Supporting Information

Multi-Resonance Thermally Activated Delayed Fluorescence Polymers for High-Efficiency and Narrowband Solution-Processed Green OLEDs

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1. Experimental Section

1.1. Materials and Methods

All raw materials and anhydrous solvents were commercially available and used without further purification. The reactions were carried out under the protection of the high-purity argon atmosphere. All reactions were heated by metal sand bath (WATTCAS, LAB-500, https://www.wattcas.com).^{1}H NMR and ^{13}C NMR spectra of the materials were measured in $CDCl_3$ solvent on the Bruker Advance 400/500 MHz spectrometer, using tetramethylsilane (TMS) as the internal standard. Molecular weights of the polymers were determined by gel permeation chromatography (GPC) on a Waters e2695 Separations Module. Tetrahydrofuran (THF) was used as the eluent and monodisperse polystyrene was used as the standard.

The samples for atomic force microscopy (AFM) test were prepared as follows: PEDOT:PSS was spin-coated onto the pre-cleaned ITO-coated glass substrates, and then sample solutions were spin-coated onto the PEDOT:PSS layer, followed by annealing at 80 ℃ under a nitrogen atmosphere for 10 min.

1.2. Synthesis

Synthesis of PhCzBN: Compound **BNCz-Br** (2.00 g, 2.78 mmol), (4-(9*H*-carbazol-9-yl)phenyl)boronic acid (0.96 g, 3.34 mmol), $Pd(PPh_3)_4$ (0.26 g, 0.22 mmol) and K_3PO_4 (2.36 g, 11.12 mmol) were added into a 250 mL two-necked flask under argon atmosphere, charged with super dried THF (50 mL) and H_2O(50 mL). Then the mixture was stirred at 70 ºC for 12 h. After cooling to room temperature, the mixture was extracted with CH_2Cl_2 and dried over anhydrous Na_2SO_4. The solvent was removed by rotary evaporation. Subsequently, the resulting crude product was purified by silica gel column chromatography (eluent: petroleum ether/dichloromethane = 8:1, v/v), giving **PhCzBN** as a yellow solid (1.1 g, yield 45%). ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 9.16 (d, *J* = 1.7, 2H), 8.64 (s, 2H), 8.53 (d, *J* = 8.9, 2H), 8.50 (d, *J* = 1.7, 2H), 8.30 (d, *J* = 2.0, 2H), 8.20 (dd, *J* = 10.0, 8.2, 4H), 7.85 (d, *J* = 8.4, 2H), 7.74 (dd, *J* = 8.8, 2.0, 2H), 7.63 (d, *J* = 8.2, 2H), 7.50 (t, *J* = 7.6, 2H), 7.36 (t, *J* = 7.4, 2H), 1.69 (s, 18H), 1.55 (s, 18H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 145.45, 145.01, 144.75, 141.76, 140.86, 140.83, 138.32, 137.79, 129.80, 129.22, 127.67, 127.19, 126.09, 124.56, 123.65, 123.58, 120.73, 120.43, 120.17, 117.37, 114.17, 109.94, 107.00, 35.19, 34.83, 32.20, 31.84, 26.92, 11.44.

***Synthesis of target polymers*:** The polymerization was performed according to the general procedures of

superacid-catalyzed Friedel-Crafts polyhydroxyalkylation described as follows: In a two-neck round bottom flask, different ratios of **M2** and **PhCzBN** and **M1**(161 mg, 1.00 mmol) were dissolved in 4 mL CH_2Cl_2. After cooling to 0 ºC, the trifluoromethanesulfonic acid (0.64 mL) was added dropwise into the reaction mixture followed by stirring for 12 h at room temperature under argon atmosphere. Then the reaction mixture was poured slowly into methanol and neutralized with NaOH aqueous solution to get an olive yellow fiber. After sedimentation in methanol twice, the precipitated polymer was washed with hot acetone for 3 days and continuously washed with hot *n*-hexane for another 3 days in a Soxhlet apparatus. Finally, the residue was dried under vacuum to provide an olive yellow solid.

***Synthesis of* P0: M2** (279 mg, 1.00 mmol) and **M1** (161 mg, 1.00 mmol) were used in the polymerization with the feed ratio (**M2:M1**) of 100:100, yield: 396 mg, 90%. GPC: M_n = 13300, M_w = 14859, M_w/M_n = 1.12.

***Synthesis of* P5: PhCzBN** (44 mg, 0.05 mmol), **M2** (265 mg, 0.95 mmol) and **M1** (161 mg, 1.00 mmol) were used in the polymerization with the feed ratio (**PhCzBN:M2:M1**) of 5:95:100, yield: 384 mg, 85%. According to ^{1}H NMR analysis, the percentage of **PhCzBN, M2** and **M1** repeating unit in the purified random copolymers were calculated to be 2.3%, 47.7% and 50%, with only minor deviation from the monomer feed ratio. GPC: M_n = 12143, M_w = 13446, M_w/M_n = 1.11.

***Synthesis of* P10: PhCzBN** (88 mg, 0.10 mmol), **M2** (251 mg, 0.90 mmol) and **M1** (161 mg, 1.00 mmol) were used in the polymerization with the feed ratio (**PhCzBN:M2:M1**) of 10:90:100, yield: 419 mg, 87%. According to ^{1}H NMR analysis, the percentage of **PhCzBN, M2** and **M1** repeating unit in the purified random copolymers were calculated to be 5.0%, 45.0% and 50%, almost the same with the monomer feed ratio. GPC: M_n = 11394, M_w = 12409, M_w/M_n = 1.09.

***Synthesis of* P15: PhCzBN** (132 mg, 0.15 mmol), **M2** (237 mg, 0.85 mmol) and **M1** (161 mg, 1.00 mmol) were used in the polymerization with the feed ratio (**PhCzBN:M2:M1**) of 15:85:100, yield: 410 mg, 80%. According to ^{1}H NMR analysis, the percentage of **PhCzBN, M2** and **M1** repeating unit in the purified random copolymers were calculated to be 7.4%, 42.6% and 50%, with only minor deviation from the monomer feed ratio. GPC: M_n = 11458, M_w = 13259, M_w/M_n = 1.16.

***Synthesis of* P20: PhCzBN** (176 mg, 0.20 mmol), **M2** (224 mg, 0.80 mmol) and **M1** (161 mg, 1.00 mmol) were used in the polymerization with the feed ratio (**PhCzBN:M2:M1**) of 20:80:100, yield: 472 mg, 87%. According to ^{1}H NMR analysis, the percentage of **PhCzBN, M2** and **M1** repeating unit in the purified

random copolymers were calculated to be 10.0%, 40.0% and 50%, almost the same with the monomer feed ratio. GPC: M_n = 12706, M_w = 13824, M_w/M_n = 1.09.

1.3. Quantum Chemical Calculations

All of the simulation calculations were carried out with Gaussian 16 program package. Density functional theory (DFT) calculations on the geometrical and electronic properties of the ground-state were performed based on B3LYP density functional method with basis set 6-31G(d,p). The density functional dispersion correction was conducted by Grimme's D3 version with Becke-Johnson damping function. Time-dependent DFT (TD-DFT) calculations were also carried out by this method.

The SOCs between S_1 and T_n (n = 1, 2, 3) states were calculated with PySOC by considering that the three Tn substrates (m = 1, 0, -1) are degenerate, i.e. $\langle S_1 | \hat{H}_{soc} | T_1 \rangle = \sqrt{\sum_{m=0,\pm1} \langle S_1 | \hat{H}_{so} | T_1{}^m \rangle^2}$, where The $\hat{H}_{soc}$ represents the interaction of the SOC. All SOCs were obtained at the TD-DFT level of theory using the B3LYP functional and the 6-31G(d,p) basis set.

1.4. Thermal and Electrochemical Characterization

Thermogravimetric analysis (TGA) measurements were conducted on a TGA-Q50 Instrument (TA Instruments, America), with a heating rate of 20 °C/min under an argon atmosphere. The thermal decomposition temperatures (T_d) were determined by the recorded temperature at 5% weight loss. Differential scanning calorimetry (DSC) was performed at a heating rate of 10 °C/min using a TA DSC-Q200 (TA Instruments, America) under argon atmosphere. Heating/cooling/re-heating scans were performed, and the DSC curves were obtained from the second heating scan.

Cyclic voltammetry (CV) measurements were carried out on a CHI600 electrochemical analyzer (Chenhua, China) at room temperature, with a conventional three-electrode system consisting of a glassy carbon working electrode, a platinum wire auxiliary electrode, and an Ag/AgCl standard electrode was used as the reference electrode. Dichloromethane and 0.1 M tetrabutylammonium hexafluorophosphate (Bu_4NPF_6) were used as the solvent and supporting electrolyte, respectively. The sweep speed was set as 50 mV s^{-1}. The onset of oxidation potential was adopted for the calculation of HOMO energy level based on the equation E_{HOMO} (eV) = – (4.80 – $E_{Fc/Fc+}$ + E_{ox}) eV. The LUMO energy levels of the compounds were then deduced from the HOMO levels and the UV-Vis absorption onsets of the longer wavelength.

1.5. Photophysical Characterization

UV-vis absorption spectra were obtained on a Shimadzu UV-2600 spectrophotometer (Shimadzu, Japan) at room temperature. Room-temperature photoluminescence spectra were measured on a Hitachi F-7100 fluorescence spectrophotometer (Hitachi, Japan). Phosphorescence spectra were measured both in toluene and neat film states at 77 K. The film samples were prepared by spin-coating using chlorobenzene as solvent. The PL lifetimes were measured by a single photon counting spectrometer from Edinburgh Instruments (FLS920) with a Picosecond Pulsed UV-LASTER (LASTER377) as the excitation source. The solid state absolute photoluminescence quantum yields (Φ_{PL}s) were measured on a Hamamatsu UV-NIR absolute PL quantum yield spectrometer (C13534, Hamamatsu Photonics) equipped with a calibrated integrating sphere, and all the samples were excited at 320 nm. During the Φ_{PL} measurements, the integrating sphere was purged with pure and dry nitrogen to maintain an inert environment.

1.6. Analysis of Rate Constants

The estimation of rate constants pertaining to radiative decay (k_r) and nonradiative decay (k_{nr}) transitioning from S_1 to S_0, as well as the rate constants associated with intersystem crossing (k_{ISC}) and reverse intersystem crossing (k_{RISC}), can be accomplished by employing the subsequent equations.

$$k_r = \Phi_p k_p + \Phi_d k_d \approx \Phi_p k_p \quad \text{.....Eq.(1)}$$

$$k_{nr} = \frac{1 - \Phi_{PL}}{\Phi_{PL}} k_r \quad \text{.....Eq.(2)}$$

$$k_{ISC} = k_p - k_r - k_{nr} \quad \text{.....Eq.(3)}$$

$$k_{RISC} = (k_p k_d \Phi_d)/(k_{ISC} \Phi_p) \quad \text{.....Eq.(4)}$$

Where 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 (r_p) and delayed components (r_d) in the transient PL spectra. r_p and r_d were determined using τ_p and τ_d and fitting parameter (A_p, A_d) as follows.

$$I(t) = A_p e^{-\frac{1}{\tau_p}} + A_d e^{-\frac{1}{\tau_d}} \quad \text{.....Eq.(5)}$$

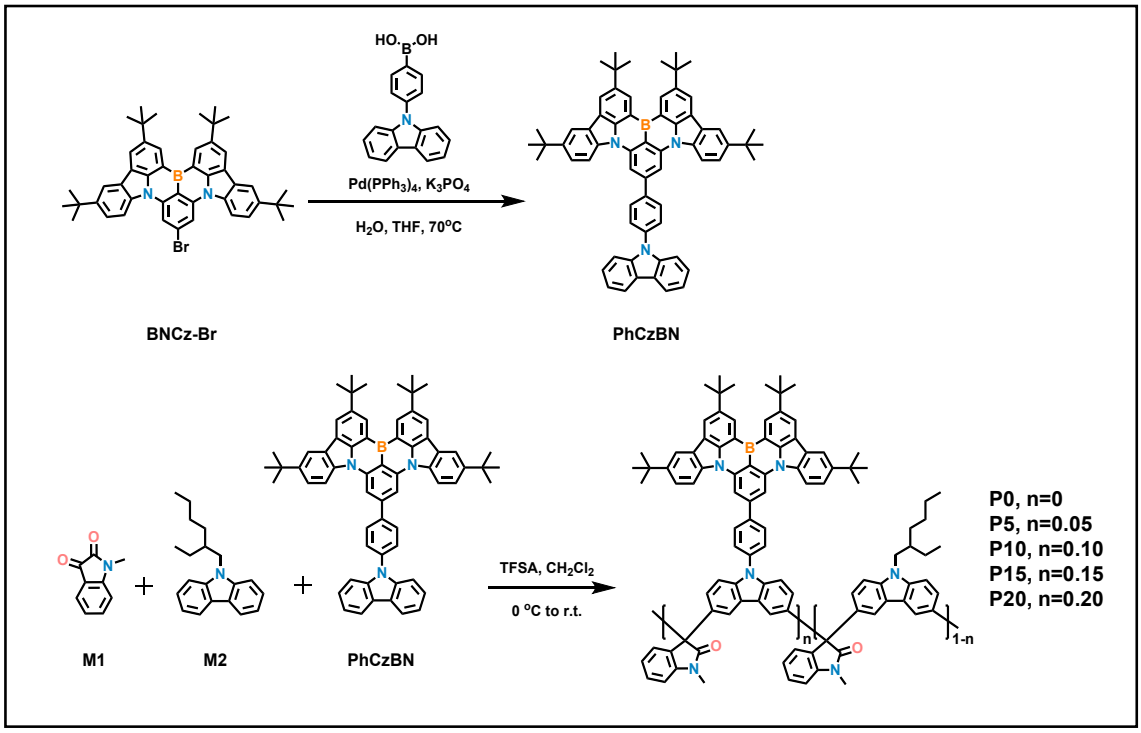
$$r_p = A_p \tau_p / (A_p \tau_p + A_d \tau_d) \quad \text{.....Eq.(6)}$$

$r_d = A_d\tau_d/(A_p\tau_p + A_d\tau_d)$ ……Eq.(7)

1.7. Device Fabrication and Measurement

The ITO-coated glass substrates were ultrasonicated sequentially in acetone and ethanol, followed by the treatment in a UV-ozone oven for 20 min. Afterwards, PEDOT:PSS was spin-coated onto the ITO substrates at ambient temperature at a speed of 4000 rpm for 30 s (~35 nm). The PEDOT:PSS coated ITO substrates were baked at 120 °C for 10 min and then transferred to a glove box with N_2 atmosphere. The emissive layer (using chlorobenzene as the solvent, 10 mg/mL) was spin-coated onto the PEDOT:PSS layer at a speed of 3000 rpm for 30 s (~35 nm), followed by an annealing process (55 °C for 10 min). Then, the exciton blocking layer (DPEPO, 10 nm), electron-transporting layer (TmPyPB, 50 nm), electron injecting layer (Liq, 1 nm) and cathode (aluminum, 100 nm) were consecutively evaporated in a vacuum chamber under 2×10^{-4} pa. The devices were tested in ambient environment without encapsulation. The current density-voltage-luminance (*J*-*V*-*L*), *L*-EQE curves, and electroluminescence spectra were measured using a Keithley 2400 source meter coupled with an absolute EQE measurement system (C9920-12, Hamamatsu Photonics, Japan).

2. Schemes, Figures and Tables



Scheme S1. Synthetic route of **PhCzBN** and **P0**-**P20** polymers.

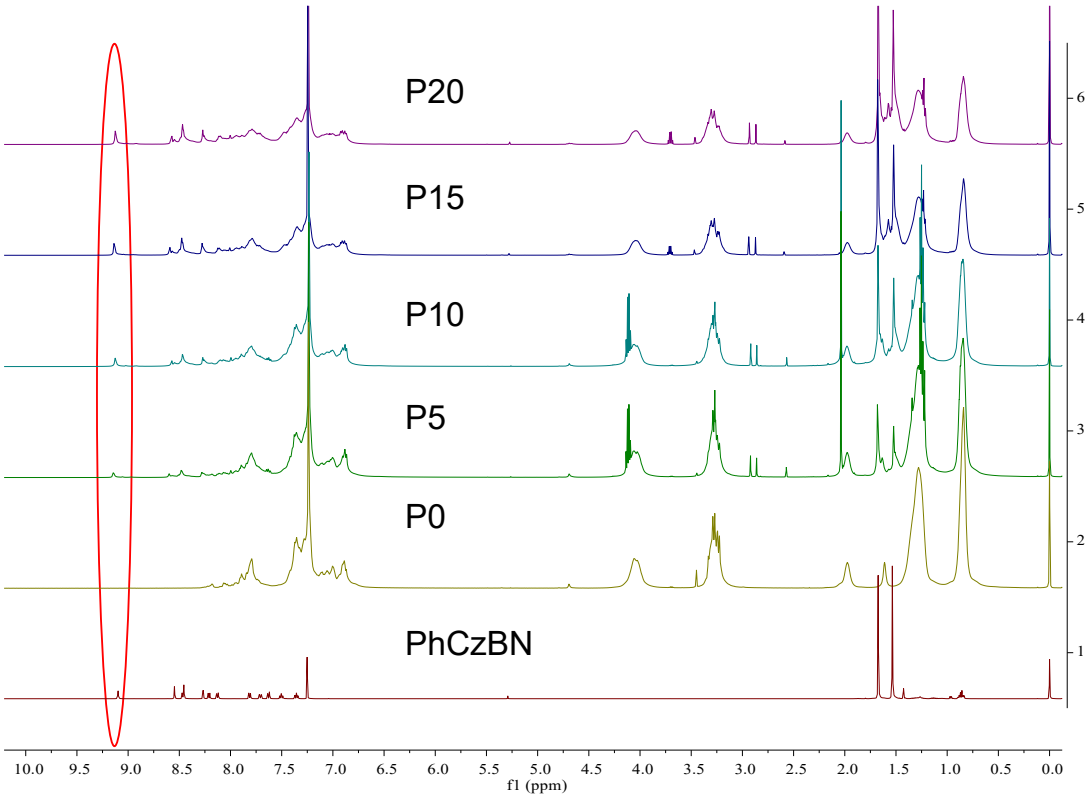


Figure S1. ^{1}H NMR spectrum of **PhCzBN** and **P0-P20** polymers in $CDCl_3$ (500 MHz, 25 °C). The red circle represents the characteristic peak of the MR-TADF moiety located at 9.12 ppm.

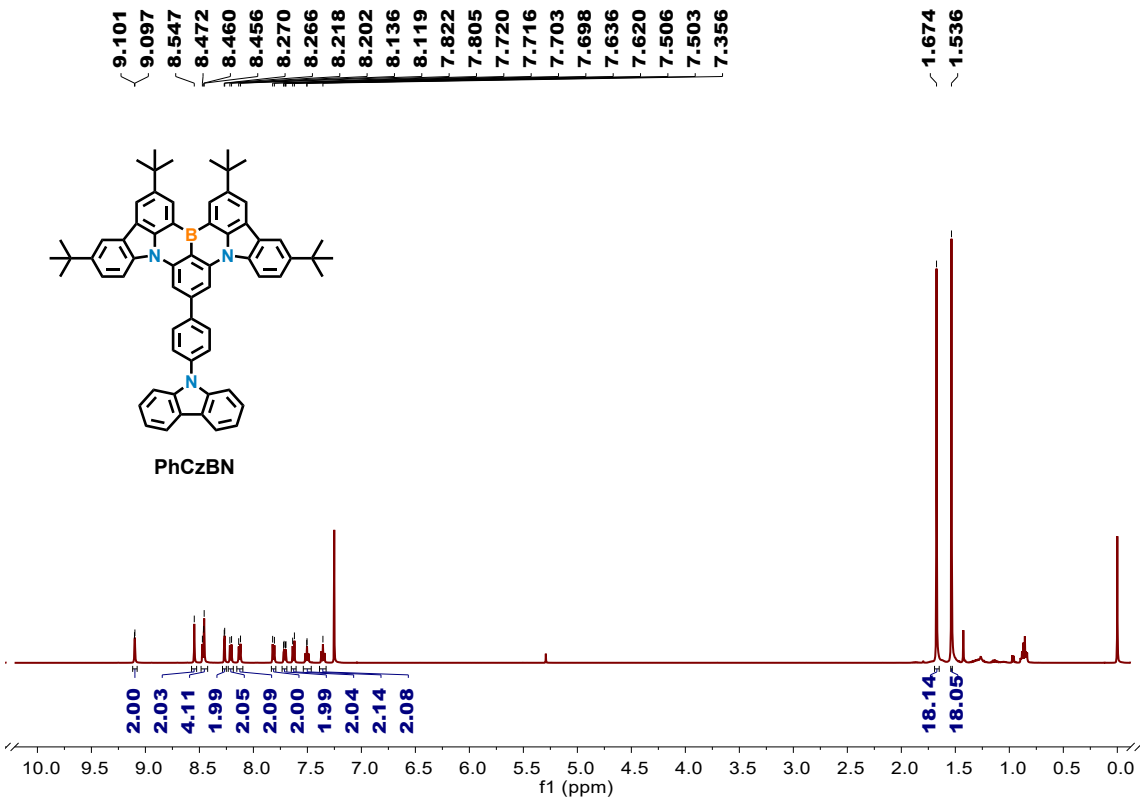


Figure S2. ^{1}H NMR spectrum of **PhCzBN** in $CDCl_3$ (400 MHz, 25 °C).

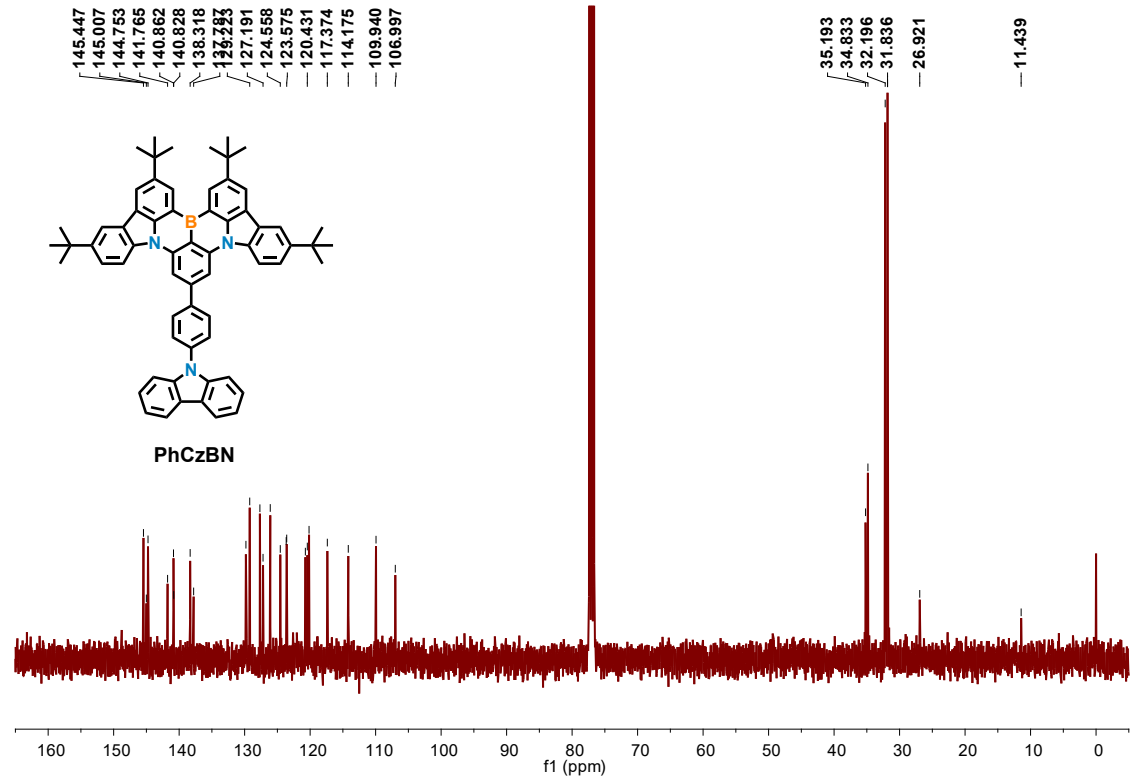


Figure S3. ^{13}C NMR spectrum of **PhCzBN** in $CDCl_3$ (100 MHz, 25 °C).

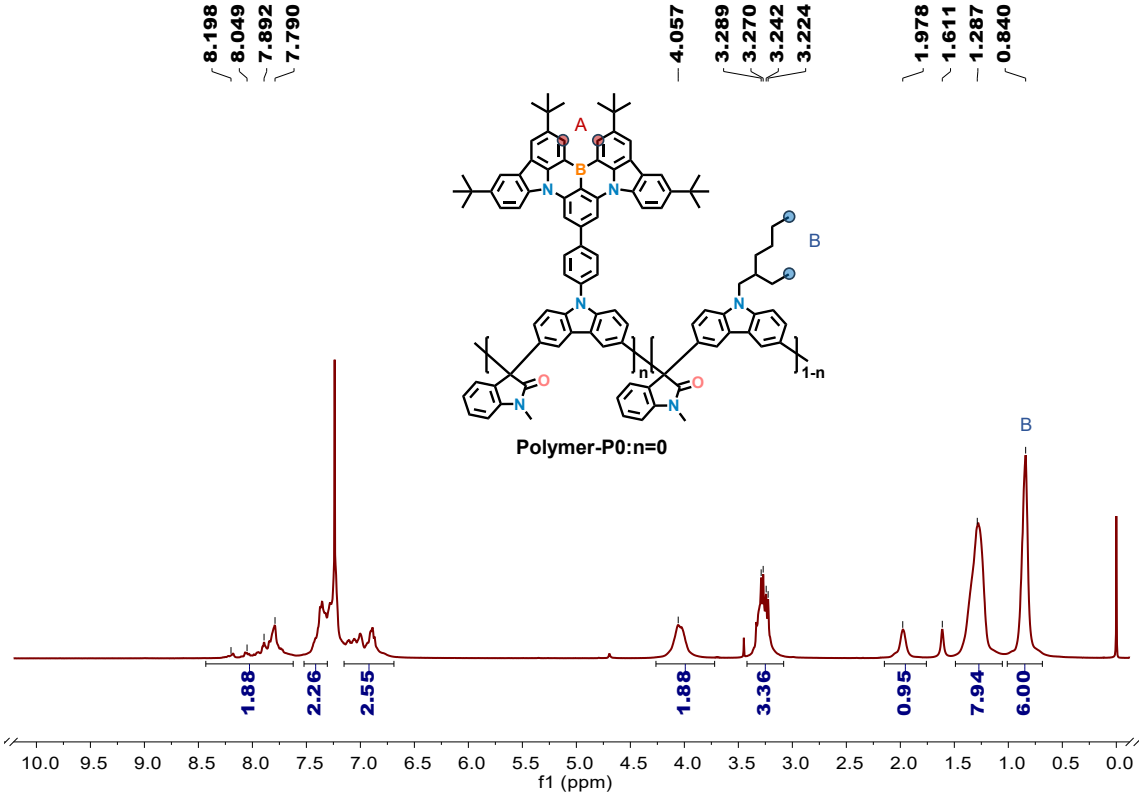


Figure S4. ^{1}H NMR spectrum of **P0** in $CDCl_3$ (500 MHz, 25 °C).

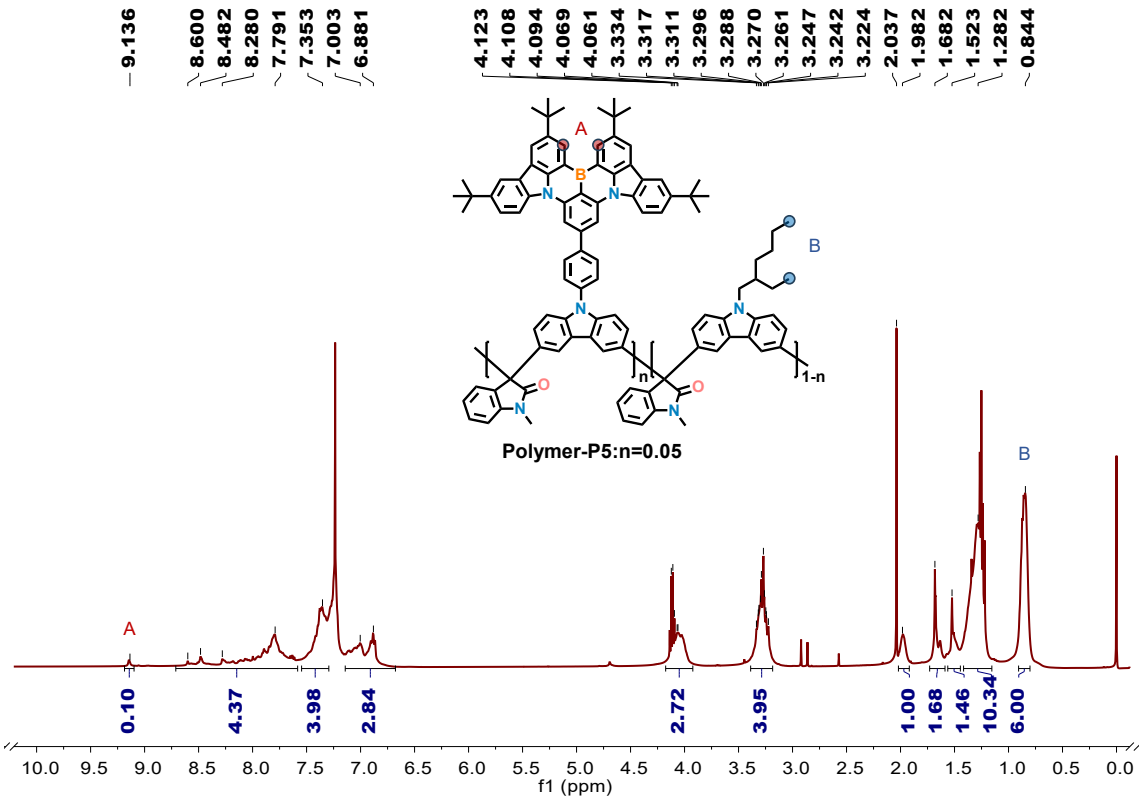


Figure S5. ^{1}H NMR spectrum of **P5** in $CDCl_3$ (500 MHz, 25 °C).

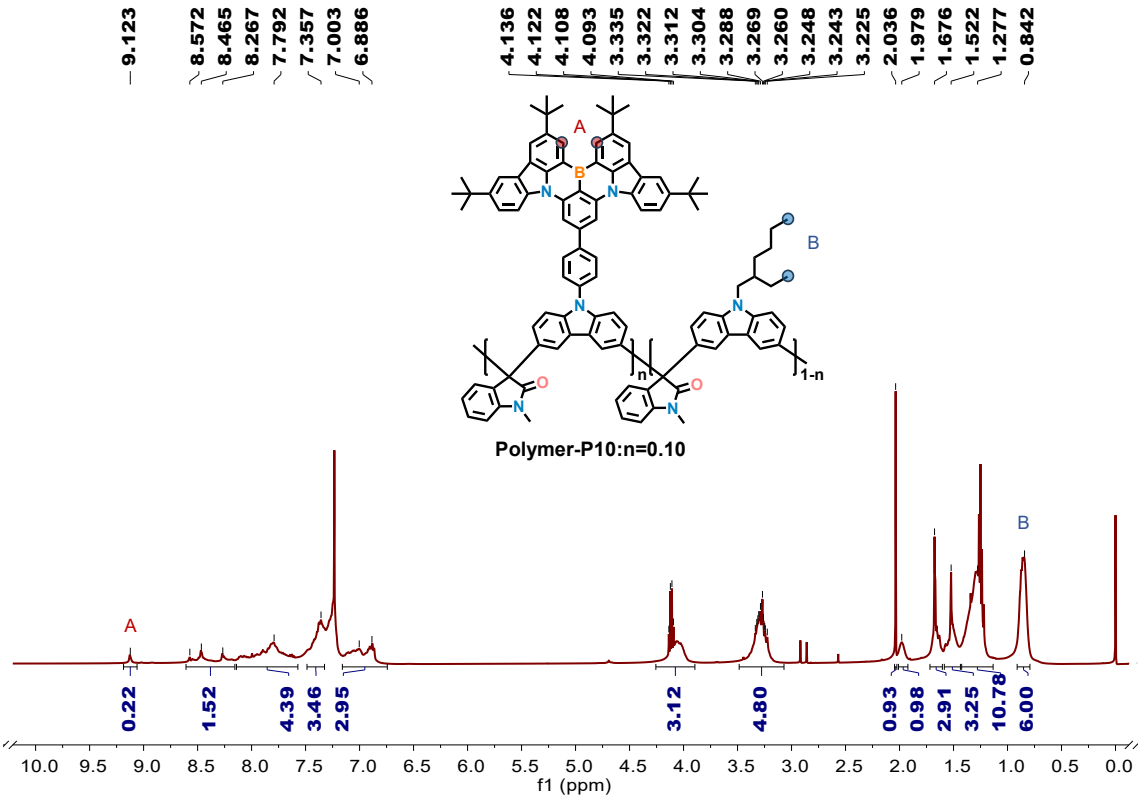


Figure S6. ^{1}H NMR spectrum of **P10** in $CDCl_3$ (500 MHz, 25 °C).

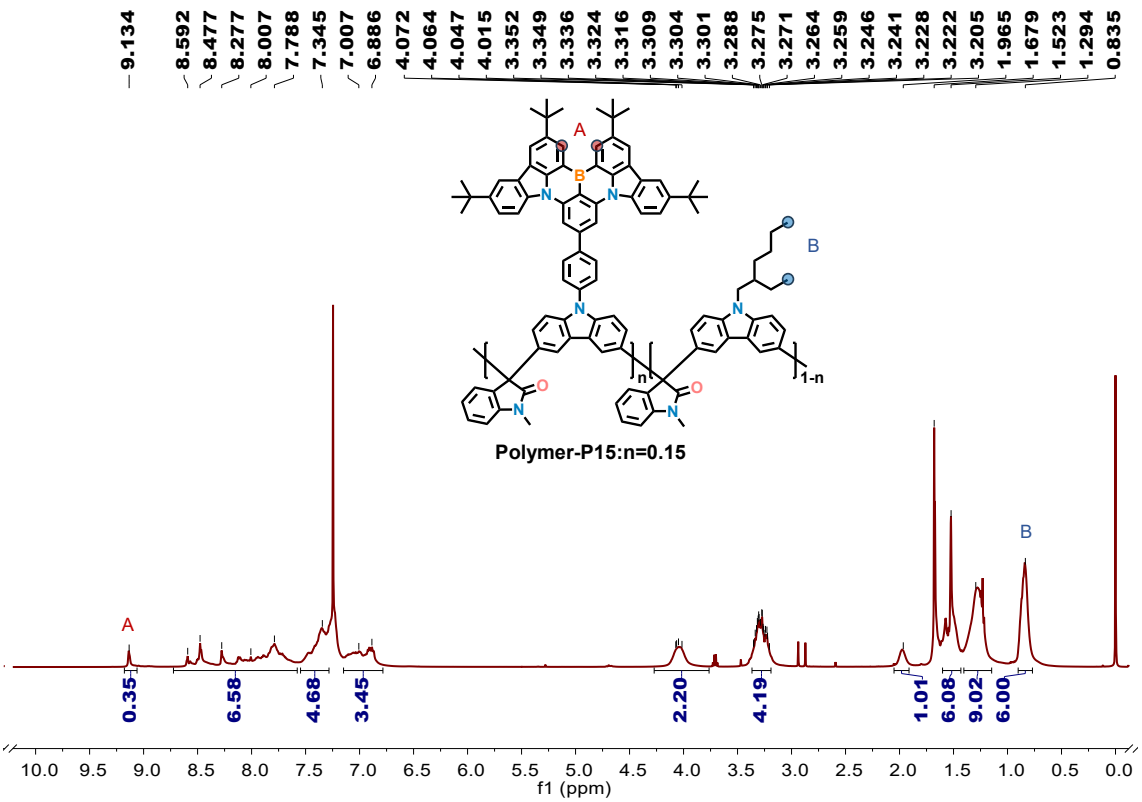


Figure S7. ^{1}H NMR spectrum of **P15** in $CDCl_3$ (500 MHz, 25 °C).

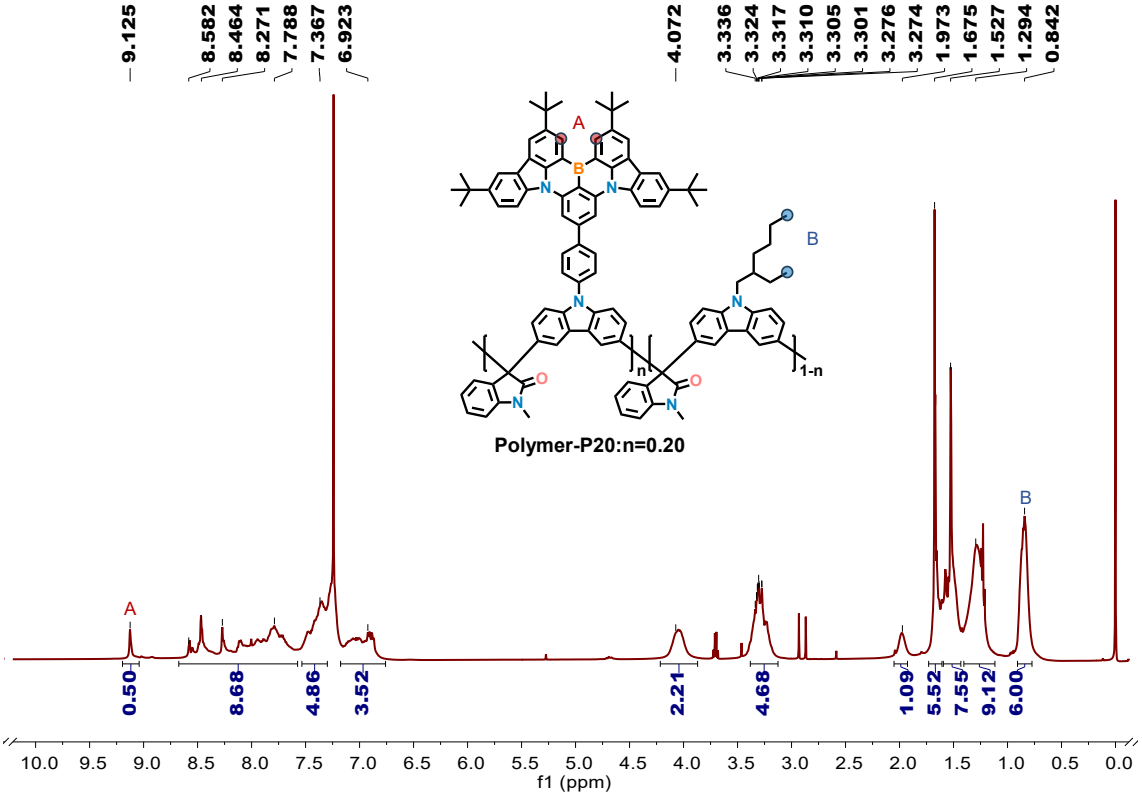


Figure S8. ^{1}H NMR spectrum of **P20** in $CDCl_3$ (500 MHz, 25 ^{o}C).

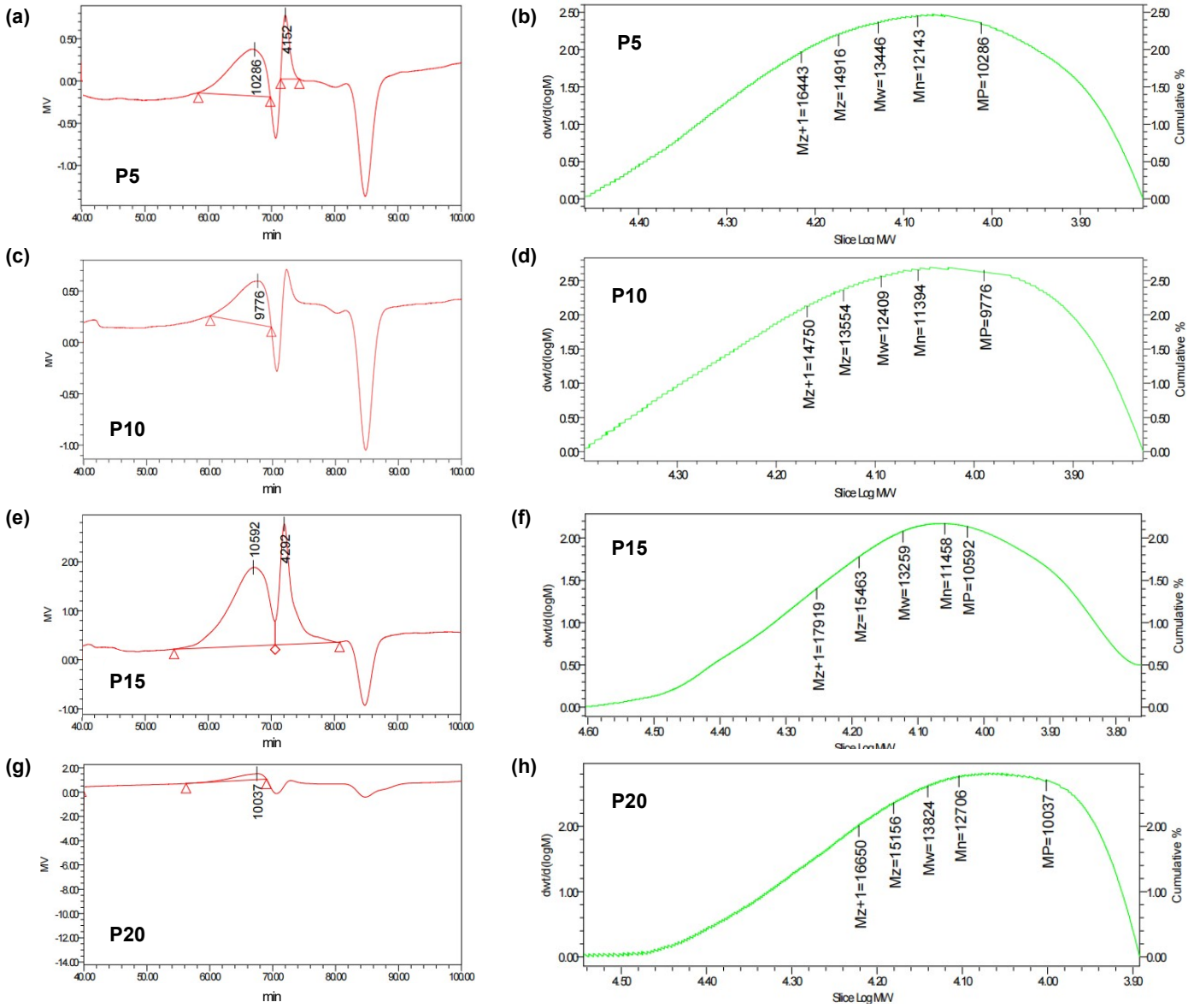


Figure S9. GPC chromatograms of (a) **P5**, (c) **P10**, (e) **P15**, (g) **P20** as a function of retention time, and schematic diagram of average molecular weights (M_{z+1}, M_z, M_w, M_n, M_p) from the GPC spectra for (b) **P5**, (d) **P10**, (f) **P15**, (h) **P20**.

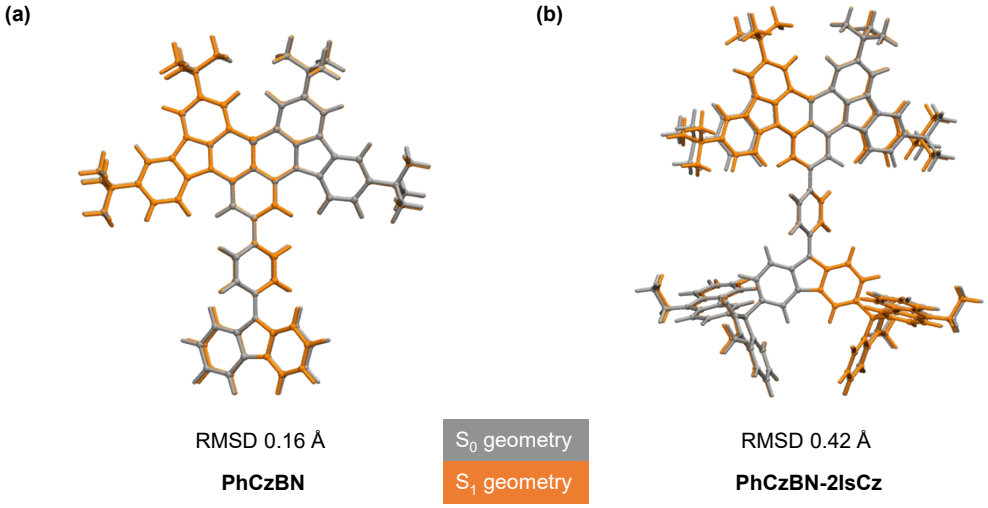


Figure S10. Comparison of the optimized conformations in the S_0 (gray) and S_1 (yellow) states with RMSD values for (a) **PhCzBN** and (b) **PhCzBN-2IsCz**.

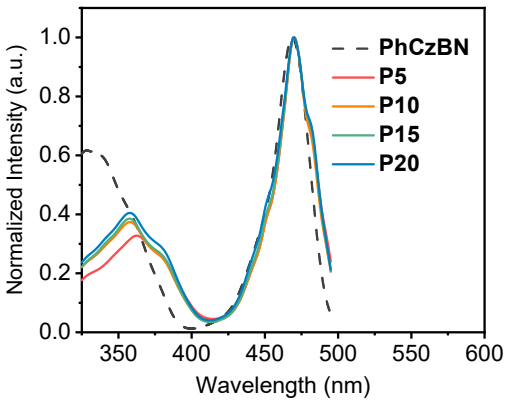


Figure S11. Excitation spectra of the **PhCzBN** and **P5-P20** polymers measured at corresponding peak wavelengths in toluene (1×10^{-5} M).

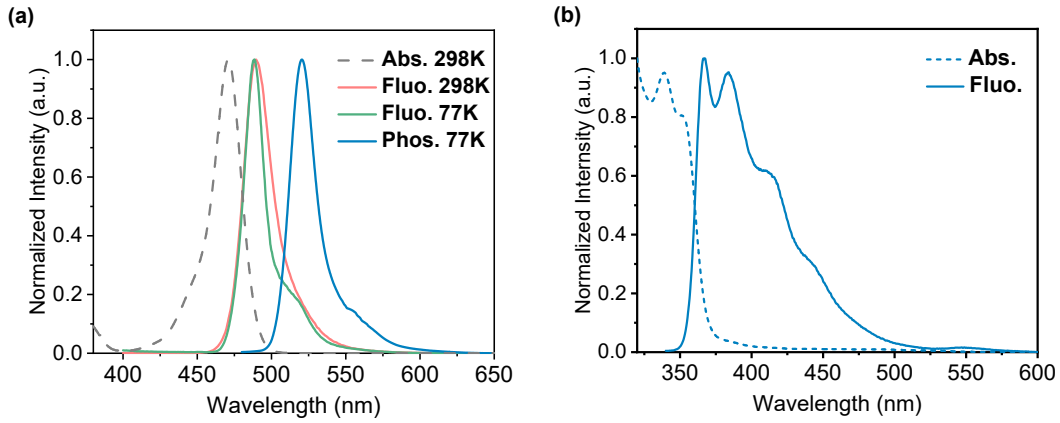


Figure S12. (a) UV-vis absorption (298 K), fluorescence (298 K and 77 K), and phosphorescence (77 K) spectra of **PhCzBN** in toluene (1×10^{-5} M), . (b) UV-vis absorption (298 K), and fluorescence (298 K) spectra of **P0** (polymer without the **PhCzBN** unit) in toluene (1×10^{-5} M).

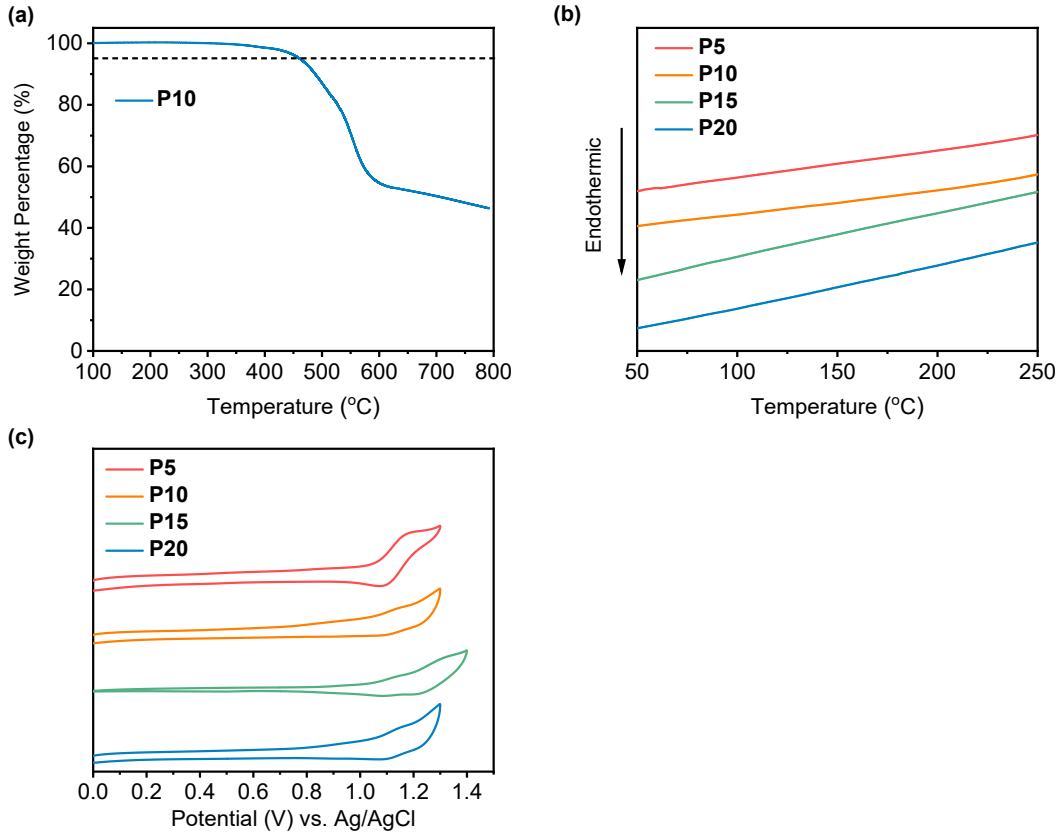


Figure S13. (a) Thermal gravimetric analysis (TGA) curves of **P10** at a heating rate of 10 °C min^{-1}, (b) Differential scanning calorimetry (DSC) curves of **P5**-**P20** polymers at a heating rate of 10 °C min^{-1}, (c) the oxidation curves obtained from the cyclic voltammetry (CV) measurement for **P5**-**P20** polymers. The HOMO energy levels of the polymers were calculated as -5.36, -5.38, -5.41, and -5.43 eV for **P5**, **P10**, **P15**, and **P20**,

respectively, based on the oxidation onsets. Based on the HOMO values and energy gaps (E_g) deduced from absorption edges, the LUMO energy levels were calculated to be -2.89, -2.90, -2.92, and -2.89 eV, respectively.

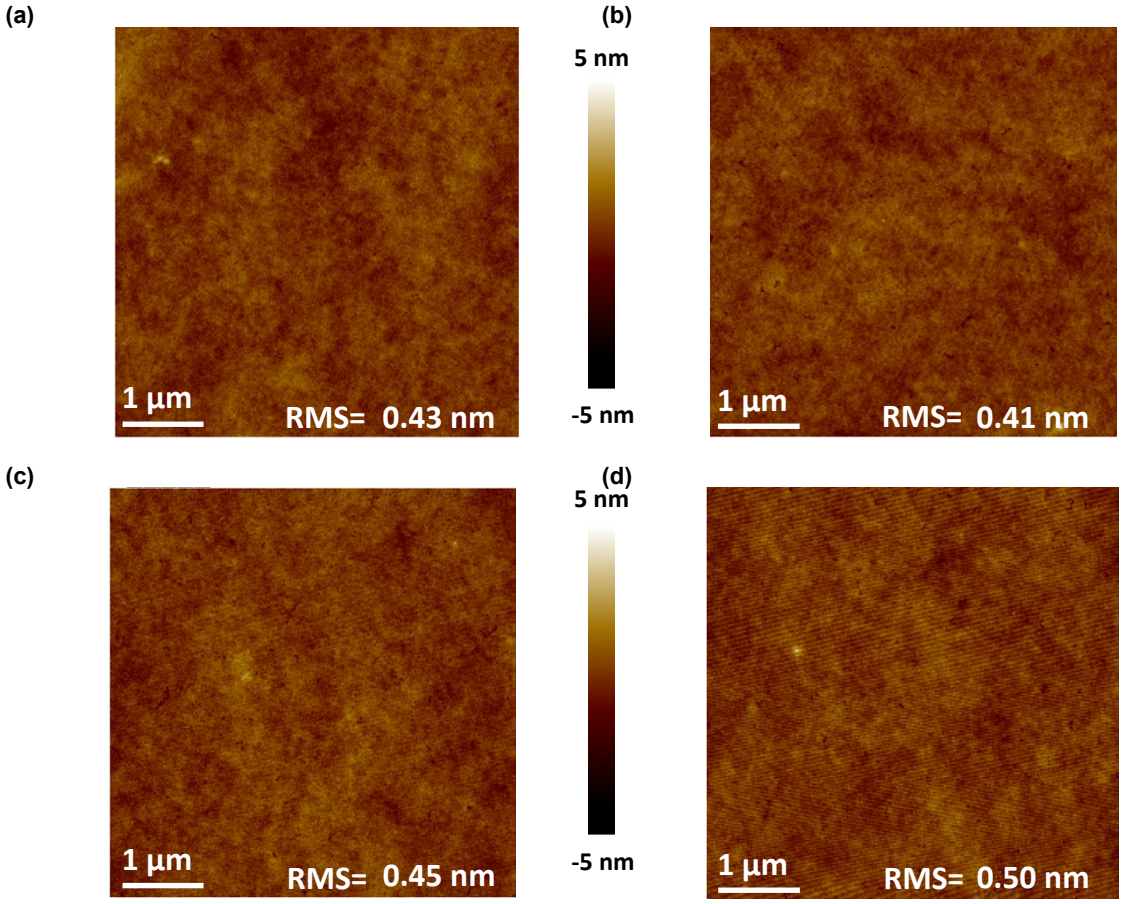


Figure S14. AFM images of the solution-processed films based on (a) **P5**, (b) **P10**, (c) **P15** and (d) **P20**. Note: The doping concentration was 10 wt% with mCP host, and the films were prepared by spin-coating onto the PEDOT:PSS coated ITO substrates, annealed at a temperature of 50 °C before measurement.

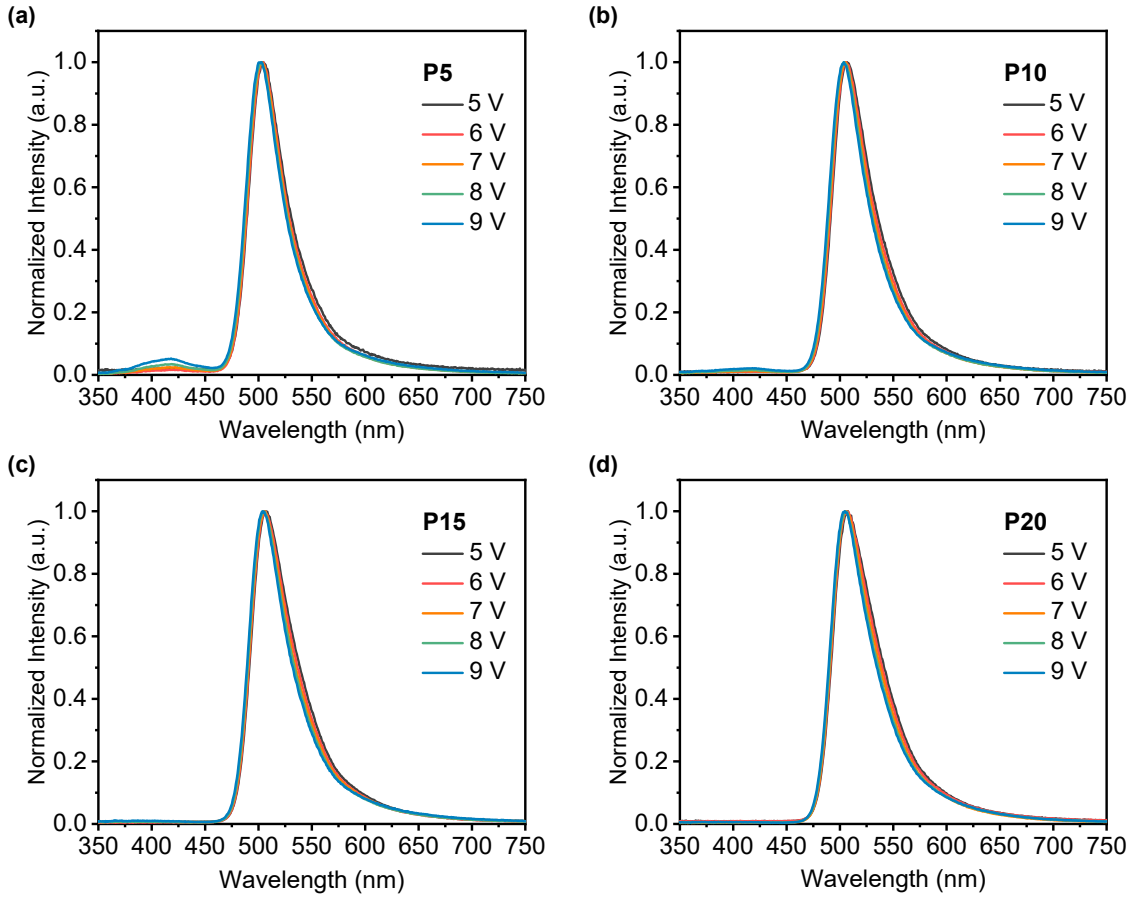


Figure S15. Electroluminescence spectra of the devices based on (a) **P5**, (b) **P10**, (c) **P15** and (d) **P20** at different voltages.

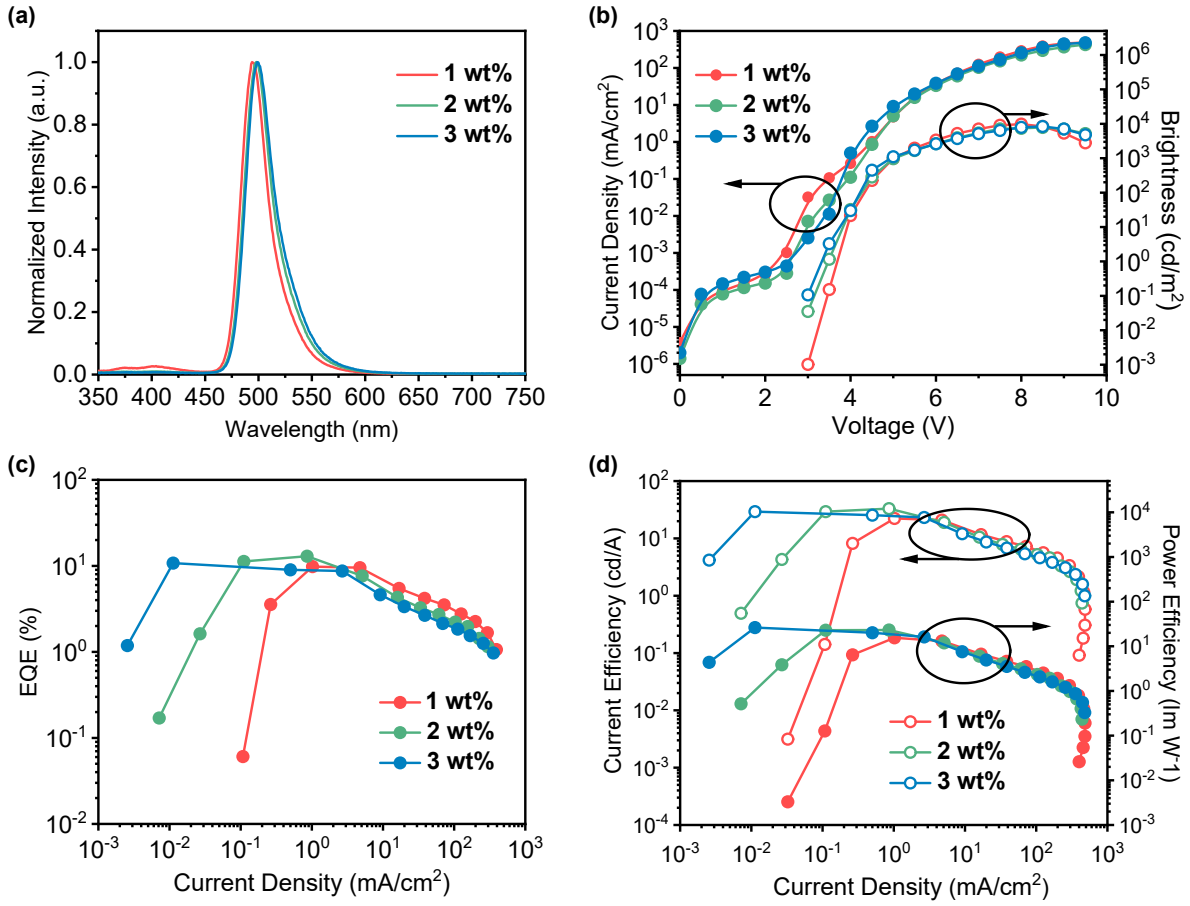


Figure S16. Electroluminescence performance of **PhCzBN** based devices: (a) electroluminescence spectra, (b) current density-voltage-luminance, (c) external quantum efficiency-current density, (d) current efficiency-current density-power efficiency characteristics. Device structure: ITO/PEDOT: PSS (35 nm)/mCP: 1-3 wt% **PhCzBN** (35 nm)/DPEPO (10 nm)/TmPyPB (50 nm)/Liq (2 nm)/Al (100 nm).

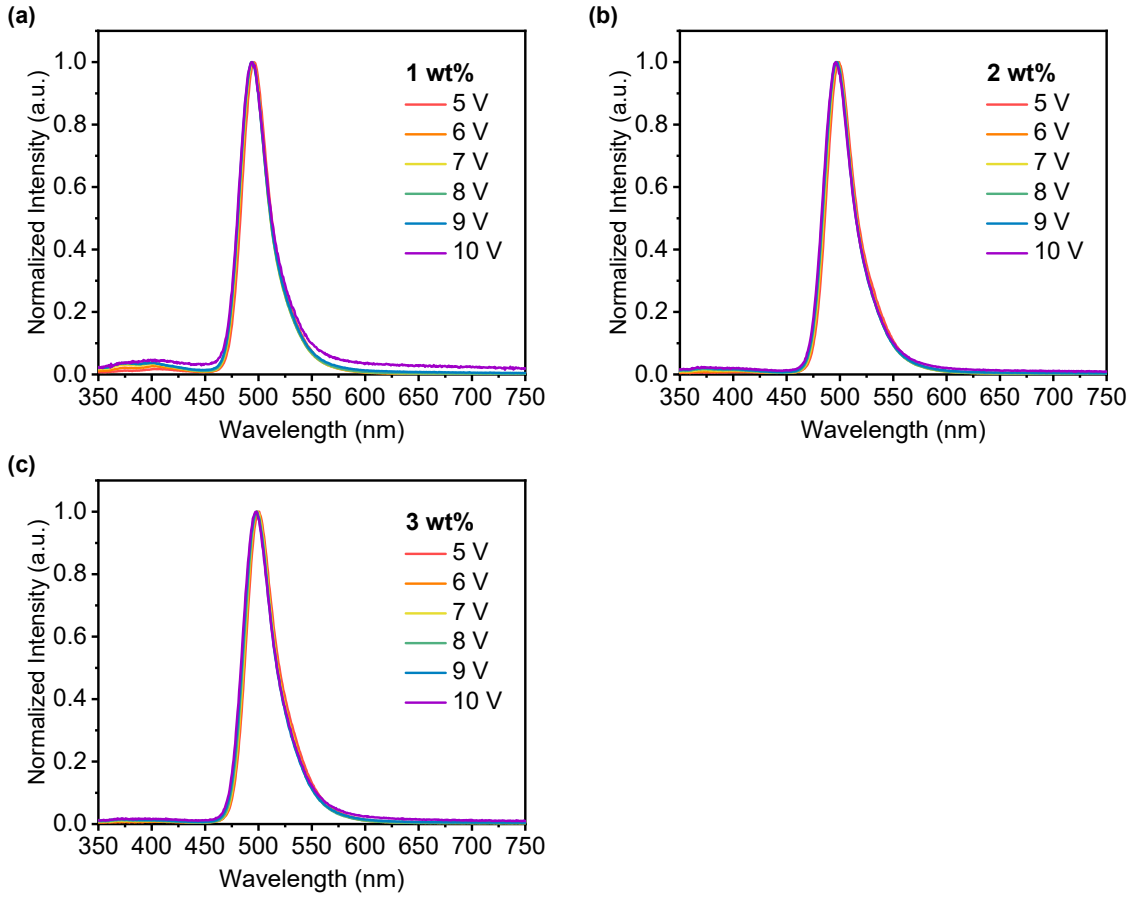


Figure S17. Voltage-dependent electroluminescence spectra of the devices based on **PhCzBN** with doping concentrations of (a) 1 wt%, (b) 2 wt%, and (c) 3 wt%.

Table S1. Photophysical data of **P5**, **P10**, **P15**, and **P20** in dilute solution (1×10^{-5} M).

emitter	λ_{abs} [a] (nm)	λ_{PL} [b] (nm)	FWHM[c] (nm)	λ_{Phos} [d] (nm)	S_1[e] (eV)	T_1[f] (eV)	ΔE_{ST} [g] (eV)
PhCzBN	471	490	23	520	2.63	2.47	0.16
P5	471	500	34	518	2.63	2.47	0.16
P10	471	503	35	519	2.62	2.46	0.16
P15	472	505	37	520	2.60	2.45	0.15
P20	472	506	38	520	2.58	2.44	0.14

[a] Absorption peaks; [b] emission peaks; [c] emission full width at half maximum; [d] phosphorescence peak; [e] singlet energy levels obtained from onset of photoluminescence spectra; [f] triplet energy levels obtained from 77 K PL in toluene; [g] singlet-triplet energy gap.

Table S2. Photophysical properties of **P5**-**P20** doped in mCP films with 10 wt% concentration.

Emitter	λ_{em}[a] (nm)	FWHM[b] (nm)	Φ_{PL}[c] (%)	τ_{PF}[d] (ns)	τ_{DF}[e] (μs)	$k_{r,S}$[f] (10^7 s^{-1})	$k_{nr,S}$[g] (10^7 s^{-1})	k_{ISC}[h] (10^7 s^{-1})	k_{RISC}[i] (10^4 s^{-1})
P5	500	34	71	5.4	14.3	9.7	4.0	4.9	9.5
P10	503	35	73	5.3	13.0	10.6	3.9	4.4	10.0
P15	505	37	61	5.2	11.7	9.2	5.9	4.1	10.9
P20	506	38	55	5.2	10.8	8.6	7.1	3.5	11.3

[a] Emission peak; [b] full-width at half-maximum; [c] photoluminescence quantum yield; [d] prompt fluorescence lifetime; [e] delayed fluorescence lifetime; [f] radiative decay rate constant of singlet exciton; [g] non-radiative decay rate constant of singlet exciton; [h] rate constant of intersystem crossing; [i] rate constant of reverse intersystem crossing.

Table S3. Summary of the device performances of the solution-processed TADF OLEDs.

Dopant	V_{on} (V)	EQE[a] (%)	CE[b] (cd A^{-1})	PE[c] (lm W^{-1})	L[d] (cd m^{-2})	λ_{EL}[e] (nm)	FWHM (nm)	CIE[f] (x,y)
PhCzBN	3.5	13.0/12.2/7.6	33.1	23.1	7843	497	31	(0.11, 0.57)
P5	3.9	15.0/8.5/1.2	43.6	30.4	1152	502	40	(0.19,0.60)
P10	3.9	19.4/6.2/1.5	60.2	37.8	1644	505	42	(0.20, 0.62)
P15	3.9	13.7/6.8/-	43.0	31.8	947	506	44	(0.23, 0.63)
P20	3.9	12.1/6.5/	38.5	26.9	1020	508	47	(0.23, 0.63)

[a] External quantum efficiency at maximum/100/1000 cd m^{-2}; [b] maximum current efficiency; [c] maximum power efficiency; [d] maximum brightness; [e] electroluminescence peak at ~500 cd m^{-2}; [f] the 1931 Commission Internationale de L'Eclairage (CIE) coordinates of devices measured at a brightness of 1000 cd m^{-2}.

Table S4. Summary of TD-DFT data for of the MR-TADF unit and polymer model compound.

Compound	Transition	Wavelength (nm)	Energy (eV)	Oscillator Strength	Coefficient of Orbital
PhCzBN	S_0-S_1	440.22	2.8164	0.3838	HOMO→LUMO (0.9821)
	S_0-T_1	515.41	2.4055	0.0000	HOMO→LUMO (0.9476)
	S_0-T_2	439.68	2.8199	0.0000	HOMO-5→LUMO+2 (0.0619) HOMO-4→LUMO (0.6304) HOMO-4→LUMO+1 (0.0504) HOMO-4→LUMO+2 (0.0507) HOMO-2→LUMO+2 (0.0454) HOMO→LUMO (0.0206)
	S_0-T_3	436.57	2.8399	0.0000	HOMO-6→LUMO (0.0691) HOMO-5→LUMO (0.1131) HOMO-5→LUMO+1 (0.0224) HOMO-5→LUMO+2 (0.0266) HOMO-4→LUMO+2 (0.0736) HOMO-2→LUMO (0.4020) HOMO-1→LUMO (0.1290) HOMO-1→LUMO+1 (0.0239)
PhCzBN-2IsCz	S_0-S_1	440.29	2.8160	0.3693	HOMO→LUMO (0.9823)
	S_0-T_1	515.11	2.4070	0.0000	HOMO→LUMO (0.9474)
	S_0-T_2	439.48	2.8212	0.0000	HOMO-11→LUMO+2 (0.0604) HOMO-9→LUMO (0.6302) HOMO-9→LUMO+1 (0.0459) HOMO-9→LUMO+2 (0.0556) HOMO-7→LUMO+2 (0.0428) HOMO→LUMO (0.0205)
	S_0-T_3	437.11	2.8364	0.0000	HOMO-12→LUMO (0.0761) HOMO-11→LUMO (0.0903) HOMO-11→LUMO+2 (0.0260) HOMO-9→LUMO+2 (0.0567) HOMO-7→LUMO (0.3617) HOMO-3→LUMO (0.0742) HOMO-1→LUMO (0.1189)

Table S5. Cartesian coordinates of **PhCzBN** at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-3.519165	1.057582	0.246202
2	6	0	-4.862964	1.040910	0.235065
3	6	0	-5.614338	-0.051434	-0.009879
4	6	0	-4.842164	-1.131493	-0.244216
5	6	0	-3.498127	-1.125456	-0.241198
6	6	0	-2.754992	-0.027216	0.005038
7	6	0	-1.391655	-0.014682	0.007279
8	6	0	-0.669747	1.122253	0.007753
9	6	0	0.672887	1.220095	0.042127
10	6	0	1.282961	0.010157	-0.003453
11	6	0	0.695996	-1.211795	-0.038122
12	6	0	-0.647940	-1.137574	0.007170
13	7	0	1.359899	-2.324871	-0.038725
14	7	0	1.314340	2.345924	0.046820
15	6	0	2.637761	-2.376376	0.092195
16	6	0	3.127922	-3.617494	0.141282
17	6	0	2.056329	-4.391019	-0.018930
18	6	0	0.999603	-3.563807	-0.141875
19	6	0	0.930507	3.574975	0.175591
20	6	0	1.966241	4.427438	0.045661
21	6	0	3.050299	3.678304	-0.146669
22	6	0	2.588041	2.426288	-0.105291
23	5	0	2.869174	0.026837	-0.023874
24	6	0	3.534280	-1.392111	0.206050
25	6	0	4.835400	-1.643868	0.413565
26	6	0	5.317156	-2.901153	0.477998
27	6	0	4.424641	-3.898975	0.320818
28	6	0	2.007124	-5.728452	-0.061114
29	6	0	0.836181	-6.358693	-0.258093
30	6	0	-0.231335	-5.558326	-0.429444
31	6	0	-0.155058	-4.215731	-0.382006
32	6	0	4.337461	3.987839	-0.347593
33	6	0	5.246444	3.010615	-0.537282
34	6	0	4.792246	1.742735	-0.479764
35	6	0	3.501196	1.461467	-0.249117
36	6	0	-0.233759	4.194389	0.452051
37	6	0	-0.335135	5.533503	0.523750
38	6	0	0.709990	6.361722	0.344080
39	6	0	1.890692	5.763459	0.111161
40	6	0	6.719908	3.356882	-0.785814
41	6	0	6.833053	4.196145	-2.077359
42	6	0	7.265136	4.167559	0.410898
43	6	0	7.636410	2.122556	-0.955174
44	6	0	0.538840	7.881570	0.443413

45	6	0	0.059018	8.248818	1.864755
46	6	0	1.838419	8.674609	0.175087
47	6	0	-0.504837	8.350073	-0.594812
48	6	0	6.802464	-3.213818	0.698706
49	6	0	7.697626	-1.959141	0.827040
50	6	0	6.961303	-4.029543	2.000435
51	6	0	7.337029	-4.033122	-0.497216
52	6	0	0.769740	-7.888915	-0.312363
53	6	0	1.640443	-8.395630	-1.483070
54	6	0	1.298529	-8.471412	1.017376
55	6	0	-0.656684	-8.446723	-0.520937
56	7	0	-6.903887	-0.061739	-0.018991
57	6	0	-7.671382	-1.079947	0.185230
58	6	0	-8.966364	-0.730901	0.094017
59	6	0	-8.974500	0.575491	-0.164422
60	6	0	-7.683711	0.944490	-0.235357
61	6	0	-7.452394	-2.357111	0.559137
62	6	0	-8.463335	-3.228508	0.723070
63	6	0	-9.737996	-2.847207	0.556896
64	6	0	-9.999704	-1.568560	0.253253
65	6	0	-10.017975	1.396951	-0.340686
66	6	0	-9.771352	2.679347	-0.640938
67	6	0	-8.500210	3.080368	-0.786890
68	6	0	-7.478717	2.224834	-0.606620
69	1	0	-3.083807	2.027857	0.532592
70	1	0	-5.320819	1.986450	0.556780
71	1	0	-5.280205	-2.084779	-0.570647
72	1	0	-3.043512	-2.087993	-0.523884
73	1	0	-1.232268	2.039999	-0.113821
74	1	0	-1.194673	-2.063935	0.131587
75	1	0	5.508780	-0.789155	0.528108
76	1	0	4.749201	-4.948893	0.353848
77	1	0	2.933283	-6.308888	0.059035
78	1	0	-1.221511	-5.994182	-0.635838
79	1	0	-1.110396	-3.724873	-0.596035
80	1	0	4.640727	5.044291	-0.372665
81	1	0	5.480045	0.903284	-0.619915
82	1	0	-1.172331	3.678504	0.681652
83	1	0	-1.324912	5.958116	0.760970
84	1	0	2.807947	6.352682	-0.018713
85	1	0	7.893391	4.447923	-2.305982
86	1	0	6.423458	3.639071	-2.950622
87	1	0	6.286695	5.162633	-2.009844
88	1	0	8.343682	4.410583	0.278606

89	1	0	7.163816	3.592470	1.359581
90	1	0	6.740394	5.138249	0.549091
91	1	0	7.342069	1.501174	-1.831115
92	1	0	8.693579	2.425141	-1.130930
93	1	0	7.643356	1.480743	-0.044934
94	1	0	-0.050666	9.350559	1.983630
95	1	0	-0.930276	7.804227	2.111240
96	1	0	0.785506	7.898068	2.632968
97	1	0	1.663361	9.772419	0.241466
98	1	0	2.238337	8.480963	-0.846135
99	1	0	2.631060	8.441878	0.921624
100	1	0	-0.193193	8.068774	-1.626607
101	1	0	-1.513278	7.915619	-0.418418
102	1	0	-0.632046	9.456043	-0.571800
103	1	0	8.764499	-2.237802	0.982404
104	1	0	7.670291	-1.332061	-0.093036
105	1	0	7.411532	-1.329623	1.699939
106	1	0	8.031370	-4.256269	2.209107
107	1	0	6.433122	-5.007545	1.960500
108	1	0	6.560156	-3.466323	2.873717
109	1	0	6.829937	-5.016775	-0.607257
110	1	0	7.201814	-3.476272	-1.452441
111	1	0	8.423311	-4.251754	-0.386323
112	1	0	1.596251	-9.504841	-1.570579
113	1	0	1.293840	-7.967323	-2.451099
114	1	0	2.714217	-8.130588	-1.364481
115	1	0	1.237257	-9.583190	1.026391
116	1	0	0.704160	-8.094722	1.880890
117	1	0	2.364228	-8.215315	1.206374
118	1	0	-1.093447	-8.121937	-1.492262
119	1	0	-0.656912	-9.560211	-0.538021
120	1	0	-1.343800	-8.144829	0.301726
121	1	0	-6.461672	-2.759826	0.806678
122	1	0	-8.250431	-4.266789	1.031764
123	1	0	-10.561345	-3.564637	0.709416
124	1	0	-11.043581	-1.232175	0.156154
125	1	0	-11.058000	1.044481	-0.260460
126	1	0	-10.603120	3.383915	-0.807174
127	1	0	-8.298529	4.121667	-1.092818
128	1	0	-6.490687	2.642969	-0.839029

Table S6. Cartesian coordinates of **PhCzBN** at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.581096	1.056024	0.528445
2	6	0	-4.969037	1.045950	0.536333
3	6	0	-5.669393	-0.041666	-0.001408
4	6	0	-4.952259	-1.118700	-0.538232
5	6	0	-3.564292	-1.107920	-0.528880
6	6	0	-2.840989	-0.020360	-0.000040
7	6	0	-1.372497	-0.009078	0.000242
8	6	0	-0.656201	1.195113	-0.076937
9	6	0	0.747207	1.212332	0.012019
10	6	0	1.513979	0.012625	-0.001744
11	6	0	0.765016	-1.198328	-0.014244
12	6	0	-0.637640	-1.203029	0.077105
13	7	0	1.472982	-2.404187	-0.057868
14	7	0	1.436287	2.428359	0.054227
15	6	0	2.868021	-2.452283	0.131968
16	6	0	3.295100	-3.786752	0.209431
17	6	0	2.119159	-4.610408	0.001364
18	6	0	1.013307	-3.732606	-0.202538
19	6	0	0.957898	3.750616	0.197155
20	6	0	2.048726	4.642678	-0.004879
21	6	0	3.236904	3.837643	-0.212347
22	6	0	2.830344	2.496544	-0.135725
23	5	0	3.049263	0.024177	-0.002561
24	6	0	3.719670	-1.341661	0.185432
25	6	0	5.083463	-1.661988	0.395001
26	6	0	5.560577	-2.977604	0.506483
27	6	0	4.653054	-4.051518	0.402625
28	6	0	1.943922	-5.985342	-0.081566
29	6	0	0.687940	-6.532477	-0.393661
30	6	0	-0.369979	-5.645109	-0.651847
31	6	0	-0.224424	-4.257942	-0.573845
32	6	0	4.590959	4.122638	-0.405151
33	6	0	5.514939	3.062547	-0.509499
34	6	0	5.058294	1.740239	-0.398931
35	6	0	3.698705	1.399132	-0.189830
36	6	0	-0.290599	4.259355	0.567179
37	6	0	-0.450457	5.640057	0.644579
38	6	0	0.598336	6.546681	0.386700
39	6	0	1.857744	6.020507	0.076487
40	6	0	6.999270	3.392297	-0.726499

41	6	0	7.158831	4.181038	-2.044540
42	6	0	7.507645	4.252305	0.451388
43	6	0	7.877928	2.132779	-0.812011
44	6	0	0.332193	8.053732	0.481224
45	6	0	-0.136580	8.403692	1.910793
46	6	0	1.585261	8.887225	0.168033
47	6	0	-0.770290	8.439170	-0.529546
48	6	0	7.049741	-3.284106	0.723755
49	6	0	7.908947	-2.011095	0.807470
50	6	0	7.221364	-4.068500	2.042912
51	6	0	7.571164	-4.137858	-0.453014
52	6	0	0.526465	-8.055693	-0.468140
53	6	0	1.471197	-8.617580	-1.553277
54	6	0	0.893344	-8.671074	0.900307
55	6	0	-0.910635	-8.476434	-0.815375
56	7	0	-7.082910	-0.052119	-0.002293
57	6	0	-7.892991	-1.082981	0.487946
58	6	0	-9.253410	-0.721187	0.309112
59	6	0	-9.262592	0.584962	-0.316680
60	6	0	-7.907408	0.966720	-0.493673
61	6	0	-7.528118	-2.281377	1.103920
62	6	0	-8.550578	-3.130422	1.521527
63	6	0	-9.902692	-2.795977	1.337768
64	6	0	-10.259750	-1.592379	0.737136
65	6	0	-10.281061	1.441249	-0.746105
66	6	0	-9.940922	2.649949	-1.346303
67	6	0	-8.593623	3.004237	-1.528245
68	6	0	-7.559352	2.170337	-1.109212
69	1	0	-3.059605	1.890082	0.986485
70	1	0	-5.521775	1.865812	0.981516
71	1	0	-5.492138	-1.946813	-0.983928
72	1	0	-3.029908	-1.934145	-0.986266
73	1	0	-1.197654	2.110264	-0.253133
74	1	0	-1.164908	-2.126220	0.254593
75	1	0	5.781894	-0.842915	0.484656
76	1	0	5.002081	-5.076619	0.463333
77	1	0	2.797070	-6.635168	0.083596
78	1	0	-1.339605	-6.031196	-0.938399
79	1	0	-1.060520	-3.631620	-0.848436
80	1	0	4.924530	5.152911	-0.465471
81	1	0	5.768973	0.931829	-0.489393
82	1	0	-1.118798	3.621711	0.839697
83	1	0	-1.424573	6.020692	0.931392
84	1	0	2.704513	6.674801	-0.090164

85	1	0	8.211894	4.430919	-2.214979
86	1	0	6.804937	3.589517	-2.894541
87	1	0	6.590830	5.115247	-2.028129
88	1	0	8.566005	4.499949	0.313678
89	1	0	7.402072	3.712830	1.397687
90	1	0	6.952854	5.190547	0.537913
91	1	0	7.585839	1.491479	-1.649252
92	1	0	8.921901	2.423712	-0.964114
93	1	0	7.828212	1.540344	0.106837
94	1	0	-0.331990	9.478244	1.993491
95	1	0	-1.056096	7.875633	2.177482
96	1	0	0.628555	8.136873	2.646212
97	1	0	1.344607	9.952310	0.236573
98	1	0	1.956680	8.694896	-0.843337
99	1	0	2.394356	8.684559	0.876613
100	1	0	-0.459503	8.202866	-1.551860
101	1	0	-1.704775	7.906838	-0.332250
102	1	0	-0.977978	9.513164	-0.473770
103	1	0	8.957233	-2.285857	0.959866
104	1	0	7.850199	-1.420681	-0.112128
105	1	0	7.607234	-1.373227	1.643901
106	1	0	8.278192	-4.301631	2.213630
107	1	0	6.668057	-5.011512	2.027741
108	1	0	6.858311	-3.481433	2.892121
109	1	0	7.031166	-5.084826	-0.538031
110	1	0	7.457098	-3.601540	-1.400105
111	1	0	8.633260	-4.368677	-0.315034
112	1	0	1.371030	-9.706460	-1.616820
113	1	0	1.232406	-8.193568	-2.533409
114	1	0	2.518510	-8.390383	-1.336479
115	1	0	0.790765	-9.761044	0.866110
116	1	0	0.235238	-8.289415	1.686919
117	1	0	1.923554	-8.440543	1.184977
118	1	0	-1.217570	-8.101189	-1.796584
119	1	0	-0.976555	-9.568155	-0.843913
120	1	0	-1.628238	-8.119901	-0.069885
121	1	0	-6.486867	-2.538806	1.258878
122	1	0	-8.293622	-4.069237	2.002396
123	1	0	-10.674036	-3.481826	1.672930
124	1	0	-11.304859	-1.328543	0.605861
125	1	0	-11.322355	1.162077	-0.616241
126	1	0	-10.721808	3.324376	-1.682549
127	1	0	-8.349841	3.946705	-2.008825
128	1	0	-6.521800	2.443070	-1.262795

Table S7. Cartesian coordinates of the model compound **PhCzBN-2IsCz** at the optimized S_0 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.353760	0.793900	0.747180
2	6	0	0.010348	0.814077	0.728283
3	6	0	-0.762224	-0.075803	0.073814
4	6	0	-0.010656	-1.003479	-0.552735
5	6	0	1.333308	-1.031816	-0.545010
6	6	0	2.097037	-0.127233	0.101013
7	6	0	3.460325	-0.137816	0.097008
8	6	0	4.199383	0.905243	0.520356
9	6	0	5.543419	0.968082	0.569876
10	6	0	6.134369	-0.140622	0.060196
11	6	0	5.528487	-1.251739	-0.427031
12	6	0	4.186005	-1.184942	-0.339833
13	7	0	6.176067	-2.287193	-0.861043
14	7	0	6.201138	2.002683	0.989354
15	6	0	7.454724	-2.395525	-0.781594
16	6	0	7.928056	-3.565530	-1.217439
17	6	0	6.843498	-4.211024	-1.640767
18	6	0	5.796946	-3.391098	-1.420704
19	6	0	5.836376	3.095049	1.578947
20	6	0	6.881938	3.925684	1.761095
21	6	0	7.952628	3.295627	1.281369
22	6	0	7.473570	2.123836	0.856371
23	5	0	7.720423	-0.132072	0.024705
24	6	0	8.367240	-1.536470	-0.317795
25	6	0	9.667280	-1.858649	-0.245416
26	6	0	10.132030	-3.048992	-0.674229
27	6	0	9.223003	-3.904653	-1.182661
28	6	0	6.775605	-5.431238	-2.188175
29	6	0	5.593610	-5.930267	-2.589115
30	6	0	4.534723	-5.117556	-2.422585
31	6	0	4.630153	-3.894848	-1.868945
32	6	0	9.241053	3.648047	1.187603
33	6	0	10.132895	2.807095	0.626599
34	6	0	9.661844	1.614260	0.211500
35	6	0	8.370419	1.276852	0.343098
36	6	0	4.684621	3.572413	2.089878
37	6	0	4.602266	4.786744	2.661997

38	6	0	5.655759	5.614483	2.787408
39	6	0	6.825113	5.139236	2.325786
40	6	0	11.607091	3.210861	0.497996
41	6	0	11.711987	4.472868	-0.386134
42	6	0	12.181586	3.509134	1.900657
43	6	0	12.503792	2.123948	-0.139801
44	6	0	5.505774	6.986787	3.453243
45	6	0	5.052218	6.796779	4.917242
46	6	0	6.811302	7.814251	3.477107
47	6	0	4.452829	7.817589	2.686385
48	6	0	11.615838	-3.433457	-0.617806
49	6	0	12.530051	-2.329019	-0.037649
50	6	0	11.782437	-4.685444	0.270810
51	6	0	12.121207	-3.737900	-2.045652
52	6	0	5.505657	-7.323591	-3.221420
53	6	0	6.352015	-7.350855	-4.513126
54	6	0	6.046351	-8.372983	-2.224679
55	6	0	4.068986	-7.749923	-3.600057
56	7	0	-2.051206	-0.043266	0.049341
57	6	0	-2.848298	-1.033367	-0.180150
58	6	0	-4.129032	-0.633952	-0.142985
59	6	0	-4.098954	0.666116	0.140088
60	6	0	-2.800722	0.990986	0.243538
61	6	0	-2.691138	-2.360737	-0.353453
62	6	0	-3.739886	-3.177162	-0.562110
63	6	0	-5.009772	-2.733556	-0.570175
64	6	0	-5.190747	-1.421673	-0.350684
65	6	0	-5.123023	1.514617	0.290076
66	6	0	-4.878241	2.814788	0.517844
67	6	0	-3.586470	3.182581	0.588354
68	6	0	-2.577655	2.307150	0.429767
69	7	0	-5.192866	8.363197	-2.244670
70	6	0	-5.472129	7.458932	-1.393202
71	6	0	-5.095456	6.290433	-1.929186
72	6	0	-4.586136	6.572302	-3.135668
73	6	0	-4.660692	7.906405	-3.308710
74	6	0	-6.031048	7.479407	-0.176051
75	6	0	-6.189763	6.316878	0.479942
76	6	0	-5.791055	5.137962	-0.039710
77	6	0	-5.256121	5.133299	-1.276649
78	6	0	-4.074355	5.750964	-4.061746
79	6	0	-3.620880	6.289385	-5.204296
80	6	0	-3.686930	7.617181	-5.395907
81	6	0	-4.203470	8.429062	-4.456836

82	6	0	-5.501917	9.775062	-1.917683
83	6	0	-5.177416	10.933832	-2.865617
84	7	0	-7.370408	-3.459674	-2.748212
85	6	0	-8.152734	-2.958840	-1.883298
86	6	0	-6.263150	-3.914100	-2.335029
87	6	0	-6.168941	-3.684231	-0.815652
88	6	0	-7.541691	-3.055889	-0.692916
89	7	0	-7.413100	3.578580	2.476362
90	6	0	-8.124458	3.181990	1.502723
91	6	0	-6.238771	3.972604	2.214345
92	6	0	-5.994220	3.828549	0.701766
93	6	0	-7.379717	3.301207	0.393205
94	6	0	-8.141417	-2.609311	0.420410
95	6	0	-9.359926	-2.053190	0.320604
96	6	0	-9.967728	-1.952075	-0.873840
97	6	0	-9.370244	-2.407477	-1.987968
98	6	0	-7.875584	2.953290	-0.803209
99	6	0	-9.129915	2.477718	-0.869710
100	6	0	-9.873696	2.357014	0.243308
101	6	0	-9.377950	2.711004	1.441118
102	6	0	-7.748704	-3.507627	-4.172797
103	6	0	-7.944404	3.575157	3.852032
104	8	0	-5.415512	4.393197	2.995405
105	8	0	-5.398280	-4.444096	-2.995243
106	7	0	-6.015218	-8.032807	2.516914
107	6	0	-5.545947	-7.507662	3.577895
108	6	0	-5.344690	-6.208662	3.310111
109	6	0	-5.721705	-6.019516	2.038638
110	6	0	-6.146249	-7.202737	1.559345
111	6	0	-5.254063	-7.997986	4.791588
112	6	0	-4.759880	-7.161422	5.720605
113	6	0	-4.561210	-5.860762	5.443774
114	6	0	-4.853021	-5.367243	4.228667
115	6	0	-5.718378	-4.902612	1.300893
116	6	0	-6.135630	-4.949127	0.022095
117	6	0	-6.581688	-6.128686	-0.451567
118	6	0	-6.584076	-7.248026	0.293239
119	6	0	-6.341902	-9.478218	2.513510
120	6	0	-6.907461	-10.193964	1.282860
121	1	0	1.807247	1.566887	1.387312
122	1	0	-0.428917	1.572507	1.389932
123	1	0	-0.463538	-1.747586	-1.221478
124	1	0	1.771092	-1.821391	-1.175857
125	1	0	3.650868	1.808324	0.760130

126	1	0	3.623651	-2.080149	-0.573530
127	1	0	10.354088	-1.117386	0.174163
128	1	0	9.532965	-4.890349	-1.558188
129	1	0	7.695302	-6.020347	-2.314868
130	1	0	3.535857	-5.435216	-2.760529
131	1	0	3.677982	-3.354174	-1.861445
132	1	0	9.558804	4.633963	1.555895
133	1	0	10.335873	0.884122	-0.246810
134	1	0	3.743083	3.013852	2.125967
135	1	0	3.621763	5.097793	3.059581
136	1	0	7.748387	5.727486	2.410468
137	1	0	12.772037	4.784574	-0.524358
138	1	0	11.281185	4.287312	-1.396592
139	1	0	11.180148	5.347077	0.049749
140	1	0	13.261387	3.775957	1.848553
141	1	0	12.086250	2.620931	2.566176
142	1	0	11.672881	4.361141	2.402797
143	1	0	12.187868	1.879051	-1.179122
144	1	0	13.562262	2.462861	-0.209307
145	1	0	12.515479	1.187325	0.462800
146	1	0	4.958358	7.774043	5.442663
147	1	0	4.061310	6.298126	4.997554
148	1	0	5.785801	6.179013	5.484023
149	1	0	6.651632	8.808184	3.953366
150	1	0	7.193184	8.014905	2.450369
151	1	0	7.611995	7.313397	4.066945
152	1	0	4.745275	7.942209	1.618839
153	1	0	3.441443	7.355440	2.705698
154	1	0	4.340526	8.834935	3.125115
155	1	0	13.595124	-2.653647	-0.020295
156	1	0	12.497904	-1.398315	-0.648580
157	1	0	12.265518	-2.077811	1.014465
158	1	0	12.852065	-4.982864	0.356307
159	1	0	11.239631	-5.570095	-0.129118
160	1	0	11.402555	-4.495608	1.300572
161	1	0	11.598370	-4.600836	-2.513423
162	1	0	11.980223	-2.857304	-2.713131
163	1	0	13.205591	-3.990616	-2.047030
164	1	0	6.292057	-8.342371	-5.016233
165	1	0	5.996575	-6.583398	-5.237893
166	1	0	7.430805	-7.157968	-4.322832
167	1	0	5.970037	-9.403638	-2.639114
168	1	0	5.469893	-8.350243	-1.271707
169	1	0	7.117996	-8.215851	-1.972451

170	1	0	3.622237	-7.076108	-4.365671
171	1	0	4.053517	-8.772579	-4.040537
172	1	0	3.398264	-7.780068	-2.711648
173	1	0	-1.722266	-2.872334	-0.287094
174	1	0	-3.552248	-4.255570	-0.703094
175	1	0	-6.200565	-0.990809	-0.333714
176	1	0	-6.154862	1.145121	0.217849
177	1	0	-3.342887	4.246871	0.749970
178	1	0	-1.580585	2.765438	0.417182
179	1	0	-6.365319	8.419459	0.290453
180	1	0	-6.665969	6.353035	1.473060
181	1	0	-4.949582	4.189022	-1.751804
182	1	0	-4.020940	4.662815	-3.901066
183	1	0	-3.193137	5.639680	-5.986318
184	1	0	-3.310019	8.045726	-6.340443
185	1	0	-4.227228	9.502304	-4.677857
186	1	0	-6.600560	9.841953	-1.717426
187	1	0	-4.983741	10.018508	-0.956465
188	1	0	-5.482162	11.906859	-2.413944
189	1	0	-4.083723	11.012803	-3.059994
190	1	0	-5.738254	10.851688	-3.824110
191	1	0	-7.637952	-2.683628	1.396853
192	1	0	-9.862201	-1.671723	1.225566
193	1	0	-10.967199	-1.489804	-0.939983
194	1	0	-9.881690	-2.319530	-2.959317
195	1	0	-7.261309	3.042570	-1.712468
196	1	0	-9.549692	2.178548	-1.844815
197	1	0	-10.900852	1.960974	0.172667
198	1	0	-9.999264	2.605516	2.344267
199	1	0	-6.970027	-3.950445	-4.830903
200	1	0	-8.668660	-4.121481	-4.307716
201	1	0	-7.939399	-2.479670	-4.557843
202	1	0	-7.221833	3.938842	4.614394
203	1	0	-8.840004	4.234197	3.922045
204	1	0	-8.230540	2.541566	4.153813
205	1	0	-5.408725	-9.059053	5.041700
206	1	0	-4.514010	-7.547539	6.724495
207	1	0	-4.154707	-5.191727	6.220950
208	1	0	-4.688907	-4.301636	4.004736
209	1	0	-5.378810	-3.953477	1.742851
210	1	0	-6.967366	-6.197518	-1.481844
211	1	0	-6.960323	-8.165018	-0.174806
212	1	0	-5.410304	-10.034405	2.786320
213	1	0	-7.078547	-9.659154	3.335814

214	1	0	-7.073674	-11.275077	1.500003
215	1	0	-7.899871	-9.783924	0.987645
216	1	0	-6.200027	-10.157190	0.423612

Table S8. Cartesian coordinates of **PhCzBN-2IsCz** at the optimized S_1 geometry.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.284425	-0.631805	1.026702
2	6	0	0.103599	-0.625509	1.033751
3	6	0	0.810344	0.001409	-0.000648
4	6	0	0.100547	0.626530	-1.033994
5	6	0	-1.287522	0.629109	-1.025050
6	6	0	-2.016686	-0.002493	0.001213
7	6	0	-3.485905	-0.004746	0.002180
8	6	0	-4.208374	-1.067263	0.564684
9	6	0	-5.612660	-1.028059	0.645527
10	6	0	-6.371502	-0.009310	0.003418
11	6	0	-5.616037	1.011239	-0.639851
12	6	0	-4.212564	1.056071	-0.560101
13	7	0	-6.315919	2.018634	-1.311199
14	7	0	-6.308173	-2.038167	1.316100
15	6	0	-7.711109	2.166783	-1.179123
16	6	0	-8.129497	3.345592	-1.814648
17	6	0	-6.948476	3.931266	-2.420119
18	6	0	-5.847861	3.071479	-2.129516
19	6	0	-5.837134	-3.093858	2.129646
20	6	0	-6.933833	-3.953041	2.422109
21	6	0	-8.117649	-3.368155	1.822834
22	6	0	-7.703454	-2.187593	1.187438
23	5	0	-7.908079	-0.010853	0.005086
24	6	0	-8.569337	1.254093	-0.552913
25	6	0	-9.931309	1.644923	-0.546216
26	6	0	-10.399840	2.825879	-1.143177
27	6	0	-9.485956	3.680234	-1.793130
28	6	0	-6.764645	5.057455	-3.211459
29	6	0	-5.505186	5.353225	-3.759561
30	6	0	-4.452390	4.457361	-3.509802
31	6	0	-4.606670	3.317972	-2.716437
32	6	0	-9.473843	-3.704611	1.805261
33	6	0	-10.391602	-2.850746	1.159580

34	6	0	-9.927399	-1.668846	0.562492
35	6	0	-8.565239	-1.275980	0.564782
36	6	0	-4.590718	-3.342886	2.711841
37	6	0	-4.438687	-4.481277	3.498520
38	6	0	-5.493706	-5.382195	3.751071
39	6	0	-6.750806	-5.086940	3.211077
40	6	0	-11.878193	-3.237032	1.144304
41	6	0	-12.044106	-4.599486	0.436602
42	6	0	-12.390813	-3.347083	2.597027
43	6	0	-12.749260	-2.205338	0.407654
44	6	0	-5.235978	-6.620724	4.617490
45	6	0	-4.762662	-6.177372	6.019340
46	6	0	-6.495400	-7.485860	4.785923
47	6	0	-4.140492	-7.484789	3.954948
48	6	0	-11.887022	3.209307	-1.123091
49	6	0	-12.753486	2.177084	-0.381756
50	6	0	-12.052811	4.572559	-0.416824
51	6	0	-12.404974	3.316247	-2.574185
52	6	0	-5.334131	6.609973	-4.621700
53	6	0	-6.276674	6.524768	-5.842405
54	6	0	-5.695255	7.854013	-3.780400
55	6	0	-3.894844	6.777214	-5.134880
56	7	0	2.223182	0.003193	-0.001585
57	6	0	3.040751	1.127253	-0.174065
58	6	0	4.394893	0.720296	-0.112777
59	6	0	4.396761	-0.708564	0.107600
60	6	0	3.043692	-1.118850	0.170156
61	6	0	2.699663	2.472412	-0.340843
62	6	0	3.732054	3.393861	-0.463671
63	6	0	5.089888	3.006305	-0.418354
64	6	0	5.417039	1.664647	-0.244500
65	6	0	5.421355	-1.650390	0.238441
66	6	0	5.097648	-2.992830	0.412684
67	6	0	3.740814	-3.383726	0.459244
68	6	0	2.706051	-2.464835	0.337289
69	7	0	5.802044	-7.980145	-3.560752
70	6	0	5.921939	-7.184963	-2.426626
71	6	0	5.568911	-5.849585	-2.756905
72	6	0	5.194455	-5.853556	-4.155683
73	6	0	5.338918	-7.192893	-4.610434
74	6	0	6.308629	-7.529189	-1.130556
75	6	0	6.354744	-6.519096	-0.173882
76	6	0	6.016245	-5.187005	-0.479252
77	6	0	5.621836	-4.857298	-1.777092

78	6	0	4.754601	-4.867586	-5.043142
79	6	0	4.459591	-5.222385	-6.356790
80	6	0	4.599794	-6.551957	-6.788390
81	6	0	5.037928	-7.554538	-5.925284
82	6	0	5.942975	-9.423825	-3.591692
83	6	0	4.643559	-10.152891	-3.243653
84	7	0	7.172828	4.266513	-2.715685
85	6	0	8.106892	3.652106	-1.870887
86	6	0	6.030874	4.638671	-2.027168
87	6	0	6.160656	4.097277	-0.570567
88	6	0	7.578428	3.549461	-0.576616
89	7	0	7.186587	-4.246813	2.708135
90	6	0	8.118110	-3.630744	1.861753
91	6	0	6.044504	-4.621832	2.021390
92	6	0	6.171193	-4.081147	0.564250
93	6	0	7.587684	-3.530001	0.568133
94	6	0	8.347297	3.015346	0.442940
95	6	0	9.639972	2.554364	0.152492
96	6	0	10.145690	2.646725	-1.144372
97	6	0	9.386056	3.205982	-2.180579
98	6	0	8.353955	-2.994613	-0.452711
99	6	0	9.645955	-2.530514	-0.164227
100	6	0	10.153625	-2.621064	1.132001
101	6	0	9.396662	-3.181530	2.169505
102	6	0	7.384004	4.563747	-4.114422
103	6	0	7.400303	-4.542790	4.106754
104	8	0	5.113665	-5.242907	2.500844
105	8	0	5.097990	5.257908	-2.505029
106	7	0	5.788179	7.992786	3.557424
107	6	0	5.326961	7.204108	4.606880
108	6	0	5.184188	5.864876	4.151290
109	6	0	5.557689	5.862443	2.752253
110	6	0	5.908477	7.198576	2.422660
111	6	0	5.026342	7.564386	5.922190
112	6	0	4.590300	6.560548	6.784894
113	6	0	4.451782	5.231070	6.352458
114	6	0	4.746418	4.877629	5.038361
115	6	0	5.611482	4.870893	1.771729
116	6	0	6.004501	5.202091	0.473856
117	6	0	6.340765	6.534914	0.169175
118	6	0	6.293771	7.544282	1.126562
119	6	0	5.927154	9.436628	3.589337
120	6	0	4.626491	10.164181	3.242788
121	1	0	-1.811822	-1.088463	1.857838

122	1	0	0.650493	-1.081034	1.851682
123	1	0	0.645100	1.083627	-1.852612
124	1	0	-1.817193	1.084584	-1.855388
125	1	0	-3.671743	-1.941652	0.895073
126	1	0	-3.679290	1.932565	-0.890605
127	1	0	-10.634545	0.999077	-0.041166
128	1	0	-9.828397	4.586529	-2.280666
129	1	0	-7.613893	5.701606	-3.414727
130	1	0	-3.479968	4.631325	-3.951881
131	1	0	-3.773842	2.637191	-2.618259
132	1	0	-9.813184	-4.612284	2.292442
133	1	0	-10.633249	-1.023758	0.060087
134	1	0	-3.757443	-2.662923	2.611868
135	1	0	-3.465690	-4.662872	3.941627
136	1	0	-7.601975	-5.726503	3.409526
137	1	0	-13.098924	-4.895494	0.420053
138	1	0	-11.687247	-4.544549	-0.596490
139	1	0	-11.481987	-5.389235	0.942513
140	1	0	-13.450868	-3.624024	2.607609
141	1	0	-12.280759	-2.391532	3.119016
142	1	0	-11.841481	-4.103058	3.164730
143	1	0	-12.453262	-2.100657	-0.640664
144	1	0	-13.795070	-2.527260	0.427732
145	1	0	-12.695737	-1.218937	0.878677
146	1	0	-4.572906	-7.052554	6.650026
147	1	0	-3.838911	-5.594570	5.970461
148	1	0	-5.522865	-5.560613	6.508457
149	1	0	-6.260917	-8.360311	5.400286
150	1	0	-6.869713	-7.847008	3.822964
151	1	0	-7.300427	-6.937155	5.284640
152	1	0	-4.454830	-7.813923	2.959753
153	1	0	-3.202056	-6.934758	3.844572
154	1	0	-3.938697	-8.373644	4.562371
155	1	0	-13.799882	2.497237	-0.398398
156	1	0	-12.700126	1.190123	-0.851583
157	1	0	-12.453453	2.074355	0.665593
158	1	0	-13.108134	4.866461	-0.396838
159	1	0	-11.494171	5.362666	-0.926038
160	1	0	-11.692066	4.519923	0.615026
161	1	0	-11.859262	4.072547	-3.144956
162	1	0	-12.294953	2.360184	-3.095215
163	1	0	-13.465592	3.591049	-2.581245
164	1	0	-6.169429	7.417680	-6.467691
165	1	0	-6.041902	5.648021	-6.453695

166	1	0	-7.325188	6.451652	-5.541102
167	1	0	-5.585599	8.763355	-4.381119
168	1	0	-5.038485	7.937649	-2.909118
169	1	0	-6.726566	7.813382	-3.419428
170	1	0	-3.591330	5.940737	-5.772031
171	1	0	-3.822159	7.690837	-5.732445
172	1	0	-3.178455	6.861118	-4.311820
173	1	0	1.665146	2.793819	-0.367129
174	1	0	3.498654	4.441687	-0.608863
175	1	0	6.452505	1.349151	-0.204600
176	1	0	6.456013	-1.332358	0.197600
177	1	0	3.510113	-4.432116	0.604685
178	1	0	1.672355	-2.788796	0.364507
179	1	0	6.558631	-8.550259	-0.862865
180	1	0	6.642855	-6.775604	0.839404
181	1	0	5.341346	-3.836626	-2.014378
182	1	0	4.640124	-3.840876	-4.708363
183	1	0	4.113772	-4.467214	-7.055218
184	1	0	4.358608	-6.807334	-7.815710
185	1	0	5.135172	-8.579064	-6.268712
186	1	0	6.291578	-9.706788	-4.589641
187	1	0	6.740519	-9.698586	-2.894627
188	1	0	4.787907	-11.237351	-3.276589
189	1	0	4.307011	-9.878168	-2.240090
190	1	0	3.853320	-9.886597	-3.951131
191	1	0	7.950331	2.957637	1.451496
192	1	0	10.249073	2.125795	0.941450
193	1	0	11.147615	2.287386	-1.358041
194	1	0	9.786195	3.288604	-3.185263
195	1	0	7.955518	-2.938322	-1.460765
196	1	0	10.253012	-2.100952	-0.954220
197	1	0	11.155013	-2.259328	1.344143
198	1	0	9.798332	-3.262721	3.173695
199	1	0	6.486982	5.066408	-4.476975
200	1	0	8.250554	5.220940	-4.247975
201	1	0	7.546188	3.644011	-4.686402
202	1	0	6.504875	-5.047210	4.470801
203	1	0	8.268469	-5.198006	4.239506
204	1	0	7.561238	-3.622375	4.677995
205	1	0	5.122305	8.588814	6.266270
206	1	0	4.349449	6.814841	7.812561
207	1	0	4.107578	4.474894	7.050595
208	1	0	4.633252	3.850981	4.702948
209	1	0	5.332792	3.849619	2.008527

210	1	0	6.627891	6.792525	-0.844117
211	1	0	6.542089	8.565906	0.859416
212	1	0	6.276091	9.719331	4.587243
213	1	0	6.723810	9.713007	2.891896
214	1	0	4.769377	11.248813	3.276444
215	1	0	4.289603	9.889755	2.239256
216	1	0	3.837130	9.896266	3.950634
