-1.02
				Emission[j]				
PP-TAzBN	Toluene	4.19	1.10	0.12	1.76	1.21	57.2	1.30
MM-TAzBN	Toluene	4.19	1.10	-0.12	1.76	1.21	-57.2	-1.30
				Absorption[i]				
PP-TAzBN	Solid	3.75	2.19	0.08	1.41	4.81	66.2	1.88
MM-TAzBN	Solid	3.76	2.20	-0.08	1.41	4.82	-65.2	-1.85
				Emission[j]				
PP-TAzBN	Solid	3.35	1.95	0.10	1.12	3.82	63.3	2.26
MM-TAzBN	Solid	3.35	1.95	-0.10	1.12	3.82	-63.3	-2.26

[a]Calculated for the isomers at TD-B3LYP-GD3BJ/6-3G(d) level. [b]Transition electric dipole moment (TEDM). [c]Transition magnetic dipole moment (TMDM).[d]cos$\theta_{\boldsymbol{\mu},\boldsymbol{m}}$ represents the angle of TEDM and TMDM. [e]Electric dipole strength, D = $|\boldsymbol{\mu}|^2$. [f]Magnetic dipole strength, G = $|\boldsymbol{m}|^2$. [g]Rotatory strength, R = $|\boldsymbol{\mu}||\boldsymbol{m}|\cos\theta_{\boldsymbol{\mu},\boldsymbol{m}}$. [i]Dissymmerty factor calculated as follows: [h] $g_{abs/PL} = \frac{4|\mu||m|cos\theta_{\mu,m}}{|\mu|^2 + |m|^2}$. [i]The geometry optimized in the S_0 state. [j]The geometry optimized in the S_1 state.

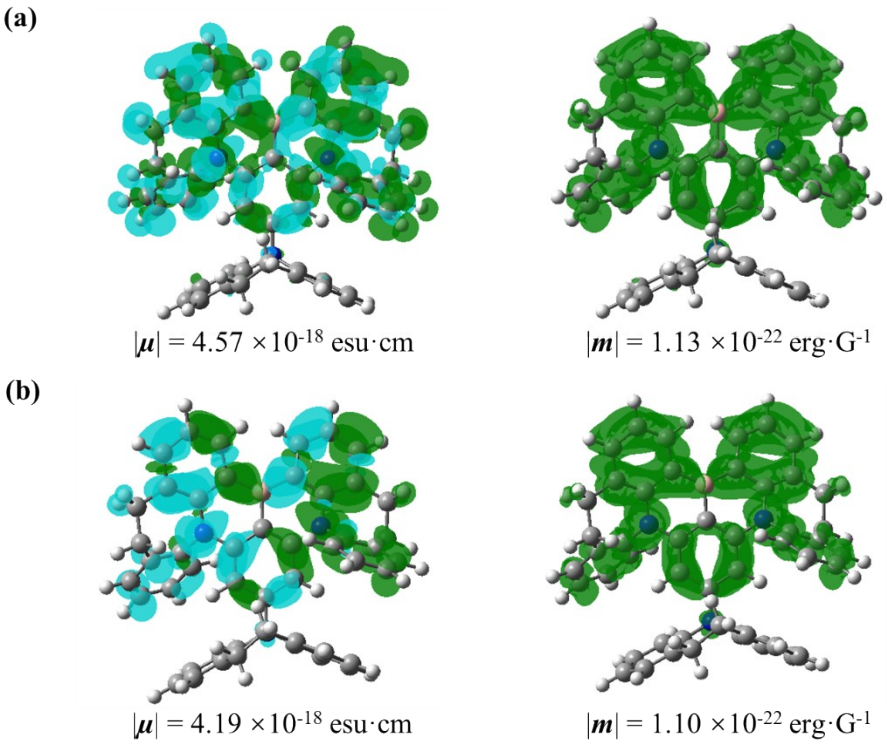


Fig. S16 The TEDM (ρ^{μ}_{total}) and TMDM (ρ^{m}_{total}) densities of *MM*-TAzBN for the (a) $S_0 \rightarrow S_1$ and (b) $S_1 \rightarrow S_0$ transition displayed with an isosurface value of 0.002 au at the TD-B3LYP-GD3BJ/6-31G(d) level of theory in toluene. The spatial integrals of the TEDM and TMDM densities correspond to the $|\boldsymbol{\mu}|$ and $|\boldsymbol{m}|$ values, respectively.

9. OLED device performance

Table S8 Summary of OLED characteristics of the control devices.

Emitter	x wt%	V_{on}[a] [V]	L_{max}[b] [cd/m^2 , V]	EQE_{max}[c] [%]	$EQE_{300/500/1000}$[d] [%]	CE[e] [cd/A]	PE[f] [lm/W]	λ_{max}[g] [nm]	CIE[h] [x, y]	FWHM[i] [nm]
TTABN	2	3.3	1334, 14.0	19.2	10.2/8.4/4.8	19.3	16.9	464	(0.14, 0.13)	31
	10	2.8	1275, 12.0	10.4	6.8/5.4/1.6	10.7	8.4	466	(0.15, 0.15)	30
	20	2.6	382, 9.0	8.5	1.5/-/-	13.9	10.9	466	(0.14, 0.15)	30
	30	2.6	451, 12.0	5.0	0.5/-/-	5.8	4.9	466	(0.14, 0.15)	30
TAzBN	2	3.3	3648, 16.0	26.0	19.0/17.2/16.2	37.1	31.7	475	(0.12, 0.21)	45
	5	3.0	3060, 10.0	26.6	22.2/18.6/17.6	41.2	32.4	478	(0.12, 0.24)	44
	10	2.9	2892, 9.0	27.3	25.0/21.4/16.6	47.8	42.9	482	(0.13, 0.29)	45
	30	2.6	1679, 13.0	16.3	14.3/12.5/8.2	33.7	31.5	486	(0.14, 0.36)	49
	50	2.6	1128, 13.0	8.1	5.9/4.2/1.0	18.2	16.3	489	(0.16, 0.40)	53

[a]The operating voltage at a brightness of 1 cd m^{-2}. [b]Maximum luminance. [c]EQE, maximum external quantum efficiency. [d]EQE at brightness of 300/500/1000 cd m^{-2}. [e]CE, maximum current efficiency. [f]PE, maximum power efficiency. [g]The EL emission wavelength at maximum intensity. [h]CIE coordinates at 8 V. [i]FWHM value.

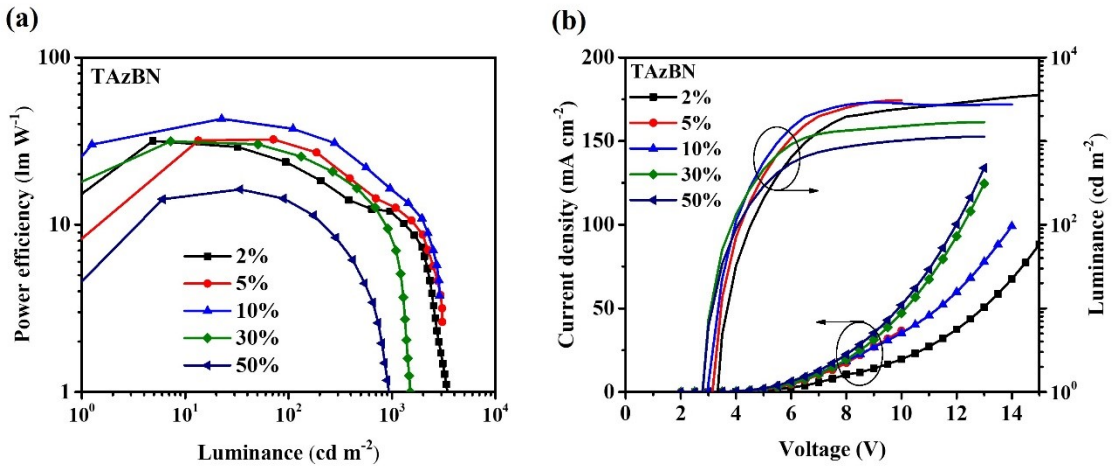


Fig. S17 (a) PE-luminance curves, (b) current density–voltage–luminance (J–V–L) characteristics, with different dopant concentrations of 2-50%.

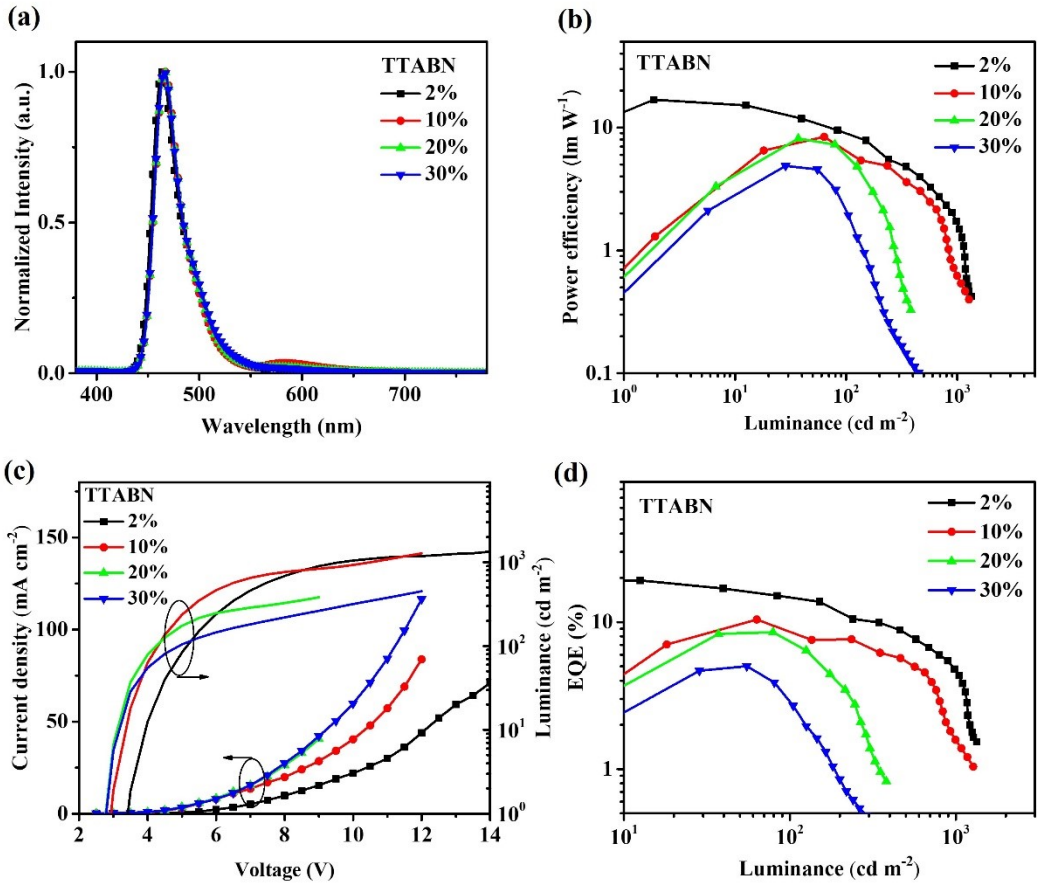


Fig. S18 Electroluminescence characteristics of blue OLEDs. (a) Electroluminescence (EL) spectra, (b) PE-luminance curves, (c) current density–voltage–luminance (J–V–L) characteristics, and (d) EQE versus luminescence with different dopant concentrations of 2%, 10%, 20% and 30%.

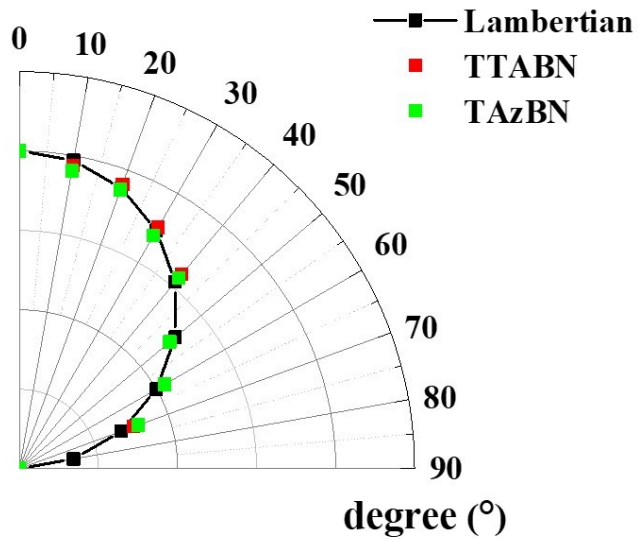


Fig. S19 Angle-dependent EL pattern of TTABN and TAzBN-based devices (2 wt% doped in mCPCN). The black line and symbol present the luminous intensity of a Lambertian distribution.

Table S9 Summary of MR-OLED performances without sensitizers.

Compound	Ref.	Host	λ_{EL}[a]	FWHM[b]	wt%[c]	EQE_{max}[d]	EQE_{1000}[e]	Roll-off[f]
TAzBN	this work	mCPCN	475	45	2	26	16.2	38
TAzBN	this work	mCPCN	478	44	5	26.6	17.6	34
TAzBN	this work	mCPCN	482	45	10	27.3	16.6	39
TAzBN	this work	mCPCN	486	49	30	16.3	8.2	50
TAzBN	this work	mCPCN	489	53	50	8.1	1.0	88
BBCZ-DB	[12]	mCBP	469	27	1	29.3	-	-
BBCZ-SB	[12]	mCBP	487	26	1	27.8	-	-
BBCz-R	[12]	mCBP	515	54	1	31.8	-	-
BBCz-G	[12]	mCBP	549	48	1	29.3	-	-
BBCz-Y	[12]	mCBP	616	26	1	22	-	-
BN1	[13]	mCB	506	36	1	24.3	12.9	47
BN2	[13]	mCB	545	46	1	24.5	7.6	69
BN3	[13]	mCB	548	43	1	24.7	8.9	64
D-SBON	[14]	mCBP	466	28	4	13.7	6.7	51
D-SBSN	[14]	mCBP	492	31	4	17.6	12.0	32
D-DBON	[14]	mCBP	510	29	4	26.7	12.0	55
D-DBSN	[14]	mCBP	556	43	4	21.8	16.9	22
BNO1	[15]	DMIC-TRZ	609	37	1	14.9	3.3	78
BNO2	[15]	DMIC-TRZ	629	39	1	12	4.4	63
BNO3	[15]	DMIC-TRZ	616	38	1	15.1	4.3	72
RBNO1	[16]	DMIC-TRZ	632	53	1	17.2	3.0	83
RBNO2	[16]	DMIC-TRZ	645	49	1	15.1	3.4	77
PTZBNO	[17]	DMIC-TRZ	617	59	1	13.6	6.3	54
PXZBNO	[17]	DMIC-TRZ	630	53	1	11.8	3.9	67
CNCz-BNCz	[18]	CBP	584	49	1	23	10.8	53
TCZ-F-DABNA	[19]	PhCzBCz	568	55	1	31.6	15.4	51
TCZ-F-DABNA	[19]	PhCzBCz	576	57	2	32.6	12.7	61
TCZ-F-DABNA	[19]	PhCzBCz	580	61	4	34.1	10.2	70
TCZ-F-DABNA	[19]	PhCzBCz	584	61	6	37.9	7.5	80
TCZ-F-DABNA	[19]	PhCzBCz	588	61	8	39.2	7.8	80
TCZ-F-DABNA	[19]	PhCzBCz	592	61	10	37.1	9.7	74
TCZ-F-DABNA	[19]	PhCzBCz	592	61	20	35.5	11.8	67
TCZ-F-DABNA	[19]	PhCzBCz	592	62	30	30.6	11.0	64
TCZ-F-DABNA	[19]	PhCzBCz	592	62	40	22.6	9.2	59
BN-R	[20]	NPB/DMFBD-TRZ	617	47	1	22	15.4	30
BN-R	[20]	NPB/DMFBD-TRZ	620	46	3	17.8	4.9	72
BN-R	[20]	NPB/DMFBD-TRZ	627	48	10	17.5	2.2	87
BN-R	[20]	NPB/DMFBD-TRZ	629	49	20	16.2	1.8	89

BN-R	[20]	NPB/DMFBD-TRZ	630	50	30	13.6	1.6	88
BN-R	[20]	NPB/DMFBD-TRZ	631	50	40	13.6	10.4	1
BNIP-tBuCz	[21]	DMIC-TRZ	566	69	1	32.2	29.6	8
BNIP-tBuDPAC	[21]	DMIC-TRZ	544	58	1	39.4	23.3	41
BNIP-CzDPA	[21]	DMIC-TRZ	584	64	1	32.4	15.2	53
BNDIP	[21]	DMIC-TRZ	582	62	1	34.1	25.5	25
B4N6-Me	[22]	DMIC-TRZ	588	27	1	30.4	6.2	80
VTCzBN	[23]	2,6-DCzppy	499	38	4	31.7	19.8	38
TCz-VTCzBN	[23]	2,6-DCzppy	524	37	4	32.2	16.0	50
tCzPhB-FL	[24]	CBP	535	26	2	26.2	-	-
tCzPhB-Ph	[24]	CBP	527	24	2	29.3	-	-
AZA-BN	[25]	mCBP	528	31	2	19.8	10.8	45
AZA-BN	[25]	mCBP	528	31	4	25.7	9.0	65
AZA-BN	[25]	mCBP	529	33	6	20.6	6.7	67
AZA-BN	[25]	mCBP	531	35	8	16.8	4.4	74
BN-STO	[26]	DMIC-TRZ	517	34	1	40.1	28.1	30
BN-XTO	[26]	DMIC-TRZ	513	34	1	37.3	18.6	50
BN-TP-N1	[27]	PhCzBCz	532	34	3	34.9	13.9	60
BN-TP-N2	[27]	PhCzBCz	534	35	3	31.3	22.3	29
BN-TP-N3	[27]	PhCzBCz	524	34	3	37.3	19.8	47
BN-TP-N4	[27]	PhCzBCz	528	36	3	36.5	21.2	42
DBTN-2	[28]	SF3-TRZ	520	29	2.5	35.2	20.4	42
ω-DABNA	[29]	DOBNA-Ph	512	25	0.5	31.1	29.4	5
t-DAB-DPA	[30]	mCBP:mCBP-CN	559	26	3	27.6	9.2	67
t-DAB-DPA	[30]	mCBP:mCBP-CN	559	26	5	27.9	8.1	71
t-DAB-DPA	[30]	mCBP:mCBP-CN	559	26	7	27.4	7.6	72
t-DAB-DPA	[30]	mCBP:mCBP-CN	560	26	10	25.9	7.6	71
t-DABNA	[30]	mCBP:mCBP-CN	564	26	3	28.4	4.4	85
t-DABNA	[30]	mCBP:mCBP-CN	564	26	5	23.9	3.4	86
t-DABNA	[30]	mCBP:mCBP-CN	564	26	7	24.8	3.2	87
t-DABNA	[30]	mCBP:mCBP-CN	565	26	10	21.3	2.7	87
mICz-DABNA	[31]	mCBP-CN	466	26	3	26.4	-	-
BFCz-DABNA	[31]	mCBP-CN	463	26	3	28	-	-
pBP-DABNA-Me	[32]	mCBP:DPEPO	464	23	5	23.4	-	-
pBP-DABNA-Me	[32]	mCBP:DPEPO	464	23	10	22.4	-	-
pBP-DABNA-Me	[32]	mCBP:DPEPO	464	23	20	22.1	-	-
pBP-DABNA-Me	[32]	mCBP:DPEPO	464	23	100	20.6	-	-
V-DABNA-Mes	[33]	polymer C	480	27	1	22.9	10.9	52
ν-DABNA	[34]	mCBP	472	17	3	24.6	14.9	39
BOBO-Z	[34]	mCBP	445	18	3	13.6	3.3	76
BOBS-Z	[34]	mCBP	456	23	3	26.9	15.0	44

BSBS-Z	[34]	mCBP	463	22	3	26.8	15.9	41
DTBA-BN2	[35]	26DCzPPy	495	47	1	26.4	22.0	17
DTBA-BN2	[35]	26DCzPPy	497	47	3	31.2	25.6	18
DTBA-BN2	[35]	26DCzPPy	499	47	5	27.9	25.1	10
DTBA-BN2	[35]	26DCzPPy	502	47	10	23.4	20.4	13
DTBA-BN2	[35]	26DCzPPy	506	48	20	21.5	18.6	13
DTBA-B2N3	[35]	26DCzPPy	475	28	3	30.9	20.5	34

[a]EL Emission peak. [b]Full-width at half-maximum of EL. [c]Dopant concentration. [d]Maximum external quantum efficiency. [e]External quantum efficiency at 1000 cd m^{-2}. [f]Efficiency roll-off at 1000 cd m^{-2}.

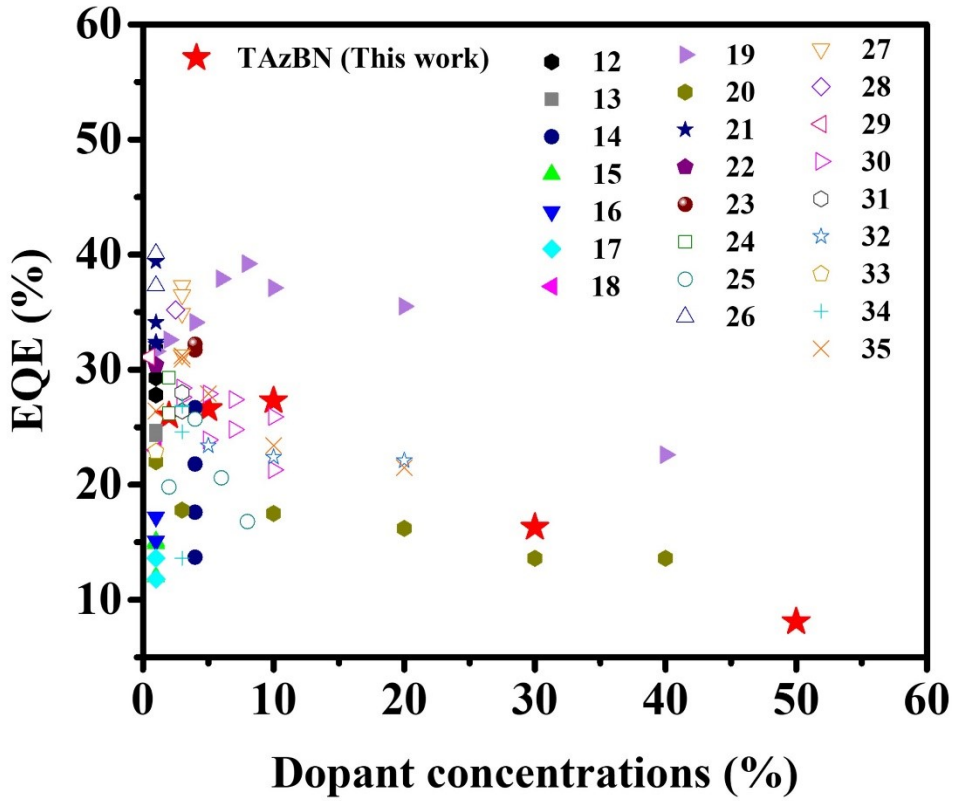


Fig. S20 Summary the maximum external quantum efficiency of MR emitters at different dopant concentrations.

10. NMR spectra

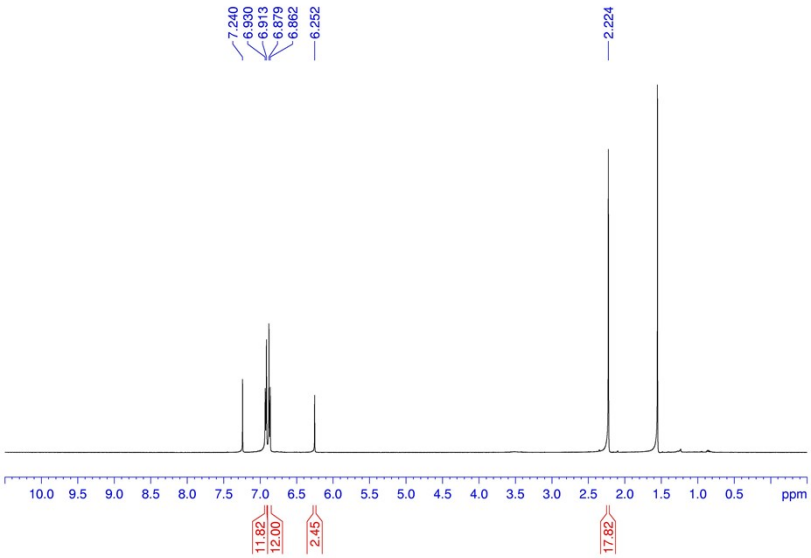


Fig. S21 ^{1}H NMR of N^1, N^1, N^3, N^3, N^5, N^5-hexa-*p*-tolylbenzene-1,3,5-triamine.

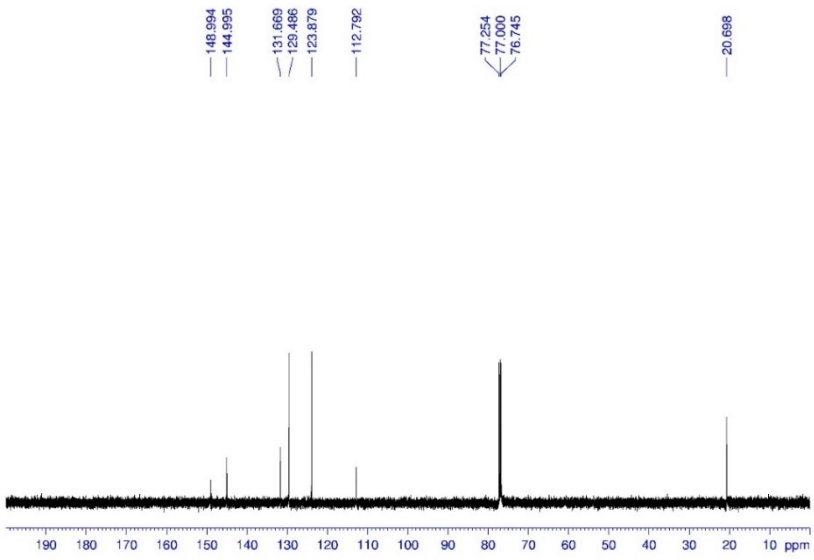


Fig. S22 ^{13}C NMR of N^1, N^1, N^3, N^3, N^5, N^5-hexa-*p*-tolylbenzene-1,3,5-triamine.

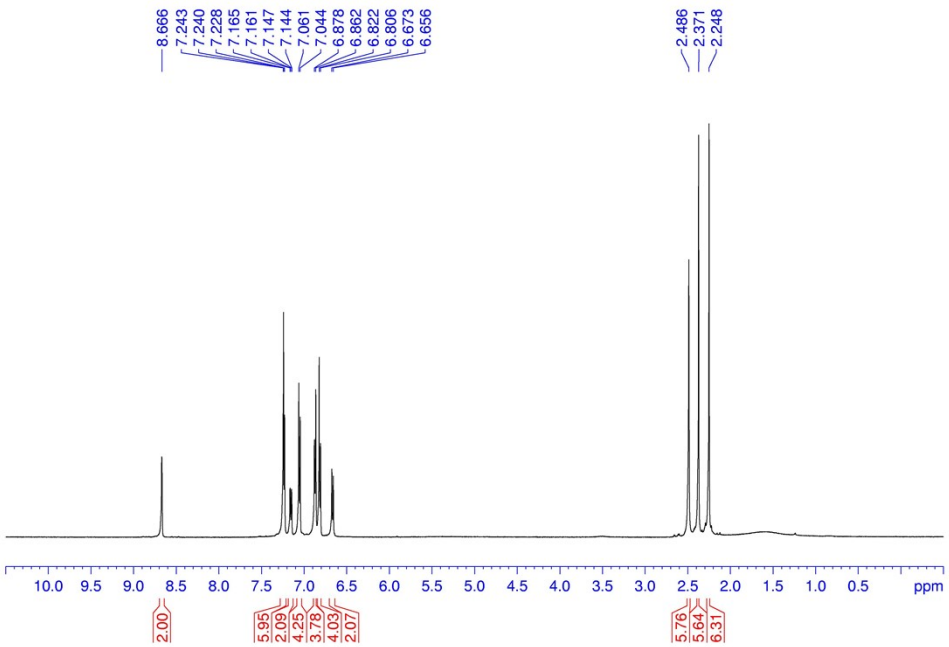


Fig. S23 [1]H NMR of TTABN.

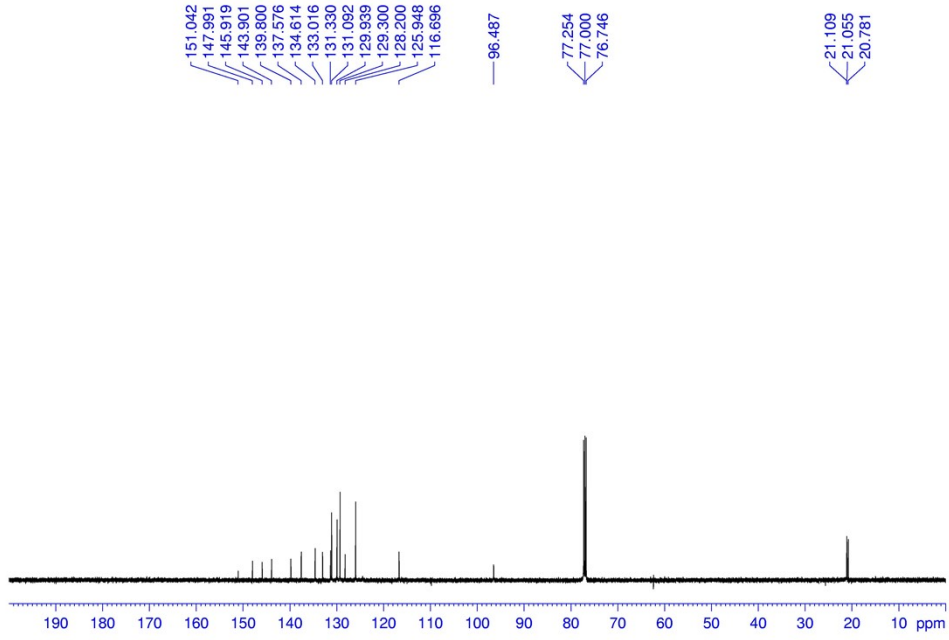


Fig. S24 [13]C NMR of TTABN.

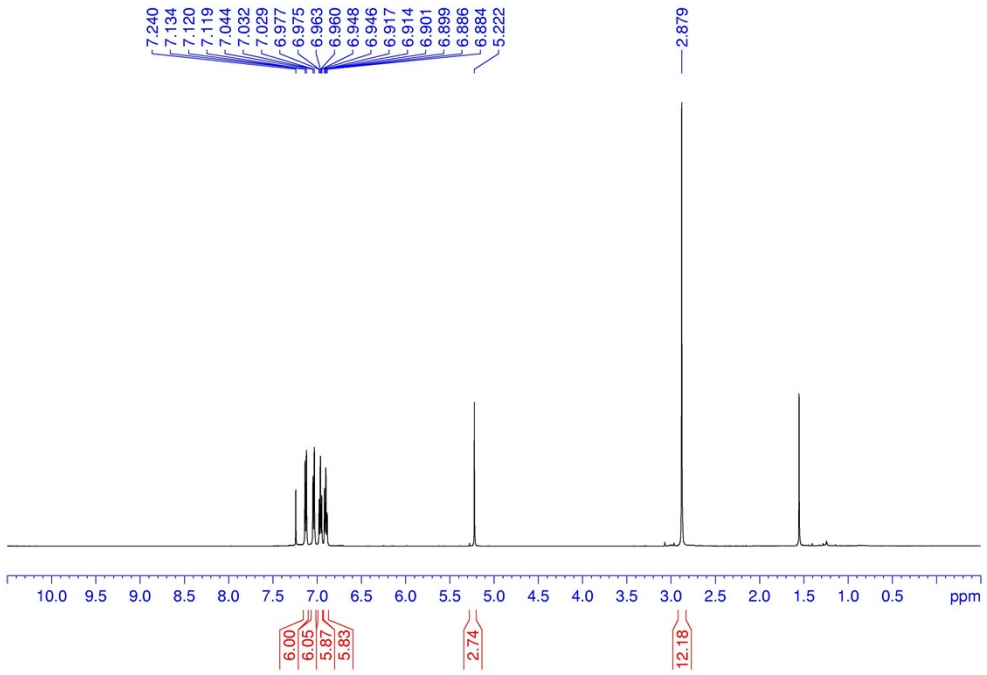


Fig. S25 [1]H NMR of 1,3,5-tris(10,11-dihydro-5*H*-dibenzo[*b*,*f*]azepin-5-yl)benzene

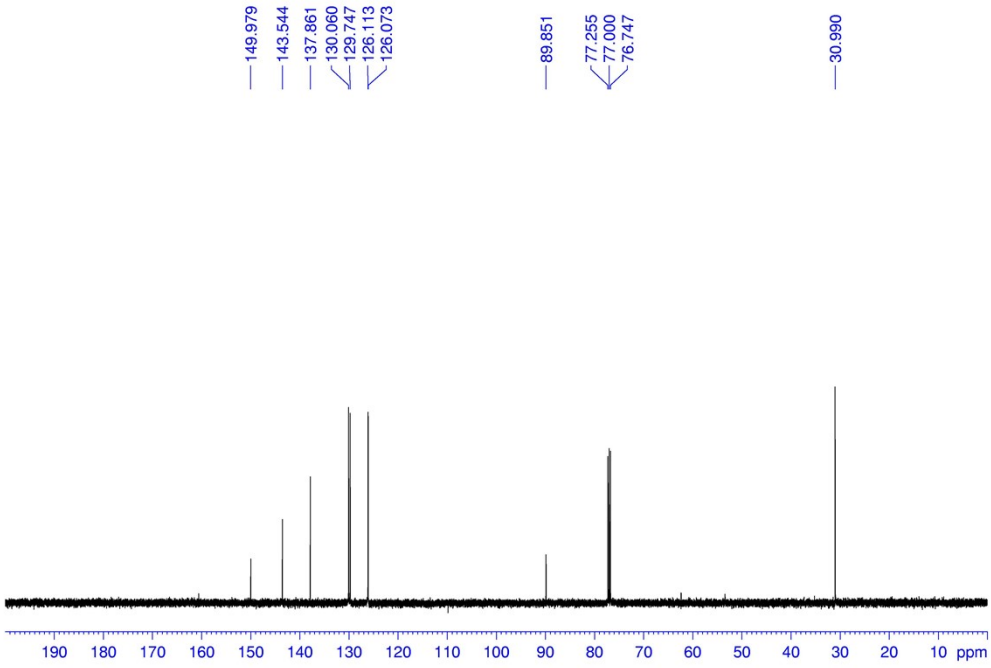


Fig. S26 [13]C NMR of 1,3,5-tris(10,11-dihydro-5*H*-dibenzo[*b*,*f*]azepin-5-yl)benzene

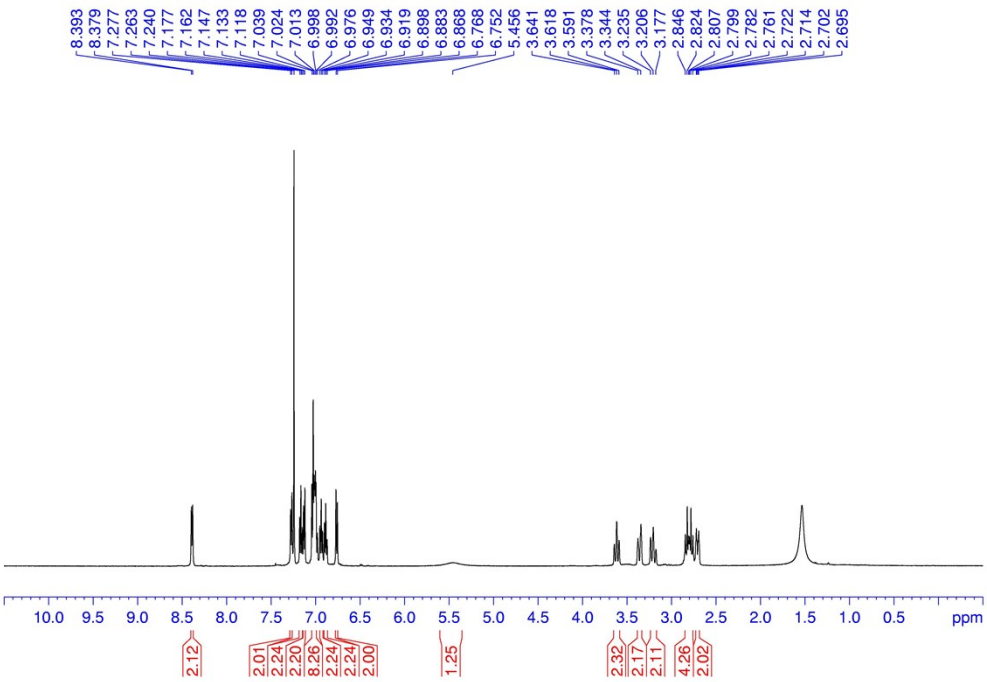


Fig. S27 [1]H NMR of TAzBN.

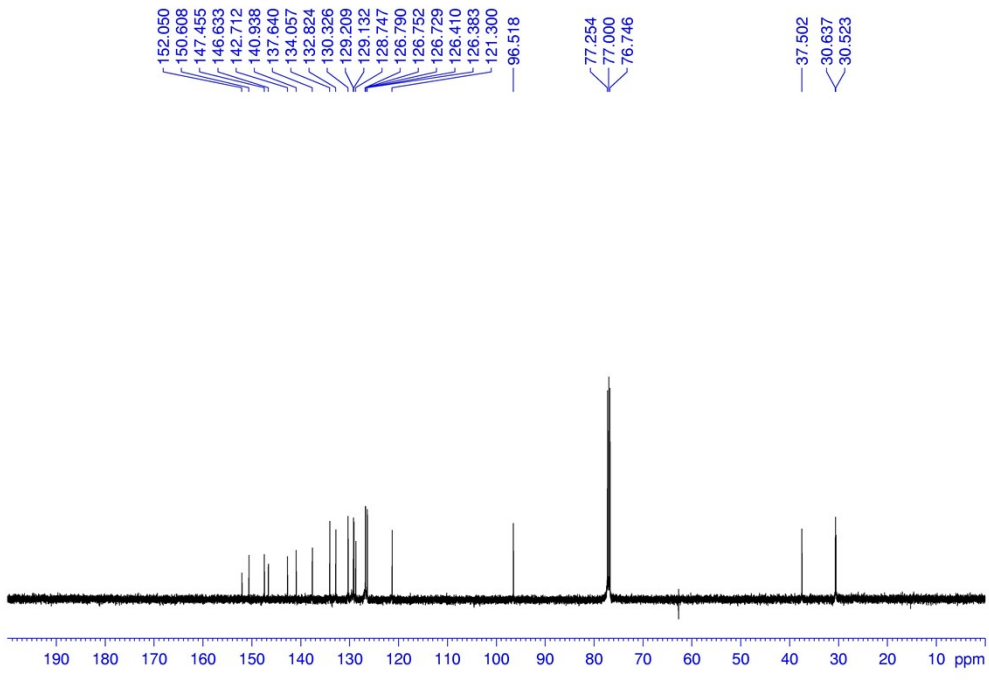


Fig. S28 [13]C NMR of TAzBN.

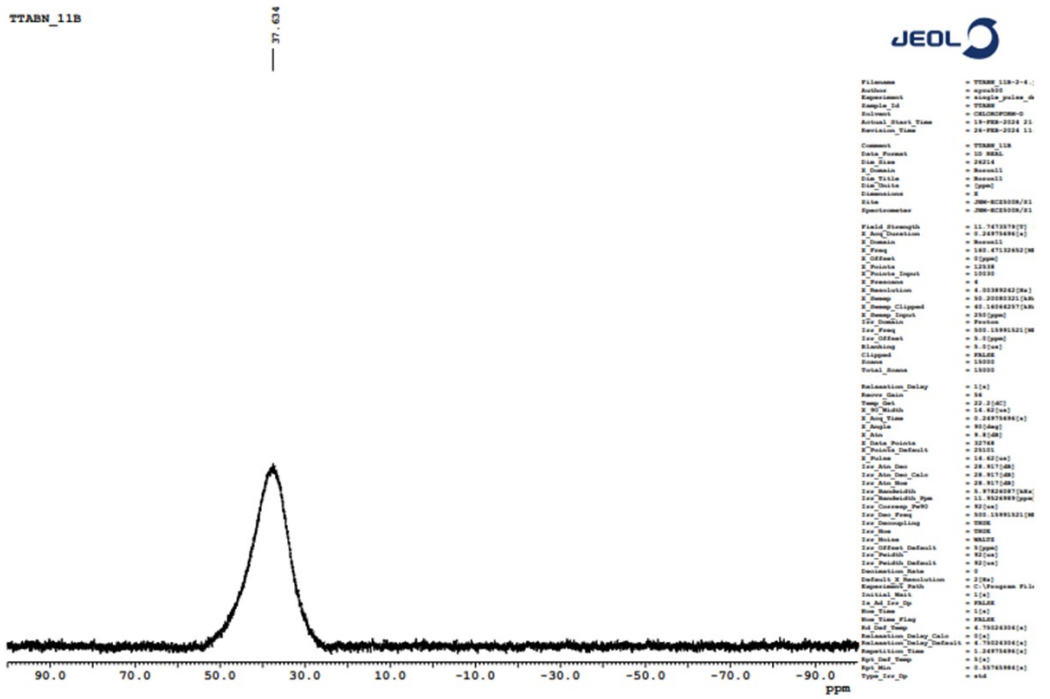


Fig. S29 ^{11}B spectra of TTABN.

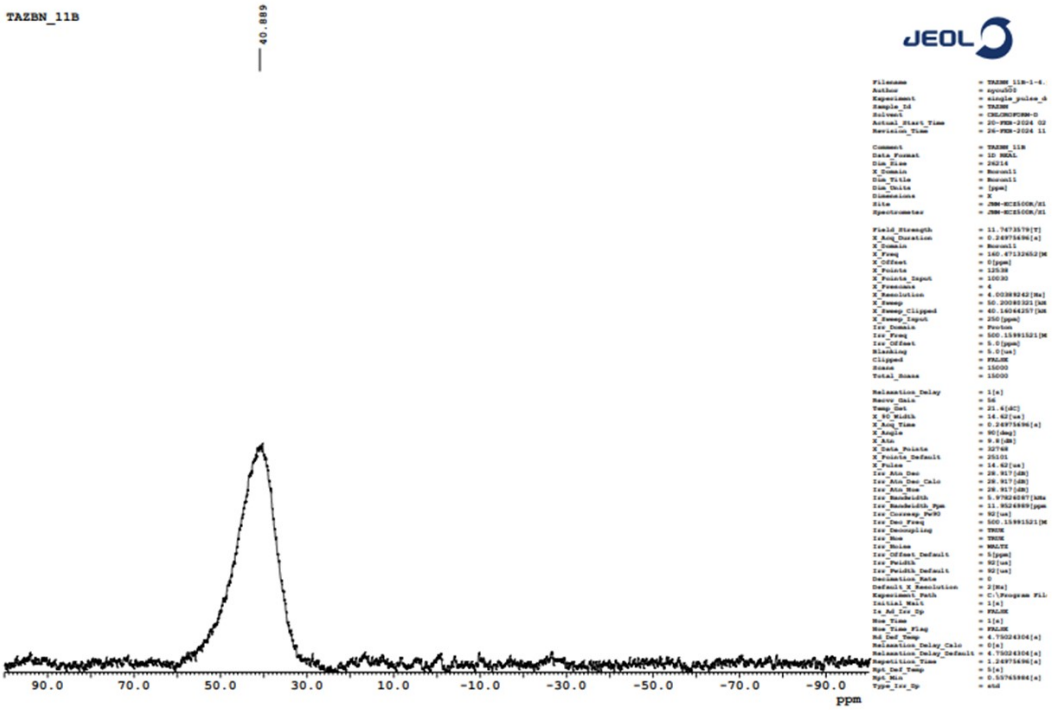


Fig. S30 ^{11}B spectra of TAzBN.

11. HPLC data

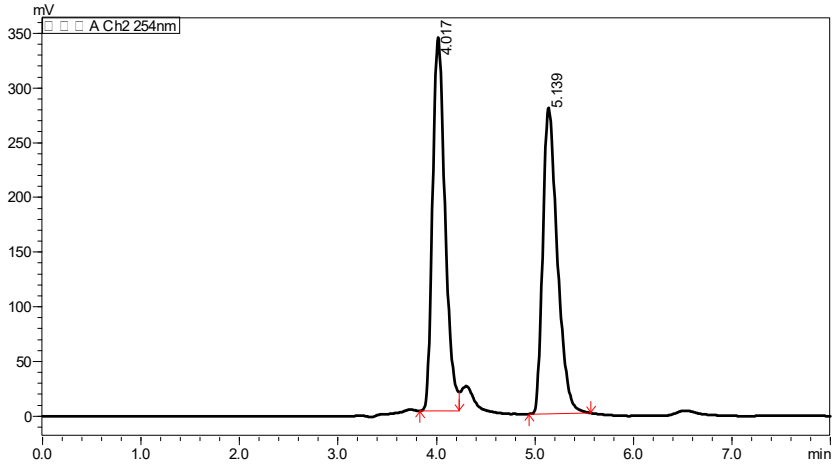


Fig. S31 HPLC profile of TAzBN eluted by Hexane/DCM (V/V = 50/50) using Daicel Chiralpak IE column. The flow rate is 1.0 ml/min.

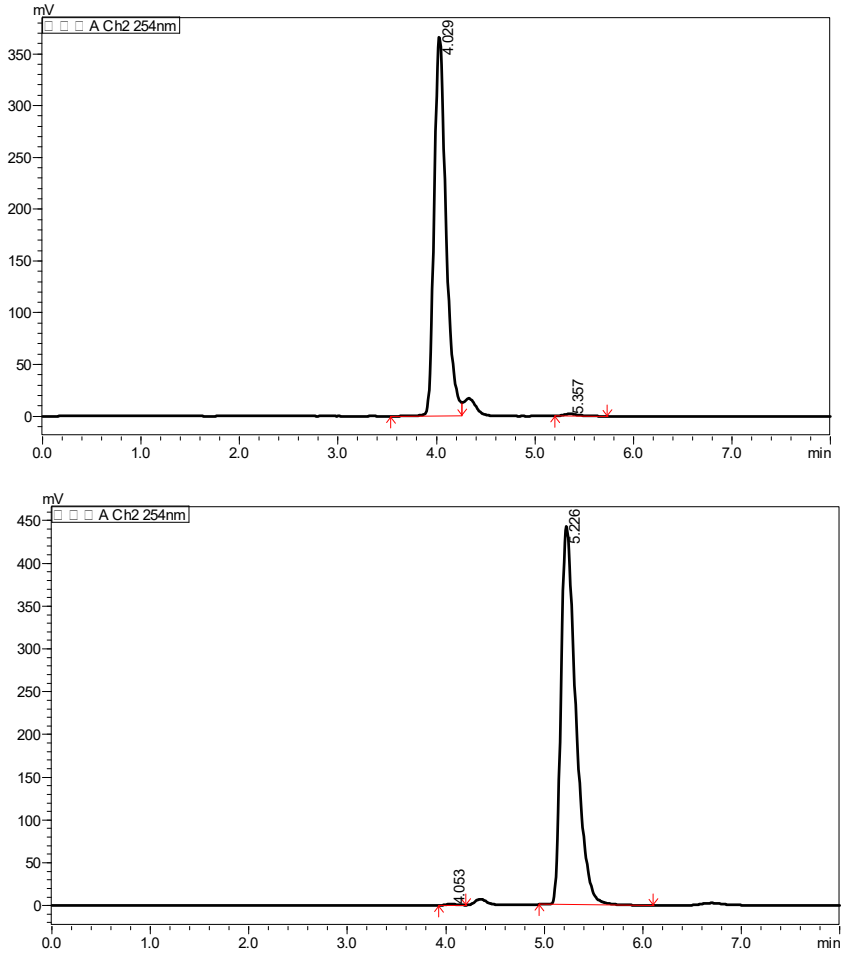


Fig. S32 HPLC profile of TAzBN eluted by Hexane/DCM (V/V = 50/50) using Daicel Chiralpak IE column. The flow rate is 1.0 ml/min. The ee% of both enantiomers are over 98%.

12. Calculated absorption properties

Table S10 Absorption properties of TTABN based on the optimized ground-state geometries by TD-DFT at B3LYP/6-31G (d) in toluene

Functional	State	Main configuration transition		E_{VA} (eV)[a]	λ_{VA} (nm)[b]	f[c]
B3LYP	S1	HOMO→LUMO	0.70073	3.0586	405.37	0.2710
	S2	HOMO-1→LUMO	0.69732	3.2447	382.12	0.3956
	S3	HOMO→LUMO+1	0.68563	3.7070	334.46	0.0381
PBE0	S_1	HOMO→LUMO	0.69884	3.1698	391.14	0.2887
	S_2	HOMO-1→LUMO	0.69064	3.4037	364.26	0.4550
	S_3	HOMO-1→LUMO+4	-0.11228	3.8579	321.38	0.0407
		HOMO→LUMO+1	0.67793			
BMK	S_1	HOMO→LUMO	0.69452	3.3556	369.49	0.3793
	S_2	HOMO-1→LUMO	0.65894	3.6767	337.22	0.5619
		HOMO→LUMO+1	0.16673			
	S_3	HOMO-4→LUMO	0.10405	4.1816	296.50	0.0210
		HOMO-1→LUMO+2	-0.19725			
		HOMO→LUMO+1	0.61996			
		HOMO→LUMO+8	0.17316			
CAM-B3LYP	S_1	HOMO→LUMO	0.68452	3.5665	347.63	0.3938
	S_2	HOMO-3→LUMO	0.14073	4.0030	309.73	0.6478
		HOMO-1→LUMO	0.61498			
		HOMO-1→LUMO+1	0.21009			
		HOMO-1→LUMO+11	-0.10820			
	S_3	HOMO-4→LUMO	0.14470	4.4118	281.03	0.0141
		HOMO-1→LUMO+2	-0.18013			
		HOMO-1→LUMO+3	0.10117			
		HOMO→LUMO+1	0.55560			
		HOMO→LUMO+7	0.16966			
		HOMO→LUMO+8	0.12297			
		HOMO→LUMO+12	0.12361			
M06-2X	S_1	HOMO→LUMO	0.68758	3.5133	352.89	0.3754
	S_2	HOMO-3→LUMO	0.11914	3.9204	316.26	0.6532
		HOMO-1→LUMO	0.62690			
		HOMO-1→LUMO+1	0.20983			
		HOMO-1→LUMO+1	-0.10187			
	S_3	HOMO-4→LUMO	-0.12081	4.3286	286.43	0.0352
		HOMO-1→LUMO+2	-0.13359			
		HOMO-1→LUMO+4	0.11308			
		HOMO→LUMO+1	0.59221			
		HOMO→LUMO+7	0.18535			
		HOMO→LUMO+12	0.10823			
ωB97X-D	S_1	HOMO→LUMO	0.67848	3.6195	342.55	0.3763
	S_2	HOMO-3→LUMO	0.16226	4.1369	299.70	0.6016
		HOMO-1→LUMO	0.58587			
		HOMO-1→LUMO+2	0.21401			
		HOMO-1→LUMO+7	0.12634			
		HOMO-1→LUMO+11	-0.10335			
	S_3	HOMO-2→LUMO	0.60260	4.4568	278.19	0.0521

	HOMO→LUMO+3	0.13063
	HOMO→LUMO+6	-0.12457
	HOMO→LUMO+10	-0.19481

[a]Absorption energy. [b]Absorption wavelength. [c]Oscillator strength.

Table S11 Absorption properties of TAzBN based on the optimized ground-state geometries by TD-DFT at B3LYP/6-31G (d) in toluene

Functional	State	Main configuration transition		E_{VA} (eV)[a]	λ_{VA} (nm)[b]	f[c]
B3LYP	S_1	HOMO→LUMO	0.70073	3.0268	409.62	0.2395
	S_2	HOMO-1→LUMO	0.66508	3.5341	350.83	0.3025
		HOMO→LUMO+1	-0.20286			
	S_3	HOMO-2→LUMO	0.19047	3.7557	330.13	0.1000
		HOMO-1→LUMO	0.19103			
		HOMO→LUMO+1	0.63000			
PBE0	S_1	HOMO→LUMO	0.70186	3.0268	427.57	0.1948
	S_2	HOMO-1→LUMO	0.69051	3.4153	363.02	0.4404
	S_3	HOMO-2→LUMO	0.69551	3.6622	338.56	0.0247
BMK	S_1	HOMO→LUMO	0.69407	3.3633	368.63	0.3223
	S_2	HOMO-2→LUMO	-0.14526	3.9620	312.94	0.3747
		HOMO-1→LUMO	0.63867			
		HOMO→LUMO+1	0.19729			
	S_3	HOMO-2→LUMO	0.65229	4.1981	295.33	0.0019
		HOMO-1→LUMO	0.10450			
		HOMO→LUMO+9	-0.10288			
CAM-B3LYP	S_1	HOMO→LUMO	0.68356	3.5761	346.70	0.3392
	S_2	HOMO-2→LUMO	-0.18023	4.1284	300.32	0.4446
		HOMO-1→LUMO	0.62841			
		HOMO→LUMO+1	0.14982			
	S_3	HOMO-2→LUMO	0.59488	4.3857	282.70	0.0014
		HOMO-1→LUMO	0.10369			
		HOMO→LUMO+1	0.17320			
		HOMO→LUMO+9	0.12701			
M06-2X	S_1	HOMO→LUMO	0.68633	3.5369	350.55	0.3352
	S_2	HOMO-2→LUMO	-0.18404	4.0601	305.37	0.4922
		HOMO-1→LUMO	0.63636			
		HOMO→LUMO+1	0.13818			
	S_3	HOMO-2→LUMO	0.61899	4.3420	285.54	0.0027
		HOMO-1→LUMO	0.13822			
		HOMO→LUMO+9	-0.11233			
ωB97X-D	S_1	HOMO→LUMO	0.67787	3.6168	342.80	0.3478
	S_2	HOMO-2→LUMO	-0.24617	4.1692	297.38	0.4325
		HOMO-1→LUMO	0.60345			
		HOMO→LUMO+1	0.13614			
	S_3	HOMO-2→LUMO	0.55391	4.4139	280.90	0.000
		HOMO-1→LUMO	0.15901			
		HOMO→LUMO+1	0.19912			
		HOMO→LUMO+9	0.14015			

[a]Vertical absorption energy. [b]Vertical absorption wavelength. [c]Oscillator strength.

Table S12 Calculated vertical absorption and singlet-triplet splitting energies of TTABN and TAzBN based on the optimized ground-state geometries in toluene and the solid phase.

Method	$\Delta E_{VA}(S_1)$[a] [nm]	$\Delta E_{VA}(T_1)$[b] [eV]	$\Delta E_{VA}(T_2)$[b] [eV]	$\Delta E_{VA}(T_3)$[b] [eV]	$\Delta E_{S1T1\text{-}VA}$[c] [eV]	$\Delta E_{S1T2\text{-}VA}$[c] [eV]	$\Delta E_{S1T3\text{-}VA}$[c] [eV]
TTABN (Toluene)							
B3LYP	2.82	2.61	2.90	3.16	0.45	0.16	-0.10
PBE0	3.06	2.69	2.92	3.10	0.48	0.25	0.07
BMK	3.17	2.83	3.18	3.40	0.52	0.18	-0.05
CAM-B3LYP	3.36	2.98	3.09	3.19	0.59	0.48	0.37
M06-2X	3.57	3.00	3.37	3.37	0.51	0.15	0.15
ωB97X-D	3.51	3.06	3.23	3.39	0.56	0.39	0.23
TAzBN (Toluene)							
B3LYP	2.87	2.66	2.98	3.21	0.37	0.05	-0.18
PBE0	3.03	2.57	2.81	3.18	0.33	0.09	-0.28
BMK	2.90	2.93	3.23	3.51	0.44	0.14	-0.15
CAM-B3LYP	3.36	3.04	3.10	3.32	0.54	0.48	0.25
M06-2X	3.58	3.10	3.34	3.70	0.44	0.19	-0.17
ωB97X-D	3.54	3.11	3.21	3.46	0.51	0.41	0.16
TTABN (Solid)							
B3LYP	3.05	2.62	2.95	3.17	0.43	0.10	-0.12
PBE0	3.16	2.69	2.95	3.14	0.47	0.21	0.02
BMK	3.37	2.85	3.20	3.44	0.51	0.16	-0.08
CAM-B3LYP	3.58	2.99	3.08	3.24	0.58	0.50	0.34
M06-2X	3.52	3.00	3.35	3.60	0.52	0.16	-0.08
ωB97X-D	3.61	3.04	3.19	3.38	0.57	0.42	0.23
TAzBN (Solid)							
B3LYP	3.03	2.62	2.95	3.17	0.43	0.10	-0.12
PBE0	3.15	2.69	2.95	3.14	0.47	0.21	0.02
BMK	3.37	2.85	3.20	3.44	0.51	0.16	-0.08
CAM-B3LYP	3.59	2.99	3.08	3.24	0.58	0.50	0.34
M06-2X	3.54	3.00	3.35	3.60	0.52	0.16	-0.08
ωB97X-D	3.63	3.04	3.19	3.38	0.57	0.42	0.23

[a]The vertical absorption energy of S_1. [a]The vertical absorption energy of $T_1/T_2/T_3$. [c]The vertical absorption energy gap between S_1 and $T_1/T_2/T_3$.

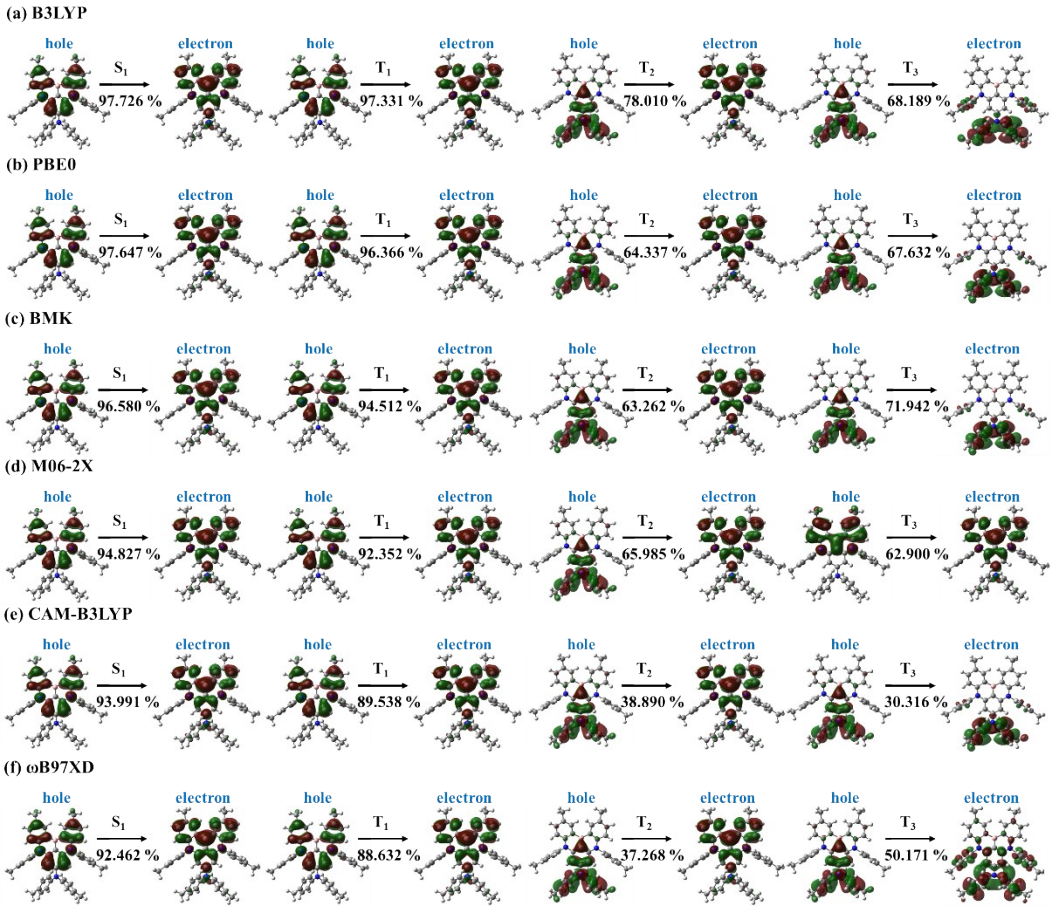


Fig. S33 Hole and electron natural transition orbitals (NTOs) in the S_1, T_1, T_2 and T_3 states of TTABN by TD-DFT based on the optimized ground-state geometries in toluene. The percentages are the predominant hole and electron wave functions with the largest weight.

Fig. S34 Hole and electron natural transition orbitals (NTOs) in the S_1, T_1, T_2 and T_3 states of TAzBN by TD-DFT based on the optimized ground-state geometries in toluene. The percentages are the predominant hole and electron wave functions with the largest weight.

13. Optimized geometries and vibrational frequencies

Table S13 Cartesian coordinates of optimized S_0 and S_1 states of TTABN in toluene at B3LYP/6-31G(d) by (TDA)-DFT, respectively.

Elements	X	Y	Z	X	Y	Z
		S_0			S_1	
C	-0.73713	-1.21892	-0.13608	0.75744	-1.19842	0.15244
C	1.34398	0.01161	0.00151	-1.36553	0.00920	-0.00110
H	-5.64495	-0.82537	0.59276	5.70505	-0.86958	-0.48397
C	-3.64604	-1.42974	0.08005	3.67450	-1.41962	-0.02730
C	-5.01022	-1.67473	0.36306	5.04486	-1.69845	-0.25256
C	-2.81360	-2.56735	-0.11106	2.83327	-2.56877	0.16156
C	-4.74037	-4.03173	0.12392	4.74956	-4.06576	0.02112
C	-5.58361	-2.94052	0.39658	5.60019	-2.98520	-0.22592
N	2.76210	0.02414	0.00209	-2.78065	0.01857	-0.00141
H	-5.14852	-5.04077	0.12168	5.14602	-5.07737	0.06008
C	-0.75829	1.20580	0.13759	0.77325	1.18860	-0.15295
C	-1.48339	-0.01297	0.00065	1.49912	-0.00975	-0.00004

C	-2.85798	2.51786	0.11190	2.86720	2.53128	-0.16178
C	-5.03868	1.58699	-0.36204	5.06705	1.63174	0.25247
H	-5.65849	0.72666	-0.59165	5.71622	0.79423	0.48399
C	-5.63408	2.84258	-0.39570	5.63944	2.91098	0.22543
C	-3.67043	1.36586	-0.07906	3.69307	1.37110	0.02737
C	-4.81000	3.94838	-0.12332	4.80324	4.00270	-0.02171
H	-5.23567	4.95015	-0.12126	5.21309	5.00895	-0.06089
C	0.66403	-1.20153	-0.16100	-0.66482	-1.18836	0.18438
H	1.23347	-2.10914	-0.29804	-1.22145	-2.10027	0.34570
C	0.64294	1.21280	0.16332	-0.64902	1.19735	-0.18580
H	1.19643	2.13017	0.30071	-1.19341	2.11660	-0.34727
B	-2.99580	-0.02616	0.00054	3.03269	-0.01991	0.00016
C	3.47272	1.08938	-0.61907	-3.48533	1.06177	0.66247
C	3.08702	1.57137	-1.87985	-3.07289	1.51530	1.92534
C	4.58674	1.66804	0.00654	-4.61103	1.65544	0.07159
C	3.79275	2.60845	-2.48442	-3.76486	2.53988	2.56682
H	2.23495	1.12573	-2.38340	-2.21355	1.05662	2.40476
C	5.29462	2.69278	-0.61881	-5.30419	2.66598	0.73435
H	4.89954	1.30710	0.98138	-4.94374	1.31732	-0.90479
C	4.91101	3.19065	-1.87082	-4.89433	3.13644	1.98933
H	3.47653	2.96096	-3.46403	-3.42828	2.86988	3.54735
H	6.15800	3.12144	-0.11441	-6.17718	3.10626	0.25731
C	3.49190	-1.02985	0.62038	-3.49965	-1.01657	-0.66261
C	4.61033	-1.59326	-0.01228	-4.62820	-1.59927	-0.06524
C	3.11569	-1.52265	1.87927	-3.09361	-1.48017	-1.92337
C	5.33302	-2.61118	0.60619	-5.33164	-2.60645	-0.72132
H	4.90891	-1.23108	-0.99112	-4.94913	-1.26069	0.91493
C	3.83683	-2.55351	2.47736	-3.79636	-2.50196	-2.55854
H	2.25377	-1.09693	2.38330	-2.22567	-1.03822	-2.40301
C	4.96378	-3.11442	1.86088	-4.93287	-3.08152	-1.97862
H	6.19500	-3.03287	0.09343	-6.20209	-3.04315	-0.23628
H	3.52309	-2.91967	3.45267	-3.46002	-2.84498	-3.53458
N	-1.46393	2.40935	0.27815	1.45745	2.39400	-0.29571
C	-0.70959	3.61084	0.53788	0.68897	3.59326	-0.53539
C	-0.47953	4.01695	1.85382	0.43901	4.00573	-1.84540
C	-0.21004	4.37635	-0.51882	0.20364	4.34625	0.53632
C	0.24462	5.18195	2.10725	-0.30329	5.16390	-2.07781
H	-0.87337	3.42111	2.67200	0.82850	3.42125	-2.67359
C	0.51339	5.53887	-0.25523	-0.53757	5.50168	0.29166
H	-0.39367	4.05907	-1.54108	0.40998	4.02513	1.55289
C	0.75601	5.96023	1.05985	-0.80645	5.92877	-1.01663
H	0.41410	5.49097	3.13598	-0.49345	5.47733	-3.10142
H	0.89523	6.12847	-1.08529	-0.91292	6.08064	1.13196
C	1.56766	7.20351	1.33937	-1.63672	7.16433	-1.27375
H	2.63939	6.97090	1.39493	-2.70759	6.92239	-1.29565
H	1.43884	7.95207	0.55052	-1.48995	7.91553	-0.49064
H	1.28439	7.66097	2.29293	-1.38640	7.62181	-2.23633
C	5.65870	4.32823	-2.52645	-5.62708	4.26065	2.68342
H	6.69864	4.37317	-2.18603	-6.68588	4.28191	2.40410
H	5.66416	4.22857	-3.61757	-5.56657	4.16573	3.77308
H	5.19863	5.29840	-2.29374	-5.20289	5.23937	2.42030

C	5.76661	-4.20214	2.53573	-5.71521	-4.15926	-2.69212
H	6.24590	-4.85996	1.80248	-6.16879	-4.86119	-1.98370
H	6.56458	-3.78190	3.16315	-6.53146	-3.73285	-3.29110
H	5.13786	-4.82077	3.18520	-5.07828	-4.73169	-3.37483
C	-7.04685	-3.14732	0.71079	7.08158	-3.18739	-0.43637
H	-7.55054	-2.19415	0.90154	7.45107	-2.58810	-1.27746
H	-7.57195	-3.64106	-0.11727	7.65783	-2.88218	0.44807
H	-7.18500	-3.77971	1.59733	7.31978	-4.23719	-0.63755
C	-7.10077	3.02373	-0.70967	7.12343	3.09348	0.43567
H	-7.25017	3.65514	-1.59507	7.37562	4.14004	0.63667
H	-7.58731	2.06204	-0.90216	7.48501	2.48945	1.27682
H	-7.63467	3.50648	0.11924	7.69548	2.78048	-0.44878
N	-1.42166	-2.43454	-0.27717	1.42552	-2.41284	0.29533
C	-0.64633	-3.62256	-0.53713	0.64097	-3.60185	0.53419
C	-0.40860	-4.02398	-1.85305	0.38444	-4.01122	1.84381
C	-0.13338	-4.37938	0.51953	0.14632	-4.34796	-0.53818
C	0.33672	-5.17565	-2.10661	-0.37379	-5.15933	2.07527
H	-0.81279	-3.43507	-2.67120	0.78110	-3.43231	2.67251
C	0.61117	-5.52834	0.25585	-0.61072	-5.49315	-0.29450
H	-0.32300	-4.06572	1.54182	0.35778	-4.02928	-1.55447
C	0.86188	-5.94475	-1.05938	-0.88646	-5.91691	1.01355
H	0.51217	-5.48115	-3.13537	-0.56907	-5.47039	3.09863
H	1.00368	-6.11104	1.08580	-0.99352	-6.06658	-1.13522
C	1.69629	-7.17297	-1.33844	-1.73369	-7.14123	1.26903
H	1.43675	-7.62325	-2.30207	-1.50592	-7.59011	2.24114
H	2.76537	-6.92448	-1.37144	-2.80229	-6.88859	1.26758
H	1.56424	-7.93249	-0.56059	-1.57990	-7.90276	0.49723
C	-3.45466	3.79958	0.11818	3.42681	3.81663	-0.20436
H	-2.85307	4.68224	0.29394	2.80143	4.68476	-0.36671
C	-3.38785	-3.85929	-0.11760	3.37577	-3.86147	0.20390
H	-2.77097	-4.73129	-0.29356	2.73891	-4.72123	0.36616

Table S14 Cartesian coordinates of optimized T_1 and T_2 states of TTABN in toluene at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z	X	Y	Z
		T_1			T_2	
C	0.74619	-1.19826	0.16062	0.70730	-1.22202	0.14486
C	-1.37091	0.00586	-0.00078	-1.38367	-0.00564	0.00134
H	5.69008	-0.85792	-0.47546	5.61402	-0.75116	-0.62410
C	3.66314	-1.41083	-0.01125	3.63107	-1.38487	-0.09340
C	5.03230	-1.68669	-0.23825	4.99265	-1.61152	-0.39519
C	2.82593	-2.56362	0.18697	2.82299	-2.54598	0.09975
C	4.74728	-4.05553	0.05283	4.77035	-3.98022	-0.18710
C	5.59266	-2.96826	-0.20513	5.58670	-2.87732	-0.44413
N	-2.79288	0.01158	-0.00147	-2.80143	-0.01033	0.00176
H	5.14993	-5.06440	0.09492	5.19028	-4.98415	-0.20363
C	0.75586	1.19298	-0.16129	0.69918	1.22450	-0.14424
C	1.49695	-0.00565	-0.00030	1.44595	0.00367	-0.00013

C	2.84664	2.54144	-0.18788	2.80629	2.56221	-0.10198
C	5.04588	1.64667	0.23719	4.98261	1.64174	0.39018
H	5.69693	0.81263	0.47452	5.60975	0.78540	0.61842
C	5.61668	2.92358	0.20350	5.56863	2.91129	0.43793
C	3.67445	1.38192	0.01052	3.62208	1.40633	0.09028
C	4.78016	4.01763	-0.05473	4.74491	4.00890	0.18159
H	5.19104	5.02316	-0.09732	5.15850	5.01548	0.19716
C	-0.66417	-1.19046	0.18681	-0.68345	-1.23029	0.13715
H	-1.22269	-2.10325	0.34278	-1.24389	-2.14464	0.27432
C	-0.65453	1.19653	-0.18779	-0.69158	1.22367	-0.13499
H	-1.20568	2.11377	-0.34393	-1.25818	2.13429	-0.27168
B	3.01227	-0.01178	-0.00024	2.95952	0.00856	-0.00105
C	-3.48885	0.94968	0.80539	-3.49995	0.93898	0.76986
C	-3.01489	1.28552	2.08428	-2.97532	1.36781	2.00874
C	-4.65876	1.57594	0.34349	-4.70641	1.50623	0.30363
C	-3.69004	2.22003	2.86617	-3.65460	2.31670	2.75765
H	-2.11842	0.80593	2.46455	-2.05753	0.92446	2.37697
C	-5.33184	2.49475	1.14482	-5.36523	2.45882	1.06615
H	-5.04067	1.33540	-0.64360	-5.09946	1.21308	-0.66368
C	-4.86203	2.84431	2.41855	-4.85833	2.88715	2.30659
H	-3.30284	2.45661	3.85516	-3.24968	2.61813	3.72016
H	-6.23811	2.96051	0.76302	-6.28708	2.89330	0.68816
C	-3.49591	-0.92348	-0.80598	-3.49481	-0.96361	-0.76639
C	-4.66376	-1.54885	-0.33723	-4.69501	-1.54170	-0.29674
C	-3.02592	-1.26460	-2.08469	-2.96777	-1.39065	-2.00435
C	-5.34059	-2.46914	-1.13341	-5.34693	-2.50051	-1.05675
H	-5.03577	-1.31270	0.65471	-5.08417	-1.25653	0.67455
C	-3.70489	-2.20075	-2.86161	-3.64056	-2.34655	-2.75123
H	-2.12456	-0.79476	-2.46560	-2.04984	-0.94648	-2.37111
C	-4.87934	-2.81770	-2.41067	-4.84154	-2.92157	-2.30089
H	-6.24108	-2.93972	-0.74383	-6.26021	-2.94796	-0.67302
H	-3.31659	-2.44656	-3.84785	-3.23021	-2.65159	-3.71020
N	1.44590	2.40572	-0.32045	1.40938	2.42979	-0.31918
C	0.67117	3.59758	-0.57869	0.64957	3.61412	-0.60999
C	0.41940	3.98764	-1.89489	0.42943	3.99169	-1.93721
C	0.17893	4.36253	0.48113	0.12577	4.40144	0.42044
C	-0.32651	5.13946	-2.14550	-0.30252	5.14329	-2.22739
H	0.81159	3.39206	-2.71383	0.84354	3.38311	-2.73584
C	-0.56599	5.51129	0.21820	-0.60547	5.55121	0.12191
H	0.38342	4.05660	1.50272	0.30356	4.11225	1.45217
C	-0.83419	5.91815	-1.09666	-0.83480	5.94093	-1.20508
H	-0.51598	5.43707	-3.17392	-0.45852	5.42918	-3.26519
H	-0.94488	6.10102	1.04931	-1.00015	6.15849	0.93347
C	-1.66836	7.14687	-1.37312	-1.65033	7.17253	-1.52451
H	-2.73873	6.90225	-1.38381	-2.71572	6.92752	-1.63106
H	-1.51877	7.91348	-0.60561	-1.56803	7.92423	-0.73244
H	-1.42453	7.58583	-2.34590	-1.32868	7.63296	-2.46458
C	-5.57646	3.87289	3.26384	-5.56531	3.94749	3.11104
H	-6.65803	3.85427	3.09023	-6.64518	3.93475	2.93142
H	-5.40339	3.70312	4.33211	-5.39300	3.81701	4.18433
H	-5.23109	4.89129	3.03803	-5.20297	4.94974	2.84418

C	-5.63344	-3.80100	-3.27515	-5.57688	-3.94247	-3.13069
H	-6.13491	-4.56469	-2.67023	-6.07561	-4.68665	-2.50078
H	-6.40959	-3.30126	-3.87105	-6.35410	-3.46501	-3.74310
H	-4.96594	-4.31147	-3.97776	-4.90104	-4.46696	-3.81323
C	7.07421	-3.16996	-0.41170	7.06131	-3.03756	-0.73700
H	7.49686	-2.39534	-1.06078	7.39786	-2.32735	-1.50162
H	7.61855	-3.12543	0.54201	7.67599	-2.85957	0.15658
H	7.28861	-4.14653	-0.85981	7.29214	-4.04805	-1.09266
C	7.09987	3.11327	0.40975	7.04259	3.08106	0.72870
H	7.32221	4.08777	0.85851	7.26721	4.09263	1.08529
H	7.51651	2.33482	1.05813	7.38507	2.37215	1.49188
H	7.64355	3.06512	-0.54416	7.65704	2.90835	-0.16607
N	1.42640	-2.41653	0.31987	1.42555	-2.42255	0.31904
C	0.64203	-3.60200	0.57854	0.67384	-3.61169	0.61139
C	0.38838	-3.99033	1.89486	0.45900	-3.99070	1.93902
C	0.14208	-4.36234	-0.48102	0.15254	-4.40209	-0.41799
C	-0.36716	-5.13580	2.14587	-0.26541	-5.14674	2.23068
H	0.78652	-3.39841	2.71358	0.87119	-3.37972	2.73680
C	-0.61252	-5.50463	-0.21771	-0.57124	-5.55615	-0.11800
H	0.34798	-4.05774	-1.50273	0.32624	-4.11169	-1.45008
C	-0.88275	-5.90964	1.09734	-0.79530	-5.94733	1.20950
H	-0.55806	-5.43213	3.17439	-0.41742	-5.43366	3.26878
H	-0.99770	-6.09059	-1.04859	-0.96439	-6.16551	-0.92872
C	-1.72728	-7.13120	1.37408	-1.60306	-7.18366	1.53036
H	-1.49125	-7.56862	2.34945	-1.28311	-7.63710	2.47437
H	-2.79584	-6.87864	1.37870	-2.67089	-6.94637	1.62958
H	-1.57980	-7.90152	0.60985	-1.51063	-7.93845	0.74232
C	3.41003	3.82981	-0.23866	3.38071	3.84209	-0.07594
H	2.78236	4.69529	-0.40657	2.77096	4.72163	-0.24216
C	3.37877	-3.85659	0.23710	3.40546	-3.82217	0.07237
H	2.74405	-4.71697	0.40471	2.80149	-4.70559	0.23908

Table S15 Cartesian coordinates of optimized T_3 state of TTABN in toluene at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z
B	0.72542	-1.20173	0.15482
C	-1.36490	0.00236	-0.00066
C	5.66657	-0.83194	-0.54013
C	3.65354	-1.40036	-0.03689
C	5.01843	-1.66351	-0.28427
H	2.82552	-2.55071	0.16800
H	4.77377	-4.04040	0.01356
H	5.60046	-2.96037	-0.25741
C	-2.79229	0.00486	-0.00100
H	5.17966	-5.04746	0.06085
C	0.72966	1.19909	-0.15564
H	1.46779	-0.00264	-0.00048
H	2.83465	2.54051	-0.16954

C	5.02461	1.64537	0.28140
N	5.66989	0.81148	0.53693
C	5.61135	2.94013	0.25406
C	3.65861	1.38716	0.03491
H	4.78844	4.02313	-0.01650
C	5.19797	5.02869	-0.06418
H	-0.67368	-1.20419	0.16942
C	-1.23791	-2.11582	0.30746
C	-0.66943	1.20652	-0.17035
H	-1.23045	2.12011	-0.30854
C	2.99622	-0.00540	-0.00077
H	-3.48980	0.92274	0.82299
H	-3.00939	1.24024	2.10547
H	-4.66960	1.54558	0.38061
C	-3.68922	2.15073	2.90910
H	-2.10503	0.76265	2.46823
C	-5.34553	2.44340	1.20305
C	-5.05456	1.32173	-0.60906
H	-4.87098	2.77224	2.48021
C	-3.29858	2.37219	3.90023
C	-6.25774	2.90892	0.83564
C	-3.49309	-0.91190	-0.82370
N	-4.66929	-1.53796	-0.37541
C	-3.01477	-1.23277	-2.10568
C	-5.34543	-2.43928	-1.19329
C	-5.04583	-1.31999	0.61883
C	-3.69497	-2.14720	-2.90513
C	-2.10692	-0.76195	-2.46857
H	-4.87731	-2.76525	-2.47390
H	-6.25079	-2.91270	-0.81893
H	-3.30176	-2.37672	-3.89332
C	1.44807	2.41552	-0.32029
H	0.67548	3.60409	-0.58883
H	0.42291	3.98236	-1.90846
H	0.17521	4.37541	0.46306
C	-0.32595	5.12998	-2.17054
C	0.81720	3.38025	-2.72162
H	-0.57206	5.52017	0.18929
C	0.37627	4.07727	1.48763
H	-0.83853	5.91558	-1.12948
C	-0.51286	5.41937	-3.20185
C	-0.95375	6.11628	1.01467
H	-1.67565	7.13973	-1.41770
C	-2.74574	6.89362	-1.42214
H	-1.52501	7.91570	-0.65973
H	-1.43561	7.56776	-2.39631
H	-5.58832	3.77696	3.35082
C	-6.65892	3.81352	3.12238
H	-5.47774	3.53734	4.41425
H	-5.19145	4.79139	3.20629
N	-5.63069	-3.72601	-3.36346

C	-6.18162	-4.46840	-2.77562
C	-6.36457	-3.20216	-3.99146
H	-4.95467	-4.26276	-4.03796
C	7.07453	-3.12970	-0.51381
H	7.35382	-2.73065	-1.49819
C	7.67329	-2.58233	0.22669
C	7.37276	-4.18212	-0.47812
H	7.08618	3.10409	0.50954
H	7.38828	4.15538	0.47338
H	7.36456	2.70428	1.49387
C	7.68247	2.55429	-0.23115
H	1.43950	-2.42067	0.31964
C	0.66279	-3.60626	0.58954
H	0.41071	-3.98320	1.90963
C	0.15787	-4.37584	-0.46142
C	-0.34235	-5.12778	2.17309
H	0.80859	-3.38247	2.72205
C	-0.59366	-5.51745	-0.18628
H	0.35849	-4.07870	-1.48637
C	-0.85972	-5.91149	1.13300
C	-0.52887	-5.41618	3.20475
H	-0.97925	-6.11204	-1.01093
C	-1.70142	-7.13215	1.42263
H	-1.46487	-7.55839	2.40287
H	-2.77070	-6.88255	1.42397
H	-1.55168	-7.91059	0.66701
C	3.41000	3.83393	-0.21825
H	2.78794	4.69857	-0.40795
C	3.39616	-3.84621	0.21615
C	2.77103	-4.70862	0.40601

Table S16 Cartesian coordinates of optimized S_0 and S_1 states of *PP*-TAzBN in toluene at B3LYP/6-31G(d) by DFT and TDA-DFT, respectively.

Elements	X	Y	Z	X	Y	Z
		S_0			S_1	
B	-0.15194	2.91632	0.09185	-0.22363	2.96791	0.08943
C	-0.07488	1.43308	-0.09542	-0.11207	1.45854	-0.09773
C	-1.24616	0.66109	-0.25241	-1.24604	0.65981	-0.23265
C	-1.18156	-0.71979	-0.43286	-1.15705	-0.74204	-0.43519
H	-2.08451	-1.29544	-0.56785	-2.05452	-1.32025	-0.59666
C	0.06736	-1.36375	-0.42089	0.09552	-1.37538	-0.43132
N	0.11937	-2.75854	-0.56149	0.17733	-2.77084	-0.58182
C	-1.07118	-3.50815	-0.27981	-0.99582	-3.53815	-0.27499
C	-1.35998	-3.82194	1.05526	-1.26079	-3.85283	1.06493
C	-2.55479	-4.48509	1.34239	-2.44329	-4.53037	1.37031
C	-3.44600	-4.82065	0.32083	-3.34587	-4.87776	0.36294
H	-4.37762	-5.32491	0.56109	-4.26700	-5.39370	0.61806
C	-3.13948	-4.51454	-1.00561	-3.06414	-4.56879	-0.96831

H	-3.82848	-4.77950	-1.80206	-3.76172	-4.84321	-1.75390
H	-2.79166	-4.73336	2.37400	-2.66084	-4.78157	2.40538
C	-0.33484	-3.47474	2.10122	-0.22546	-3.49564	2.09759
C	0.94459	-4.31663	1.94386	1.06362	-4.31747	1.91704
H	0.66496	-5.37613	2.03051	0.79777	-5.38197	1.98228
C	1.77160	-4.14585	0.67726	1.88113	-4.10619	0.65095
C	3.03841	-4.75247	0.65847	3.17084	-4.66312	0.62611
H	3.35652	-5.31164	1.53568	3.51199	-5.21452	1.49944
C	3.90031	-4.63638	-0.42707	4.02586	-4.50723	-0.45962
H	4.87956	-5.10525	-0.39432	5.02261	-4.93766	-0.43079
C	3.50190	-3.90885	-1.55116	3.59772	-3.78907	-1.57905
H	4.16467	-3.79939	-2.40423	4.25383	-3.64958	-2.43277
C	2.24026	-3.32786	-1.57018	2.31421	-3.25817	-1.59293
H	1.90242	-2.75771	-2.42968	1.95274	-2.69906	-2.45025
H	1.60128	-4.11074	2.79833	1.72180	-4.12146	2.77241
H	-0.74564	-3.66024	3.09931	-0.61965	-3.69231	3.10005
H	-0.08710	-2.40786	2.04900	0.00666	-2.42480	2.04976
C	-1.94461	-3.85794	-1.30707	-1.88185	-3.89834	-1.28832
H	-1.68860	-3.59397	-2.32844	-1.64341	-3.63461	-2.31406
C	1.37717	-3.43479	-0.47014	1.45685	-3.40548	-0.49257
C	1.24625	-0.61998	-0.24587	1.24277	-0.59059	-0.25457
H	2.20286	-1.11823	-0.20708	2.21494	-1.05580	-0.19192
N	-2.50166	1.29387	-0.20169	-2.51461	1.24357	-0.20078
C	-3.55477	0.49400	0.36376	-3.52730	0.41651	0.37864
C	-4.70314	0.20146	-0.37527	-4.68932	0.09885	-0.33539
C	-5.64938	-0.67474	0.16737	-5.59551	-0.80180	0.22945
H	-6.54532	-0.90146	-0.40512	-6.49544	-1.05751	-0.32386
C	-5.44926	-1.26314	1.41471	-5.34980	-1.38891	1.47156
H	-6.18471	-1.95635	1.81256	-6.06052	-2.09800	1.88551
C	-4.30523	-0.95036	2.15342	-4.19027	-1.06190	2.17836
H	-4.14561	-1.39276	3.13224	-3.99388	-1.50666	3.14909
C	-4.91834	0.93621	-1.66341	-4.92235	0.77630	-1.65098
H	-5.80606	0.55212	-2.17643	-5.80032	0.34777	-2.14518
H	-4.06227	0.80426	-2.33643	-4.06298	0.62488	-2.31654
C	-5.11486	2.42808	-1.35429	-5.14598	2.27562	-1.42694
H	-5.52405	2.92438	-2.24216	-5.50971	2.71876	-2.36268
H	-5.88835	2.51223	-0.57813	-5.96552	2.39438	-0.70346
C	-3.87606	3.21226	-0.93702	-3.95021	3.10521	-0.98125
C	-3.96013	4.59323	-1.14225	-4.12458	4.49681	-1.14307
H	-4.89960	4.99503	-1.51594	-5.08518	4.85732	-1.50214
C	-2.88208	5.45249	-0.94833	-3.09300	5.39188	-0.89033
C	-1.67071	4.91386	-0.54314	-1.85350	4.91354	-0.48220
H	-0.80247	5.55861	-0.46317	-1.03381	5.61226	-0.36261
H	-2.98244	6.51471	-1.15197	-3.24667	6.45765	-1.04170
C	-3.36361	-0.06913	1.63064	-3.28108	-0.16086	1.63371
H	-2.45921	0.16751	2.18150	-2.37334	0.10428	2.16546
C	-2.65035	2.68282	-0.45442	-2.71658	2.64284	-0.49114
C	1.16851	0.76571	-0.10282	1.12608	0.81865	-0.12476
N	2.35203	1.51268	0.03883	2.29403	1.56682	0.03477
C	3.48554	0.99016	-0.67501	3.42470	1.05995	-0.67968
C	3.36463	0.75552	-2.04913	3.28615	0.79427	-2.04983

C	4.40429	0.14932	-2.74868	4.33156	0.20694	-2.75608
H	4.30350	-0.03316	-3.81457	4.22183	0.00958	-3.81821
C	5.57319	-0.21770	-2.07654	5.51804	-0.11954	-2.09456
H	6.38660	-0.69575	-2.61475	6.33658	-0.58335	-2.63711
C	5.69732	0.04169	-0.71286	5.65271	0.15511	-0.73292
H	6.60991	-0.22799	-0.18730	6.57362	-0.10060	-0.21533
H	2.44332	1.03119	-2.55180	2.35632	1.05486	-2.54453
C	4.65515	0.64011	0.00338	4.61126	0.74017	-0.00862
C	4.78049	1.03917	1.44214	4.72129	1.09182	1.44320
H	3.93552	0.65787	2.02837	3.88093	0.66457	2.00486
H	5.69778	0.62547	1.87354	5.64310	0.67678	1.86357
C	4.82538	2.57234	1.52498	4.73004	2.61599	1.60238
H	5.16642	2.86471	2.52519	5.00445	2.85835	2.63706
H	5.59821	2.92483	0.82765	5.53985	3.01991	0.97771
C	3.51862	3.31362	1.26571	3.43660	3.36090	1.30323
C	3.46200	4.60451	1.80100	3.40990	4.68444	1.79497
H	4.35337	4.99093	2.29075	4.30566	5.07551	2.27079
C	2.30453	5.37793	1.78625	2.26416	5.46534	1.71400
C	1.15583	4.83982	1.22716	1.10885	4.93369	1.15343
H	0.22737	5.39745	1.28026	0.19890	5.52197	1.16841
H	2.29628	6.36342	2.24297	2.26324	6.47535	2.11693
C	2.35649	2.80389	0.62915	2.28801	2.86744	0.66138
C	-1.52055	3.54285	-0.26860	-1.60795	3.53929	-0.26168
C	1.14626	3.56916	0.62457	1.06335	3.63071	0.60655

Table S17 Cartesian coordinates of optimized T_1 and T_2 states of *PP*-TAzBN in toluene at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z	X	Y	Z
		T_1			T_2	
B	-0.23848	2.96030	0.09159	-0.45877	2.93901	0.07696
C	-0.12147	1.46473	-0.09527	-0.23634	1.42602	0.01371
C	-1.25249	0.65294	-0.23862	-1.33293	0.52622	-0.11353
C	-1.15568	-0.74014	-0.44335	-1.13032	-0.84233	-0.20202
H	-2.05037	-1.32528	-0.59824	-1.97387	-1.50765	-0.31657
C	0.09872	-1.37052	-0.43607	0.19095	-1.36350	-0.12929
N	0.18557	-2.77018	-0.59186	0.41284	-2.73148	-0.23977
C	-0.97972	-3.53886	-0.26054	-0.67668	-3.66596	-0.20027
C	-1.22879	-3.84326	1.08498	-0.84091	-4.42085	0.96568
C	-2.40650	-4.51968	1.41060	-1.89729	-5.33355	1.01825
C	-3.32123	-4.87667	0.41759	-2.76877	-5.47848	-0.06222
H	-4.23859	-5.39136	0.68848	-3.59100	-6.18512	-0.00116
C	-3.05594	-4.57874	-0.91944	-2.58331	-4.72205	-1.22088
H	-3.76269	-4.86047	-1.69424	-3.25526	-4.83826	-2.06548
H	-2.61074	-4.76264	2.45042	-2.03899	-5.92926	1.91606
C	-0.18076	-3.47840	2.10175	0.17568	-4.26147	2.06283
C	1.10546	-4.30156	1.90846	1.53382	-4.85553	1.65118
H	0.83927	-5.36585	1.97688	1.39284	-5.92825	1.46058
C	1.90951	-4.08936	0.63398	2.24403	-4.25328	0.44755

C	3.20318	-4.63663	0.60032	3.54455	-4.70992	0.18566
H	3.55526	-5.18326	1.47239	3.96300	-5.47078	0.84012
C	4.04908	-4.47632	-0.49184	4.31671	-4.20480	-0.85589
H	5.04932	-4.89909	-0.46979	5.32502	-4.57601	-1.01209
C	3.60690	-3.76268	-1.60874	3.79006	-3.21520	-1.69031
H	4.25560	-3.61912	-2.46750	4.37820	-2.79954	-2.50204
C	2.31920	-3.24220	-1.61383	2.49875	-2.75951	-1.47217
H	1.94682	-2.68736	-2.46930	2.06871	-1.99701	-2.11179
H	1.77289	-4.10587	2.75673	2.21664	-4.79063	2.50737
H	-0.56164	-3.66844	3.11067	-0.16541	-4.77358	2.96791
H	0.05072	-2.40797	2.04275	0.29475	-3.20139	2.31598
C	-1.87836	-3.90964	-1.25918	-1.52703	-3.81436	-1.29523
H	-1.65274	-3.65416	-2.28992	-1.36052	-3.21732	-2.18599
C	1.46941	-3.39474	-0.50783	1.72638	-3.26277	-0.40979
C	1.24174	-0.58061	-0.25212	1.28857	-0.48684	0.06985
H	2.21620	-1.04323	-0.19886	2.28747	-0.88126	0.18219
N	-2.52861	1.23534	-0.20031	-2.62676	1.06924	-0.12713
C	-3.54357	0.39674	0.36741	-3.63289	0.31008	0.54641
C	-4.68812	0.06412	-0.36423	-4.75431	-0.14810	-0.15311
C	-5.59215	-0.84787	0.18757	-5.70309	-0.92139	0.52414
H	-6.48079	-1.11453	-0.37858	-6.58007	-1.27166	-0.01485
C	-5.35862	-1.42732	1.43475	-5.52906	-1.25426	1.86658
H	-6.06568	-2.14552	1.83920	-6.27033	-1.86364	2.37564
C	-4.21672	-1.08068	2.16046	-4.40028	-0.79925	2.55445
H	-4.03032	-1.52013	3.13551	-4.26182	-1.04497	3.60342
C	-4.91821	0.75435	-1.67393	-4.91791	0.28398	-1.57978
H	-5.78780	0.32325	-2.18038	-5.74618	-0.25858	-2.04812
H	-4.05283	0.62404	-2.33590	-4.00866	0.05780	-2.15081
C	-5.16212	2.24727	-1.42522	-5.20337	1.78944	-1.64235
H	-5.53617	2.70110	-2.35118	-5.48354	2.05277	-2.67094
H	-5.97842	2.34214	-0.69495	-6.09494	1.99095	-1.03104
C	-3.97482	3.08636	-0.97163	-4.08526	2.73656	-1.22942
C	-4.15442	4.47227	-1.12863	-4.31418	4.09084	-1.57338
H	-5.11313	4.83199	-1.49301	-5.26716	4.34954	-2.02918
C	-3.12325	5.37244	-0.87071	-3.35095	5.06944	-1.37377
C	-1.88212	4.90164	-0.46763	-2.12163	4.71022	-0.83113
H	-1.06722	5.60585	-0.34793	-1.34034	5.45760	-0.74089
H	-3.28280	6.43766	-1.02009	-3.54622	6.09814	-1.66615
C	-3.30982	-0.16981	1.62747	-3.45584	-0.01661	1.89597
H	-2.41129	0.10459	2.16991	-2.57373	0.34678	2.41387
C	-2.73461	2.62557	-0.48254	-2.87591	2.40714	-0.60040
C	1.12146	0.82068	-0.12068	1.07683	0.88014	0.08943
N	2.29035	1.58023	0.03402	2.15789	1.77102	0.14967
C	3.42869	1.07227	-0.67422	3.32708	1.36338	-0.56599
C	3.30189	0.82255	-2.04660	3.22029	1.06653	-1.93052
C	4.35169	0.23502	-2.74686	4.32630	0.59450	-2.63178
H	4.25217	0.04770	-3.81176	4.24025	0.37417	-3.69203
C	5.52748	-0.10819	-2.07501	5.54679	0.42165	-1.97138
H	6.34796	-0.57395	-2.61295	6.41416	0.05475	-2.51269
C	5.64968	0.15286	-0.71023	5.65001	0.72976	-0.61594
H	6.56385	-0.11140	-0.18516	6.59763	0.60074	-0.09883

H	2.37704	1.08913	-2.54720	2.26438	1.20620	-2.42552
C	4.60395	0.74036	0.00716	4.54285	1.19299	0.10354
C	4.70721	1.10115	1.45745	4.61134	1.58556	1.54933
H	3.86243	0.68414	2.01989	3.81799	1.08285	2.11672
H	5.62522	0.68651	1.88619	5.57035	1.27845	1.97995
C	4.72337	2.62770	1.59784	4.45979	3.10554	1.68965
H	5.00402	2.88292	2.62722	4.69366	3.38800	2.72445
H	5.53015	3.01983	0.96228	5.23283	3.58265	1.06988
C	3.43046	3.37430	1.29617	3.10322	3.71196	1.35983
C	3.39865	4.69280	1.78562	2.93714	5.04621	1.80407
H	4.28958	5.08792	2.26678	3.78531	5.53969	2.27286
C	2.24623	5.46992	1.70371	1.72606	5.71020	1.68310
C	1.09218	4.93505	1.14892	0.64018	5.04652	1.11816
H	0.18111	5.52143	1.16699	-0.32584	5.53933	1.08499
H	2.24253	6.47966	2.10734	1.61989	6.72765	2.05101
C	2.27894	2.87323	0.65469	2.02409	3.08937	0.71534
C	-1.62587	3.52803	-0.25438	-1.84119	3.38726	-0.41743
C	1.04736	3.63126	0.60519	0.74578	3.73357	0.60810

Table S18 Cartesian coordinates of optimized T_3 state of *PP*-TAzBN in toluene at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z
B	-0.04182	2.97739	0.06492
C	-0.01668	1.49422	-0.10210
C	-1.20899	0.78198	-0.28378
C	-1.19143	-0.65826	-0.48845
H	-2.09727	-1.17522	-0.76465
C	0.02649	-1.34897	-0.40893
N	0.03148	-2.74549	-0.55851
C	-1.19938	-3.45118	-0.34816
C	-1.57971	-3.75485	0.96586
C	-2.80585	-4.38938	1.17717
C	-3.63884	-4.70418	0.10146
H	-4.59530	-5.18629	0.28264
C	-3.24402	-4.40466	-1.20278
H	-3.88821	-4.65334	-2.04093
H	-3.11290	-4.63114	2.19167
C	-0.60960	-3.44107	2.07267
C	0.64637	-4.32823	1.99315
H	0.32382	-5.37724	2.05593
C	1.55838	-4.18164	0.78288
C	2.80699	-4.82277	0.84556
H	3.05237	-5.39064	1.74038
C	3.74107	-4.72734	-0.18139
H	4.70383	-5.22129	-0.08554
C	3.43710	-3.98801	-1.32663
H	4.15850	-3.89070	-2.13188
C	2.19428	-3.37440	-1.42810

H	1.93042	-2.79214	-2.30437
H	1.25391	-4.14915	2.88906
H	-1.08728	-3.60978	3.04379
H	-0.32095	-2.38383	2.03594
C	-2.01621	-3.77753	-1.42823
H	-1.68810	-3.52363	-2.43141
C	1.25865	-3.46088	-0.38690
C	1.22037	-0.65785	-0.16457
H	2.13701	-1.19296	0.02593
N	-2.44909	1.41542	-0.20422
C	-3.47632	0.59750	0.37525
C	-4.69362	0.36754	-0.28541
C	-5.56828	-0.58674	0.22921
H	-6.51182	-0.76195	-0.28145
C	-5.24433	-1.32725	1.37555
H	-5.93106	-2.08215	1.74612
C	-4.03616	-1.08971	2.03024
H	-3.77461	-1.65286	2.92112
C	-5.03266	1.21792	-1.47059
H	-5.98808	0.90031	-1.90017
H	-4.27020	1.12157	-2.25459
C	-5.13399	2.68222	-1.02231
H	-5.66919	3.25560	-1.78739
H	-5.76242	2.71825	-0.12155
C	-3.82106	3.40393	-0.76011
C	-3.86061	4.78508	-0.96489
H	-4.80856	5.22780	-1.26114
C	-2.73368	5.59875	-0.85669
C	-1.52257	5.01402	-0.52895
H	-0.62928	5.62722	-0.49898
H	-2.80490	6.66384	-1.05711
C	-3.14972	-0.13896	1.53360
H	-2.20737	0.05742	2.03298
C	-2.57766	2.81662	-0.39958
C	1.19555	0.79419	-0.06462
N	2.41494	1.46427	0.03568
C	3.48836	0.82052	-0.66658
C	3.22928	0.34951	-1.97041
C	4.17305	-0.42991	-2.63314
H	3.96829	-0.77738	-3.64185
C	5.37057	-0.76631	-2.00084
H	6.10499	-1.38578	-2.50676
C	5.62330	-0.29597	-0.70401
H	6.55644	-0.54904	-0.20720
H	2.29525	0.61994	-2.45062
C	4.69267	0.48687	-0.02515
C	4.96157	1.06468	1.32955
H	4.17458	0.78287	2.04114
H	5.91054	0.68368	1.72000
C	5.03183	2.59304	1.21093
H	5.51994	3.00064	2.10324

H	5.69080	2.83777	0.36633
C	3.70538	3.32111	1.05565
C	3.69605	4.62830	1.54805
H	4.62176	5.02167	1.96126
C	2.54772	5.41771	1.57902
C	1.36355	4.88251	1.10230
H	0.45150	5.46302	1.17869
H	2.58053	6.41808	2.00068
C	2.49173	2.79219	0.53694
C	-1.40275	3.63528	-0.27218
C	1.29395	3.58710	0.55635

Table S19 Cartesian coordinates of optimized S_0 and S_1 states of TTABN as the QM layer in the solid phase at B3LYP/6-31G(d).

Elements	X	Y	Z	X	Y	Z
		S_0			S_1	
B	5.47148	2.99372	1.85444	5.43750	2.98427	1.84806
C	4.91536	1.56312	1.59869	4.89791	1.56464	1.59259
C	3.66306	1.25602	1.02307	3.64645	1.23237	1.01657
C	3.12458	-0.02713	0.95448	3.12038	-0.06585	0.97795
C	1.75877	-0.27126	0.35497	1.75072	-0.31423	0.39353
H	1.53147	-1.34064	0.29780	1.52566	-1.38327	0.32709
H	0.96760	0.19901	0.95347	0.96680	0.15191	1.00537
H	1.68119	0.13977	-0.65947	1.66226	0.11199	-0.61409
C	3.88320	-1.06920	1.50702	3.87390	-1.10292	1.53556
H	3.48390	-2.08143	1.52186	3.47748	-2.11447	1.57151
C	5.15051	-0.84268	2.02143	5.15620	-0.85148	2.04069
H	5.71420	-1.67831	2.41641	5.72759	-1.67515	2.44918
H	3.08254	2.06696	0.59681	3.05772	2.02955	0.57513
C	5.70589	0.45476	2.02091	5.69111	0.44313	2.01221
N	7.03949	0.63038	2.43562	7.04803	0.63615	2.40383
C	7.84389	-0.52413	2.73406	7.85058	-0.51467	2.71544
C	8.30267	-0.75724	4.02907	8.34003	-0.71326	4.00741
H	7.98909	-0.10626	4.83919	8.04310	-0.04351	4.80826
C	9.20706	-1.79220	4.26202	9.24295	-1.74961	4.24771
H	9.59883	-1.93134	5.26033	9.65217	-1.86804	5.24253
C	9.65789	-2.62616	3.23446	9.66468	-2.61143	3.23256
C	9.15146	-2.40654	1.94713	9.12628	-2.42413	1.94949
H	9.46040	-3.03851	1.12004	9.41400	-3.07974	1.13329
C	10.66728	-3.71431	3.50190	10.67392	-3.69871	3.50094
H	10.22348	-4.71485	3.41624	10.23181	-4.69923	3.40669
H	11.08907	-3.61934	4.50556	11.09009	-3.60860	4.50735
H	11.50197	-3.66270	2.79459	11.51232	-3.64325	2.79755
C	8.25904	-1.36990	1.70411	8.22565	-1.39799	1.69946
H	7.86987	-1.20260	0.71306	7.80397	-1.26367	0.71644
C	7.69678	1.87221	2.42048	7.68029	1.87952	2.41136
C	9.08573	1.92116	2.58368	9.09648	1.92439	2.55883
H	9.66851	1.01563	2.62930	9.67447	1.01371	2.55311

C	9.74050	3.15844	2.65338	9.76361	3.15395	2.66328
C	9.00763	4.35031	2.57097	9.01181	4.33207	2.59886
C	7.62040	4.29959	2.37088	7.60215	4.27495	2.38347
N	6.88712	5.49400	2.31027	6.88585	5.46490	2.32469
C	5.50917	5.55023	2.01946	5.49127	5.54254	2.01745
C	4.88066	6.80972	1.94393	4.89250	6.80424	1.94590
C	3.52427	6.90603	1.67670	3.52562	6.92759	1.66700
C	2.72140	5.76904	1.52467	2.72472	5.79601	1.51228
C	1.24108	5.87659	1.24636	1.24848	5.91387	1.22494
H	0.64252	5.52872	2.09744	0.64636	5.53474	2.06058
H	0.94775	5.26951	0.38120	0.96488	5.32864	0.34119
H	0.95381	6.91201	1.03520	0.96048	6.95446	1.04344
C	3.35570	4.53318	1.60945	3.33535	4.53995	1.60165
H	2.74022	3.64746	1.50779	2.70445	3.66432	1.50126
H	3.08094	7.89139	1.57838	3.09608	7.91711	1.56350
H	5.45373	7.71802	2.08099	5.47588	7.70391	2.09482
C	7.56843	6.70853	2.68861	7.56731	6.68199	2.70197
C	7.68614	7.06755	4.03386	7.68748	7.04262	4.04596
H	7.24689	6.43618	4.79782	7.24937	6.41420	4.81262
C	8.38770	8.21901	4.39261	8.38910	8.19647	4.39917
H	8.47382	8.48301	5.44455	8.48014	8.46123	5.45040
C	8.99252	9.03156	3.42456	8.98638	9.00945	3.42715
C	8.86916	8.65544	2.08035	8.85601	8.63200	2.08345
H	9.32953	9.26606	1.30756	9.31078	9.24292	1.30756
C	9.73755	10.28913	3.80435	9.72997	10.26943	3.80202
H	9.10839	11.17929	3.67062	9.09870	11.15757	3.66538
H	10.06146	10.26649	4.84959	10.05383	10.25125	4.84732
H	10.62539	10.42556	3.17888	10.61739	10.40582	3.17574
C	8.15697	7.51509	1.71561	8.14306	7.49075	1.72253
H	8.04732	7.23267	0.67643	8.02504	7.20999	0.68374
H	9.52146	5.29440	2.67271	9.51366	5.28400	2.69035
N	11.14199	3.19474	2.82134	11.16419	3.18632	2.82108
C	11.84118	2.06798	3.35256	11.85804	2.05841	3.35604
C	11.45347	1.48477	4.56921	11.46501	1.47701	4.57169
H	10.61734	1.90479	5.11962	10.63328	1.90303	5.12484
C	12.12352	0.36694	5.05623	12.13103	0.35726	5.06048
H	11.80273	-0.07674	5.99399	11.80956	-0.08294	5.99942
C	13.21298	-0.19334	4.37544	13.22004	-0.20659	4.38158
C	13.93374	-1.40210	4.92784	13.93801	-1.41518	4.93711
H	13.29304	-2.29352	4.92500	13.29947	-2.30803	4.92506
H	14.82553	-1.63626	4.33861	14.83616	-1.64508	4.35618
H	14.25337	-1.24076	5.96479	14.24662	-1.25570	5.97753
C	13.60646	0.41320	3.17719	13.61600	0.39670	3.18236
H	14.45879	0.01389	2.63232	14.46740	-0.00625	2.63893
C	12.93360	1.52219	2.66621	12.94809	1.50741	2.66928
H	13.25403	1.96981	1.73073	13.27108	1.95358	1.73401
C	11.93335	4.30051	2.38325	11.95128	4.29429	2.37984
C	11.86859	4.79615	1.07291	11.88430	4.78763	1.06882
H	11.15785	4.38164	0.36903	11.18086	4.36608	0.36148
C	12.71895	5.82155	0.67058	12.72820	5.81849	0.66703
H	12.66952	6.17095	-0.35599	12.67778	6.16633	-0.35986

C	13.65264	6.39114	1.54587	13.65796	6.39393	1.54314
C	13.69044	5.90906	2.85779	13.69637	5.91425	2.85607
H	14.38580	6.35228	3.56683	14.38851	6.36167	3.56551
C	14.59885	7.46763	1.07855	14.59957	7.47370	1.07501
H	14.07857	8.26143	0.53462	14.07561	8.26661	0.53363
H	15.13166	7.92604	1.91735	15.13358	7.93220	1.91284
H	15.35092	7.06082	0.39402	15.35015	7.06940	0.38747
C	12.84630	4.88074	3.27098	12.85678	4.88262	3.26982
H	12.87442	4.51585	4.29142	12.88309	4.52017	4.29112
C	4.74333	4.36420	1.80675	4.72420	4.34552	1.80264
C	6.93380	3.05807	2.23762	6.92422	3.04882	2.23356

Table S20 Cartesian coordinates of optimized T_1 and T_2 states of TTABN as the QM layer in the solid phase at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z	X	Y	Z
		T_1			T_2	
B	5.44309	2.98642	1.85340	5.47328	3.00161	1.83958
C	4.89421	1.56640	1.60170	4.92253	1.57590	1.57602
C	3.64413	1.23527	1.02756	3.67525	1.26851	0.98606
C	3.11976	-0.06340	0.98063	3.12554	-0.02047	0.92888
C	1.74932	-0.30818	0.39793	1.75991	-0.24899	0.32438
H	1.52430	-1.37653	0.32301	1.50340	-1.31336	0.30270
H	0.96818	0.15295	1.01686	0.97709	0.26646	0.89647
H	1.65830	0.12779	-0.60506	1.70356	0.12884	-0.70493
C	3.87478	-1.10754	1.52749	3.86433	-1.06079	1.48643
H	3.47825	-2.11909	1.55414	3.46138	-2.07114	1.50805
C	5.15549	-0.85952	2.02772	5.14309	-0.82987	2.01125
H	5.73180	-1.68568	2.42367	5.69769	-1.66654	2.41791
H	3.04986	2.03321	0.59585	3.10560	2.07816	0.54240
C	5.69278	0.43954	2.01093	5.69554	0.45626	2.00999
N	7.03864	0.62836	2.39901	7.03349	0.63596	2.46354
C	7.84513	-0.52110	2.71400	7.83645	-0.51821	2.74519
C	8.31922	-0.72618	4.00884	8.30448	-0.76095	4.03606
H	8.01454	-0.05983	4.80955	7.98926	-0.11785	4.85213
C	9.22052	-1.76164	4.25330	9.20769	-1.79920	4.25981
H	9.61961	-1.88407	5.25130	9.59754	-1.95000	5.25754
C	9.65757	-2.61617	3.23712	9.65264	-2.62875	3.22628
C	9.13625	-2.42085	1.95070	9.14044	-2.40050	1.94240
H	9.43420	-3.07028	1.13337	9.44272	-3.03100	1.11119
C	10.66593	-3.70304	3.51209	10.65753	-3.72346	3.48507
H	10.21943	-4.70303	3.43572	10.21403	-4.72201	3.37822
H	11.09068	-3.60010	4.51360	11.06819	-3.64738	4.49517
H	11.49835	-3.65944	2.80148	11.50059	-3.66258	2.78794
C	8.23854	-1.39265	1.69637	8.24674	-1.36239	1.70955
H	7.83047	-1.25084	0.70910	7.84687	-1.19439	0.72269
C	7.68437	1.87980	2.39998	7.71406	1.86708	2.42176
C	9.08716	1.92488	2.54488	9.09856	1.91219	2.54069
H	9.66531	1.01371	2.55953	9.68474	1.00632	2.53777

C	9.75692	3.15346	2.65296	9.76056	3.16284	2.61976
C	8.99852	4.33229	2.60045	9.01860	4.37139	2.56540
C	7.60150	4.27717	2.38867	7.64003	4.32287	2.37903
N	6.87454	5.47646	2.33389	6.88626	5.50681	2.34300
C	5.49332	5.54967	2.02185	5.49750	5.56239	2.02899
C	4.88822	6.81341	1.94559	4.87607	6.81161	1.94394
C	3.52592	6.93395	1.66676	3.50675	6.91166	1.66727
C	2.72700	5.79737	1.51372	2.71667	5.77598	1.51901
C	1.25073	5.91285	1.22774	1.23758	5.87149	1.23126
H	0.65166	5.53850	2.06755	0.63635	5.50592	2.07353
H	0.96689	5.32054	0.34905	0.95707	5.27029	0.35726
H	0.96105	6.95171	1.03988	0.94064	6.90635	1.03003
C	3.33873	4.54295	1.60346	3.35354	4.53338	1.61364
H	2.70740	3.66825	1.50046	2.73932	3.64602	1.51609
H	3.09294	7.92143	1.56091	3.06583	7.89680	1.56090
H	5.47200	7.71306	2.09304	5.44597	7.72215	2.08245
C	7.56138	6.69131	2.70950	7.56361	6.71896	2.71698
C	7.68370	7.05245	4.05295	7.68548	7.08675	4.06015
H	7.24525	6.42556	4.82062	7.24088	6.46294	4.82729
C	8.38783	8.20492	4.40437	8.39117	8.23799	4.41292
H	8.47864	8.47135	5.45517	8.47613	8.50932	5.46329
C	8.98806	9.01469	3.43147	8.99736	9.04396	3.44031
C	8.85830	8.63468	2.08858	8.87264	8.66075	2.09817
H	9.31549	9.24270	1.31188	9.33171	9.26836	1.32182
C	9.73475	10.27334	3.80440	9.74189	10.30418	3.81232
H	9.10549	11.16284	3.66727	9.10813	11.19195	3.68494
H	10.05959	10.25542	4.84937	10.07672	10.28352	4.85430
H	10.62190	10.40657	3.17720	10.62252	10.44471	3.17743
C	8.14356	7.49443	1.72930	8.15690	7.52046	1.74026
H	8.02763	7.21131	0.69084	8.04399	7.23411	0.70199
H	9.50090	5.28324	2.70562	9.53189	5.31232	2.69959
N	11.16125	3.19085	2.82152	11.15700	3.19702	2.77758
C	11.85279	2.06706	3.36195	11.84735	2.10091	3.35439
C	11.45180	1.47830	4.57227	11.38884	1.48686	4.53558
H	10.61427	1.90001	5.11999	10.52271	1.89299	5.04680
C	12.11689	0.35849	5.06187	12.05322	0.37702	5.03854
H	11.79001	-0.08495	5.99752	11.69819	-0.08158	5.95539
C	13.21104	-0.20280	4.38879	13.17425	-0.17076	4.39213
C	13.92832	-1.41136	4.94564	13.87215	-1.38546	4.95447
H	13.28807	-2.30316	4.94183	13.21336	-2.26311	4.95613
H	14.82258	-1.64632	4.36048	14.76272	-1.63971	4.37220
H	14.24424	-1.24855	5.98350	14.18741	-1.22006	5.99219
C	13.61286	0.40439	3.19342	13.61785	0.45211	3.21530
H	14.46594	0.00225	2.65161	14.47991	0.04862	2.68977
C	12.94806	1.51680	2.68095	12.98157	1.57632	2.70549
H	13.27568	1.96498	1.74819	13.33254	2.03609	1.78758
C	11.94813	4.29230	2.37188	11.94559	4.29053	2.33295
C	11.87209	4.79335	1.06377	11.82510	4.83145	1.04192
H	11.16094	4.37782	0.36056	11.08593	4.44114	0.35456
C	12.71713	5.82269	0.65987	12.68330	5.84804	0.64287
H	12.66134	6.17365	-0.36569	12.61651	6.22187	-0.37252

C	13.65495	6.39311	1.53057	13.64802	6.38760	1.50829
C	13.70129	5.90825	2.84146	13.72113	5.87398	2.80935
H	14.39849	6.35254	3.54814	14.43223	6.30363	3.51012
C	14.59583	7.47295	1.06094	14.58713	7.46900	1.04436
H	14.07304	8.26092	0.51126	14.06298	8.25469	0.49391
H	15.12302	7.93864	1.89932	15.11215	7.93359	1.88422
H	15.35297	7.06773	0.38108	15.34534	7.06431	0.36537
C	12.86221	4.87757	3.25698	12.89374	4.83480	3.21525
H	12.89234	4.51331	4.27749	12.93434	4.44799	4.22610
C	4.72544	4.34841	1.80454	4.74354	4.36440	1.81404
C	6.91362	3.05033	2.22906	6.95123	3.06750	2.22571

Table S21 Cartesian coordinates of optimized T_3 state of TTABN as the QM layer in the solid phase at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z
B	5.46296	2.99167	1.86214
C	4.90788	1.57055	1.60488
C	3.66219	1.24865	1.02280
C	3.12397	-0.06005	0.96530
C	1.75922	-0.28596	0.36891
H	1.50159	-1.34895	0.33330
H	0.98231	0.22724	0.95205
H	1.69937	0.11150	-0.65316
C	3.86815	-1.10110	1.51162
H	3.46967	-2.11209	1.53644
C	5.14758	-0.85619	2.02836
H	5.71279	-1.68107	2.44258
H	3.07726	2.04760	0.57983
C	5.69928	0.44798	2.01730
N	7.02901	0.62158	2.42018
C	7.83546	-0.52802	2.72247
C	8.30797	-0.74616	4.01602
H	8.00085	-0.08689	4.82173
C	9.21032	-1.78175	4.25293
H	9.60559	-1.91493	5.25110
C	9.65252	-2.62613	3.22961
C	9.13594	-2.41874	1.94420
H	9.43693	-3.05994	1.12127
C	10.66204	-3.71352	3.49950
H	10.21952	-4.71432	3.41085
H	11.08015	-3.61964	4.50482
H	11.49928	-3.66064	2.79509
C	8.23863	-1.38697	1.69793
H	7.83683	-1.23277	0.70995
C	7.70205	1.87933	2.41301
C	9.08981	1.91665	2.55836
H	9.67241	1.00921	2.57965
C	9.74905	3.15705	2.64018

C	9.00574	4.35201	2.57817
C	7.62296	4.28791	2.38619
N	6.86833	5.49611	2.33538
C	5.50456	5.55509	2.02121
C	4.88529	6.82417	1.93940
C	3.51886	6.94046	1.66311
C	2.72834	5.80566	1.51568
C	1.25520	5.90241	1.22395
H	0.65783	5.51136	2.05827
H	0.98414	5.30958	0.34083
H	0.95100	6.93786	1.04177
C	3.35467	4.54229	1.61332
H	2.72255	3.66629	1.52691
H	3.08482	7.92652	1.55057
H	5.46959	7.72491	2.07581
C	7.55550	6.70774	2.71050
C	7.67808	7.06965	4.05412
H	7.23710	6.44361	4.82110
C	8.38606	8.21939	4.40679
H	8.47419	8.48729	5.45756
C	8.99229	9.02595	3.43470
C	8.86598	8.64472	2.09215
H	9.32715	9.25085	1.31619
C	9.74103	10.28321	3.80826
H	9.11227	11.17379	3.67555
H	10.06971	10.26266	4.85207
H	10.62605	10.41741	3.17825
C	8.14863	7.50597	1.73240
H	8.03719	7.22003	0.69417
H	9.51455	5.29764	2.69397
N	11.15368	3.19502	2.80441
C	11.84811	2.08430	3.35923
C	11.42805	1.48517	4.55972
H	10.57632	1.89679	5.09161
C	12.09601	0.37117	5.05412
H	11.75961	-0.07904	5.98287
C	13.20091	-0.18347	4.38988
C	13.91193	-1.39427	4.94779
H	13.26070	-2.27789	4.95873
H	14.79702	-1.64393	4.35490
H	14.24044	-1.22656	5.98114
C	13.61658	0.43066	3.20135
H	14.47298	0.02930	2.66434
C	12.96020	1.54676	2.69064
H	13.29482	1.99967	1.76288
C	11.94057	4.29343	2.35901
C	11.84593	4.81324	1.05821
H	11.11914	4.41178	0.36351
C	12.69868	5.83514	0.65587
H	12.63809	6.19638	-0.36541
C	13.65019	6.39031	1.52367

C	13.70801	5.89227	2.82999
H	14.41256	6.32885	3.53387
C	14.59217	7.46917	1.05601
H	14.07043	8.25622	0.50425
H	15.11789	7.93509	1.89508
H	15.35061	7.06290	0.37811
C	12.87229	4.85913	3.24168
H	12.90787	4.48434	4.25781
C	4.73980	4.35546	1.80600
C	6.93336	3.05624	2.24500

Table S22 Cartesian coordinates of optimized S_0 and S_1 states of *PP*-TAzBN as the QM layer in the solid phase at B3LYP/6-31G(d) by DFT and TDA-DFT, respectively.

Elements	X	Y	Z	X	Y	Z
		S_0			S_1	
B	-3.10095	-7.44411	0.61569	-3.10095	7.49012	-0.60338
C	-3.12601	-6.05480	1.20243	-3.12692	6.07068	-1.20159
C	-2.05004	-5.15725	1.01881	-2.05574	5.19253	-1.05333
N	-0.89908	-5.61049	0.34129	-0.91771	5.60979	-0.35449
C	0.35779	-5.16544	0.87789	0.33317	5.15764	-0.88274
C	0.63721	-5.40001	2.22537	0.60910	5.38192	-2.23533
H	-0.05786	-6.00008	2.79645	-0.08168	5.99125	-2.80093
C	1.78228	-4.86790	2.80700	1.76142	4.86143	-2.81324
H	1.96180	-5.00592	3.86589	1.94499	5.00353	-3.87080
C	2.67560	-4.13341	2.02827	2.65975	4.13961	-2.02926
H	3.56808	-3.70309	2.46751	3.55816	3.71720	-2.46407
C	2.41812	-3.94513	0.67403	2.39956	3.95004	-0.67394
H	3.10732	-3.36340	0.07411	3.08974	3.36943	-0.07380
C	1.25941	-4.45408	0.08382	1.24027	4.45223	-0.08281
C	0.95633	-4.34110	-1.37616	0.92051	4.29541	1.36925
H	1.67651	-3.67893	-1.85967	1.64127	3.62449	1.84073
H	-0.03081	-3.89195	-1.51383	-0.06169	3.82556	1.47509
C	1.01553	-5.72352	-2.04264	0.94742	5.65162	2.08524
H	0.89355	-5.58491	-3.12192	0.76520	5.47139	3.15123
H	2.02838	-6.12574	-1.89941	1.96892	6.05329	2.01902
C	-0.00869	-6.78009	-1.63033	-0.03863	6.73437	1.65943
C	-0.05524	-7.90414	-2.46193	-0.03031	7.87719	2.48818
H	0.67819	-7.97449	-3.26361	0.71203	7.93417	3.28120
C	-1.04754	-8.87447	-2.35334	-0.98756	8.87444	2.34959
C	-2.01686	-8.72599	-1.37339	-1.95959	8.76182	1.36423
H	-2.83981	-9.42741	-1.33206	-2.74236	9.50597	1.30999
H	-1.09055	-9.70402	-3.05271	-1.00493	9.72050	3.03070
C	-0.95299	-6.69287	-0.57645	-0.97163	6.68507	0.61075
C	-2.10398	-3.83942	1.48514	-2.10402	3.84572	-1.52975
H	-1.27256	-3.16860	1.31461	-1.26332	3.18727	-1.35567
C	-3.26346	-3.38009	2.14088	-3.26102	3.36427	-2.16701
N	-3.36557	-2.04713	2.57523	-3.36533	2.02829	-2.59911

C	-2.20525	-1.21574	2.72173	-2.19969	1.20667	-2.75297
C	-1.70424	-0.48770	1.63987	-1.69073	0.48273	-1.67169
H	-2.20341	-0.55846	0.67763	-2.19050	0.54692	-0.70917
C	-0.57913	0.32089	1.80832	-0.56042	-0.31799	-1.84246
H	-0.18845	0.89364	0.97175	-0.16440	-0.88887	-1.00722
C	0.03986	0.38883	3.05600	0.05520	-0.38139	-3.09205
H	0.93374	0.98882	3.18419	0.95082	-0.97784	-3.22345
C	-0.47636	-0.32388	4.13943	-0.46671	0.32982	-4.17374
H	0.01234	-0.26148	5.10871	0.02151	0.27156	-5.14330
C	-1.61109	-1.12627	3.99139	-1.60659	1.12468	-4.02359
C	-2.25154	-1.87512	5.13475	-2.25292	1.87111	-5.16560
H	-1.59784	-1.84174	6.01422	-1.60105	1.83958	-6.04630
H	-2.36768	-2.92968	4.86211	-2.37070	2.92615	-4.89446
C	-3.62700	-1.30955	5.54491	-3.62775	1.30269	-5.57368
H	-3.47969	-0.30768	5.96911	-3.47950	0.29870	-5.99205
H	-4.00970	-1.92194	6.37269	-4.00936	1.90986	-6.40557
C	-4.72245	-1.20305	4.48933	-4.72507	1.20188	-4.51967
C	-5.96770	-0.71171	4.91850	-5.97358	0.72063	-4.95143
H	-6.09045	-0.45776	5.96941	-6.09783	0.47279	-6.00344
C	-7.04351	-0.55438	4.05157	-7.05067	0.56547	-4.08581
H	-7.99194	-0.18026	4.42773	-8.00076	0.19824	-4.46428
C	-6.88926	-0.86480	2.69835	-6.89543	0.86834	-2.73084
H	-7.70898	-0.72574	1.99944	-7.71528	0.72888	-2.03237
C	-5.66739	-1.34784	2.24739	-5.67071	1.34144	-2.27704
H	-5.52221	-1.59472	1.19998	-5.52403	1.57753	-1.22714
C	-4.58870	-1.53720	3.12746	-4.59000	1.52788	-3.15572
C	-4.32826	-4.26822	2.37502	-4.32044	4.26169	-2.37890
H	-5.19308	-3.93683	2.93096	-5.18835	3.94664	-2.94009
C	-4.25075	-5.58520	1.91815	-4.24227	5.59774	-1.89525
N	-5.29942	-6.47409	2.18864	-5.28403	6.47197	-2.18014
C	-5.14200	-7.88200	2.09507	-5.12339	7.91123	-2.11973
C	-5.91630	-8.73911	2.91809	-5.89266	8.73970	-2.95011
C	-6.68762	-8.34770	4.17851	-6.66345	8.33848	-4.20174
C	-6.66991	-6.87007	4.58709	-6.66981	6.85596	-4.58463
C	-7.31292	-6.04751	3.51256	-7.30772	6.05432	-3.49184
C	-8.58753	-5.48604	3.62461	-8.58220	5.49364	-3.59024
H	-9.12143	-5.59769	4.56203	-9.12733	5.61239	-4.52035
C	-9.14717	-4.77163	2.56666	-9.13105	4.76974	-2.53132
H	-10.13614	-4.33282	2.65402	-10.12473	4.33986	-2.61201
C	-8.42696	-4.61581	1.38196	-8.39340	4.59271	-1.36082
H	-8.83706	-4.02768	0.57017	-8.79397	3.99907	-0.54821
C	-7.17228	-5.20084	1.24383	-7.13296	5.16951	-1.23581
H	-6.61027	-5.09339	0.32442	-6.56217	5.05933	-0.32278
H	-5.63681	-6.53999	4.74737	-5.64179	6.51169	-4.75131
H	-7.19918	-6.74436	5.53358	-7.21080	6.71626	-5.52278
H	-6.28577	-8.94578	5.00765	-6.25021	8.91380	-5.04216
H	-7.73350	-8.65612	4.07187	-7.70372	8.67127	-4.10376
C	-5.88553	-10.10824	2.64085	-5.90074	10.12558	-2.67681
H	-6.50943	-10.76840	3.24139	-6.53801	10.77039	-3.27764
C	-5.03392	-10.65256	1.68488	-5.08019	10.66460	-1.69532
H	-5.02408	-11.72405	1.52299	-5.09354	11.73501	-1.51904

C	-4.15396	-9.81444	1.01340	-4.21027	9.84379	-0.98544
H	-3.40601	-10.25077	0.36335	-3.50965	10.29860	-0.29706
C	-6.61773	-5.91537	2.30906	-6.59547	5.90749	-2.29620
C	-1.99206	-7.66752	-0.44906	-1.99244	7.68802	0.44864
C	-4.17534	-8.41717	1.18682	-4.17103	8.43955	-1.17392

Table S23 Cartesian coordinates of optimized T_1 and T_2 states of *PP*-TAzBN as the QM layer in the solid phase at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z	X	Y	Z
		T_1			T_2	
B	-3.09706	7.48349	-0.60709	-3.10802	7.47609	-0.59888
C	-3.12444	6.07941	-1.19626	-3.13470	6.04902	-1.19883
C	-2.05692	5.18701	-1.04217	-2.04508	5.14424	-1.01681
N	-0.90876	5.61582	-0.34980	-0.89554	5.63779	-0.37538
C	0.34217	5.15856	-0.87998	0.35957	5.18947	-0.89741
C	0.61659	5.38758	-2.23076	0.65016	5.41518	-2.24505
H	-0.07565	5.99546	-2.79624	-0.03313	6.02601	-2.81902
C	1.76711	4.86448	-2.80987	1.79290	4.87106	-2.81904
H	1.95003	5.00770	-3.86729	1.97841	5.00307	-3.87752
C	2.66245	4.13531	-2.02894	2.67957	4.13641	-2.03208
H	3.55880	3.71109	-2.46616	3.57304	3.70098	-2.46430
C	2.40163	3.94042	-0.67525	2.41310	3.95542	-0.67882
H	3.08933	3.35510	-0.07684	3.09515	3.37128	-0.07258
C	1.24357	4.44576	-0.08287	1.25264	4.47015	-0.09639
C	0.92505	4.29344	1.37007	0.92908	4.32429	1.35746
H	1.64339	3.62074	1.84235	1.64609	3.65304	1.83526
H	-0.05904	3.82885	1.48004	-0.05651	3.86211	1.46687
C	0.96091	5.65209	2.08142	0.96110	5.68424	2.06735
H	0.78433	5.47693	3.14869	0.79891	5.51088	3.13788
H	1.98260	6.05088	2.00588	1.97914	6.09162	1.98069
C	-0.02509	6.73710	1.65881	-0.04259	6.75364	1.65232
C	-0.02043	7.87511	2.48491	-0.05261	7.89543	2.49198
H	0.71714	7.93392	3.28203	0.69925	7.96164	3.27568
C	-0.98357	8.87167	2.34510	-1.02783	8.87198	2.37268
C	-1.95618	8.75881	1.36321	-2.00387	8.73980	1.38938
H	-2.73978	9.50242	1.31173	-2.80814	9.46171	1.34392
H	-1.00273	9.71606	3.02834	-1.05698	9.71387	3.05861
C	-0.96348	6.68273	0.60838	-0.96644	6.69825	0.59878
C	-2.11261	3.84566	-1.50316	-2.10666	3.83138	-1.47565
H	-1.27367	3.18411	-1.32822	-1.27864	3.15680	-1.30235
C	-3.26404	3.36745	-2.15230	-3.25562	3.38467	-2.17808
N	-3.37111	2.02642	-2.58359	-3.34756	2.07313	-2.65165
C	-2.20454	1.20899	-2.74643	-2.19169	1.22788	-2.77707
C	-1.68962	0.48213	-1.66956	-1.70007	0.51935	-1.67912
H	-2.18666	0.54222	-0.70534	-2.19878	0.60898	-0.71848
C	-0.55893	-0.31679	-1.84638	-0.57778	-0.29528	-1.83380
H	-0.15955	-0.88983	-1.01413	-0.18979	-0.85428	-0.98722

C	0.05231	-0.37629	-3.09831	0.04346	-0.38354	-3.07899
H	0.94731	-0.97257	-3.23517	0.93712	-0.98586	-3.19471
C	-0.47430	0.33795	-4.17572	-0.46917	0.31056	-4.17589
H	0.01000	0.28273	-5.14748	0.02354	0.23319	-5.14148
C	-1.61445	1.13117	-4.01885	-1.60440	1.11535	-4.04658
C	-2.26768	1.87687	-5.15705	-2.25046	1.83896	-5.20316
H	-1.61881	1.85045	-6.04025	-1.60314	1.78331	-6.08557
H	-2.39101	2.93058	-4.88309	-2.36141	2.90077	-4.95670
C	-3.64017	1.29940	-5.55960	-3.63092	1.26668	-5.58960
H	-3.48699	0.29446	-5.97410	-3.49123	0.25947	-6.00156
H	-4.02759	1.90080	-6.39310	-4.02260	1.86813	-6.42074
C	-4.73400	1.19816	-4.50188	-4.71636	1.17652	-4.52230
C	-5.98246	0.71401	-4.93032	-5.96739	0.68200	-4.92652
H	-6.10734	0.46159	-5.98131	-6.10175	0.40360	-5.96925
C	-7.05883	0.56179	-4.06333	-7.03719	0.55503	-4.04622
H	-8.00872	0.19145	-4.43928	-7.98977	0.17519	-4.40482
C	-6.90250	0.87222	-2.71009	-6.87497	0.90785	-2.70430
H	-7.72175	0.73593	-2.01016	-7.69171	0.79712	-1.99749
C	-5.67744	1.34698	-2.25945	-5.65109	1.40410	-2.27559
H	-5.52960	1.58724	-1.21063	-5.50057	1.68772	-1.23864
C	-4.59574	1.52854	-3.13865	-4.57847	1.55154	-3.17145
C	-4.31679	4.27213	-2.37689	-4.31910	4.28664	-2.43207
H	-5.18571	3.95389	-2.93564	-5.16998	3.96492	-3.01518
C	-4.23953	5.59955	-1.89832	-4.26103	5.58361	-1.94273
N	-5.28682	6.48088	-2.18101	-5.31404	6.47731	-2.14858
C	-5.12730	7.90714	-2.11982	-5.13725	7.90736	-2.09845
C	-5.90342	8.74128	-2.94891	-5.89297	8.74204	-2.93319
C	-6.66966	8.33613	-4.20381	-6.66723	8.34206	-4.18254
C	-6.65935	6.85512	-4.59471	-6.66923	6.85952	-4.56845
C	-7.29962	6.04661	-3.50841	-7.31879	6.05226	-3.48500
C	-8.57202	5.48077	-3.61301	-8.59252	5.48924	-3.60232
H	-9.11025	5.58886	-4.54848	-9.12440	5.60579	-4.54050
C	-9.12746	4.76774	-2.55083	-9.15343	4.76692	-2.55064
H	-10.11838	4.33251	-2.63482	-10.14276	4.32952	-2.64232
C	-8.40131	4.60864	-1.37078	-8.43387	4.60266	-1.36635
H	-8.80760	4.02249	-0.55579	-8.84476	4.00885	-0.55923
C	-7.14361	5.19024	-1.24042	-7.18161	5.19105	-1.22097
H	-6.57915	5.09028	-0.32223	-6.62463	5.08594	-0.29833
H	-5.62752	6.52031	-4.75606	-5.63873	6.51754	-4.72496
H	-7.19278	6.71600	-5.53712	-7.19983	6.72445	-5.51370
H	-6.26188	8.92063	-5.03992	-6.25777	8.92271	-5.02148
H	-7.71348	8.65566	-4.10357	-7.70893	8.67055	-4.08310
C	-5.90866	10.12027	-2.67579	-5.88707	10.13375	-2.66277
H	-6.53795	10.77021	-3.27927	-6.53495	10.77803	-3.25336
C	-5.08187	10.65791	-1.69255	-5.04917	10.67266	-1.70236
H	-5.09300	11.72872	-1.51804	-5.05264	11.74298	-1.52804
C	-4.20845	9.83989	-0.98847	-4.17250	9.84094	-1.00688
H	-3.50541	10.29606	-0.30338	-3.45039	10.28720	-0.33505
C	-6.59972	5.91347	-2.30597	-6.62623	5.91896	-2.27766
C	-1.99092	7.68495	0.44835	-2.00291	7.67974	0.45637
C	-4.16512	8.43689	-1.17936	-4.17011	8.43387	-1.17627

Table S24 Cartesian coordinates of optimized T_3 state of *PP*-TAzBN as the QM layer in the solid phase at B3LYP/6-31G(d) by TDA-DFT.

Elements	X	Y	Z
B	-3.09594	7.46817	-0.60939
C	-3.12749	6.06686	-1.19739
C	-2.06404	5.16330	-1.02256
N	-0.89364	5.62313	-0.33547
C	0.35482	5.17819	-0.87544
C	0.62654	5.40589	-2.22693
H	-0.07021	6.00738	-2.79396
C	1.77225	4.87707	-2.80929
H	1.95029	5.01670	-3.86817
C	2.67008	4.14520	-2.03221
H	3.56188	3.71562	-2.47348
C	2.41466	3.95383	-0.67803
H	3.10249	3.36679	-0.08127
C	1.25782	4.46156	-0.08366
C	0.93722	4.30389	1.36887
H	1.65429	3.62934	1.84057
H	-0.04808	3.84033	1.47469
C	0.96960	5.65773	2.08914
H	0.79011	5.47866	3.15574
H	1.99054	6.06051	2.01967
C	-0.01436	6.74226	1.66898
C	-0.01222	7.88283	2.49151
H	0.72951	7.95064	3.28368
C	-0.99177	8.86322	2.35905
C	-1.97378	8.73535	1.37888
H	-2.75691	9.47990	1.32472
H	-1.01687	9.71098	3.03796
C	-0.96066	6.67130	0.61536
C	-2.11587	3.83973	-1.46384
H	-1.28757	3.16793	-1.28088
C	-3.26048	3.39114	-2.16217
N	-3.35520	2.07312	-2.64581
C	-2.19939	1.23146	-2.77142
C	-1.70563	0.52323	-1.67352
H	-2.20565	0.61234	-0.71347
C	-0.58292	-0.29120	-1.82667
H	-0.19601	-0.85058	-0.97966
C	0.03910	-0.38117	-3.07144
H	0.93210	-0.98486	-3.18659
C	-0.47286	0.31311	-4.16852
H	0.01990	0.23511	-5.13422
C	-1.60767	1.11863	-4.03943
C	-2.25097	1.84361	-5.19637
H	-1.60028	1.79260	-6.07680
H	-2.36663	2.90388	-4.94561
C	-3.62802	1.26804	-5.58858

H	-3.48448	0.26019	-5.99779
H	-4.01723	1.86682	-6.42302
C	-4.71707	1.18033	-4.52509
C	-5.96635	0.68528	-4.93358
H	-6.09560	0.40258	-5.97589
C	-7.04133	0.56306	-4.05878
H	-7.99208	0.18121	-4.42036
C	-6.88544	0.92416	-2.71792
H	-7.70513	0.81622	-2.01397
C	-5.66354	1.42100	-2.28563
H	-5.51763	1.70799	-1.24895
C	-4.58222	1.56108	-3.17424
C	-4.31886	4.29902	-2.41214
H	-5.16928	3.98723	-3.00153
C	-4.24258	5.59652	-1.91562
N	-5.30692	6.50130	-2.17856
C	-5.13060	7.90693	-2.12187
C	-5.91076	8.75785	-2.94564
C	-6.67315	8.35412	-4.20058
C	-6.67432	6.87138	-4.58441
C	-7.31907	6.06679	-3.49711
C	-8.59054	5.49810	-3.60488
H	-9.12699	5.60696	-4.54125
C	-9.14301	4.77831	-2.54661
H	-10.13139	4.33737	-2.63178
C	-8.41478	4.61916	-1.36687
H	-8.81842	4.02722	-0.55456
C	-7.16095	5.20703	-1.23260
H	-6.59453	5.10139	-0.31617
H	-5.64434	6.52944	-4.74284
H	-7.20720	6.73412	-5.52741
H	-6.25965	8.93450	-5.03754
H	-7.71412	8.68470	-4.10352
C	-5.91343	10.13604	-2.66585
H	-6.54868	10.79000	-3.25826
C	-5.06914	10.66416	-1.69562
H	-5.07252	11.73331	-1.51281
C	-4.18545	9.83329	-1.00426
H	-3.48151	10.28535	-0.31688
C	-6.61785	5.93653	-2.29476
C	-1.99975	7.66842	0.46323
C	-4.15352	8.43528	-1.19235

Table S25 Vibration frequencies of TTABN in toluene at B3LYP/6-31G(d) by (TDA)-DFT.

No.	S_0	S_1	T_1	T_2	T_3
1	9.18	9.54	8.60	8.59	7.92
2	11.34	11.38	10.53	12.07	10.11
3	17.97	17.22	16.85	15.73	16.23

4	21.29	19.82	18.69	21.66	20.51
5	25.55	25.41	23.51	27.13	24.87
6	27.33	29.80	25.36	29.49	25.61
7	27.49	32.65	31.84	31.31	30.14
8	28.01	33.34	33.99	34.25	34.10
9	31.67	35.16	34.88	34.77	34.81
10	34.70	35.72	35.88	36.28	37.43
11	38.41	37.99	36.00	37.10	38.22
12	43.59	38.94	40.07	38.28	42.92
13	45.98	41.81	42.38	42.01	45.44
14	48.19	44.01	44.16	46.44	46.56
15	49.94	45.33	45.23	47.18	48.28
16	55.75	47.70	47.69	49.18	58.24
17	56.20	48.58	48.63	51.04	64.26
18	60.60	59.20	59.08	58.57	71.13
19	68.06	65.04	64.96	62.18	74.83
20	69.36	68.31	68.96	74.60	85.83
21	81.48	76.48	76.38	82.40	92.47
22	108.83	106.91	106.30	105.98	107.53
23	108.92	108.27	108.38	107.94	108.20
24	127.57	128.36	127.08	124.85	127.96
25	142.93	140.96	141.27	138.41	139.88
26	144.86	142.91	141.69	141.57	141.88
27	154.71	151.91	152.12	154.17	153.28
28	161.60	162.22	162.03	159.99	161.27
29	169.04	168.82	170.19	175.57	171.65
30	177.19	176.78	176.77	177.55	178.60
31	198.55	185.82	189.43	194.26	186.94
32	199.05	192.61	198.32	204.25	200.91
33	211.58	206.69	209.02	214.57	211.78
34	215.01	215.00	216.28	215.85	215.09
35	220.48	220.34	224.83	225.01	220.10
36	260.27	250.33	254.46	264.80	258.67
37	266.99	261.98	264.03	266.30	264.68
38	268.18	265.10	266.58	267.54	266.03
39	302.94	296.10	295.28	302.50	296.92
40	303.22	303.13	302.77	304.22	300.69
41	314.51	312.39	313.20	311.52	310.06
42	326.58	318.73	318.20	325.94	319.12
43	333.25	331.01	328.87	327.01	329.47
44	334.45	332.56	329.97	330.19	331.30
45	350.15	347.46	347.62	347.09	345.62
46	351.14	352.62	351.18	347.70	347.26
47	351.63	353.01	352.39	353.25	351.50
48	356.68	355.74	355.97	358.04	355.81
49	374.26	373.62	372.73	374.31	372.80
50	385.68	380.59	383.77	381.12	379.31
51	414.92	393.71	397.67	403.75	387.39
52	422.46	418.57	417.55	415.54	409.43
53	424.97	421.09	421.21	423.03	416.82
54	425.96	422.40	422.32	423.92	421.07

55	426.14	423.21	423.78	425.85	423.87
56	430.70	425.33	424.71	427.15	424.64
57	431.95	427.82	428.51	429.01	426.86
58	435.61	431.88	433.62	435.50	427.88
59	454.09	436.62	438.43	447.76	446.70
60	454.23	450.36	450.66	449.42	450.24
61	458.13	458.28	456.95	463.91	457.39
62	492.97	489.44	492.86	482.03	478.26
63	496.10	494.83	493.37	498.06	495.44
64	513.54	510.19	509.66	503.96	513.26
65	518.85	515.07	516.30	509.13	516.32
66	527.96	516.92	522.76	524.05	525.68
67	530.55	526.40	524.86	526.87	528.19
68	548.50	530.20	530.02	533.95	544.44
69	559.33	550.40	549.32	561.37	551.59
70	561.46	567.27	566.19	566.86	564.01
71	569.34	570.57	568.26	570.85	568.56
72	595.43	586.02	587.52	590.93	585.64
73	601.74	592.62	593.71	594.51	593.39
74	613.76	600.11	600.73	595.17	599.25
75	623.69	600.82	604.16	601.61	600.65
76	632.33	612.61	614.20	611.27	612.48
77	637.15	616.15	614.58	615.67	619.40
78	652.46	620.34	619.26	617.20	640.30
79	656.96	652.10	650.64	645.39	646.81
80	658.39	652.46	653.05	649.23	652.13
81	660.26	657.13	657.06	657.14	656.39
82	663.01	659.76	659.43	658.40	659.52
83	667.29	660.87	660.44	664.10	659.59
84	682.31	672.24	672.47	676.82	666.01
85	711.65	702.87	701.84	704.78	704.41
86	713.04	703.99	702.06	712.34	711.18
87	723.53	712.05	719.35	713.90	714.46
88	728.24	722.41	721.12	714.79	716.43
89	744.43	724.62	722.96	728.14	720.89
90	748.77	738.43	740.08	741.14	725.39
91	752.33	743.63	743.53	749.01	742.32
92	757.04	747.36	746.43	750.64	749.87
93	792.48	757.60	762.93	774.18	763.64
94	796.16	789.49	786.77	785.74	786.19
95	797.94	790.25	793.49	791.68	791.45
96	804.90	791.79	794.86	796.80	793.10
97	806.84	795.70	796.74	800.32	795.17
98	812.85	799.68	797.11	802.42	802.99
99	826.43	806.73	806.72	808.02	807.67
100	826.79	809.57	809.49	808.43	812.99
101	827.11	830.12	829.97	811.18	829.14
102	832.85	834.51	833.39	817.97	831.60
103	836.69	836.17	837.19	826.39	832.98
104	838.91	837.13	841.90	829.30	833.80
105	839.68	843.61	845.62	834.39	835.02

106	845.99	845.83	845.64	837.31	839.27
107	846.52	846.44	851.57	838.29	842.96
108	850.04	850.84	852.35	847.79	845.42
109	854.22	852.29	853.31	848.65	848.82
110	854.53	853.07	854.43	854.42	849.48
111	855.72	855.86	872.45	854.71	853.05
112	910.44	871.84	881.10	899.14	853.09
113	921.55	889.98	900.30	899.52	865.26
114	931.03	891.78	901.92	911.98	880.98
115	937.60	894.75	903.23	914.83	881.09
116	945.46	908.17	907.14	919.95	906.46
117	947.87	919.34	919.26	926.74	908.75
118	959.63	932.27	933.91	935.55	930.98
119	960.88	938.33	937.02	938.67	940.16
120	961.14	955.01	956.49	954.96	951.99
121	961.46	959.67	958.03	965.47	958.21
122	961.73	960.08	959.14	965.74	959.15
123	962.49	960.87	959.44	967.75	960.41
124	967.14	962.43	962.04	968.90	961.37
125	967.74	967.23	968.34	969.81	961.89
126	967.82	967.32	968.40	971.18	967.46
127	970.55	968.57	969.13	972.37	967.51
128	971.59	969.82	970.44	972.95	969.08
129	988.77	977.06	976.03	986.45	969.99
130	1017.99	1017.80	1017.18	1017.93	1002.25
131	1018.02	1018.18	1017.28	1018.31	1016.91
132	1019.74	1020.32	1020.48	1018.39	1017.38
133	1019.77	1020.35	1020.52	1018.53	1019.99
134	1032.34	1025.49	1027.04	1022.72	1020.04
135	1034.88	1032.12	1031.50	1027.39	1025.08
136	1036.01	1034.49	1033.81	1027.75	1033.89
137	1037.47	1035.49	1034.84	1031.15	1034.36
138	1040.20	1038.94	1038.48	1037.51	1040.46
139	1041.13	1041.18	1041.01	1039.92	1041.19
140	1072.11	1066.33	1061.81	1040.88	1054.16
141	1073.70	1067.04	1064.75	1066.95	1059.86
142	1074.45	1069.08	1067.26	1067.89	1061.34
143	1074.91	1073.60	1073.36	1072.06	1061.53
144	1075.49	1074.08	1073.71	1073.03	1072.66
145	1076.25	1075.22	1075.21	1074.55	1073.53
146	1077.31	1075.43	1075.46	1074.89	1075.25
147	1099.39	1094.36	1086.63	1085.49	1075.37
148	1121.74	1117.51	1117.19	1119.47	1111.32
149	1141.15	1142.13	1142.50	1139.06	1140.07
150	1141.17	1142.23	1142.53	1139.10	1141.80
151	1149.19	1149.07	1150.64	1147.05	1141.85
152	1150.88	1150.34	1152.69	1154.87	1151.05
153	1172.56	1151.70	1156.43	1160.06	1153.05
154	1183.50	1170.13	1170.31	1165.34	1167.81
155	1199.98	1186.44	1181.92	1168.12	1168.85
156	1206.87	1196.38	1204.99	1189.02	1185.97

157	1207.69	1202.42	1206.29	1202.37	1202.98
158	1212.94	1205.49	1208.27	1204.29	1207.56
159	1214.27	1208.48	1211.60	1204.58	1208.05
160	1219.72	1212.05	1212.95	1207.52	1210.36
161	1235.39	1212.66	1213.03	1224.02	1214.49
162	1237.99	1219.40	1224.04	1234.39	1218.53
163	1239.95	1227.08	1232.17	1238.81	1236.19
164	1241.78	1238.29	1235.95	1239.02	1236.61
165	1243.13	1238.94	1239.37	1244.20	1239.55
166	1243.59	1241.82	1239.85	1244.43	1241.56
167	1251.96	1242.15	1242.51	1248.37	1242.60
168	1265.37	1247.22	1243.13	1265.03	1243.61
169	1280.04	1252.12	1248.62	1272.46	1257.77
170	1284.90	1267.25	1265.14	1278.05	1267.23
171	1290.14	1268.70	1271.66	1278.43	1273.91
172	1307.15	1279.96	1279.75	1289.16	1299.83
173	1311.71	1280.17	1283.13	1292.61	1299.98
174	1321.06	1306.31	1300.60	1307.35	1312.22
175	1329.60	1310.89	1310.38	1309.48	1313.02
176	1331.68	1313.95	1311.98	1326.74	1324.55
177	1331.74	1321.47	1321.92	1327.51	1331.74
178	1334.22	1330.19	1332.82	1328.11	1331.77
179	1344.59	1332.68	1333.01	1337.90	1334.12
180	1344.63	1332.95	1337.19	1342.62	1342.36
181	1348.16	1344.89	1345.18	1343.27	1344.72
182	1348.92	1344.97	1345.22	1343.35	1344.74
183	1350.83	1348.94	1346.69	1345.29	1349.26
184	1352.42	1349.14	1349.42	1348.31	1349.44
185	1355.46	1355.18	1350.21	1352.28	1354.61
186	1355.61	1355.73	1356.41	1356.56	1357.43
187	1380.63	1361.20	1363.98	1366.76	1378.75
188	1396.69	1362.04	1375.09	1382.50	1381.27
189	1438.50	1402.01	1412.37	1422.98	1391.84
190	1440.18	1418.56	1416.64	1423.34	1429.37
191	1440.33	1421.70	1433.11	1438.13	1435.35
192	1440.61	1435.39	1436.04	1438.50	1436.56
193	1440.71	1436.06	1436.88	1438.71	1440.17
194	1440.99	1440.59	1440.57	1439.12	1440.58
195	1445.74	1440.63	1440.70	1440.28	1440.65
196	1450.31	1440.88	1440.81	1440.33	1441.79
197	1450.34	1441.18	1440.99	1442.85	1449.36
198	1453.90	1449.70	1447.56	1449.04	1449.62
199	1460.44	1449.84	1450.14	1449.10	1449.79
200	1462.75	1456.56	1450.19	1460.71	1456.80
201	1469.65	1459.58	1451.08	1470.69	1463.44
202	1502.57	1460.53	1457.61	1477.30	1465.42
203	1510.27	1464.74	1466.52	1501.19	1468.96
204	1510.32	1503.32	1503.87	1509.27	1501.89
205	1512.98	1507.38	1509.57	1510.53	1501.94
206	1513.07	1509.83	1511.92	1511.64	1508.11
207	1513.65	1513.33	1512.63	1512.76	1509.64

208	1513.69	1513.48	1512.93	1512.89	1512.58
209	1515.08	1513.64	1513.02	1513.83	1512.83
210	1516.95	1513.69	1513.73	1514.15	1513.69
211	1517.05	1514.37	1513.80	1514.16	1513.76
212	1518.74	1516.64	1516.71	1516.33	1516.88
213	1519.74	1516.76	1516.73	1516.87	1516.92
214	1524.23	1518.28	1517.25	1516.92	1517.40
215	1525.03	1519.77	1518.58	1519.44	1517.91
216	1540.30	1520.62	1520.33	1522.67	1519.86
217	1555.13	1531.96	1546.30	1530.22	1529.59
218	1557.88	1552.45	1552.17	1536.24	1543.74
219	1559.34	1553.43	1552.34	1545.73	1549.89
220	1560.26	1554.74	1554.96	1559.35	1556.07
221	1587.69	1556.28	1557.47	1559.51	1558.17
222	1603.92	1560.28	1558.82	1572.50	1559.52
223	1605.83	1564.54	1559.76	1585.25	1560.21
224	1621.93	1588.50	1576.82	1590.55	1585.13
225	1626.56	1602.41	1605.87	1604.10	1597.57
226	1629.18	1616.94	1615.93	1609.91	1609.46
227	1629.23	1625.32	1625.67	1622.94	1612.66
228	1631.10	1626.59	1629.11	1625.96	1621.31
229	1664.06	1627.72	1629.30	1626.07	1628.16
230	1664.35	1627.92	1633.02	1628.22	1628.33
231	1665.37	1662.25	1662.84	1648.77	1654.41
232	1668.77	1663.21	1664.54	1665.98	1664.58
233	1670.90	1663.27	1665.08	1666.26	1665.35
234	1672.08	1669.40	1670.08	1687.79	1685.77
235	3035.52	3031.88	3033.52	3028.63	3030.70
236	3035.68	3032.18	3033.73	3028.91	3031.12
237	3036.28	3036.17	3034.38	3039.75	3034.32
238	3036.50	3036.79	3035.15	3040.08	3034.85
239	3043.37	3044.08	3044.55	3040.42	3044.05
240	3043.49	3044.21	3044.62	3040.48	3044.10
241	3083.89	3084.51	3090.47	3082.17	3077.34
242	3083.96	3084.55	3090.48	3082.28	3077.46
243	3092.65	3093.05	3090.96	3098.27	3090.95
244	3092.80	3093.19	3091.13	3098.31	3091.21
245	3101.05	3102.21	3102.62	3099.88	3101.76
246	3101.08	3102.23	3102.64	3100.18	3101.77
247	3119.41	3117.19	3119.84	3110.54	3120.08
248	3119.57	3117.36	3120.01	3110.71	3120.47
249	3120.98	3121.52	3120.06	3126.28	3123.34
250	3121.56	3122.12	3120.20	3126.31	3123.59
251	3127.74	3129.41	3129.55	3131.51	3128.56
252	3127.75	3129.43	3129.57	3132.86	3128.57
253	3172.17	3176.75	3174.87	3169.12	3175.61
254	3172.27	3177.01	3175.02	3169.23	3175.67
255	3176.06	3177.82	3175.83	3179.31	3176.69
256	3176.45	3178.12	3176.29	3179.50	3177.40
257	3177.27	3182.44	3183.85	3180.74	3185.74
258	3177.76	3182.76	3184.49	3180.77	3185.77

259	3184.37	3186.63	3187.21	3189.22	3186.28
260	3184.44	3186.72	3187.22	3192.49	3186.35
261	3184.90	3187.20	3187.68	3192.75	3188.25
262	3185.00	3187.28	3187.78	3194.96	3188.33
263	3201.09	3199.77	3202.91	3196.01	3198.19
264	3209.16	3209.45	3210.50	3207.23	3211.11
265	3209.17	3209.74	3210.92	3207.28	3211.13
266	3210.87	3211.34	3211.60	3208.66	3212.76
267	3210.94	3211.36	3211.63	3209.28	3212.79
268	3210.97	3211.54	3211.87	3209.32	3213.04
269	3211.01	3211.73	3212.39	3224.59	3213.89
270	3212.62	3212.95	3213.19	3225.99	3215.24
271	3212.83	3212.98	3213.24	3227.94	3216.06
272	3221.24	3221.97	3225.18	3228.01	3218.12
273	3237.15	3238.82	3239.15	3236.43	3243.55
274	3237.37	3238.91	3239.35	3236.96	3243.77
275	3261.19	3262.17	3253.95	3249.05	3253.83
276	3261.23	3262.60	3254.03	3249.54	3253.91

Table S26 Vibration frequencies of TTABN in the solid phase at B3LYP/6-31G(d) by (TDA)-DFT.

No.	S_0	S_1	T_1	T_2	T_3
1	63.46	65.23	65.51	63.74	64.47
2	67.12	66.83	66.86	66.87	66.99
3	70.62	71.36	72.59	72.46	72.75
4	74.27	74.44	75.36	74.33	75.37
5	75.48	76.49	76.25	80.77	78.15
6	82.52	83.81	83.98	83.33	83.91
7	85.24	86.70	86.19	85.40	86.62
8	90.01	91.44	91.51	89.37	91.59
9	96.08	96.64	96.50	96.08	97.11
10	100.72	99.75	99.61	101.23	102.13
11	106.29	107.38	106.08	104.45	105.23
12	109.07	112.52	112.24	108.76	111.31
13	113.17	113.89	113.41	110.51	113.72
14	115.57	117.68	117.60	116.69	118.10
15	119.73	120.45	120.05	119.74	122.35
16	121.67	121.50	121.77	121.53	122.86
17	125.84	125.21	125.70	127.66	126.38
18	131.27	130.38	129.96	131.13	132.21
19	135.99	132.88	134.03	137.64	136.28
20	138.80	138.54	138.61	140.53	139.38
21	140.88	147.98	146.35	141.43	146.17
22	157.10	157.49	156.86	153.04	155.19
23	168.13	168.40	167.58	168.98	169.31
24	174.83	176.41	176.28	174.91	177.86
25	177.49	182.08	180.29	176.16	182.26

26	183.10	183.19	182.53	181.89	183.00
27	189.83	189.21	188.32	188.75	190.95
28	194.01	202.29	199.05	200.92	204.82
29	204.60	204.05	203.77	203.73	207.80
30	209.32	207.23	207.07	204.32	209.99
31	217.96	215.92	215.73	218.09	217.10
32	226.12	225.35	226.10	224.98	226.60
33	233.15	228.62	229.92	230.96	230.86
34	237.23	237.69	239.06	239.04	239.28
35	249.06	250.92	252.76	251.15	252.12
36	262.99	261.94	262.59	265.78	263.89
37	275.15	264.96	265.31	272.44	269.36
38	285.53	279.57	281.22	282.86	282.34
39	315.66	311.41	312.20	313.96	311.97
40	321.59	320.01	319.55	321.08	319.27
41	327.20	325.80	326.68	326.40	325.67
42	339.38	331.38	332.84	337.83	332.25
43	342.73	341.90	341.43	342.73	342.66
44	353.09	351.81	351.05	348.04	350.60
45	353.90	352.05	351.74	353.59	351.68
46	361.29	360.88	360.88	358.02	355.76
47	366.42	366.44	365.76	363.01	362.87
48	367.99	368.99	367.54	365.05	364.84
49	386.27	385.37	385.34	385.04	385.55
50	399.30	395.85	396.21	394.82	390.77
51	421.32	403.68	403.96	405.52	400.51
52	427.22	422.39	421.22	424.01	419.36
53	430.89	427.23	427.81	429.71	425.43
54	436.21	429.73	429.39	430.99	428.61
55	439.91	433.95	434.22	432.91	433.37
56	440.92	439.69	439.36	434.94	436.71
57	443.53	440.02	439.89	437.62	441.35
58	449.87	446.00	446.21	447.63	445.80
59	458.24	453.82	452.98	451.79	455.85
60	461.06	459.32	458.95	453.50	459.03
61	468.48	468.37	465.43	477.09	473.00
62	496.45	488.17	492.17	484.38	482.98
63	500.89	496.70	496.16	503.19	500.95
64	521.45	517.23	516.41	515.87	520.74
65	526.29	523.70	522.93	521.94	523.64
66	536.20	531.43	532.08	528.80	533.84
67	540.51	537.13	535.91	535.41	538.98
68	557.02	548.18	548.68	541.68	552.33
69	574.62	558.30	557.51	569.24	571.50
70	576.18	574.08	574.30	570.87	573.92
71	577.98	579.69	579.70	575.50	579.22
72	597.87	588.84	588.94	585.13	594.57
73	607.47	593.30	593.48	592.64	598.21
74	617.58	605.52	605.80	594.08	605.52
75	625.35	610.78	612.24	605.59	607.45
76	637.48	614.77	616.55	609.79	618.94

77	641.39	619.90	620.52	614.14	622.54
78	656.32	625.80	623.71	619.39	628.47
79	660.17	655.96	655.79	651.27	648.23
80	664.64	658.66	656.48	660.98	654.18
81	666.20	662.82	663.36	662.35	662.51
82	668.67	664.19	664.18	666.10	663.10
83	670.03	666.36	667.26	666.82	666.64
84	685.52	675.81	675.51	679.35	672.07
85	715.96	704.68	704.16	707.60	709.26
86	717.41	707.01	704.54	716.89	714.80
87	730.89	715.58	722.82	718.81	721.19
88	736.35	729.88	729.69	723.15	726.73
89	748.49	732.64	732.13	727.65	730.19
90	753.16	742.74	743.43	745.46	734.45
91	758.28	744.93	745.29	748.18	746.07
92	761.31	754.43	754.11	758.00	754.60
93	797.79	765.28	768.74	776.05	768.90
94	798.39	791.43	787.14	791.68	791.83
95	802.69	797.60	797.00	796.44	795.92
96	807.61	801.27	801.98	800.01	801.61
97	813.80	806.32	803.73	803.42	805.18
98	822.93	811.99	812.22	806.59	808.56
99	828.89	812.71	814.98	814.19	812.20
100	830.90	818.90	819.39	821.14	821.43
101	836.49	828.22	833.92	823.58	827.04
102	840.51	833.43	838.37	828.53	833.48
103	841.10	836.00	842.09	831.14	836.14
104	842.68	838.32	844.92	834.98	838.38
105	844.37	845.02	851.01	839.65	841.13
106	849.80	846.07	853.14	845.15	845.93
107	856.24	852.31	856.91	848.72	853.23
108	858.73	856.27	861.42	850.68	854.76
109	862.73	861.26	869.24	856.15	856.15
110	871.84	871.50	871.54	858.02	862.40
111	880.69	877.23	879.19	878.48	866.24
112	915.43	877.65	880.96	896.65	877.90
113	925.91	894.27	899.06	904.30	887.21
114	930.77	906.80	909.65	916.55	899.35
115	942.17	911.09	914.45	922.29	908.26
116	948.17	914.92	918.73	925.08	912.92
117	954.03	920.60	920.39	930.87	920.49
118	958.08	933.74	936.20	941.01	936.69
119	963.17	945.08	943.71	942.00	942.62
120	964.33	953.01	958.75	957.46	957.36
121	965.71	958.45	959.77	959.52	961.38
122	967.13	962.25	962.85	962.63	962.60
123	970.52	966.11	966.34	969.91	966.95
124	977.32	966.52	967.58	972.91	968.82
125	978.91	976.09	977.63	975.01	969.81
126	982.41	979.75	979.21	977.64	976.49
127	986.86	980.70	981.04	983.71	977.99

128	995.82	986.90	983.58	990.20	979.77
129	1005.10	999.84	1000.83	1001.18	998.95
130	1022.64	1022.11	1022.09	1020.54	1004.98
131	1023.37	1023.17	1023.17	1022.39	1021.05
132	1027.13	1026.86	1026.30	1026.12	1022.83
133	1027.71	1027.29	1026.63	1027.45	1025.84
134	1035.23	1029.43	1027.44	1030.81	1027.36
135	1042.89	1039.69	1038.78	1031.92	1031.71
136	1044.56	1042.05	1041.21	1036.15	1038.96
137	1048.48	1046.58	1046.27	1039.86	1047.13
138	1052.25	1050.04	1050.57	1047.55	1051.56
139	1053.48	1051.45	1051.67	1052.14	1052.58
140	1077.99	1072.95	1068.88	1052.80	1063.27
141	1080.80	1075.71	1073.68	1076.66	1065.27
142	1083.39	1076.63	1074.68	1080.88	1069.82
143	1083.87	1081.14	1080.73	1081.66	1070.69
144	1084.05	1082.96	1083.42	1083.74	1078.76
145	1086.46	1084.70	1085.89	1084.86	1083.59
146	1087.59	1087.61	1087.72	1085.15	1085.62
147	1102.64	1099.66	1090.35	1090.55	1086.36
148	1122.88	1118.12	1118.09	1120.32	1113.36
149	1147.55	1146.77	1148.24	1131.73	1147.44
150	1148.49	1147.73	1148.49	1146.07	1149.16
151	1153.33	1148.42	1153.69	1151.20	1150.22
152	1164.77	1152.81	1157.21	1153.32	1153.24
153	1176.61	1164.60	1164.61	1166.75	1166.09
154	1188.52	1174.68	1175.39	1169.86	1171.09
155	1200.89	1179.03	1182.05	1188.93	1184.46
156	1214.08	1187.94	1198.43	1193.20	1191.33
157	1214.78	1202.79	1208.07	1204.34	1202.39
158	1216.34	1208.97	1211.14	1209.69	1212.35
159	1218.86	1214.52	1215.95	1215.69	1216.03
160	1232.29	1215.74	1217.83	1219.81	1217.44
161	1239.83	1219.26	1222.01	1228.89	1218.58
162	1241.96	1221.89	1229.94	1231.28	1232.97
163	1243.27	1234.18	1235.98	1240.99	1238.88
164	1245.01	1241.94	1236.14	1242.84	1241.50
165	1248.82	1242.02	1241.96	1244.75	1242.39
166	1253.63	1245.79	1242.91	1247.89	1243.89
167	1258.08	1249.99	1247.74	1252.63	1248.36
168	1271.09	1253.63	1249.19	1254.92	1253.78
169	1283.57	1253.78	1253.78	1271.05	1259.73
170	1285.98	1268.64	1266.40	1277.52	1270.03
171	1294.94	1273.69	1272.08	1279.46	1278.14
172	1309.48	1281.40	1281.54	1285.87	1294.96
173	1311.89	1287.54	1282.68	1292.29	1295.50
174	1319.14	1309.62	1305.87	1296.55	1300.29
175	1328.22	1311.05	1309.35	1303.39	1328.13
176	1335.84	1321.01	1312.78	1323.73	1331.69
177	1337.26	1324.29	1321.56	1332.91	1333.94
178	1342.04	1335.46	1335.53	1338.28	1336.01

179	1347.72	1337.45	1337.04	1340.23	1342.59
180	1348.05	1342.99	1343.29	1342.53	1347.83
181	1349.25	1347.66	1348.23	1347.13	1349.36
182	1351.16	1350.88	1349.33	1347.93	1352.19
183	1353.02	1351.04	1350.83	1352.24	1354.90
184	1354.49	1353.92	1353.71	1357.78	1357.62
185	1358.18	1356.40	1356.42	1359.23	1363.19
186	1363.78	1361.22	1361.41	1364.46	1370.32
187	1381.62	1365.96	1365.41	1370.99	1372.63
188	1396.85	1367.33	1379.61	1384.89	1378.61
189	1440.85	1404.35	1411.47	1413.78	1404.44
190	1444.68	1420.03	1420.38	1417.39	1432.05
191	1445.70	1423.70	1437.18	1434.85	1439.29
192	1446.94	1440.39	1440.27	1443.15	1440.67
193	1447.66	1442.46	1441.84	1443.50	1442.89
194	1449.08	1444.44	1444.70	1445.85	1444.02
195	1453.26	1446.56	1446.83	1446.84	1446.78
196	1454.53	1447.73	1447.80	1447.09	1447.29
197	1457.28	1453.13	1448.35	1452.99	1452.77
198	1459.41	1453.54	1450.37	1453.65	1453.65
199	1464.20	1457.37	1453.59	1458.85	1455.51
200	1465.75	1460.26	1454.10	1462.25	1459.52
201	1475.21	1465.62	1460.00	1470.20	1463.90
202	1505.97	1466.61	1461.10	1479.98	1468.82
203	1515.30	1469.44	1466.93	1499.88	1481.29
204	1517.93	1507.43	1504.47	1514.96	1511.09
205	1524.96	1517.61	1517.66	1523.19	1516.51
206	1525.09	1521.85	1520.24	1524.21	1516.56
207	1525.55	1523.40	1522.91	1524.80	1519.60
208	1527.27	1524.33	1524.62	1524.92	1521.16
209	1528.11	1525.31	1525.64	1525.25	1524.82
210	1528.46	1526.43	1525.90	1528.14	1525.18
211	1528.94	1526.59	1526.66	1528.43	1526.73
212	1530.63	1527.67	1528.25	1528.87	1527.12
213	1537.44	1528.31	1528.60	1529.70	1527.19
214	1540.84	1531.42	1533.15	1531.66	1528.90
215	1541.10	1537.47	1537.66	1533.71	1536.13
216	1542.69	1538.71	1539.90	1535.66	1537.50
217	1557.39	1539.40	1547.64	1541.57	1540.78
218	1563.31	1555.08	1549.94	1543.00	1545.69
219	1567.05	1557.90	1556.33	1553.58	1548.38
220	1567.94	1560.05	1559.07	1562.52	1560.79
221	1591.79	1560.74	1563.04	1564.28	1561.92
222	1608.03	1568.20	1563.67	1572.39	1564.72
223	1612.88	1572.25	1567.44	1586.01	1578.17
224	1625.88	1594.78	1583.48	1599.98	1598.60
225	1631.84	1606.05	1606.43	1604.04	1609.02
226	1632.33	1620.10	1621.18	1612.39	1616.15
227	1636.32	1622.60	1629.83	1618.71	1616.59
228	1640.24	1627.89	1631.45	1628.21	1629.94
229	1663.17	1628.51	1632.90	1629.50	1634.05

230	1668.12	1631.24	1635.20	1635.28	1634.45
231	1668.64	1660.40	1666.14	1648.47	1646.63
232	1672.74	1664.86	1668.70	1654.88	1668.34
233	1676.49	1665.87	1672.28	1669.98	1672.42
234	1678.08	1673.89	1673.90	1675.31	1782.01
235	3038.65	3035.63	3037.88	3033.65	3031.00
236	3043.36	3040.61	3042.77	3039.34	3037.23
237	3044.02	3044.27	3042.86	3045.77	3042.80
238	3046.39	3047.05	3047.22	3046.39	3046.54
239	3049.34	3047.71	3050.21	3048.86	3049.44
240	3075.30	3076.59	3075.67	3079.26	3076.08
241	3087.75	3083.31	3086.54	3081.11	3076.70
242	3092.87	3090.05	3092.29	3088.95	3084.67
243	3095.42	3094.38	3093.23	3096.26	3091.95
244	3107.82	3103.61	3108.46	3104.69	3107.31
245	3108.39	3107.91	3108.64	3106.55	3107.65
246	3119.84	3121.31	3123.46	3116.40	3125.21
247	3121.59	3123.90	3126.12	3117.04	3125.88
248	3130.89	3132.35	3130.85	3134.38	3130.97
249	3131.21	3133.07	3131.09	3134.45	3131.41
250	3136.64	3136.30	3137.03	3134.62	3136.27
251	3146.99	3147.05	3148.36	3144.15	3146.78
252	3147.06	3149.37	3148.46	3157.27	3150.19
253	3176.62	3181.23	3181.70	3176.33	3179.99
254	3179.65	3184.87	3182.44	3176.86	3183.34
255	3183.37	3185.48	3182.77	3188.51	3185.72
256	3183.69	3186.40	3188.89	3189.89	3188.01
257	3194.48	3194.01	3194.59	3192.94	3193.07
258	3205.89	3200.09	3202.47	3200.92	3202.12
259	3206.03	3203.10	3203.12	3211.00	3210.72
260	3215.19	3216.22	3215.54	3212.33	3216.45
261	3216.52	3216.94	3217.79	3220.44	3217.54
262	3218.12	3218.31	3220.68	3221.58	3218.07
263	3221.26	3223.47	3223.19	3221.79	3228.16
264	3223.41	3224.21	3223.34	3230.06	3228.72
265	3225.17	3226.65	3230.00	3231.65	3229.40
266	3232.76	3229.22	3230.63	3236.54	3234.18
267	3236.10	3233.79	3233.95	3240.08	3238.97
268	3239.69	3238.97	3241.13	3241.41	3241.53
269	3241.95	3245.67	3246.20	3241.72	3245.60
270	3242.04	3247.88	3250.71	3246.65	3254.81
271	3261.88	3259.70	3259.25	3255.44	3259.45
272	3262.42	3261.72	3260.48	3261.76	3262.59
273	3266.21	3268.19	3261.15	3270.51	3265.11
274	3282.68	3270.38	3274.48	3271.82	3275.97
275	3283.96	3281.92	3276.63	3277.71	3276.40
276	3343.38	3338.68	3344.89	3340.49	3344.94

Table S27. Vibration frequencies of TAzBN in toluene at B3LYP/6-31G(d) by (TDA)-DFT.

No.	S_0	S_1	T_1	T_2	T_3
1	18.05	15.96	10.24	12.84	10.05
2	22.04	22.44	20.15	16.34	13.84
3	24.23	24.89	24.00	24.33	22.89
4	30.04	33.92	34.16	30.06	27.52
5	40.61	40.21	40.29	36.30	32.65
6	48.10	49.02	49.54	50.32	47.88
7	51.55	50.95	50.96	52.32	50.10
8	56.51	55.25	54.84	55.17	54.65
9	59.24	57.79	57.00	61.41	57.05
10	67.42	68.96	68.39	63.78	68.25
11	83.85	83.02	82.44	84.49	82.62
12	88.65	92.29	91.92	89.09	88.40
13	101.55	101.31	100.85	101.97	100.10
14	107.13	102.53	103.32	105.57	105.15
15	131.54	130.02	130.13	124.28	122.60
16	145.10	142.51	142.29	138.26	140.21
17	150.49	149.79	149.51	143.58	143.74
18	152.74	153.21	152.55	153.79	155.02
19	164.26	165.64	164.41	164.30	163.15
20	181.11	180.85	180.17	179.35	167.96
21	195.56	193.37	194.06	189.51	189.39
22	197.59	195.46	195.82	196.52	202.68
23	219.48	207.96	208.30	209.81	208.41
24	232.12	227.02	227.11	221.81	219.11
25	238.21	228.23	229.08	225.79	225.73
26	251.16	248.13	248.75	243.36	249.64
27	259.76	255.77	256.44	253.58	251.85
28	281.43	281.64	281.66	280.16	276.31
29	296.47	292.36	290.75	288.31	283.94
30	299.21	295.24	296.86	298.62	286.99
31	307.35	306.50	306.92	303.78	302.62
32	322.36	321.78	322.57	321.69	321.27
33	325.06	323.73	324.62	323.49	324.91
34	335.14	332.42	331.65	335.68	338.98
35	345.12	340.59	341.91	343.14	341.39
36	355.64	350.64	350.73	354.46	352.00
37	359.51	357.14	356.87	358.93	363.93
38	369.28	369.45	369.38	365.69	372.54
39	378.62	374.46	374.11	378.71	373.49
40	394.98	390.78	386.80	390.91	389.80
41	407.22	398.54	399.54	401.37	401.32
42	433.00	415.69	416.07	411.66	420.56
43	445.81	441.78	443.04	438.76	437.17
44	448.84	445.45	445.95	440.80	439.63
45	451.16	449.60	448.78	450.07	450.73
46	470.98	470.20	470.85	462.76	464.01
47	476.59	473.72	474.23	470.41	469.11
48	479.44	477.20	477.54	475.35	475.77
49	491.25	484.25	485.52	482.43	479.46
50	495.30	489.71	490.36	487.45	485.96

51	497.41	491.82	491.96	490.38	488.93
52	508.10	505.50	505.40	499.76	500.75
53	520.73	516.34	520.32	515.88	512.99
54	529.94	527.54	527.08	525.97	524.90
55	536.84	531.15	528.79	533.45	527.63
56	545.59	534.49	533.34	534.57	528.57
57	551.53	537.88	536.55	541.25	535.94
58	557.82	553.79	554.12	550.50	543.99
59	564.52	556.90	556.91	556.34	548.58
60	570.50	561.06	559.27	557.88	561.96
61	580.45	570.54	568.90	559.47	568.10
62	583.36	576.91	574.83	570.66	572.90
63	589.46	578.12	578.39	576.57	580.29
64	594.83	587.31	587.51	581.77	583.50
65	603.62	596.94	597.62	587.01	600.13
66	609.71	601.87	601.65	600.38	602.57
67	625.14	610.68	610.03	602.88	606.96
68	634.53	612.75	612.12	607.58	615.70
69	641.12	618.44	616.01	616.11	623.65
70	647.10	631.49	629.77	634.74	637.70
71	656.62	644.36	642.16	645.51	646.05
72	660.66	651.90	651.26	648.51	650.62
73	665.45	659.78	656.81	653.63	661.90
74	691.22	682.05	676.95	684.92	681.89
75	698.09	696.00	693.74	689.70	697.23
76	702.57	696.55	695.69	716.22	698.09
77	731.35	720.70	725.07	723.64	725.44
78	736.02	730.67	730.67	729.83	732.89
79	751.45	735.06	735.26	735.68	735.76
80	757.96	746.20	747.33	745.53	741.87
81	763.16	750.86	754.74	751.78	747.13
82	764.25	756.37	758.48	759.84	757.29
83	768.06	757.82	760.87	760.31	758.94
84	769.89	764.02	764.30	762.36	761.50
85	772.09	766.49	767.59	766.55	766.07
86	773.60	770.75	770.69	769.58	769.05
87	784.29	774.10	775.51	775.98	775.01
88	786.75	777.43	777.28	778.34	776.12
89	788.08	780.10	780.59	781.84	778.52
90	791.62	786.10	786.22	783.15	785.55
91	793.02	787.91	788.77	787.32	789.62
92	801.70	790.04	790.20	791.65	790.98
93	812.61	792.28	792.38	797.74	793.11
94	822.09	818.00	817.34	814.04	816.87
95	829.89	823.79	822.48	824.78	821.25
96	832.15	829.08	829.10	829.44	821.73
97	847.92	836.75	852.79	842.22	842.54
98	849.36	859.63	867.89	857.11	846.19
99	874.87	864.58	874.61	875.25	864.00
100	877.35	874.57	875.33	877.44	872.86
101	881.12	875.53	876.85	878.16	875.25

102	887.32	878.89	881.41	881.70	877.88
103	913.71	881.98	882.50	887.57	879.74
104	917.47	887.64	887.69	889.84	887.21
105	920.99	907.89	905.21	908.56	901.83
106	932.05	914.31	914.13	909.18	913.86
107	934.48	918.43	918.93	919.96	919.69
108	938.62	926.13	927.65	922.02	925.17
109	941.62	935.93	937.59	936.50	935.90
110	944.05	939.10	938.54	937.09	937.97
111	945.92	944.83	944.62	945.61	945.26
112	948.99	948.29	948.67	946.17	945.87
113	954.15	953.21	953.93	952.74	952.46
114	958.03	954.87	954.80	955.96	953.65
115	965.20	958.01	959.52	956.45	954.75
116	967.52	959.00	963.46	959.10	956.56
117	973.70	964.88	964.89	961.72	961.55
118	978.45	972.03	976.97	968.85	968.06
119	978.77	978.22	977.14	979.12	977.06
120	980.15	980.48	980.62	979.58	981.63
121	981.51	981.44	981.63	979.91	981.71
122	986.05	982.78	984.09	983.69	982.03
123	986.56	985.88	985.45	987.78	986.79
124	990.77	988.10	987.44	991.55	988.92
125	996.84	999.52	998.92	997.81	999.07
126	1039.08	1034.63	1030.23	1029.79	1026.37
127	1053.03	1053.81	1053.86	1039.92	1049.03
128	1061.69	1057.96	1056.15	1049.32	1050.09
129	1064.26	1064.45	1063.36	1061.10	1053.57
130	1066.51	1065.47	1063.97	1062.39	1061.09
131	1068.81	1068.35	1068.13	1069.18	1069.37
132	1074.24	1073.52	1073.16	1071.14	1071.71
133	1074.63	1074.24	1074.12	1071.62	1072.03
134	1080.53	1080.49	1080.39	1081.47	1080.45
135	1107.61	1100.49	1099.42	1093.53	1091.93
136	1123.61	1122.16	1122.54	1121.39	1118.01
137	1129.50	1127.66	1126.09	1122.83	1121.65
138	1134.57	1128.40	1127.51	1129.99	1125.40
139	1141.64	1140.63	1140.70	1140.16	1139.12
140	1149.09	1142.41	1142.18	1140.98	1141.22
141	1153.87	1153.04	1149.29	1150.83	1145.16
142	1186.05	1170.99	1170.04	1175.28	1163.90
143	1189.19	1175.89	1179.40	1177.35	1172.25
144	1191.16	1187.11	1189.30	1189.05	1185.36
145	1191.38	1189.49	1191.02	1189.99	1185.94
146	1191.81	1191.26	1191.67	1190.32	1190.82
147	1194.01	1191.90	1192.12	1193.14	1191.22
148	1194.50	1192.28	1192.39	1195.32	1191.33
149	1197.75	1192.37	1194.43	1195.44	1193.57
150	1200.00	1196.60	1195.80	1195.91	1194.51
151	1201.02	1197.17	1199.00	1199.68	1199.59
152	1207.64	1201.02	1200.78	1201.70	1202.09

153	1219.58	1205.24	1201.27	1206.16	1206.56
154	1222.00	1208.60	1208.17	1210.10	1208.77
155	1228.41	1212.33	1214.69	1211.72	1217.20
156	1232.41	1229.95	1226.69	1229.58	1221.34
157	1239.28	1233.07	1229.79	1231.34	1234.81
158	1244.31	1233.47	1234.93	1232.80	1236.53
159	1252.94	1237.64	1237.74	1235.58	1239.24
160	1253.13	1240.64	1241.42	1239.60	1244.86
161	1256.54	1244.24	1248.78	1257.69	1250.11
162	1272.26	1255.39	1254.10	1262.74	1257.50
163	1273.74	1260.67	1259.77	1270.76	1264.74
164	1289.72	1271.29	1269.20	1272.37	1266.54
165	1291.49	1273.60	1271.05	1275.90	1277.78
166	1295.96	1280.35	1281.37	1288.57	1279.61
167	1307.10	1280.88	1284.60	1290.78	1292.57
168	1307.29	1295.00	1293.44	1296.24	1294.20
169	1318.47	1305.80	1301.54	1308.33	1309.79
170	1324.49	1307.19	1305.85	1315.40	1315.47
171	1325.58	1318.16	1318.65	1319.62	1316.98
172	1327.83	1319.32	1319.71	1321.37	1318.49
173	1332.52	1322.72	1322.23	1324.44	1323.24
174	1334.99	1326.88	1326.23	1329.99	1331.35
175	1344.67	1339.66	1336.87	1342.77	1339.91
176	1349.95	1342.49	1339.56	1345.32	1345.56
177	1355.18	1346.48	1345.99	1348.70	1351.19
178	1362.30	1359.84	1358.89	1361.86	1359.02
179	1364.77	1362.95	1360.74	1362.02	1361.91
180	1365.01	1364.45	1362.73	1364.18	1362.82
181	1371.75	1368.98	1367.14	1374.84	1367.36
182	1374.64	1370.63	1368.74	1376.98	1376.75
183	1381.47	1376.34	1375.61	1382.73	1377.76
184	1388.14	1379.16	1379.61	1387.52	1380.39
185	1396.74	1382.49	1382.16	1395.57	1383.69
186	1403.83	1394.03	1395.45	1399.77	1391.15
187	1405.73	1396.36	1397.92	1402.90	1402.28
188	1406.36	1406.96	1406.56	1405.43	1404.78
189	1445.01	1425.50	1422.03	1441.17	1418.47
190	1459.41	1429.11	1438.64	1455.49	1448.64
191	1482.88	1439.53	1448.07	1460.94	1459.53
192	1495.29	1482.31	1478.02	1484.70	1470.61
193	1497.30	1486.55	1481.73	1487.65	1477.89
194	1499.36	1493.87	1493.97	1495.43	1492.14
195	1500.13	1494.63	1495.87	1497.88	1496.14
196	1504.68	1495.62	1497.08	1498.33	1497.41
197	1507.72	1499.80	1499.93	1500.92	1498.63
198	1508.88	1503.03	1502.98	1501.74	1500.88
199	1512.86	1507.28	1506.95	1507.01	1502.23
200	1514.73	1508.61	1507.33	1507.88	1503.12
201	1515.65	1514.67	1515.23	1511.86	1511.38
202	1518.20	1515.50	1516.05	1513.46	1513.98
203	1520.72	1519.78	1519.53	1517.15	1514.46

204	1535.63	1530.41	1522.76	1519.92	1517.10
205	1539.83	1533.59	1534.78	1532.21	1524.26
206	1541.80	1537.54	1539.46	1539.93	1534.86
207	1544.08	1539.58	1539.57	1540.92	1538.11
208	1545.53	1541.54	1541.10	1541.82	1538.91
209	1596.79	1553.31	1553.89	1550.76	1542.56
210	1622.69	1574.14	1570.61	1565.91	1562.69
211	1624.92	1575.46	1583.35	1596.28	1569.99
212	1631.10	1600.95	1592.47	1601.78	1591.59
213	1640.03	1604.87	1599.04	1616.89	1615.54
214	1640.45	1619.84	1620.75	1622.80	1623.40
215	1641.86	1630.11	1629.62	1639.64	1637.19
216	1645.84	1634.35	1638.24	1640.80	1639.52
217	1648.78	1635.47	1638.27	1642.47	1641.03
218	1648.82	1640.77	1640.72	1650.39	1649.59
219	1659.73	1651.66	1655.23	1657.49	1656.04
220	1661.31	1652.85	1655.92	1659.13	1656.24
221	1662.32	1658.85	1658.71	1660.51	1659.55
222	1669.83	1665.58	1665.41	1787.92	1662.49
223	3027.03	3018.96	3022.99	3017.63	3015.90
224	3027.09	3019.59	3023.40	3018.06	3016.77
225	3027.50	3028.97	3028.07	3033.95	3029.89
226	3052.86	3046.26	3049.45	3043.22	3045.41
227	3053.45	3046.43	3049.64	3044.70	3046.88
228	3054.48	3053.97	3053.57	3057.19	3054.66
229	3069.93	3060.31	3065.63	3058.40	3059.12
230	3071.72	3061.33	3066.67	3058.71	3060.21
231	3071.89	3071.88	3071.24	3074.34	3069.23
232	3100.46	3100.13	3100.03	3095.91	3101.10
233	3102.21	3100.36	3101.62	3097.40	3102.39
234	3102.90	3100.55	3102.02	3108.41	3103.85
235	3169.71	3170.19	3171.39	3168.33	3174.81
236	3169.81	3171.05	3172.38	3169.05	3175.86
237	3173.70	3175.71	3174.69	3179.06	3176.19
238	3180.82	3182.08	3181.10	3180.08	3182.88
239	3181.40	3185.11	3185.40	3181.16	3183.32
240	3181.72	3185.18	3185.53	3185.97	3183.77
241	3193.26	3187.95	3188.96	3188.24	3191.24
242	3193.74	3189.25	3190.24	3188.63	3193.26
243	3193.86	3195.07	3194.18	3190.32	3194.62
244	3193.98	3195.18	3194.35	3190.94	3194.69
245	3194.48	3196.54	3197.21	3200.94	3194.92
246	3197.28	3197.71	3198.26	3203.29	3196.93
247	3205.17	3205.43	3204.83	3204.13	3207.85
248	3205.56	3205.85	3205.27	3204.18	3208.32
249	3206.58	3209.37	3209.84	3204.74	3208.55
250	3206.90	3210.14	3210.56	3211.13	3208.64
251	3213.60	3215.05	3215.52	3213.99	3211.18
252	3216.24	3216.77	3216.19	3214.40	3218.78
253	3217.46	3217.55	3216.86	3215.61	3219.46
254	3217.66	3219.73	3220.83	3216.19	3220.12

255	3218.00	3220.51	3221.54	3221.59	3220.71
256	3226.18	3232.41	3233.12	3227.46	3224.51
257	3264.22	3265.03	3259.88	3258.42	3250.03
258	3265.35	3267.21	3262.24	3261.19	3265.32

Table S28 Vibration frequencies of TAzBN in the solid phase at B3LYP/6-31G(d) by (TDA)-DFT.

No.	S_0	S_1	T_1	T_2	T_3
1	72.96	71.38	72.43	72.95	72.62
2	73.94	77.03	76.29	76.07	75.46
3	81.87	81.66	81.55	81.61	82.18
4	87.29	89.05	89.18	87.02	87.27
5	91.17	91.30	91.16	90.45	90.56
6	103.93	104.71	104.51	104.33	104.18
7	106.46	105.79	105.73	106.39	106.35
8	108.32	110.10	110.19	110.59	110.12
9	117.07	113.36	114.21	115.82	115.07
10	120.79	118.85	118.87	120.07	118.68
11	122.62	121.66	121.37	123.28	122.23
12	124.99	124.23	123.67	125.66	125.05
13	136.37	133.21	133.97	135.29	135.21
14	151.86	147.63	148.09	150.07	148.51
15	159.20	157.83	157.79	160.35	157.59
16	165.80	165.48	164.91	161.72	162.56
17	172.38	171.52	171.31	172.48	172.63
18	180.18	178.44	178.63	179.34	178.52
19	183.37	185.65	184.48	183.93	183.45
20	201.48	203.22	201.69	202.86	200.14
21	208.91	208.76	208.31	204.36	205.84
22	222.32	219.66	220.63	215.28	220.24
23	227.28	227.11	226.98	226.69	228.44
24	240.77	233.35	233.60	233.96	234.07
25	245.39	242.45	243.54	241.60	243.91
26	254.42	248.27	249.52	250.36	248.31
27	281.01	266.50	267.09	270.74	261.60
28	288.70	287.10	287.01	286.22	285.49
29	303.73	299.29	297.01	299.31	295.64
30	310.32	303.15	303.88	305.92	299.89
31	314.08	309.51	308.13	314.33	307.20
32	333.29	331.58	332.61	331.88	330.95
33	342.57	343.56	343.79	341.98	342.16
34	347.98	345.96	345.79	346.55	347.87
35	355.99	353.83	354.71	355.93	354.87
36	365.28	362.59	362.08	364.81	363.88
37	370.57	366.61	366.54	369.38	367.27
38	383.02	380.53	380.62	372.03	380.83
39	394.28	390.41	390.18	392.79	390.73
40	403.42	398.86	394.81	399.22	395.48
41	412.61	404.33	404.90	404.02	404.56

42	439.19	427.96	426.44	422.09	430.92
43	447.64	446.35	446.12	443.94	444.83
44	455.43	451.84	452.11	448.59	446.27
45	459.04	454.77	453.71	455.03	453.26
46	469.23	467.46	467.63	466.43	467.77
47	474.00	471.00	471.55	470.74	469.82
48	481.85	479.39	480.10	477.92	478.33
49	488.13	481.46	482.26	483.73	483.01
50	492.83	484.23	484.86	486.62	486.84
51	497.80	493.61	493.09	494.76	493.66
52	505.26	501.02	500.67	501.45	502.33
53	526.14	520.05	523.57	519.39	520.80
54	531.12	529.63	527.87	527.65	526.04
55	544.75	539.01	537.65	539.26	534.85
56	554.54	540.63	540.27	542.34	535.39
57	557.70	546.69	545.85	548.77	542.84
58	560.37	556.79	557.31	556.57	550.30
59	568.46	559.86	558.79	561.12	556.92
60	573.06	562.27	563.24	561.63	566.59
61	585.20	572.28	570.85	570.67	574.39
62	586.55	582.19	579.12	576.29	578.98
63	594.54	585.89	584.46	583.30	585.75
64	608.80	589.47	589.41	590.90	590.53
65	613.46	598.05	600.85	591.89	607.03
66	618.25	611.49	611.24	608.84	610.71
67	624.73	616.16	613.97	611.28	611.98
68	634.00	618.13	618.13	616.47	619.96
69	637.84	620.90	619.48	620.54	623.17
70	646.94	631.68	629.79	635.88	633.54
71	659.15	643.90	641.38	647.35	648.26
72	660.25	655.32	654.69	649.47	653.48
73	665.85	661.39	658.20	653.42	660.69
74	691.67	680.21	673.32	686.49	679.04
75	697.96	695.96	694.77	689.68	695.80
76	704.68	699.19	697.23	717.29	698.02
77	732.11	724.55	730.18	728.31	727.99
78	734.83	731.17	731.70	731.00	733.31
79	756.03	734.04	734.28	732.45	737.72
80	760.76	748.29	749.88	745.82	746.80
81	761.81	757.89	760.61	758.01	755.41
82	772.44	761.52	762.27	760.05	760.90
83	777.94	765.17	768.95	763.71	764.49
84	782.52	770.14	771.76	769.66	768.24
85	783.35	776.12	779.01	778.32	775.46
86	787.16	781.15	781.04	780.13	780.25
87	792.31	784.58	784.16	781.26	785.48
88	793.49	785.80	785.26	788.16	788.51
89	795.72	791.12	793.23	793.15	791.61
90	804.80	793.88	794.48	796.12	794.12
91	807.78	796.16	797.26	800.81	794.49
92	811.69	806.70	807.18	806.39	805.26

93	817.97	808.25	808.08	808.48	806.41
94	823.87	817.42	816.97	815.18	816.16
95	827.34	825.13	825.22	819.60	820.18
96	835.06	826.72	825.49	828.87	823.07
97	839.68	828.30	845.34	833.44	829.53
98	844.83	848.16	867.65	846.35	838.97
99	877.75	862.49	869.31	875.61	864.57
100	880.30	877.00	877.15	876.16	873.20
101	894.39	878.12	879.75	879.48	875.44
102	902.04	879.75	881.19	887.74	877.38
103	912.69	893.35	892.78	893.25	889.08
104	917.52	900.84	900.59	898.09	898.55
105	920.66	910.96	908.95	907.95	905.71
106	928.34	912.18	913.83	910.92	913.31
107	934.39	917.70	918.76	917.63	918.08
108	942.02	922.22	922.18	920.77	923.90
109	943.15	933.00	935.04	935.12	936.55
110	944.36	937.92	937.34	935.40	937.13
111	948.88	946.62	946.64	945.40	944.56
112	956.28	951.62	951.69	951.61	950.91
113	960.34	956.83	957.49	956.87	955.07
114	964.38	959.42	959.21	958.41	957.42
115	965.14	964.36	964.06	963.76	960.14
116	967.07	968.44	969.18	964.90	963.13
117	980.61	968.78	972.68	966.68	965.68
118	988.62	973.27	978.44	970.40	969.63
119	989.46	987.70	986.86	988.54	985.20
120	990.21	989.75	988.81	989.50	988.60
121	991.89	990.45	989.72	992.45	989.84
122	1000.63	1000.04	1001.69	1000.08	998.94
123	1008.46	1012.22	1011.67	1008.45	1009.27
124	1016.06	1015.70	1016.46	1017.76	1015.67
125	1016.70	1020.31	1018.82	1021.58	1018.65
126	1042.29	1040.01	1035.39	1031.17	1027.72
127	1048.26	1048.25	1047.58	1043.58	1043.42
128	1055.39	1050.30	1048.99	1046.52	1046.63
129	1062.05	1060.23	1059.53	1056.24	1054.69
130	1066.23	1062.67	1062.32	1061.07	1060.02
131	1071.12	1070.93	1070.74	1071.10	1070.98
132	1079.61	1079.39	1079.28	1079.23	1078.79
133	1083.35	1083.13	1083.02	1080.96	1081.90
134	1086.05	1083.54	1083.38	1082.16	1083.41
135	1105.73	1099.09	1098.14	1091.06	1095.12
136	1123.37	1120.90	1121.66	1119.19	1114.88
137	1131.50	1125.38	1124.01	1123.01	1119.73
138	1132.09	1127.01	1126.06	1129.64	1122.25
139	1142.68	1142.05	1142.31	1141.71	1141.55
140	1150.82	1144.79	1144.60	1144.37	1144.07
141	1158.74	1157.65	1155.38	1155.65	1151.24
142	1181.49	1162.41	1170.51	1169.22	1160.89
143	1191.82	1170.19	1175.32	1171.24	1168.99

144	1198.20	1183.65	1192.32	1189.71	1191.23
145	1200.20	1192.54	1193.94	1193.72	1193.24
146	1203.29	1194.13	1196.58	1196.68	1195.16
147	1204.72	1198.40	1197.99	1198.44	1199.13
148	1206.74	1201.09	1198.65	1200.00	1200.43
149	1208.49	1202.74	1201.68	1201.01	1204.93
150	1210.06	1205.56	1204.27	1204.35	1205.71
151	1210.69	1207.62	1206.49	1206.62	1208.71
152	1215.05	1209.17	1208.44	1209.67	1210.17
153	1222.05	1210.97	1211.11	1209.94	1214.64
154	1227.37	1214.25	1214.20	1214.55	1217.42
155	1229.37	1218.15	1219.79	1219.85	1221.35
156	1234.92	1230.65	1228.22	1230.77	1224.59
157	1242.33	1232.66	1233.61	1232.02	1234.61
158	1252.31	1234.96	1236.75	1235.42	1237.89
159	1257.10	1236.68	1240.04	1237.96	1242.84
160	1260.27	1243.08	1246.76	1246.11	1245.36
161	1263.91	1248.08	1247.31	1250.52	1254.27
162	1274.00	1253.66	1250.98	1257.18	1256.83
163	1276.56	1257.97	1257.67	1261.94	1267.03
164	1286.54	1272.97	1270.93	1272.94	1273.15
165	1288.48	1275.36	1275.85	1277.40	1275.06
166	1292.01	1277.77	1277.59	1283.53	1279.10
167	1306.15	1280.13	1282.42	1285.08	1284.80
168	1308.61	1289.87	1288.92	1293.19	1290.61
169	1315.26	1302.12	1297.96	1300.49	1307.64
170	1317.99	1306.86	1302.74	1315.17	1317.79
171	1327.22	1315.40	1316.42	1319.52	1319.72
172	1328.99	1317.82	1318.36	1321.43	1321.92
173	1332.66	1328.05	1327.64	1326.98	1326.80
174	1337.51	1332.53	1331.86	1332.62	1334.16
175	1338.16	1337.95	1336.79	1340.20	1338.64
176	1342.99	1340.44	1340.18	1342.30	1341.13
177	1349.63	1342.88	1340.80	1347.48	1351.82
178	1359.08	1356.69	1353.91	1359.64	1357.17
179	1368.31	1358.98	1357.82	1366.25	1359.64
180	1373.21	1364.40	1359.45	1371.01	1365.00
181	1378.36	1368.48	1368.62	1377.30	1369.27
182	1384.16	1373.88	1373.78	1381.97	1380.48
183	1386.48	1380.80	1382.17	1387.45	1385.91
184	1388.10	1386.49	1386.02	1387.97	1386.95
185	1400.04	1387.25	1386.67	1390.56	1391.21
186	1402.72	1396.91	1396.88	1399.76	1398.23
187	1405.33	1403.80	1403.14	1405.40	1405.09
188	1405.72	1406.13	1405.80	1405.62	1410.52
189	1445.74	1416.00	1418.78	1438.14	1417.78
190	1461.56	1424.87	1436.98	1453.55	1432.75
191	1478.36	1440.45	1437.87	1458.89	1447.26
192	1494.04	1481.78	1472.00	1483.76	1463.36
193	1502.13	1487.78	1482.95	1490.15	1469.25
194	1505.30	1493.00	1493.15	1497.45	1490.92

195	1506.11	1501.39	1501.35	1498.74	1500.73
196	1508.56	1502.73	1503.63	1503.65	1504.25
197	1510.26	1503.83	1505.65	1505.82	1505.64
198	1515.03	1506.28	1506.24	1508.10	1505.92
199	1518.54	1517.64	1516.93	1509.11	1509.16
200	1521.30	1520.33	1518.14	1516.62	1511.63
201	1523.16	1522.24	1520.62	1520.09	1516.15
202	1523.57	1523.18	1522.33	1521.09	1519.77
203	1526.39	1526.15	1522.91	1523.63	1523.25
204	1530.93	1528.77	1526.91	1525.83	1525.11
205	1536.07	1536.04	1535.79	1532.45	1529.10
206	1540.08	1538.18	1536.37	1537.31	1531.69
207	1550.90	1540.37	1540.11	1539.89	1537.38
208	1552.40	1544.56	1546.68	1548.00	1546.07
209	1590.14	1548.43	1550.43	1549.46	1547.11
210	1623.91	1567.18	1569.82	1566.00	1557.25
211	1626.70	1575.27	1579.34	1588.24	1569.82
212	1629.40	1599.28	1588.98	1600.84	1585.26
213	1637.25	1606.36	1598.52	1612.36	1618.94
214	1639.09	1618.58	1615.93	1624.93	1625.79
215	1640.81	1628.53	1627.81	1639.50	1638.55
216	1644.67	1639.00	1638.79	1646.76	1645.71
217	1653.24	1643.18	1646.69	1648.63	1647.21
218	1656.06	1645.05	1646.96	1653.02	1649.15
219	1656.49	1655.71	1655.53	1658.64	1656.49
220	1663.62	1659.54	1660.91	1664.17	1662.16
221	1667.25	1661.13	1662.32	1668.69	1666.78
222	1671.89	1663.36	1665.76	1703.09	1675.52
223	3035.54	3027.52	3031.80	3024.97	3027.65
224	3040.69	3034.76	3040.85	3032.23	3034.31
225	3042.79	3043.54	3042.15	3047.57	3045.62
226	3062.69	3060.74	3062.07	3059.58	3062.94
227	3068.93	3063.13	3063.52	3066.70	3065.70
228	3071.83	3074.84	3073.50	3076.74	3079.84
229	3096.67	3078.44	3085.20	3081.52	3079.99
230	3097.49	3084.10	3089.62	3082.37	3086.44
231	3108.81	3106.96	3106.23	3109.62	3109.20
232	3122.32	3111.84	3114.28	3109.70	3111.00
233	3157.55	3152.62	3154.65	3146.41	3155.02
234	3166.74	3158.78	3161.14	3152.86	3160.32
235	3167.30	3175.03	3176.43	3172.43	3179.81
236	3167.72	3176.08	3177.63	3173.53	3180.93
237	3176.83	3179.57	3177.64	3184.59	3183.22
238	3188.34	3190.80	3189.87	3195.44	3193.21
239	3192.58	3193.77	3192.85	3198.45	3196.47
240	3192.76	3194.09	3193.03	3199.00	3197.61
241	3202.82	3202.50	3201.90	3202.79	3205.15
242	3206.84	3204.98	3204.93	3206.32	3206.12
243	3207.99	3206.57	3207.73	3207.96	3207.16
244	3208.65	3208.39	3208.08	3212.54	3211.35
245	3215.74	3216.17	3215.39	3220.32	3219.80

246	3232.50	3222.84	3222.61	3227.33	3226.00
247	3233.51	3233.48	3233.75	3231.49	3232.56
248	3235.54	3234.77	3234.44	3232.94	3234.38
249	3238.43	3240.35	3239.09	3243.09	3240.72
250	3243.32	3246.84	3240.03	3244.42	3242.05
251	3248.86	3247.54	3246.26	3247.38	3245.09
252	3248.94	3249.99	3252.07	3250.32	3249.83
253	3254.10	3254.96	3255.57	3253.89	3253.83
254	3258.81	3261.38	3255.75	3257.58	3255.08
255	3262.49	3261.44	3261.67	3259.88	3260.40
256	3265.88	3271.87	3270.38	3268.80	3265.43
257	3266.31	3274.23	3273.25	3269.56	3271.76
258	3280.11	3287.01	3286.07	3280.20	3284.00

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