Supporting Information

Triazole Functionalized 5,9-Dioxa-13*b*-boranaphtho[3,2,1-*de*]anthracene：A New Family of Multi-Stimuli Responsive Materials

Guoyun Meng,[a] Tai Peng,*[b] Yonggang Shi,[a] Haijun Li,[c] Xiang Wang,[c] Xiaodong Yin,[a] Deng-Tao Yang,*[c] Suning Wang [ac] and Nan Wang*[a]

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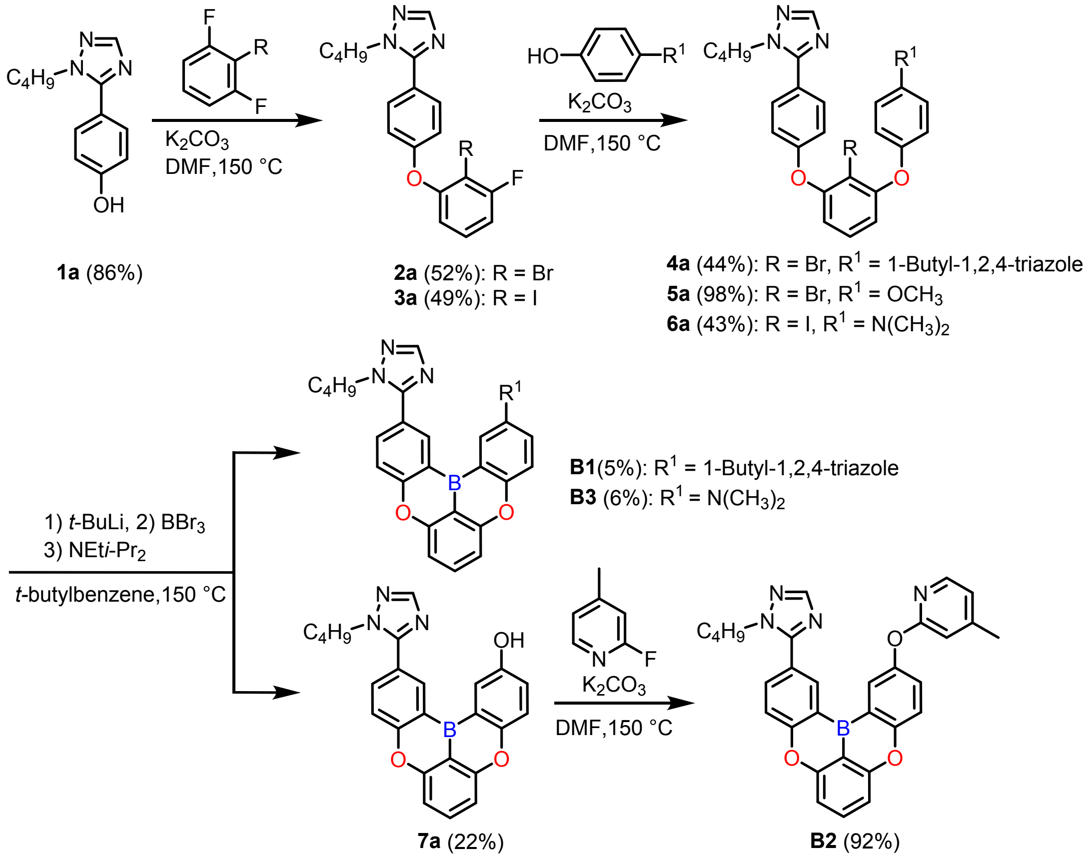
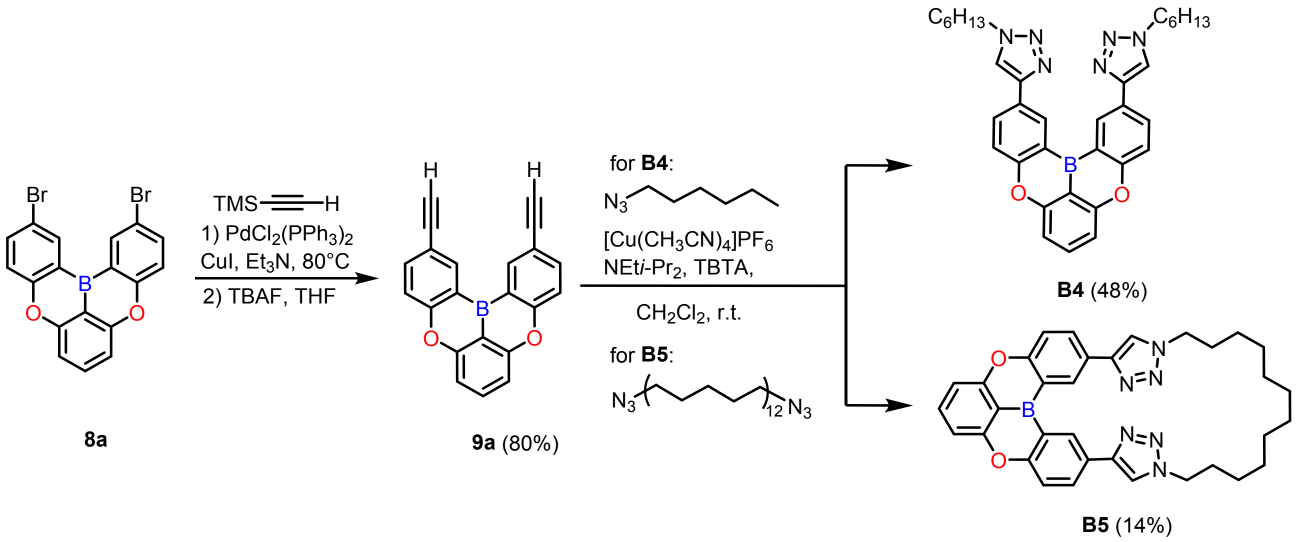
S1 General Information



Scheme S1. Synthetic routes of **B1–B3**.



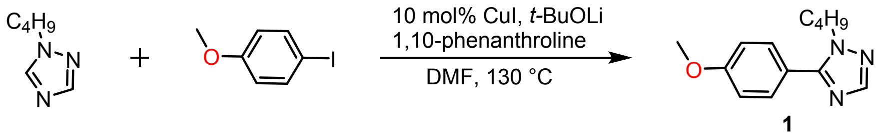
Scheme S2. Synthetic routes of **B4–B5**.

All reactions and operations were carried out using standard Schlenk techniques using dried and degassed solvents under an inert N_2 atmosphere. The precursors **1a** and **8a** were synthesized by the literature procedure. ^1H, ^{13}C and ^{11}B NMR spectra were recorded on a Bruker Avance 400 MHz, 500 MHz or 700 MHz spectrometer. UV-visible absorption spectra were obtained on an Agilent Cary 300 UV-Vis spectrophotometer. Fluorescence spectra were recorded on an Edinburgh Instruments FLS980 spectrophotometer. Fluorescent quantum efficiencies were determined using a Hamamatsu Quantaurus-QY spectrometer (C11347). High-resolution mass spectra (HRMS) were obtained from an Agilent Q-TOF 6520 LC-MS spectrometer. The powder X-ray diffraction (PXRD) patterns were recorded on a Bruker D8 Advance diffractometer. Cyclic voltammetry and differential pulsed voltammetry were conducted on an AUTOLAB-CV-75W analyzer with a scan rate of 100 mV s^{-1}. The electrochemical cell was a standard three-compartment cell composed of a Pt working electrode, a Pt auxiliary electrode, and a Pt wire reference electrode. All measurements were performed in anhydrous and nitrogen-saturated CH_2Cl_2 / THF solutions with 0.10 M of NBu_4NPF_6 as the supporting electrolyte and 2.0 mM investigated compounds. The oxidation and reduction potentials are based on values measured from differential pulsed voltammetry and are reported relative to a ferrocene/ferrocenium (Fc/Fc^+) redox couple used as a standard.

Density Functional Theory (DFT) Calculations. TD-DFT calculations were carried out using the Gaussian 09 software24[1] at the High Performance Computing Virtual Laboratory (HPCVL) at Queen's University. All computations were performed at the B3LYP level of theory using 6-31G(d) as the basis set for all atoms.[2,3]

X-ray Crystallography. Single-crystal X-ray diffraction data were recorded on a Bruker D8 Venture X-ray single-crystal diffractometer using Mo Kα radiation (λ = 0.71073 Å) at 180 K for all compounds. Data were processed on a PC with the aid of the Bruker SHELXTL software package and corrected for absorption effects. All non-hydrogen atoms were refined anisotropically. The positions of hydrogen atoms were calculated and refined isotropically. CCDC 1967670 (**B1**), 1967673 (**B2**), and 1967674 (**B3**) contain the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.

Synthesis of compound 1



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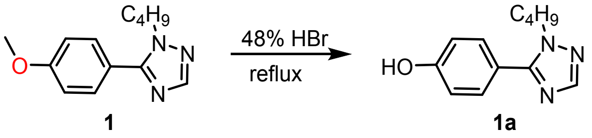
To a 50 mL Schlenk flask with a stir bar was added CuI (47.4 mg, 0.25mmol), 1-iodo-4-methoxybenzene (1.0 g, 4.3 mmol), 1,10-phenanthroline (45 mg, 0.025 mmol), 1-butyl-1,2,4-

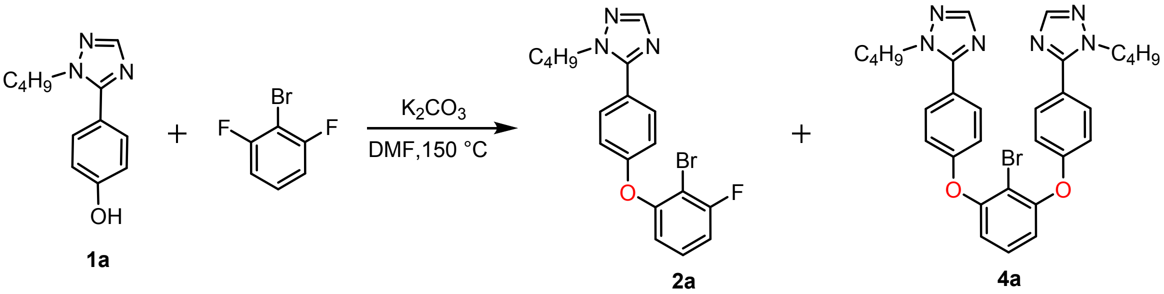
triazole (0.26 g, 2.1 mmol), *t*-BuOLi (0.5 g, 6.2 mmol), and DMF (15 mL). The resulting mixture were heated at 130 °C for 5 h. After the solvent was removed under reduced pressure, the reaction mixture was purified by flash chromatography on silica gel with petroleum ether / ethyl acetate (2:1, v/v) as eluent, and give **1** as colorless oil (0.38 g, 79%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.92 (s, 1H), 7.55 (d, *J* = 8.7 Hz, 2H), 7.01 (d, *J* = 8.7 Hz, 2H), 4.19 (t, *J* = 7.4 Hz, 2H), 3.87 (s, 3H), 1.90–1.83 (m, 2H), 1.35–1.26 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H).

Synthesis of compound 1a



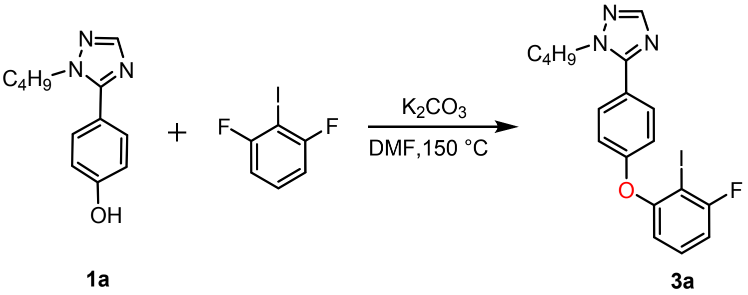
In a 50 mL flask, equipped with a stir bar, reflux condenser, and N_2 gas inlet, were placed **1** (1.16 g, 5 mmol) and 25 mL of 48% hydrobromic acid. The resulting mixture was heated to 130 °C for 24 h, and then the solution was cooled to room temperature and poured into 500 mL of vigorously stirred distilled water to afford a light brown solid (0.94 g, 86%). ^{1}H NMR (400 MHz, $CDCl_3$, δ): 10.59 (s, 1H), 7.98 (s, 1H), 7.33 (d, *J* = 8.6 Hz, 2H), 6.78 (d, *J* = 8.6 Hz, 2H), 4.17 (t, *J* = 7.4 Hz, 2H), 1.90–1.83 (m, 2H), 1.34–1.25 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, δ): 159.7, 154.9, 149.7, 130.3, 117.7, 116.4, 49.1, 32.0, 19.8, 13.6.

Synthesis of compound 2a and 4a



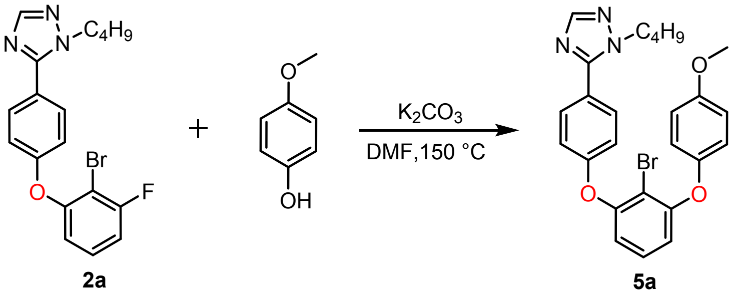
DMF (5 mL) was added to a mixture of 2-bromo-1,3-difluorobenzene (0.17 g, 0.89 mmol), K_2CO_3 (0.49 g, 3.56 mmol) and **1a** (0.43 g, 1.99 mmol) at room temperature under a nitrogen atmosphere. The reaction mixture was stirred at 160 °C for 24 h, and then cooled to room temperature. After addition of CH_2Cl_2 and water, the organic layer was washed with water twice, and then condensed in vacuo. The reaction mixture was purified by flash chromatography on silica gel with CH_2Cl_2 / ethyl acetate (1:1, v/v) as eluent to give **4a** (0.23 g, 44%) and **2a** (0.18 g, 52%) as colorless oil. Compound **4a:** ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.95 (s, 2H), 7.66–7.59 (m, 4H), 7.32 (t, *J* = 8.2 Hz, 1H), 7.17–7.09 (m, 4H), 6.91 (d, *J* = 8.2 Hz, 2H), 4.21 (t, *J* = 7.4 Hz, 4H), 1.93–1.85 (m, 4H), 1.37–1.27 (m, 4H), 0.90 (t, *J* = 7.4 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$, δ): 158.3, 154.9, 154.1, 151.0, 130.7, 129.1, 123.6, 118.3, 117.0, 109.4, 49.2, 32.2, 19.9, 13. 7; Compound **2a:** ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.94 (s, 1H), 7.63–7.58 (m, 2H), 7.11–7.06 (m, 2H), 7.00 (d, *J* = 8.2, 1H), 6.85 (d, *J* = 8.3, 1H), 4.20 (t, *J* = 7.4 Hz, 2H), 1.92–1.84 (m, 2H), 1.36–1.27 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H).

Synthesis of compound 3a



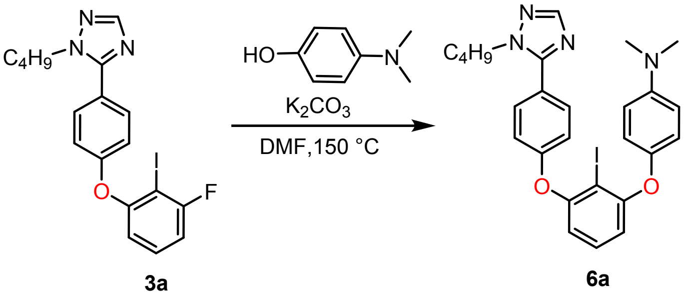
Compound **3a** was synthesized using the same procedure as that for compound **4a**, and obtained as colorless oil in 49% yield. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.95 (s, 1H), 7.64–7.58 (m, 2H), 7.31 (td, *J* = 8.2, 6.4 Hz, 1H), 7.12–7.07 (m, 2H), 6.95–6.89 (m, 1H), 6.78 (d, *J* = 8.2 Hz, 1H), 4.21 (t, *J* = 7.6 Hz, 2H), 1.92–1.85 (m, 2H), 1.36–1.27 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, δ): 164.6, 162.1, 158.2, 157.6, 157.5, 154.1, 151.0, 130.8, 131.0, 130.6, 123.7, 118.6, 115.6, 115.6, 111.8, 111.5, 49.2, 32.2, 19.9, 13.7.

Synthesis of compound 5a



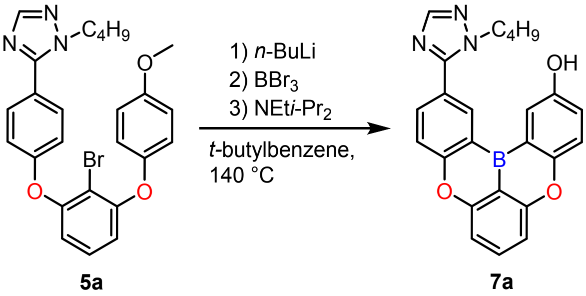
Compound **5a** was synthesized using the same procedure as that for compound **4a**, and obtained as colorless oil in 98% yield. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.04 (s, 1H), 7.66 (d, *J* = 7.9 Hz, 2H), 7.20 (t, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.92 (d, *J* = 7.9 Hz, 2H), 6.79 (d, *J* = 8.2 Hz, 1H), 6.66 (d, *J* = 8.2 Hz, 1H), 4.24 (t, *J* = 6.9 Hz, 2H), 3.82 (s, 3H), 1.94–1.87 (m, 2H), 1.38–1.28 (m, 2H), 0.91 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$, δ): 157.4, 156.6, 154.1, 153.8, 153.6, 149.6, 149.5, 130.8, 128.7, 120.9, 118.1, 115.6, 115.2, 114.1, 55.8, 49.5, 32.0, 19.9, 13.7.

Synthesis of compound 6a



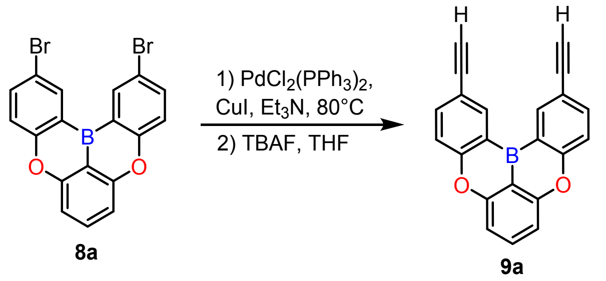
Compound **6a** was synthesized using the same procedure as that for compound **4a**, and obtained as white powder in 43% yield. ^{1}H NMR (400 MHz, CDCl$_3$, δ): 7.94 (s, 1H), 7.60 (d, J = 8.7 Hz, 2H), 7.18 (t, J = 8.2 Hz, 1H), 7.12 (d, J = 8.7 Hz, 2H), 7.00 (d, J = 9.1 Hz, 2H), 6.75 (d, J = 9.1 Hz, 2H), 6.67 (d, J = 8.1 Hz, 1H), 6.53 (d, J = 9.4 Hz, 1H), 4.21 (t, J = 7.4 Hz, 2H), 2.96 (s, 6H), 1.93–1.85 (m, 2H), 1.37–1.28 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, CDCl$_3$, δ): 160.7, 158.7, 157.3, 154.3, 151.0, 148.3, 146.9, 130.6, 130.0, 123.2, 121.2, 118.3, 114.1, 113.9, 112.4, 83.2, 49.2, 41.3, 32.2, 19.9, 13.7.

Synthesis of compound 7a



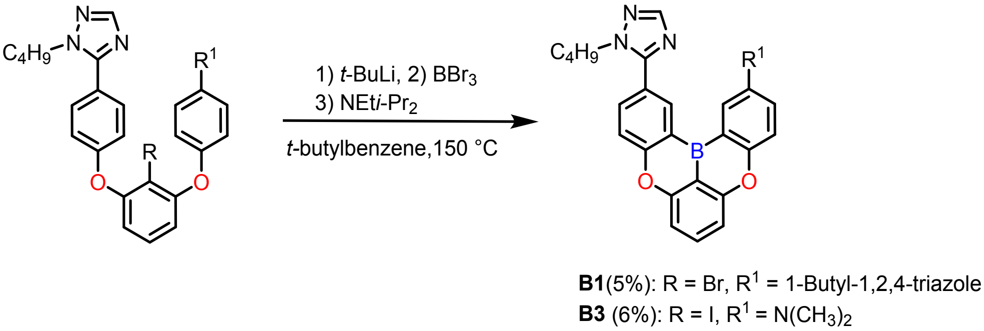
A solution of n-butyllithium in hexane (2.33 mL, 1.6 M, 1.36 mmol) was added slowly to compound **5a** (0.56 g, 1.13 mmol) in *t*-butylbenzene (10 mL) at –30 ºC under a nitrogen atmosphere. After the reaction mixture was stirred for 2 h, boron tribromide (0.21 mL, 2.26 mmol) was added at –30 ºC. After the reaction mixture was allowed to warm to room temperature, and stirred for 1 h, *N,N*-diisopropylethylamine (NEt*i*-Pr$_2$, 1.02 mL, 2.26 mmol) was added at 0 ºC. After stirring at 140 ºC for 24 h, sodium acetate aqueous solution was added at 0 ºC. The precipitate was separated by filtration, and the organic layer was washed with NH$_4$Cl aq. and brine. The crude product was purified by silica gel column chromatography using CH$_2$Cl$_2$ / ethyl acetate (5:1, v/v) as eluent to obtain the compound **7a** (0.1 g, 22% yield) as pale-yellow powder. ^{1}H NMR (400 MHz, CD$_2$Cl$_2$, δ): 8.36 (s, 1H), 8.09 (s, 1H), 7.67 (s, 1H), 7.60–7.56 (m, 2H), 7.22 (d, J = 8.4, 1H), 7.17 (d, J = 8.8, 1H), 7.09 (d, J = 8.9 Hz, 1H), 6.98–6.93 (m, 2H), 4.14 (t, J = 7.0 Hz, 2H), 1.85–1.79 (m, 2H), 1.29–1.20 (m, 2H), 0.84 (t, J = 7.3 Hz, 3H); ^{13}C NMR (101 MHz, CDCl$_3$, δ): 161.6, 157.6, 157.0, 154.7, 154.5, 152.6, 152.5, 149.9, 135.8, 134.6, 133.5, 123.5, 121.0, 119.3, 119.2, 118.9, 109.1, 108.0, 49.6, 32.2, 20.0, 13.6; ^{11}B NMR (225 MHz, $CDCl_3$, δ): 35.35; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{24}H_{21}BN_3O_3^+$, 410.1670; found, 410.1677; $[2M+H]^+$ calcd for $C_{48}H_{41}B_2N_6O_6^+$, 819.3268; found, 819.3283.

Synthesis of compound 9a



The compound **8a** was synthesized according to the literature method.[3] A 50 mL Schlenk flask was charged with compound **8a** (1.0 g, 2.34 mmol), trimethylsilylacetylene (1.5 mL, 10.76 mmol), $PdCl_2(PPh_3)_2$ (0.16 g, 0.23 mmol), PPh_3 (0.12 g, 0.47 mmol), CuI (67 mg, 0.35 mmol) and 20 mL of triethylamine. The mixture was stirred at 90 ºC for 24 h, the reaction was quenched with 1 M HCl and extracted with CH_2Cl_2, and then concentrated under reduced pressure. The solid was then purified using flash chromatography through silica using petroleum ether / CH_2Cl_2 (10:1, v/v) as eluent. The resulting white solid was dissolved in 10 mL of tetrahydrofuran and treated with tetrabutylammonium fluoride (TBAF) in THF (0.8 mL of a 1.0 M solution). After stirring overnight, the resulting mixture was concentrated under reduced pressure. After extraction with dichloromethane, the organic layer was dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The solid was then purified using flash chromatography through silica using petroleum ether / CH_2Cl_2 (20:1, v/v) as eluent. Yield, 0.2 g, 80%. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.69 (s, 2H), 7.78–7.74 (m, 3H), 7.43 (d, J = 8.7 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 3.19 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$, δ): 160.3, 157.1, 138.6, 137.2, 135.3, 118.9, 116.9, 109.0, 83.6.

Synthesis of compound B1 and B3

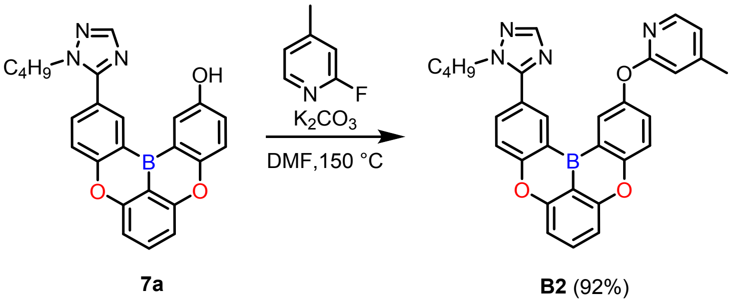


A solution of tert-butyllithium (1.3 M, 1.74 mmol) was added slowly to a solution of phenoxy derivatives (0.87 mmol) in tert-butylbenzene (10 mL) at –30 ºC under N_2 atmosphere. After stirring at –30 ºC for 2 h, BBr_3 (1.05 mmol) was added slowly at –30 ºC. Then the reaction mixture was allowed to warm to room temperature for 1 h. NEt*i*-Pr_2 (1.74 mmol) was added at 0 ºC. After stirring at 150 ºC for 24 h, sodium acetate aqueous solution was added at 0 ºC. The precipitate was separated by filtration, and the organic layer was washed with CH_2Cl_2 and brine. The crude product was purified by silica gel column chromatography using the appropriate solvents as the eluent.

B1. White solid (yield: 5%, using 5 : 1 of CH_2Cl_2 and ethyl acetate as the eluent). ^1H NMR (400 MHz, $CDCl_3$, δ): 8.02 (s, 2H), 7.84 (s, 2H), 7.63 (t, *J* = 8.1 Hz, 1H), 7.53 (d, *J* = 8.2 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.17 (d, *J* = 8.1 Hz, 2H), 4.05 (t, *J* = 7.3 Hz, 4H), 1.8–1.73 (m, 4H), 1.22–1.13 (m, 4H), 0.77 ppm (t, *J* = 7.3 Hz, 6H); ^{13}C NMR (176 MHz, $CDCl_3$, δ): 160.7, 157.1, 154.4, 149.5, 135.9, 131.8, 131.3, 119.8, 118.5, 109.9, 49.2, 31.8, 19.8, 13.5 ppm; ^{11}B NMR (225 MHz, $CDCl_3$, δ): −3.98 ppm; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{30}H_{30}BN_6O_2^+$, 517.2518; found, 517.2518; $[2M+H]^+$ calcd for $C_{60}H_{59}B_2N_{12}O_4^+$, 1033.4963; found, 1033.4976.

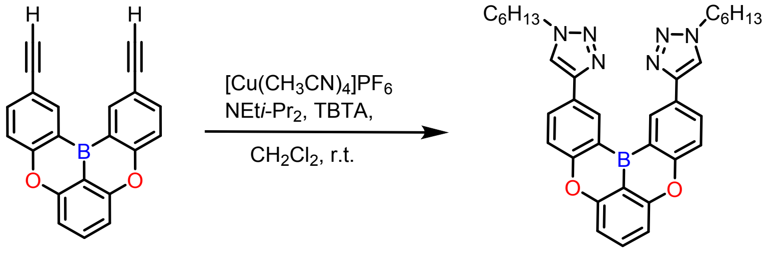
B3. Yellow solid (yield: 6%, using 50 : 1 of CH_2Cl_2 and methanol as the eluent). ^1H NMR (400 MHz, CD_2Cl_2, δ): 8.79 (s, 1H), 7.92 (s, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.80–7.76 (m, 2H), 7.63 (d, *J* = 8.6 Hz, 1H), 7.46 (d, *J* = 9.1 Hz, 1H), 7.28–7.20 (m, 3H), 4.29 (t, *J* = 7.2 Hz, 2H), 3.04 (s, 6H), 1.92–1.85 (m, 2H), 1.31–1.22 (m, 2H), 0.84 ppm (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, CD_2Cl_2, δ): 161.6, 158.0, 157.6, 154.7, 153.6, 150.8, 135.8, 134.5, 133.6, 122.5, 120.9, 119.2, 119.1, 109.4, 108.2, 49.6, 41.7, 32.3, 20.1, 13.6 ppm; ^{11}B NMR (225 MHz, CD_2Cl_2, δ): 37.60 ppm; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{26}H_{26}BN_4O_2^+$, 437.2143; found, 437.2159; $[2M+H]^+$ calcd for $C_{52}H_{51}B_2N_8O_4^+$, 873.4214; found, 873.4236.

Synthesis of compound B2



DMF (25 mL) was added to a mixture of 2-fluoro-4-methylpyridine (72 µL, 1.9 mmol), K_2CO_3 (0.16 g, 1.2 mmol) and 7a (0.24 g, 0.58 mmol) at room temperature under a N_2 atmosphere. The reaction mixture was stirred at 150 ºC for 24 h, and then cooled to room temperature. After addition of CH_2Cl_2 and water, the organic layer was washed with water twice, and then condensed in vacuo. The reaction mixture was purified by flash chromatography on silica gel with CH_2Cl_2 / methanol (100 : 1) as eluent to give B2 (0.38 g, 92%) as a white solid. ^1H NMR (400 MHz, CD_2Cl_2, δ): 7.91 (d, *J* = 4.7 Hz, 1H), 7.50 (t, *J* = 8.0 Hz, 1H), 7.38 (s, 1H), 7.32 (s, 1H), 7.26 (s, 1H), 7.21 (d, *J* = 8.7 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 1H), 7.07–7.00 (m, 3H), 6.86 (d, *J* = 4.6 Hz, 1H), 6.81 (s, 1H), 6.72 (d, *J* = 8.2 Hz, 1H), 3.77 (t, *J* = 7.2 Hz, 2H), 2.44 (s, 3H), 1.66–1.59 (m, 2H), 1.14–1.05 (m, 2H), 0.70 ppm (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (176 MHz, $CDCl_3$, δ): 165.1, 161.6, 157.7, 157.6, 155.5, 153.9, 151.6, 148.9, 147.4, 147.1, 137.3, 131.8, 130.8, 127.0, 123.1, 120.0, 118.5, 117.5, 116.5, 111.9, 110.0, 109.3, 49.9, 31.6, 21.3, 19.9, 13.4 ppm; ^{11}B NMR (225 MHz, $CDCl_3$, δ): −5.02 ppm; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{30}H_{26}BN_4O_3^+$, 501.2092; found, 501.2122; $[M+H]^+$ calcd for $C_{60}H_{51}B_2N_8O_6^+$, 1001.4112; found, 1001.4083.

Synthesis of compound B4

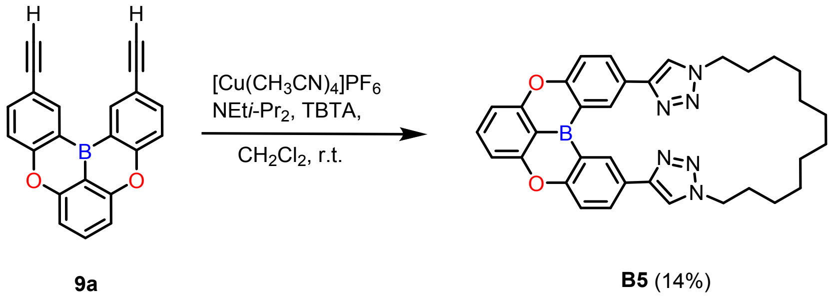


9a

B4 (48%)

To a Schlenk flask equipped with a magnetic stir bar was added **9a** (52 mg, 0.16 mmol), 1-azidohexane (67 mg, 0.51 mmol), NEt*i*-Pr$_2$ (0.11 mL, 0.64 mmol), tris[(1-benzyl-1H-1,2,3-triazol-4-yl) methyl]amine (1 mol %) and CH_2Cl_2 (10 mL). The resulting solution was bubbled with N_2 for 20 minutes. $[Cu(CH_3CN)_4]PF_6$ (1 mol %) was added as a catalyst. The resulting mixture was stirred overnight, after which the solvent was removed under reduced pressure. The crude product was dissolved in CH_2Cl_2 and washed with saturated NH_4Cl and brine. The organic layer was dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using CH_2Cl_2 / ethyl acetate (5 : 1) as eluent to give a pale yellow solid in 48% yield. ^{1}H NMR (400 MHz, $CDCl_3$, δ): 9.18 (s, 2H), 8.15 (dd, *J* = 8.7, 2.0 Hz, 2H), 7.94 (s, 2H), 7.79 (t, *J* = 8.2 Hz, 1H), 7.57 (d, *J* = 8.7 Hz, 2H), 7.22 (d, *J* = 8.2 Hz, 2H), 4.46 (d, *J* = 14.6 Hz, 4H), 2.06–1.98 (m, 4H), 1.45–1.32 (m, 12H), 0.90 ppm (t, *J* = 7.0 Hz, 6H); ^{13}C NMR (176 MHz, $CDCl_3$, δ): 160.4, 157.4, 147.5, 135.0, 131.7, 131.5, 125.6, 119.7, 119.1, 108.8, 50.7, 31.4, 30.5, 26.4, 22.6, 14.1 ppm; ^{11}B NMR (225 MHz, $CDCl_3$, δ): −3.32 ppm; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{34}H_{38}BN_6O_2^+$, 573.3144; found, 573.3151; $[2M+H]^+$ calcd for $C_{68}H_{75}B_2N_{12}O_4^+$, 1145.6215; found, 1145.6259.

Synthesis of compound B5



Prepared using the same procedure as compound **B4** except replacing 1-azidohexane with 1,12-diazidododecane (14% yield). ^{1}H NMR (400 MHz, CD_2Cl_2, δ): 9.24 (s, 2H), 8.22 (d, J = 8.7 Hz, 2H), 8.08 (s, 2H), 7.85 (t, J = 8.2 Hz, 1H), 7.63 (d, J = 8.6 Hz, 2H), 7.28 (d, J = 8.1 Hz, 2H), 4.48 (t, J = 6.9 Hz, 4H), 2.07–1.99 (m, 4H), 1.43–1.35 ppm (m, 16H); ^{13}C NMR (176 MHz, CD_2Cl_2, δ): 160.8, 157.7, 147.0, 135.5, 131.9, 120.5, 119.4, 109.1, 50.8, 30.2, 28.4, 28.4, 28.2, 26.0 ppm; ^{11}B NMR (225 MHz, CD_2Cl_2, δ): 39.15 ppm; HRMS (ESI) m/z: $[M+H]^+$ calcd for $C_{34}H_{36}BN_6O_2^+$, 571.2987; found, 571.2997.

S2 Photophysical and electrochemical properties

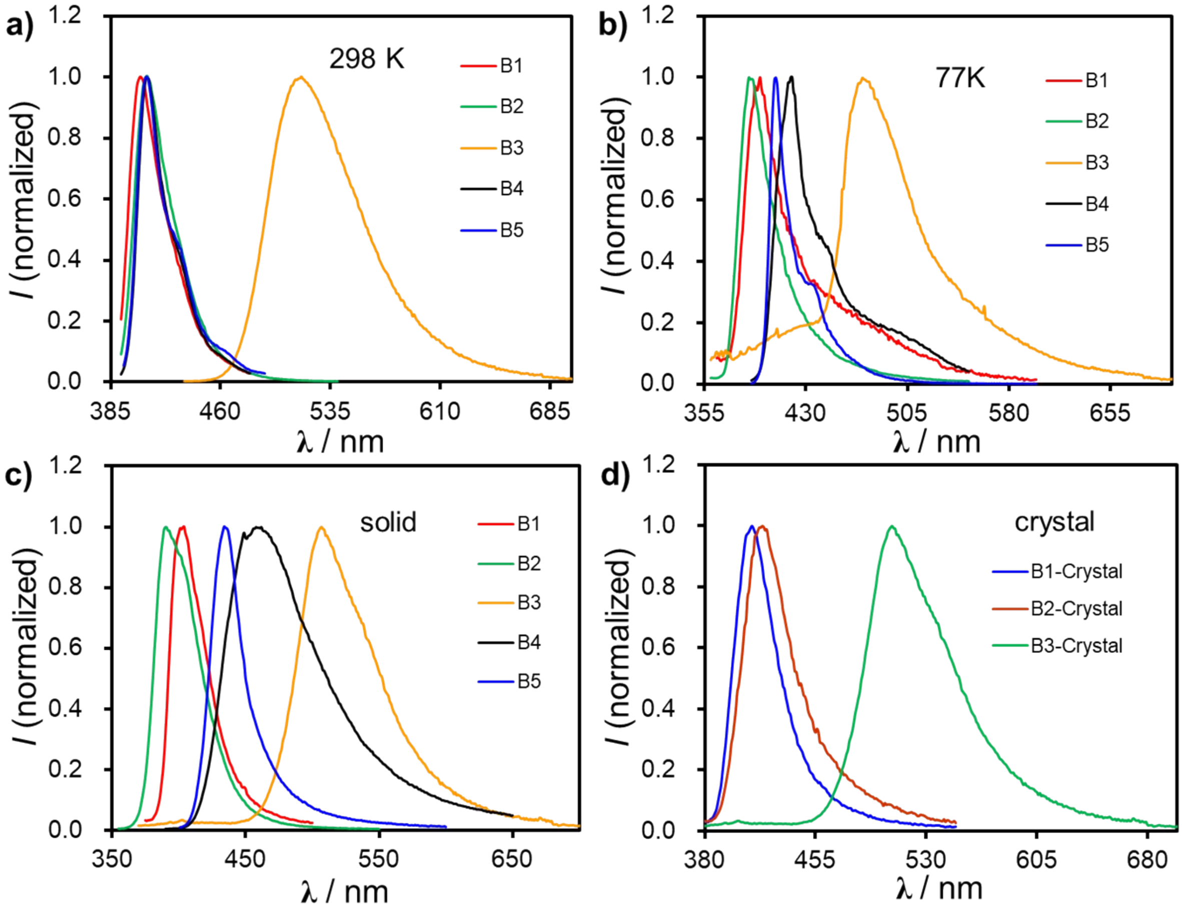


Fig. S1. Normalized emission spectra of **B1**–**B5** at a) 298 K in toluene solution, b) at 77 K in toluene matrix, c) as solid at 298 K and d) as crystal at 298 K.

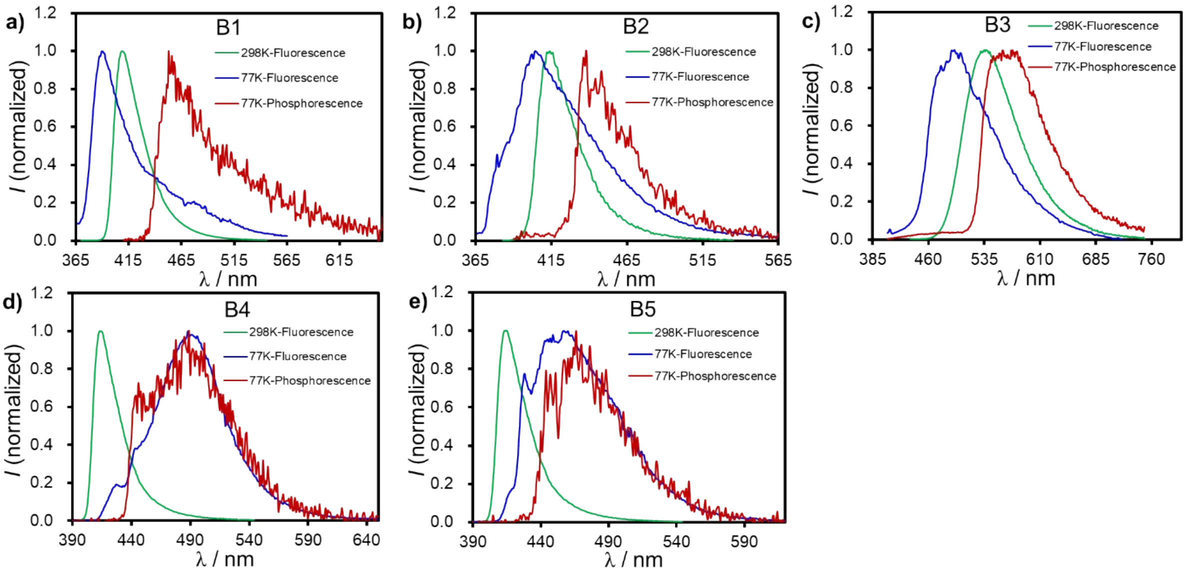


Fig. S2. Normalized fluorescence (298 K, 0.01 mM in CH_2Cl_2 and 77 K, 1 mM in CH_2Cl_2) and phosphorescence (77 K, 1 mM in CH_2Cl_2, 100 μs delay) spectra of **B1**–**B5**.

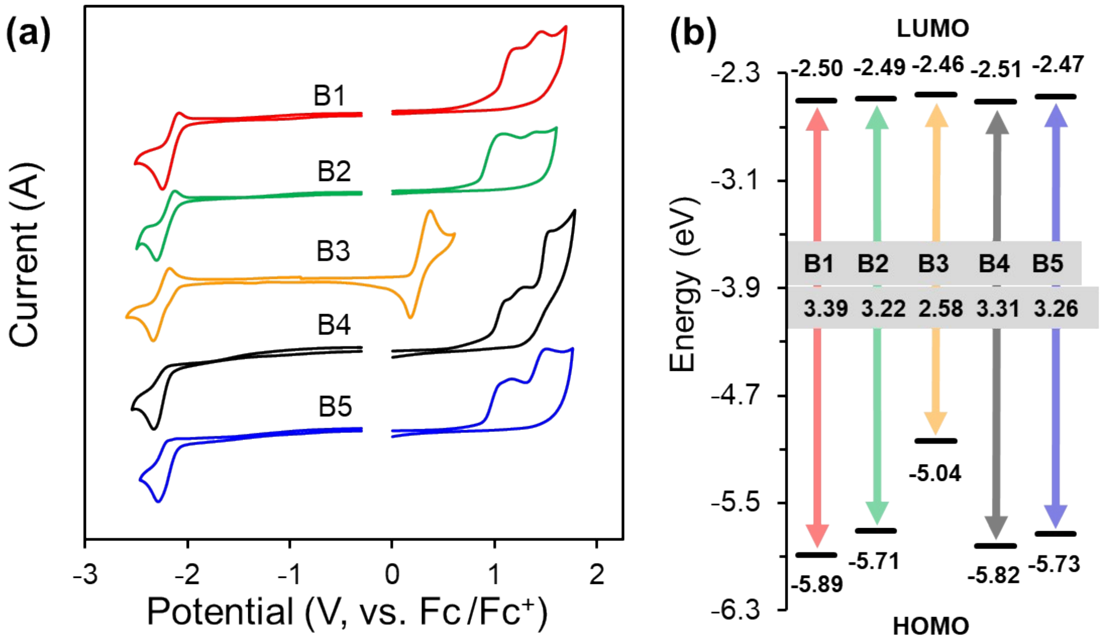


Fig. S3. a) Cyclic voltammogram (CV) diagrams of **B1**–**B5** showing the reduction (recorded in THF) and oxidation waves (recorded in CH_2Cl_2) using NBu_4NPF_6 (0.1 M) as the electrolyte with a scan rate = 100 mV s^{-1}, the reduction and oxidation waves of **B3** recorded in CH_2Cl_2; b) Experimental HOMO and LUMO energy levels (eV) obtained by differential pulse voltammetry (DPV).

Table S1. Photophysical properties of **B1−B5**.

compound	λ_{abs} a) (nm)	ε (M^{-1} cm^{-1})	λ_{em} a) (nm)	Φ_F b)	Stokes shift c) (10^3 cm^{-1})	τ_F d) (ns)	E_g e) (eV)	HOMO f)/LUMO g) (eV)
B1	390	11733	405	0.53	0.95	8.19	3.07	−5.89/−2.50
B2	391	16051	410	0.64	1.19	7.67	3.05	−5.71/−2.49
B3	430	5493	514	0.71	3.80	19.0	2.57	−5.04/−2.46
B4	398	16461	410	0.60	0.74	7.22	3.02	−5.82/−2.51
B5	398	9517	409	0.52	0.68	6.48	3.02	−5.73/−2.47

a) In toluene (0.01×10^{-3} M); b) Determined by an absolute quantum yields spectrometer; d) Stokes shift = $1/\lambda_{abs} - 1/\lambda_{em}$; d) Fluorescence lifetime measured at an emission maxima on excitation at 365 nm picosecond pulsed LED; e) Estimated from absorption edges of UV–vis spectra; f) Determined from the oxidation peaks in DPV diagrams recorded in CH_2Cl_2; g) Determined from the reduction peaks in DPV diagrams recorded in THF.

Table S2. Photophysical properties of **B1**–**B5** in CH_2Cl_2 under 77 K and 298 K.

Compound	T (K)	Fluorescence			Phosphorescence			
		λ_{em} a) [nm]	τ b) [ns]	E_S c) [eV]	λ_{em} d) [nm]	τ e) [s]	E_T c) [eV]	ΔE_{ST} c) [eV]
B1	298	409	8.7	3.03	–	–	–	0.21
	77	390	6.0	–	439	0.96	2.82	
B2	298	414	9.7	3.00	–	–	–	0.15
	77	405	8.9	–	435	0.67	2.85	
B3	298	535	11.2	2.32	–	–	–	0.11
	77	495	9.4	–	560	0.40	2.21	
B4	298	413	8.0	3.00	–	–	–	0.47
	77	491	270.4	–	490	2.70	2.53	
B5	298	413	8.0	3.00	–	–	–	0.34
	77	457	34.2	–	467	1.74	2.66	

a) Maximum wavelength of emission; b) Fluorescence lifetime measured with 365 nm picosecond pulsed LED; c) Singlet and triplet energies estimated from the emission maxima, $E_{S/T} = 1240/\lambda_{em,\,max}$, $\Delta E_{ST} = E_S - E_T$; d) Phosphorescence spectra were obtained at 77 K with a 100 μs delay time; e) Phosphorescence lifetime.

Table S3. Electrochemical data for compound **B1−B5**^{a} at 298 K

	$E_{red}^{CV,\,c}$ (V)	$E_{red}^{DPV,\,d}$ (V)	$E_{ox}^{CV,\,e}$ (V)	$E_{ox}^{DPV,\,f}$ (V)	E_{LUMO}^{g} (eV)	E_{HOMO}^{g} (eV)	E_g^{h} (eV)
B1	−2.24	−2.30	+1.17, +1.43	+1.09, +1.35	−2.50	−5.89	3.39
B2	−2.30	−2.31	+0.99, +1.33	+0.91, +1.22	−2.49	−5.71	3.22
B3^b	−2.33	−2.34	+0.27	+0.24	−2.46	−5.04	2.58
B4	−2.33	−2.29	+1.09, +1.25, +1.52	+1.02, +1.24	−2.51	−5.82	3.31
B5	−2.29	−2.33	+1.03, +1.11, +1.48	+0.93, +1.02	−2.47	−5.73	3.26

a) All potentials are relative to Fc/Fc^+ couple, oxidative scan in CH_2Cl_2 and reductive scan in THF, 0.1 M NBu_4NPF_6 as supporting electrolyte at room temperature; b) Redox peaks measured in CH_2Cl_2; c) Reduction potentials from cyclic voltammetry (CV), scan rate: 100 mV s^{-1}; d) Peak potentials determined by the reduction peak positions from differential pulse voltammetry

(DPV), scan rate: 50 mV s^{-1}; [e)] Oxidation potentials from CV, scan rate: 100 mV s^{-1}; [f)] Peak potentials determined by the first oxidation peak positions from DPV, scan rate: 50 mV s^{-1}; [g)] The HOMO and LUMO energy levels are obtained by DPV, $E_{\mathrm{LUMO}}/E_{\mathrm{HOMO}} = -(4.8 + E_{\mathrm{red}}^{\mathrm{DPV}}/E_{\mathrm{ox}}^{\mathrm{DPV}})$; [h)] The energy gap corresponds to the electrochemical energy gap, $E_g = E_{\mathrm{LUMO}} - E_{\mathrm{HOMO}}$.

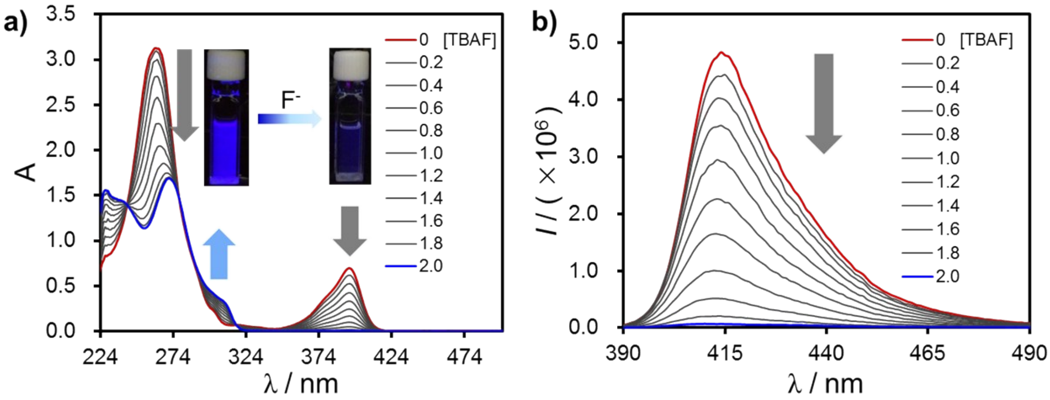


Fig. S4. a) UV-vis absorption and b) emission titrations of 5.0 x 10^{-5} M solution of **B4** in CH_2Cl_2 with TBAF. Photographs showing the emission colors of **B4** and **B4•F⁻** under irradiated with 365 nm UV light.

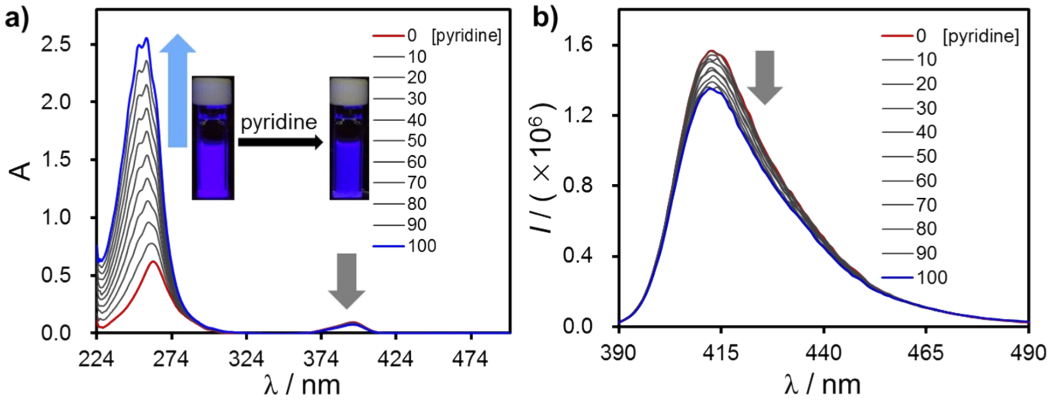


Fig. S5. a) UV-vis absorption and b) emission titrations of 1.0 x 10^{-5} M solution of **B4** in CH_2Cl_2 with pyridine. Photographs showing the emission colors of **B4** and **B4•Pyridine** under irradiated with 365 nm UV light.

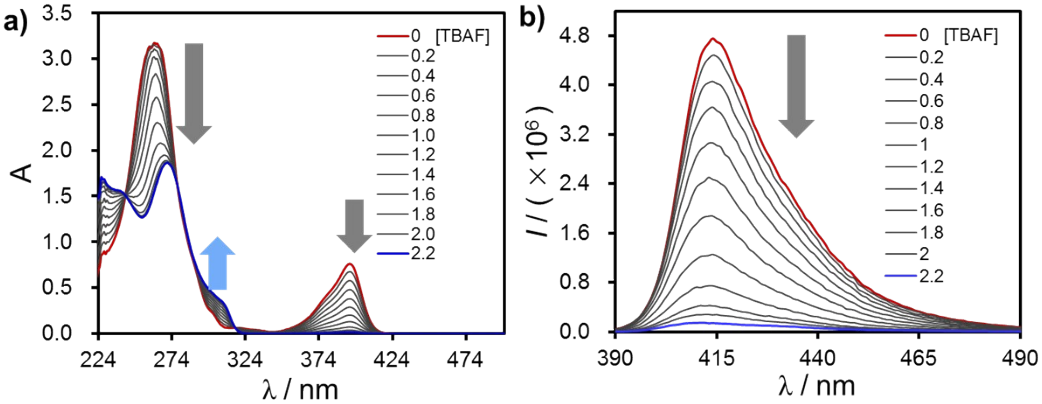


Fig. S6. a) The UV-vis absorption and b) emission titrations of 5.0 x 10^{-5} M solution of **B5** in CH_2Cl_2 with TBAF.

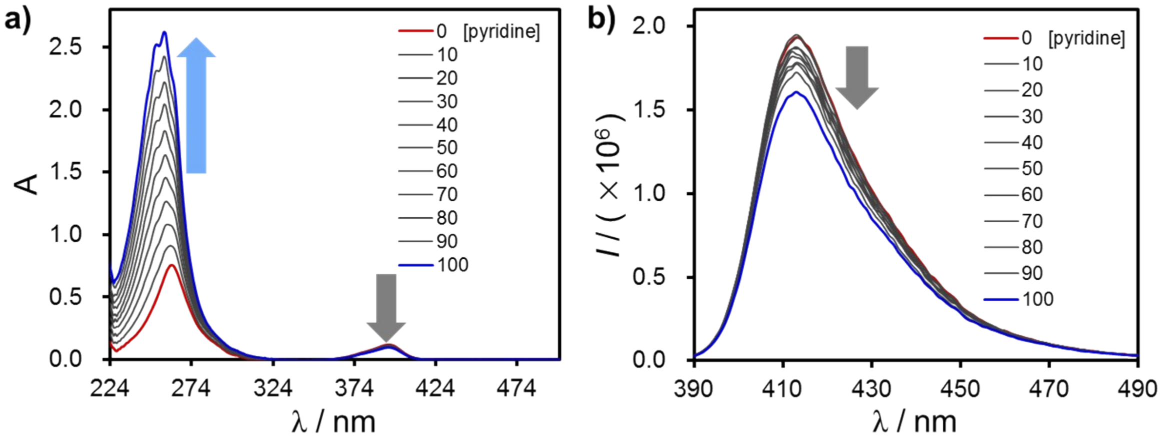


Fig. S7. a) UV-vis absorption and b) emission titrations of 1.0×10^{-5} M solution of **B5** in CH_2Cl_2 with pyridine.

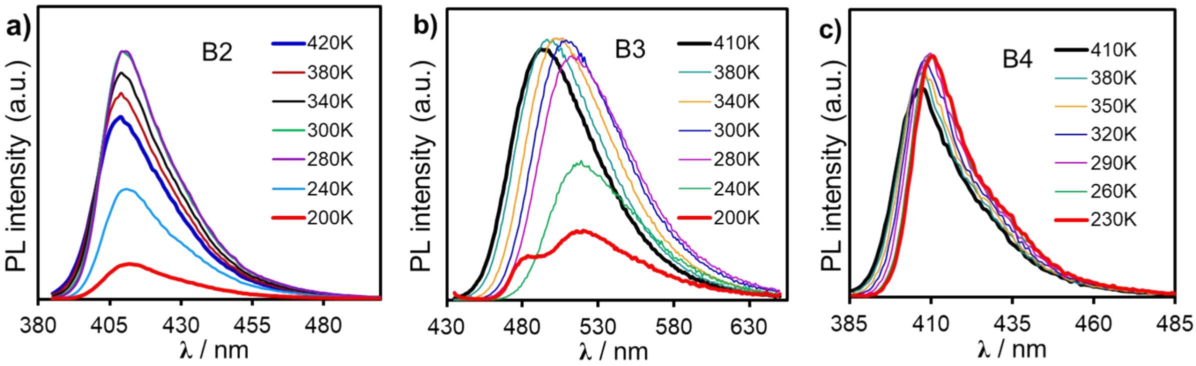


Fig. S8. Temperature-dependent fluorescence spectra of **B2** a), **B3** b) and **B4** c) in mesitylene (0.01 mM) under N_2.

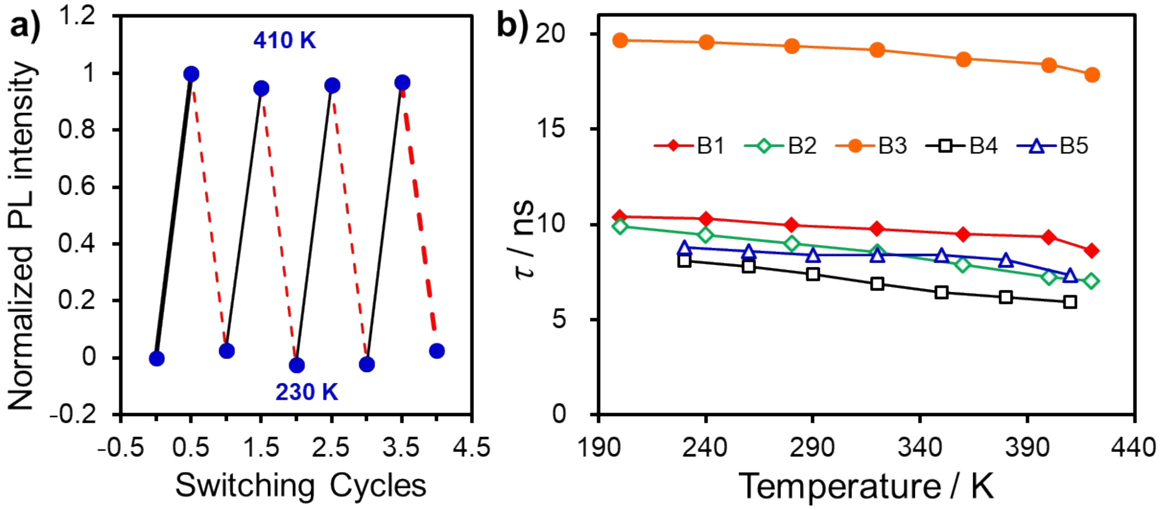


Fig. S9. a) Normalized fluorescence intensity of **B1** (blue circle) monitored at the emission maximum under the reversible emission tuning experiments in mesitylene solution. Black solid and red dashed lines denote that reversible cycling of **B1** emission between 230 K (at 408 nm) and 410 K (at 404 nm); b) The change of transient decay lifetime of **B1**, **B2**, **B3**, **B4** and **B5** in mesitylene solution (0.01 mM) between 200 K and 420 K.

S3 Temperature-dependent NMR Studies

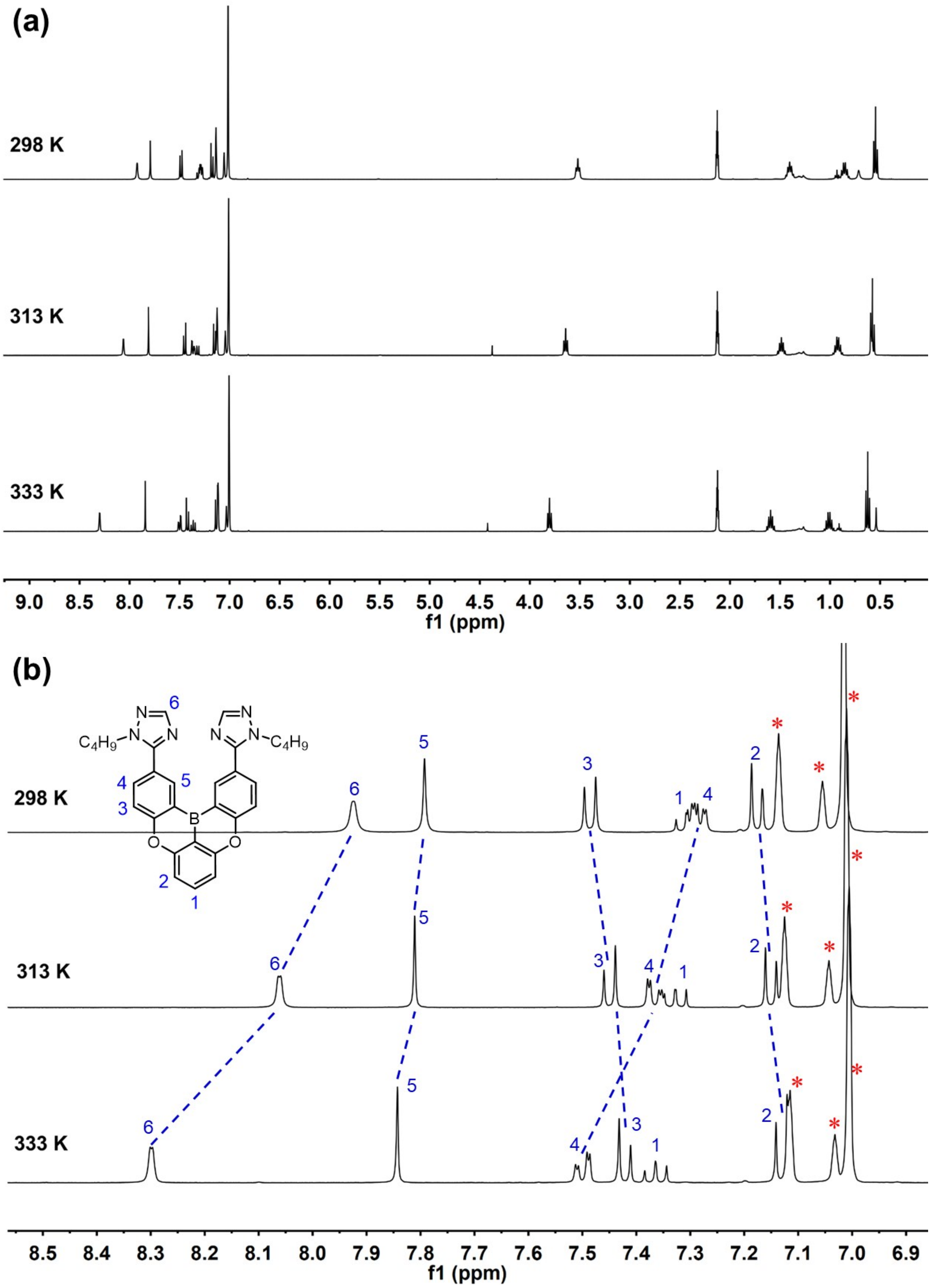


Fig. S10. Variable temperature ^{1}H NMR spectra of **B1** (400 MHz, toluene-d_8) between 298 K and 333 K: a) full and b) aromatic region, * denote the solvent residual signals.

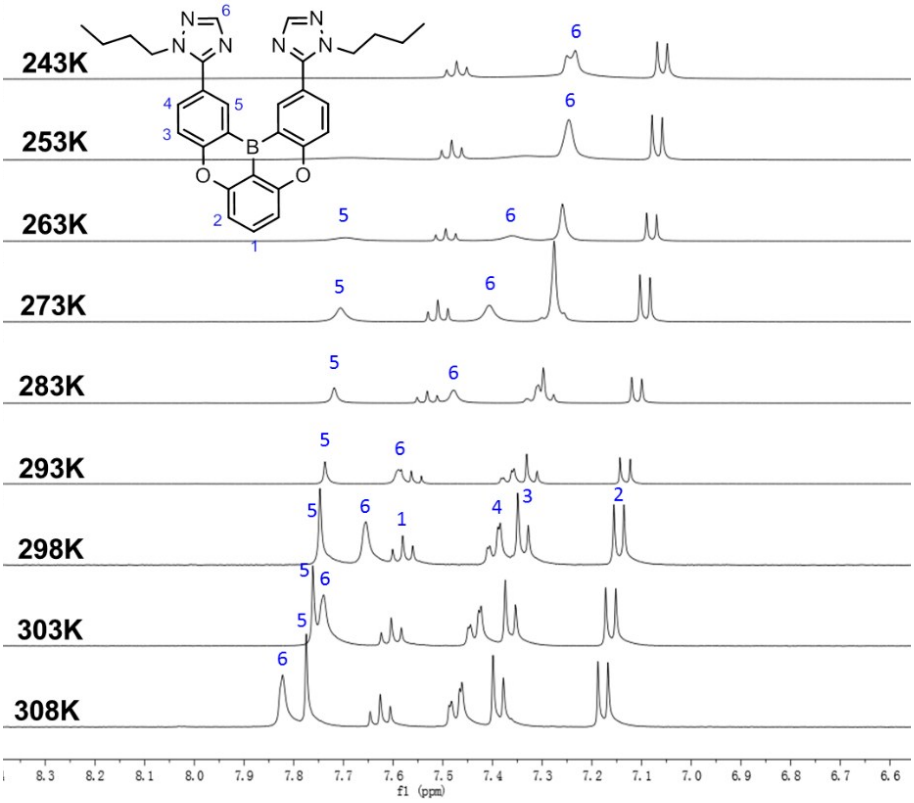


Fig. S11. Aromatic region of variable temperature ^{1}H NMR spectra of **B1** (500 MHz, CD_2Cl_2) between 243 K and 308 K.

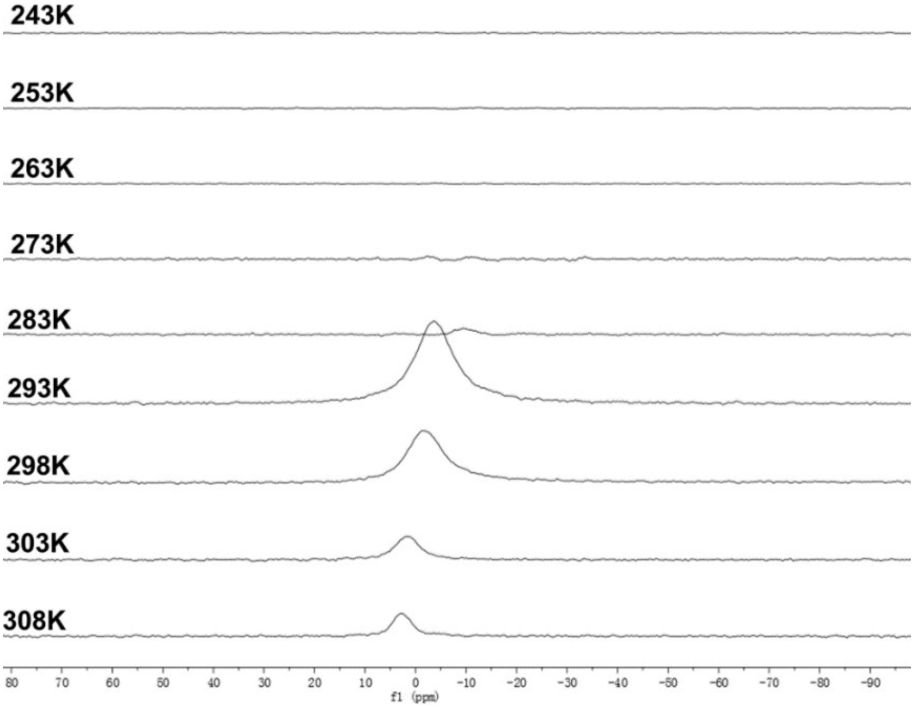


Fig. S12. Variable temperature ^{11}B NMR spectra of **B1** (161 MHz, CD_2Cl_2) between 243 K and 308 K.

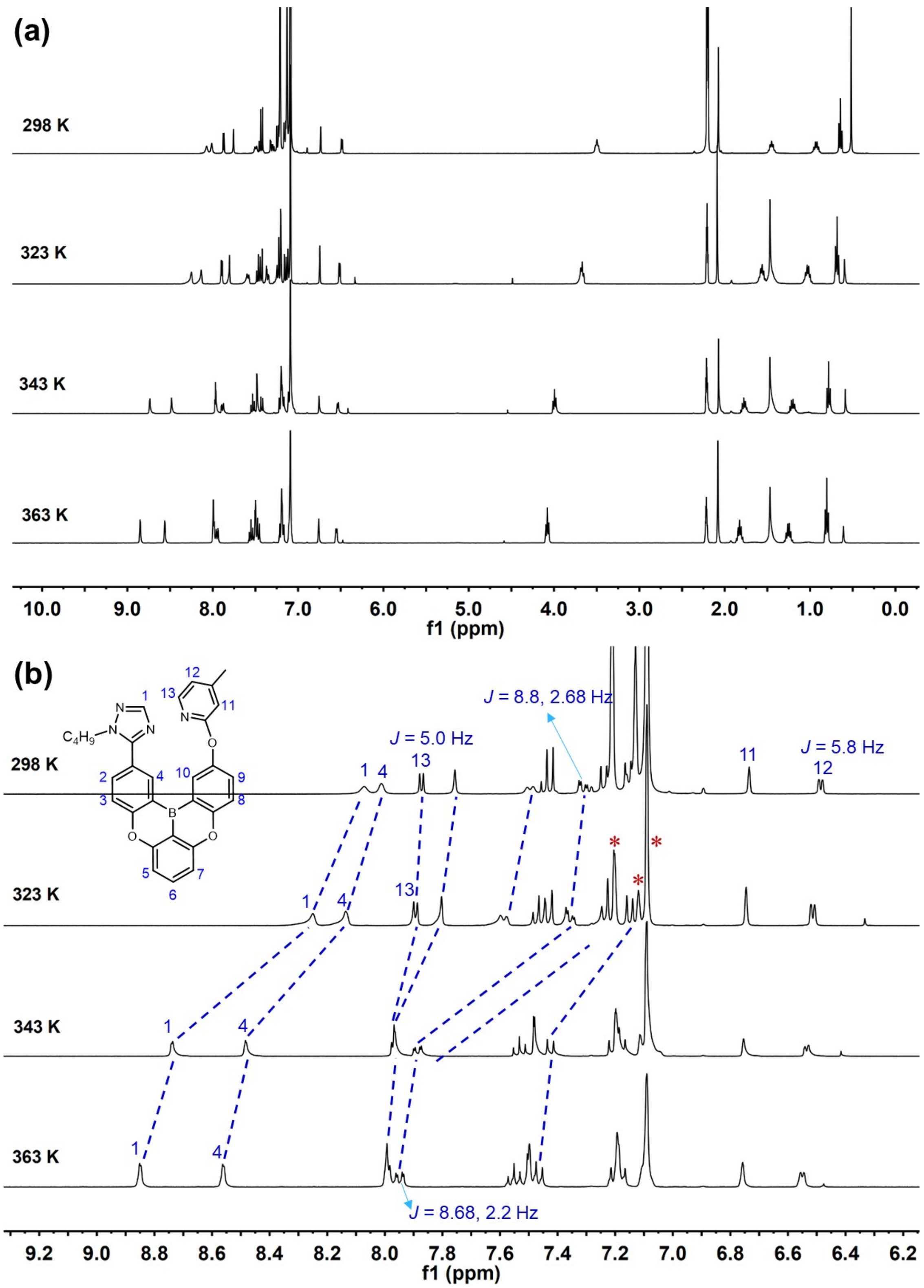


Fig. S13. Variable temperature ^{1}H NMR spectra of **B2** (400 MHz, toluene-d_8) between 298 K and 363 K: a) full and b) aromatic region, * denote the solvent residual signals.

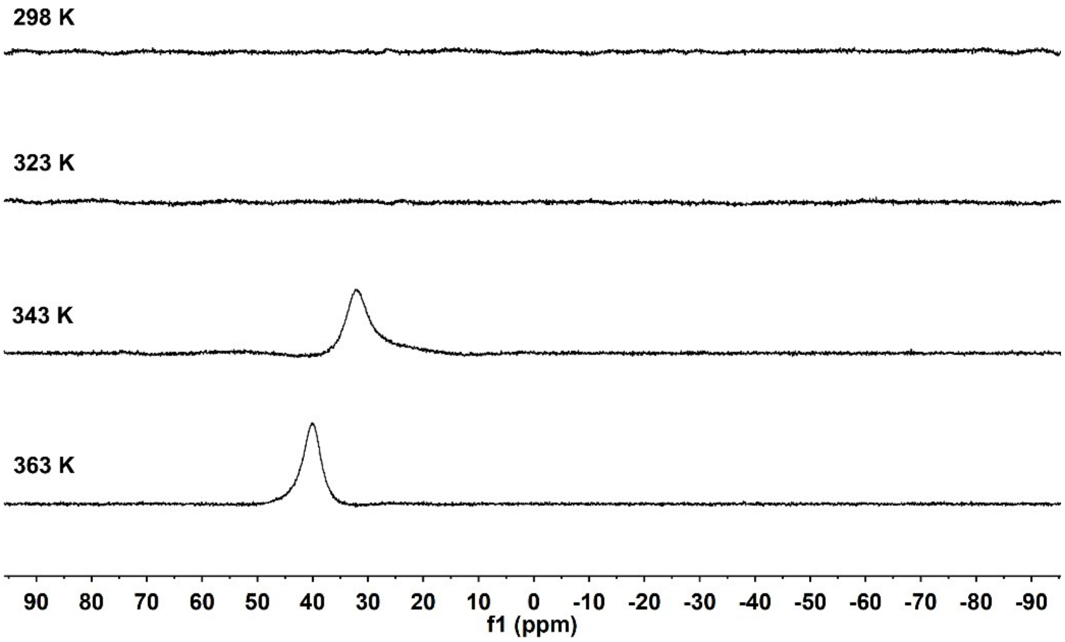


Fig. S14. Variable temperature ^{11}B NMR spectra of **B2** (128 MHz, toluene-d_8) between 298 K and 363 K.

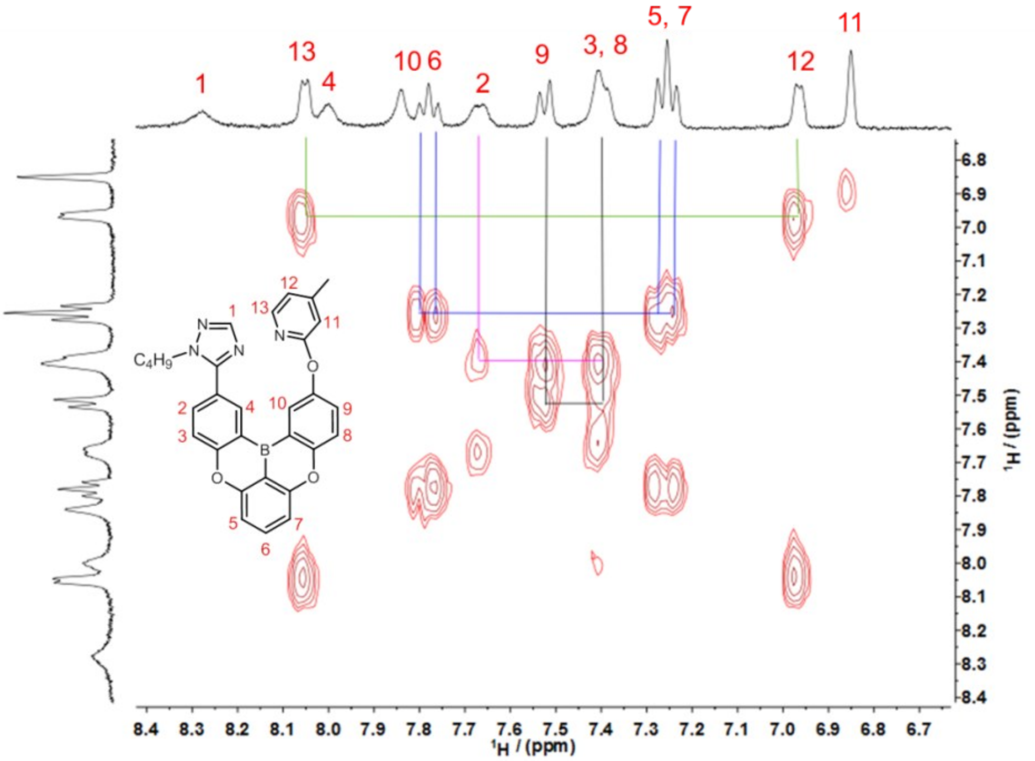


Fig. S15. The aromatic region of the COSY NMR spectrum of **B2** in CD_2Cl_2 with the 1D spectral assignment.

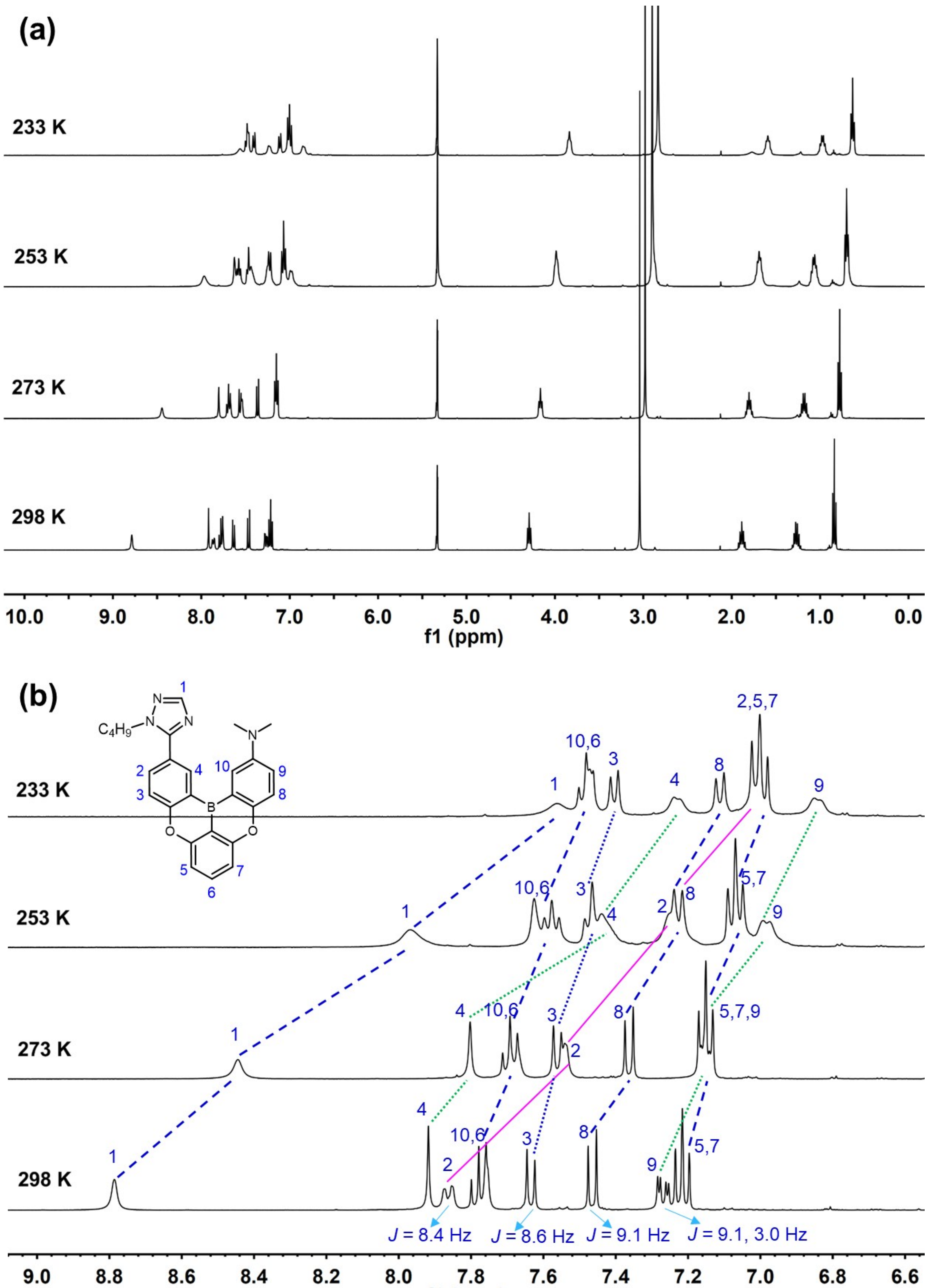


Fig. S16. Variable temperature ^{1}H NMR spectra of **B3** (400 MHz, CD_2Cl_2) between 233 K and 298 K: a) full and b) aromatic region.

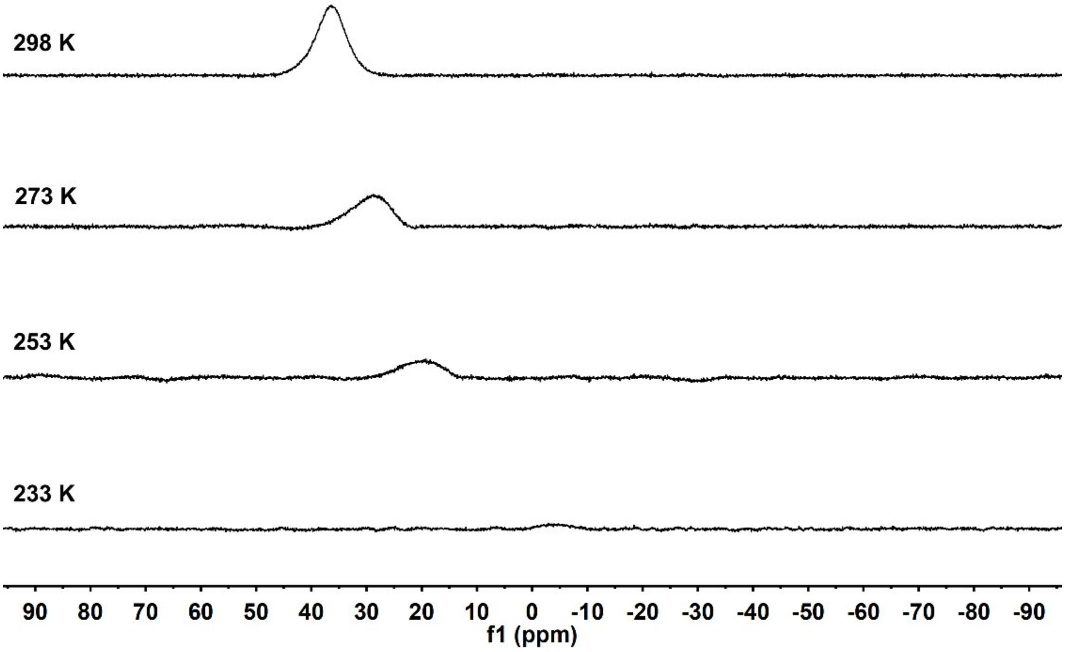


Fig. S17. Variable temperature ^{11}B NMR experiments for **B3** (128 MHz, CD_2Cl_2) between 233 K and 298 K.

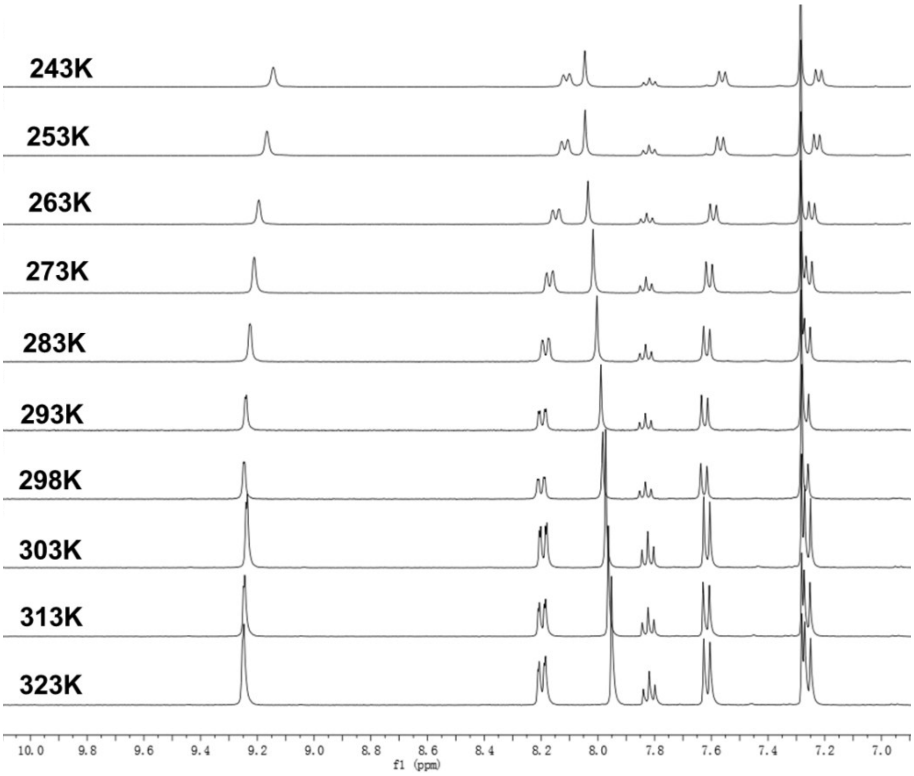


Fig. S18. Aromatic region of the variable temperature ^{1}H NMR experiments for **B4** (500 MHz, $CDCl_3$) between 243 K and 323 K.

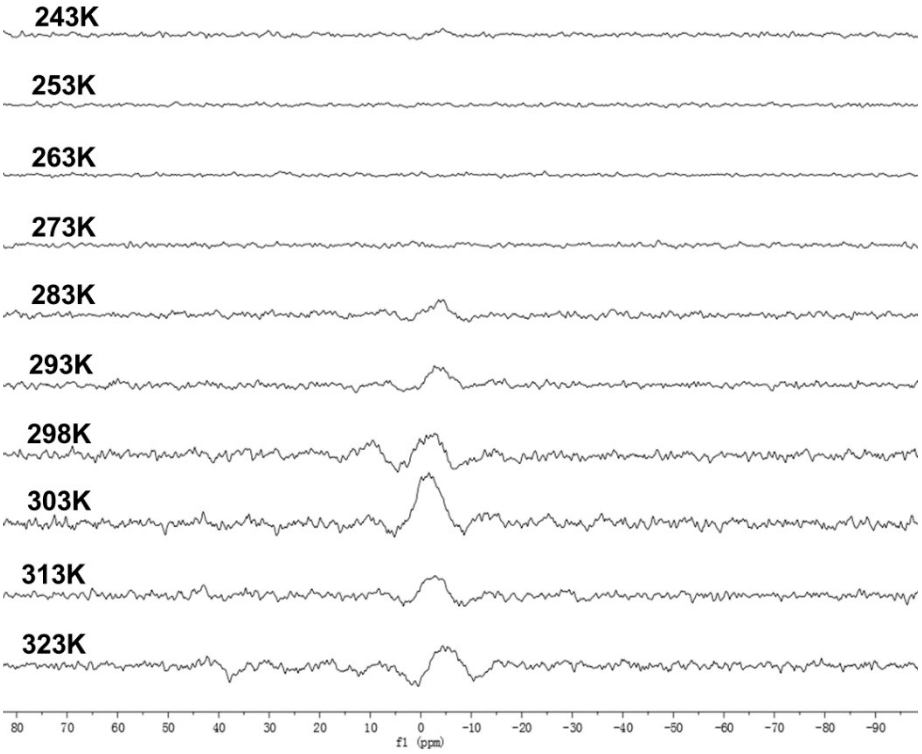


Fig. S19. Variable temperature ^{11}B NMR spectra of **B4** (161 MHz, $CDCl_3$) between 243 K and 323 K.

S4 Mechanoresponsive emission properties

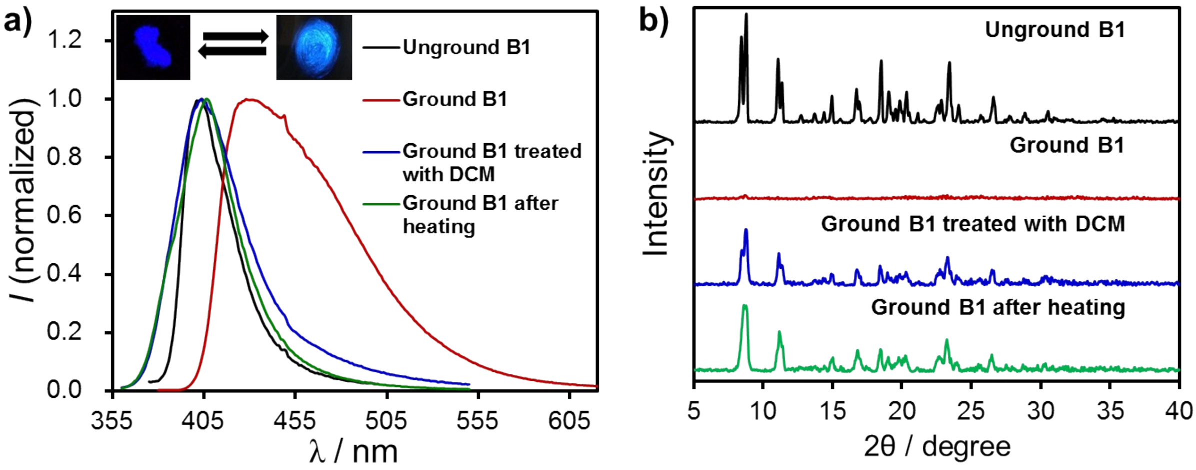


Fig. S20. a) Emission spectra of **B1** with unground (black line), ground (red line), ground **B1** treated with DCM (blue line) and ground **B1** after heating at 130 °C for 5 min (green line), respectively; b) Powder XRD patterns of **B1** with unground, ground, ground **B1** treated with DCM and ground **B1** after heating at 130 °C for 5 min, respectively. (The photographs show the fluorescence color in the crystalline state (left) and as amorphous film (right)).

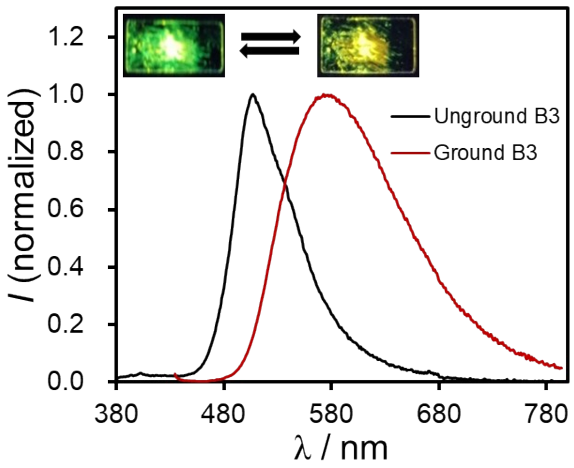


Fig. S21. Normalized emission spectra of **B3** as pristine crystalline solid and ground powder. (The photographs show the fluorescence color in the crystalline state (left) and as amorphous film (right)).

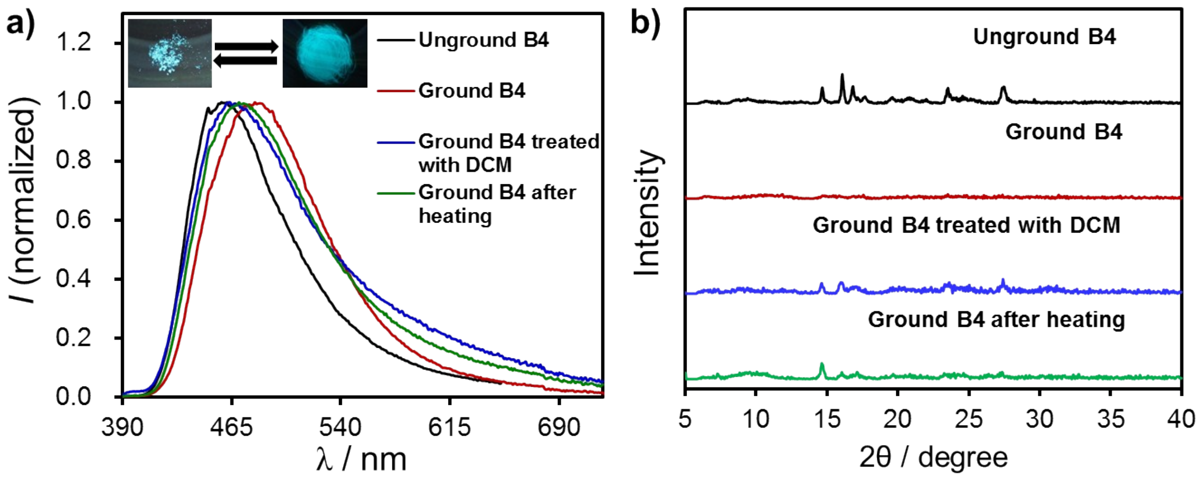


Fig. S22. a) Emission spectra change of **B4** with unground (black line), ground (red line), ground **B4** treated with DCM (blue line) and ground **B4** after heating at 150 ºC for 5 min (green line), respectively; b) Powder XRD patterns (right) of **B4** with unground, ground, ground **B4** treated with DCM and ground **B4** after heating at 150 ºC for 5 min, respectively. (The photographs show the fluorescence color in the crystalline state (left) and as amorphous film (right)).

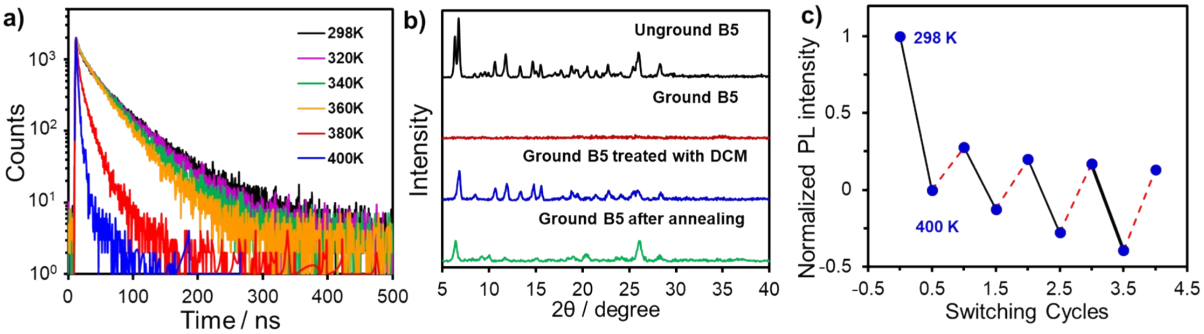


Fig. S23. a) Temperature-dependent transient decay spectra of **B5** as amorphous film; b)

Powder XRD patterns of **B5** as pristine crystalline solid, ground powder, recrystallized solid, and annealed solid after heating at 130 ºC for 5 min, respectively; c) Normalized fluorescence intensity of **B5** (blue circle) monitored at the emission maximum under the reversible emission tuning experiments. Black solid and red dashed lines denote that reversible cycling of **B5** emission between 298 K (at 473 nm) and 400 K (at 437 nm).

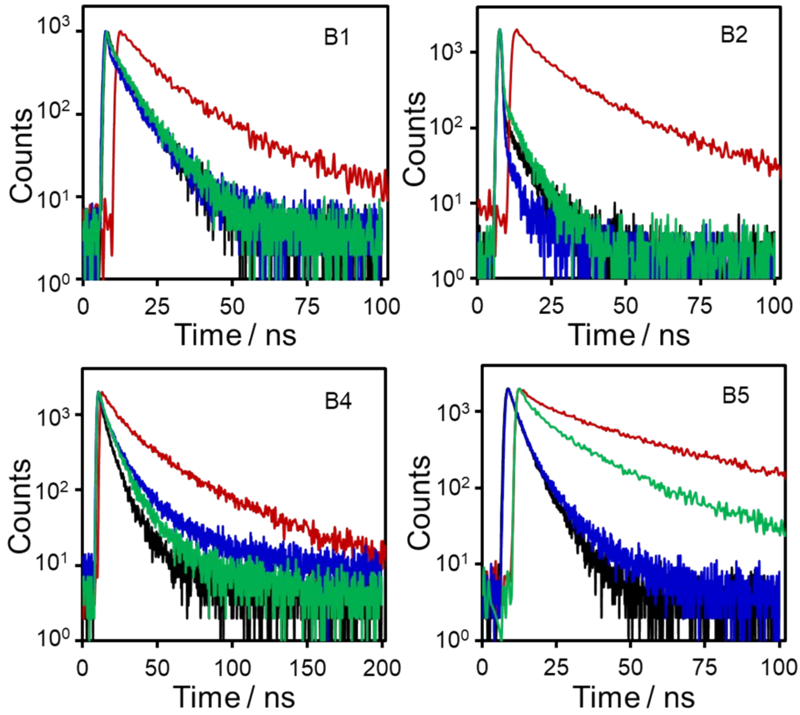


Fig. S24. Transient decay spectra of **B1**–**B5** with unground (black line), ground (red line), ground compounds treated with solvent (blue line) and ground compounds after heating for 5 min (green line), respectively.

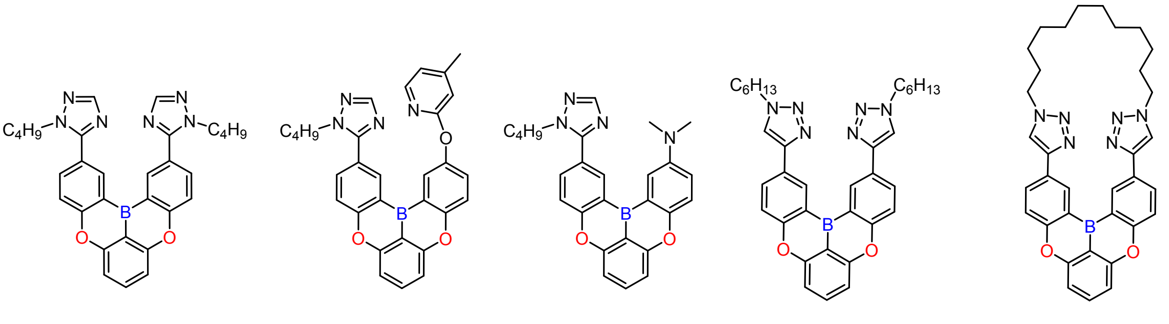
Table S4. Photophysical properties of **B1**−**B5** in the different states.

compd	Toluene, 77 K[a]		5 w.t% PMMA, 298 K			Unground powder			Ground powder	
	λ_{em} (nm)	τ (ns)[b]	λ_{em} (nm)	τ (ns)	Φ_F[c]	λ_{em} (nm)	τ (ns)	Φ_F[c]	λ_{em} (nm)	τ (ns)
B1	396	8.15	407	9.83	0.75	404	7.13	0.65	448	22.44
B2	388	N.d.	416	9.92	0.73	390	3.96	0.66	467	21.17
B3	473	3.18	497	52.0	0.51	507	16.91	0.45	573	16.14
B4	419	10.29	423	7.08	0.06	459	8.84	0.03	480	31.75
B5	408	8.04	422	4.65	0.15	435	4.91	0.15	473	42.86

[a] In toluene (0.05 mM) at 77 K; [b] Fluorescence lifetime measured at a maximum λ_{max} on excitation at 365 nm picosecond pulsed LED; [c] Determined by an absolute quantum yields spectrometer; N.d. = Not determined.

S5 DFT/TD-DFT Computational data

DFT and TD-DFT calculations were performed using the Gaussian 09 suite of programs[1] on the High Performance Computing Virtual Laboratory (HPCVL) at Queen's University. Geometry optimizations and vertical excitations of all compounds were obtained at the B3LYP/6-31g(d)[2,3] level of theory.



B1 **B2** **B3** **B4** **B5**

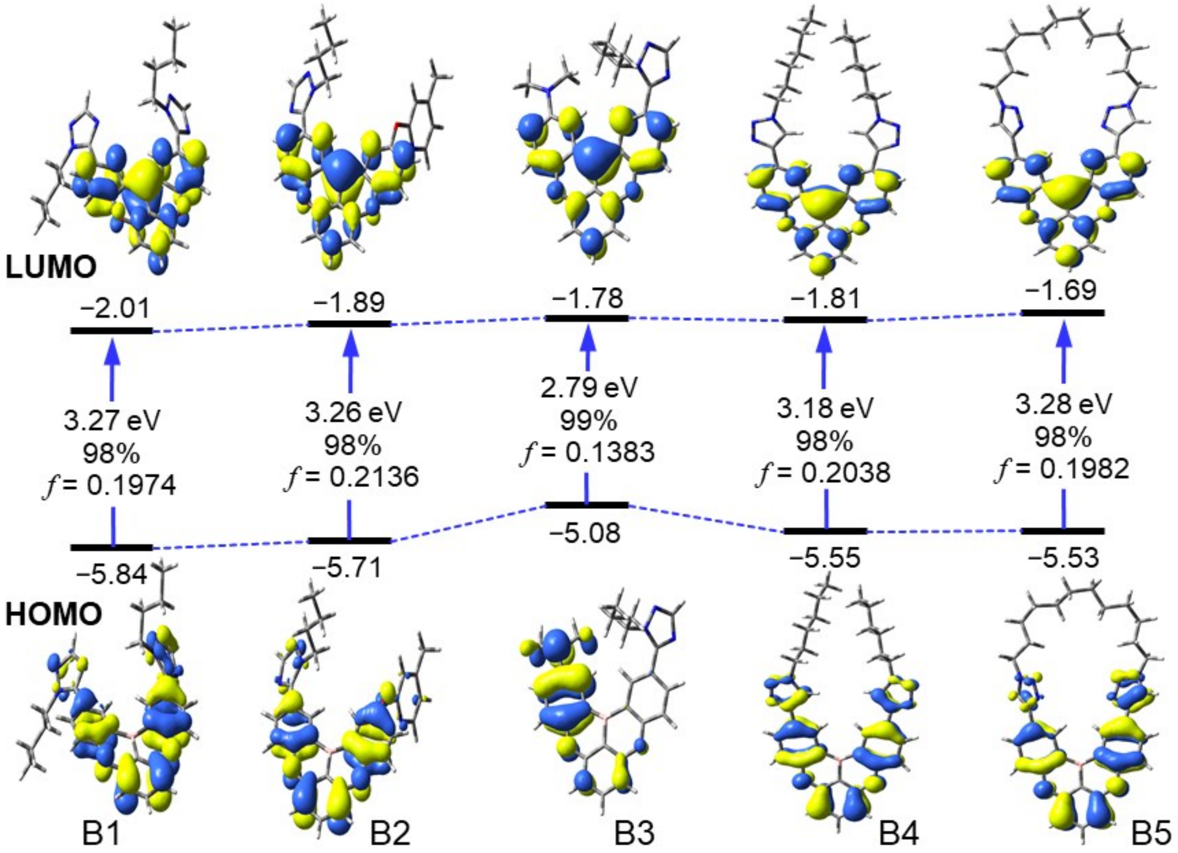
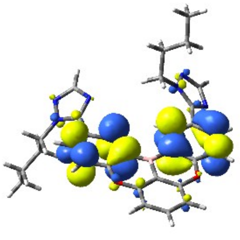
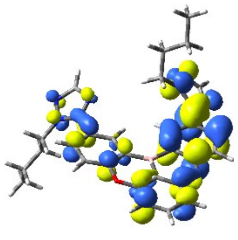
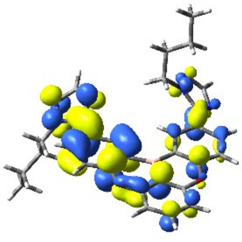
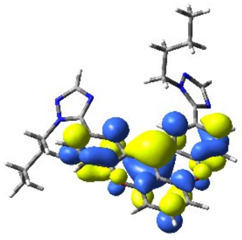
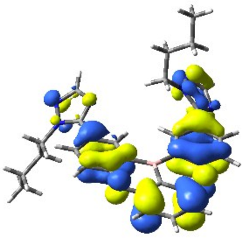
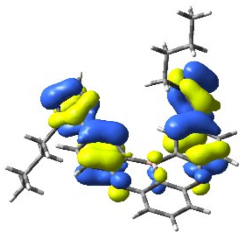
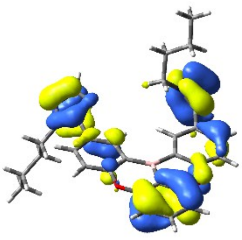
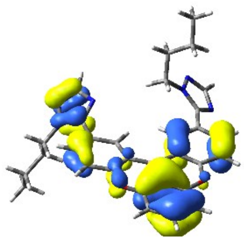


Fig. S25. TD-DFT calculated $S_0 \rightarrow S_1$ transition energies (eV), oscillator strength (*f*), and orbital diagrams for **B1–B5** (isovalue = 0.03, B3LYP / 6-31G(d)).

Table S5 TD-DFT calculated electronic transitions for **B1** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
B1	S_1	HOMO → LUMO (98%)	378.87 (3.27)	0.1974
	S_2	HOMO-1 → LUMO (97%)	319.90 (3.88)	0.0002
	S_3	HOMO → LUMO+1 (93%)	295.21 (4.20)	0.0975
	S_4	HOMO-2 → LUMO (63%)	290.68 (4.27)	0.0079
		HOMO → LUMO+2 (20%)		
		HOMO-3 → LUMO (12%)		
	S_5	HOMO-3 → LUMO (43%)	287.08 (4.32)	0.0269
		HOMO-2 → LUMO (31%)		
		HOMO → LUMO+2 (23%)		
	S_6	HOMO → LUMO+2 (46%)	272.43 (4.55)	0.8506
		HOMO-3 → LUMO (33%)		
		HOMO-4 → LUMO (14%)		
	S_7	HOMO-4 → LUMO (81%)	269.94 (4.59)	0.3896
	S_8	HOMO → LUMO+3 (80%)	264.42 (4.69)	0.0199
	S_9	HOMO-1 → LUMO+1 (36%)	254.99 (4.86)	0.3959
		HOMO-1 → LUMO+2 (44%)		
	S_{10}	HOMO-5 → LUMO (80%)	253.29 (4.89)	0.0165

Table S6 Primary orbitals which contribute to the calculated transitions of **B1** (iso = 0.03).

			
LUMO+3	LUMO+2	LUMO+1	LUMO
			
HOMO	HOMO-1	HOMO-2	HOMO-3

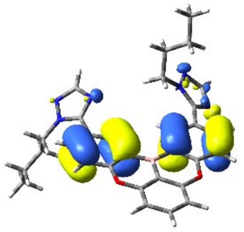
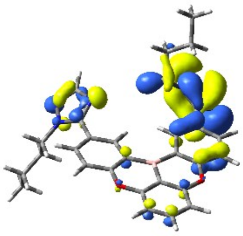
			
HOMO-4	HOMO-5		

Table S7 TD-DFT calculated electronic transitions for **B2** along with their corresponding excitation energies and oscillator strengths.

Compound	**Spin State**	**Transition Configuration**	**Excitation Energy (nm, eV)**	**Oscillator Strength**
B2	S_1	HOMO → LUMO (98%)	380.33 (3.26)	0.2136
	S_2	HOMO-1 → LUMO (96%)	318.68 (3.89)	0.0003
	S_3	HOMO-2 → LUMO (91%)	296.58 (4.18)	0.0344
	S_4	HOMO → LUMO+1 (81%)	292.19 (4.24)	0.0892
		HOMO-3 → LUMO (9%)		
	S_5	HOMO-3 → LUMO (68%)	283.42 (4.37)	0.1067
		HOMO → LUMO+2 (14%)		
	S_6	HOMO → LUMO+2 (25%)	273.19 (4.54)	0.1824
		HOMO-3 → LUMO (9%)		
		HOMO-4 → LUMO (51%)		
	S_7	HOMO-4 → LUMO (36%)	270.96 (4.57)	0.2877
		HOMO-5 → LUMO (25%)		
		HOMO → LUMO+2 (30%)		
	S_8	HOMO-5 → LUMO (64%)	267.66 (4.63)	0.1996
		HOMO → LUMO+2 (20%)		
	S_9	HOMO → LUMO+3 (65%)	262.98 (4.71)	0.048
		HOMO → LUMO+4 (17%)		
	S_{10}	HOMO → LUMO+4 (50%)	257.73 (4.81)	0.249
		HOMO-1 → LUMO+1 (16%)		

Table S8 Primary orbitals which contribute to the calculated transitions of **B2** (iso = 0.03).

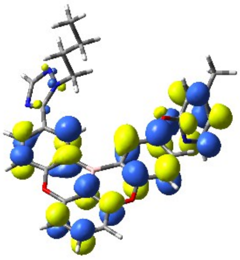
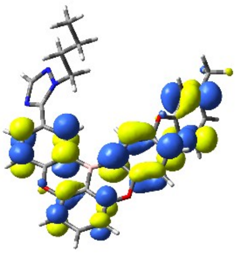
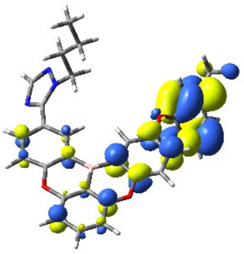
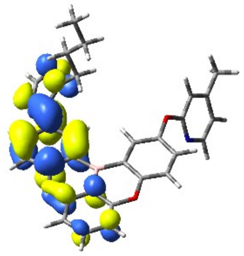
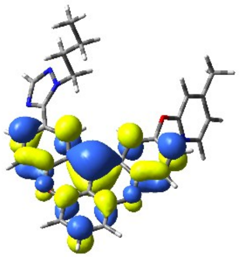
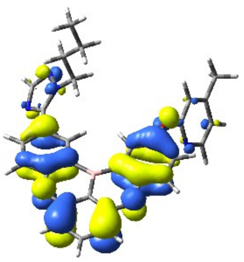
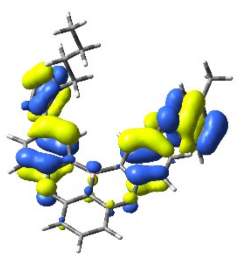
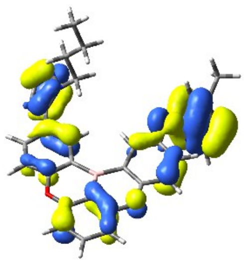
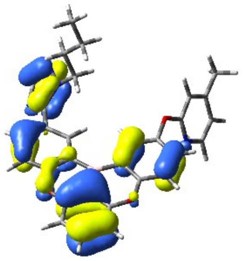
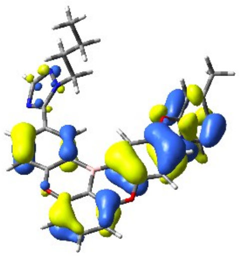
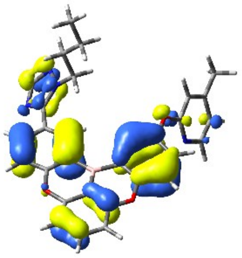
			
LUMO+4	LUMO+3	LUMO+2	LUMO+1
			
LUMO	HOMO	HOMO-1	HOMO-2
			
HOMO-3	HOMO-4	HOMO-5	

Table S9 TD-DFT calculated electronic transitions for **B3** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
B3	S_1	HOMO → LUMO (99%)	444.26 (2.79)	0.1383
	S_2	HOMO-1 → LUMO (97%)	344.69 (3.60)	0.0719
	S_3	HOMO → LUMO+1 (99%)	332.93 (3.72)	0.0226
	S_4	HOMO → LUMO+2 (82%)	301.03 (4.12)	0.0146
		HOMO-2 → LUMO (11%)		
	S_5	HOMO-2 → LUMO (71%)	292.34 (4.24)	0.0298
		HOMO → LUMO+2 (13%)		
		HOMO → LUMO+3 (13%)		
	S_6	HOMO-3 → LUMO (60%)	284.09 (4.36)	0.0153
		HOMO → LUMO+3 (28%)		

	S_7	HOMO-1 → LUMO+1 (41%)	280.99 (4.41)	0.1189
		HOMO → LUMO+3 (32%)		
		HOMO-3 → LUMO (15%)		
	S_8	HOMO-4 → LUMO (72%)	271.44 (4.57)	0.2641
		HOMO → LUMO+3 (10%)		
	S_9	HOMO-1 → LUMO+1 (41%)	264.34 (4.69)	0.7912
		HOMO-4 → LUMO (20%)		
		HOMO → LUMO+4 (19%)		
	S_{10}	HOMO → LUMO+4 (74%)	260.35 (4.76)	0.696

Table S10 Primary orbitals which contribute to the calculated transitions of **B3** (iso = 0.03).

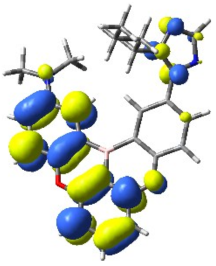
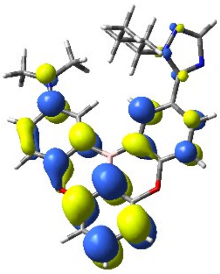
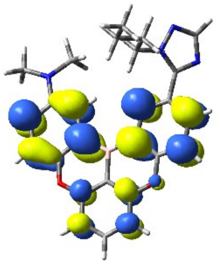
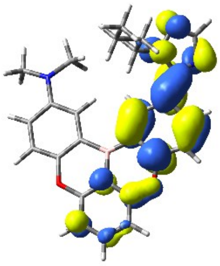
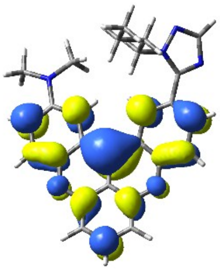
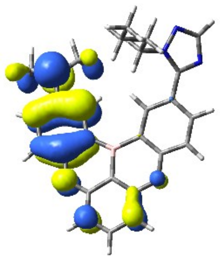
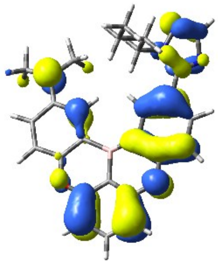
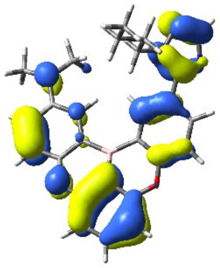
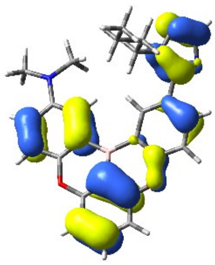
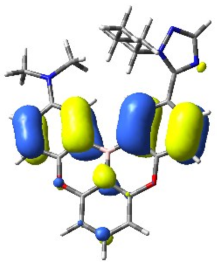
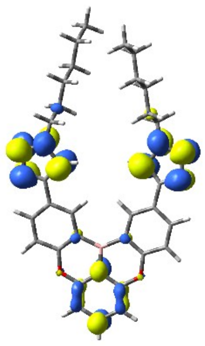
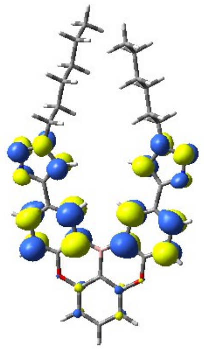
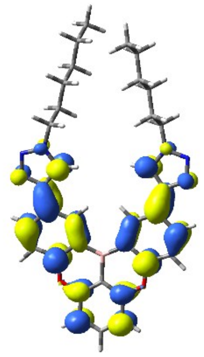
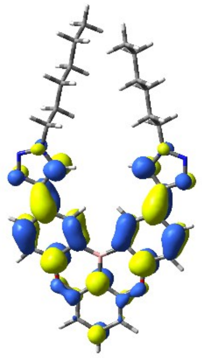
			
LUMO+4	LUMO+3	LUMO+2	LUMO+1
			
LUMO	HOMO	HOMO-1	HOMO-2
			
HOMO-3	HOMO-4		

Table S11 TD-DFT calculated electronic transitions for **B4** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
B4	S_1	HOMO → LUMO (98%)	388.81 (3.18)	0.2038
	S_2	HOMO-1 → LUMO (97%)	333.75 (3.72)	0.0026
	S_3	HOMO → LUMO+1 (94%)	297.24 (4.17	0.0743
	S_4	HOMO-2 → LUMO (94%)	291.35 (4.27)	0.0158
	S_5	HOMO → LUMO+2 (48%)	289.98 (4.28)	0.0491
		HOMO-3 → LUMO (47%)		
	S_6	HOMO-3 → LUMO (18%)	274.69 (4.51)	0.4244
		HOMO → LUMO+2 (35%)		
		HOMO → LUMO+3 (33%)		
		HOMO-1 → LUMO+1 (11%)		
	S_7	HOMO → LUMO+2 (14%)	271.99 (4.56)	0.5268
		HOMO → LUMO+3 (53%)		
		HOMO-3 → LUMO (27%)		
	S_8	HOMO-4 → LUMO (95%)	271.88 (4.56)	0.2309
	S_9	HOMO-1 → LUMO+2 (72%)	259.88 (4.77)	0.1459
		HOMO → LUMO+4 (14%)		
	S_{10}	HOMO-1 → LUMO+1 (85%)	257.62 (4.81)	1.3444

Table S12 Primary orbitals which contribute to the calculated transitions of **B4** (iso = 0.03).

			
LUMO+4	LUMO+3	LUMO+2	LUMO+1

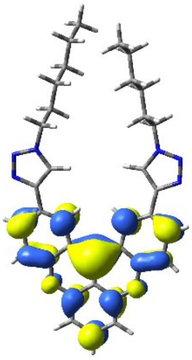
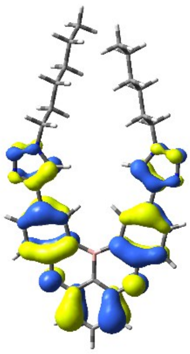
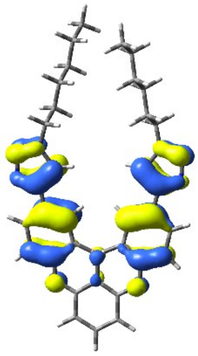
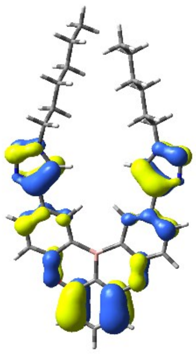
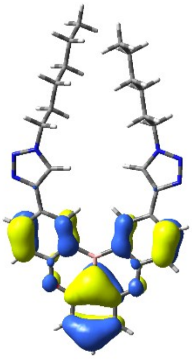
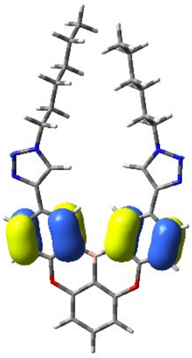
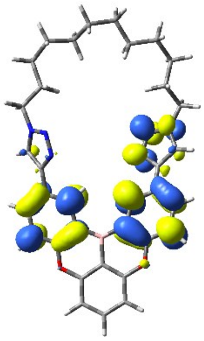
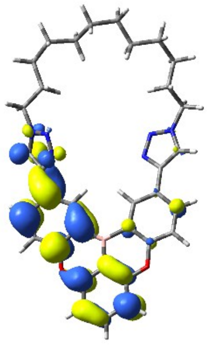
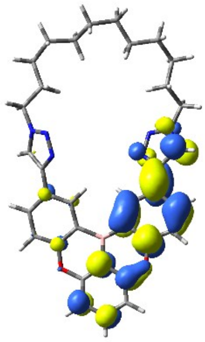
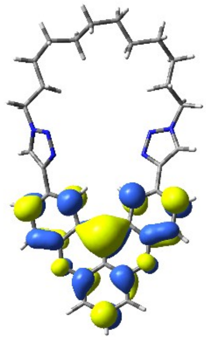
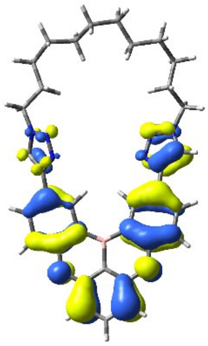
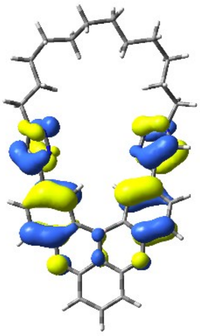
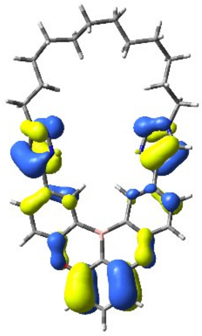
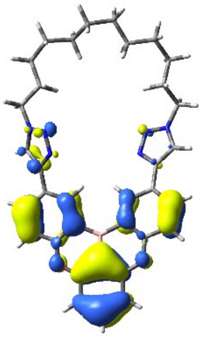
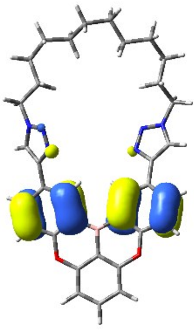
			
LUMO	HOMO	HOMO-1	HOMO-2
			
HOMO-3	HOMO-4		

Table S13 TD-DFT calculated electronic transitions for **B5** along with their corresponding excitation energies and oscillator strengths.

Compound	Spin State	Transition Configuration	Excitation Energy (nm, eV)	Oscillator Strength
B5	S_1	HOMO → LUMO (98%)	377.84 (3.28)	0.1982
	S_2	HOMO-1 → LUMO (97%)	327.11 (3.79)	0.003
	S_3	HOMO → LUMO+1 (49%)	288.19 (4.30)	0.0404
		HOMO-2 → LUMO (36%)		
		HOMO-3 → LUMO (11%)		
	S_4	HOMO → LUMO+1 (21%)	286.01 (4.33)	0.0326
		HOMO-2 → LUMO (58%)		
		HOMO-3 → LUMO (15%)		
	S_5	HOMO → LUMO+1 (15%)	284.15 (4.36)	0.0403
		HOMO → LUMO+2 (37%)		
		HOMO-3 → LUMO (39%)		
	S_6	HOMO-4 → LUMO (91%)	271.75 (4.56)	0.3324
	S_7	HOMO → LUMO+2 (51%)	268.77 (4.61)	0.839
		HOMO → LUMO+3 (10%)		

		HOMO-3 → LUMO (28%)		
	S_8	HOMO → LUMO+3 (70%)	262.34 (4.73)	0.1392
		HOMO-1 → LUMO+1 (11%)		
	S_9	HOMO-1 → LUMO+1 (44%)	253.92 (4.88)	0.2119
		HOMO-1 → LUMO+2 (41%)		
	S_{10}	HOMO-5 → LUMO (35%)	249.65 (4.96)	0.3351

Table S14 Primary orbitals which contribute to the calculated transitions of **B5** (iso = 0.03).

			
LUMO+3	LUMO+2	LUMO+1	LUMO
			
HOMO	HOMO-1	HOMO-2	HOMO-3
			
HOMO-4			

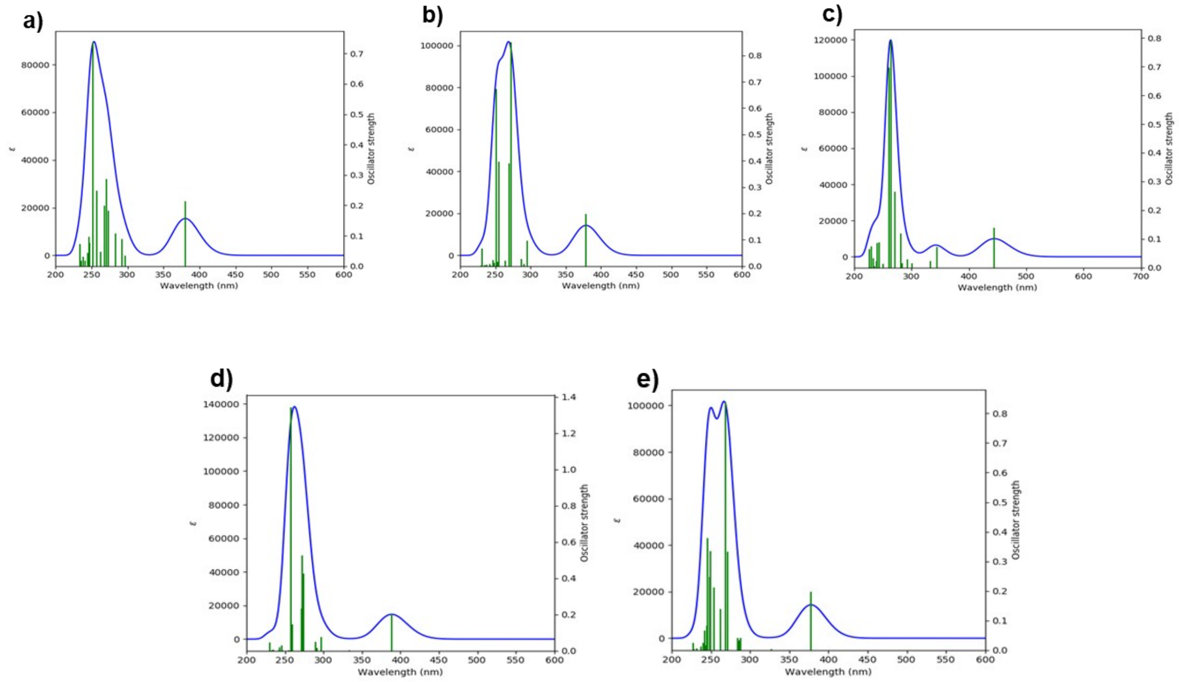


Fig. S26. Predicted UV/Vis spectra of a) **B1**, b) **B2**, c) **B3**, d) **B4** and e) **B5** based on TD-DFT calculation.

S6 ^{1}H NMR, ^{13}C NMR and ^{11}B NMR spectra for isolated compounds

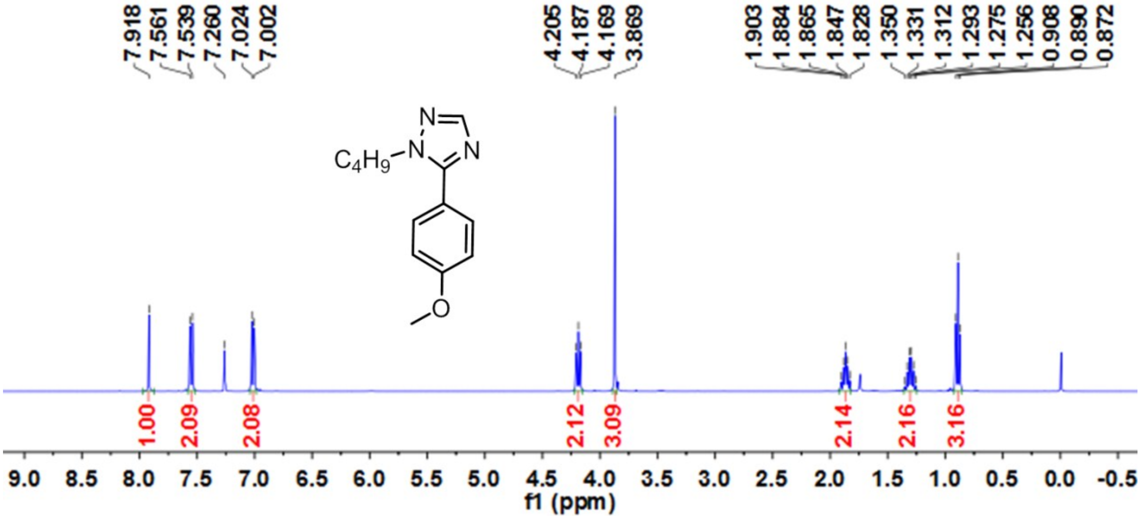


Fig. S27. ^{1}H NMR spectrum of **1** (400 MHz, $CDCl_3$)

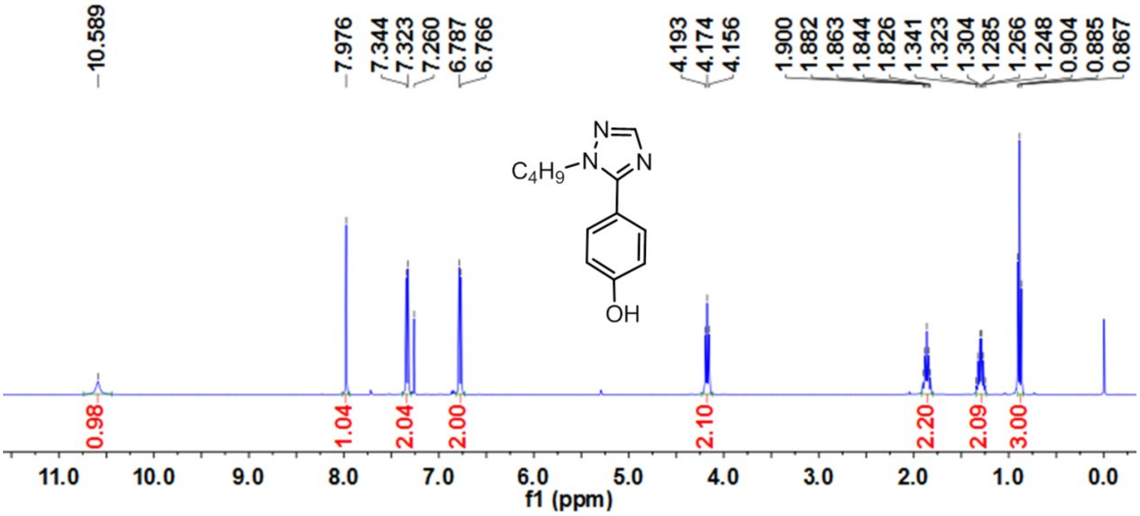


Fig. S28. ^{1}H NMR spectrum of **1a** (400 MHz, $CDCl_3$)

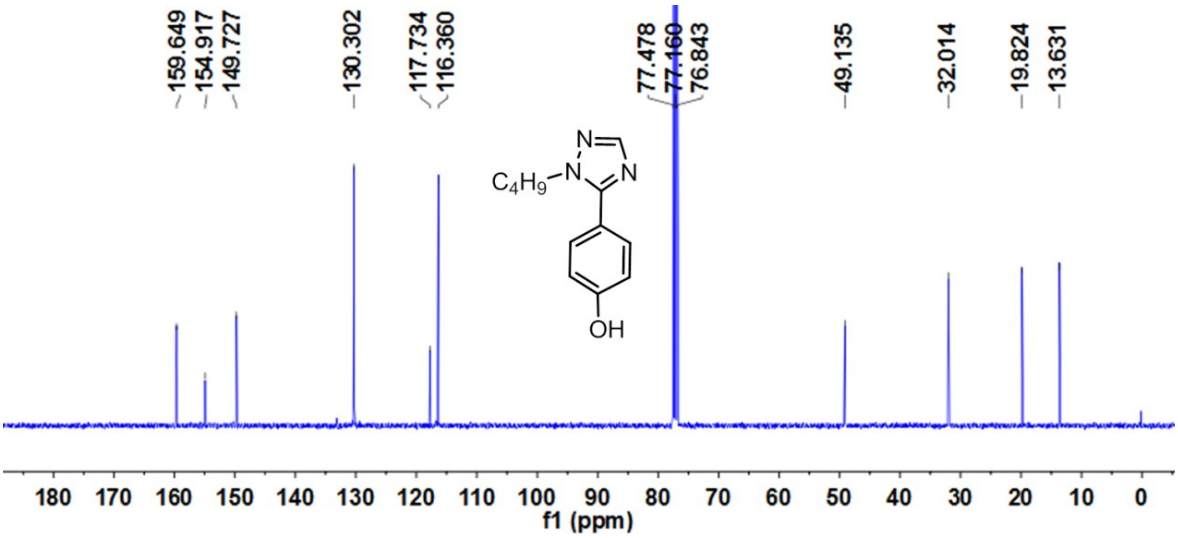


Fig. S29. ^{13}C NMR spectrum of **1a** (101 MHz, $CDCl_3$)

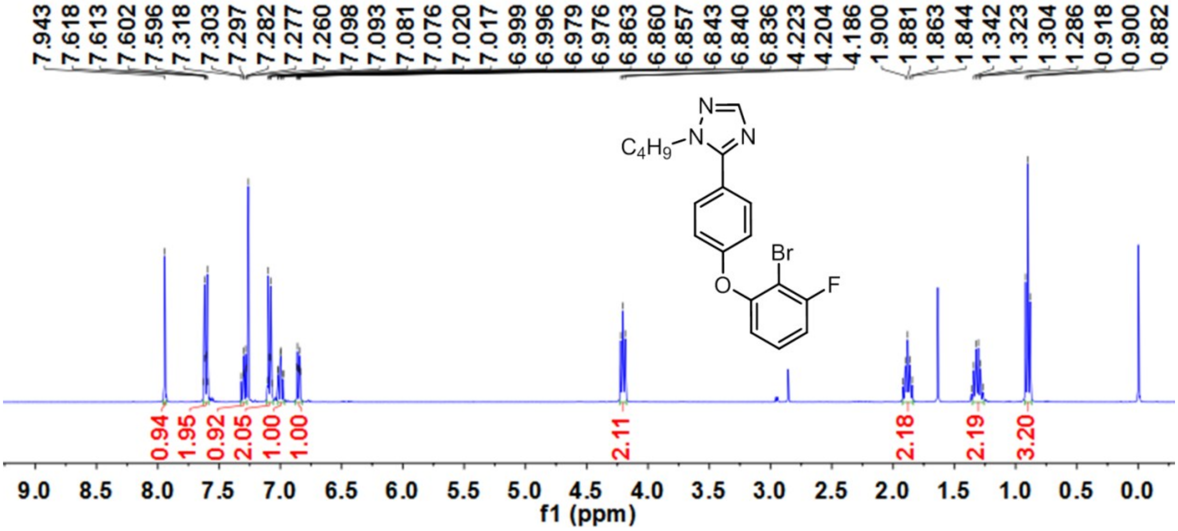


Fig. S30. ^{1}H NMR spectrum of **2a** (400 MHz, $CDCl_3$)

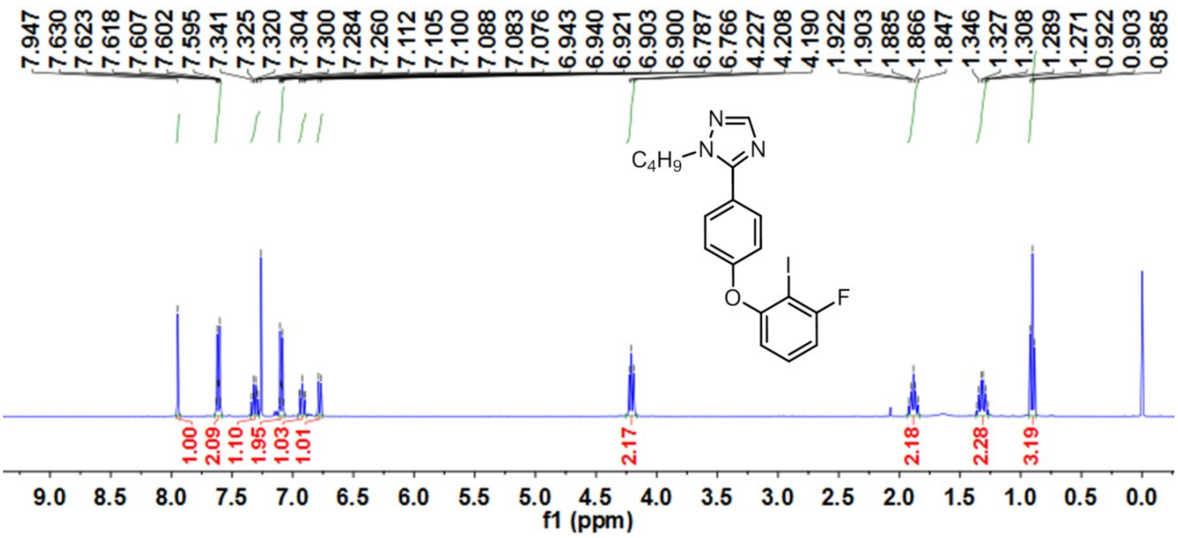


Fig. S31. ^{1}H NMR spectrum of **3a** (400 MHz, $CDCl_3$)

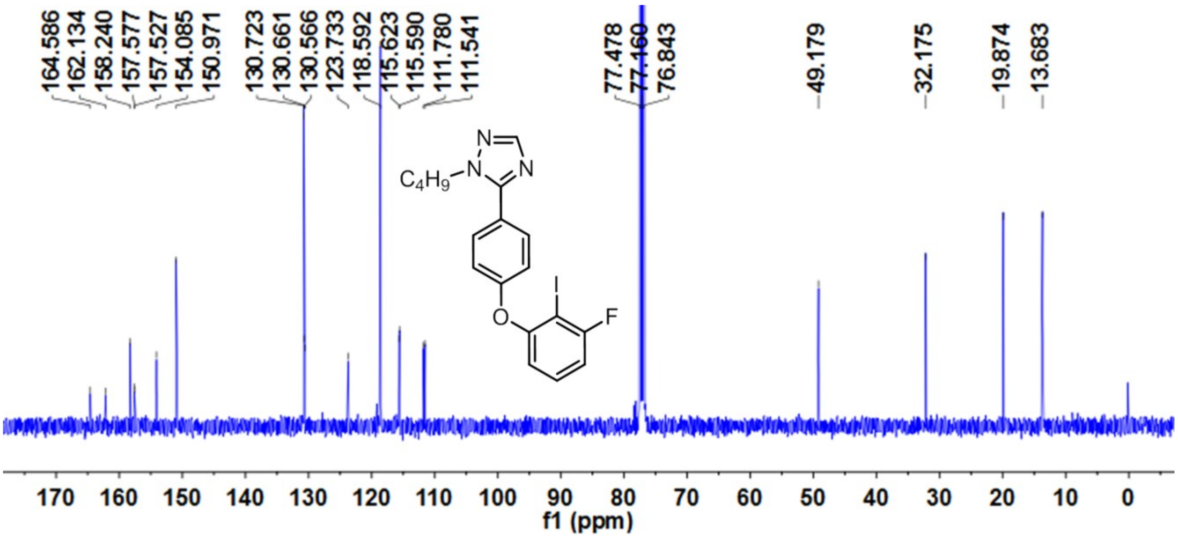


Fig. S32. ^{13}C NMR spectrum of **1a** (101 MHz, $CDCl_3$)

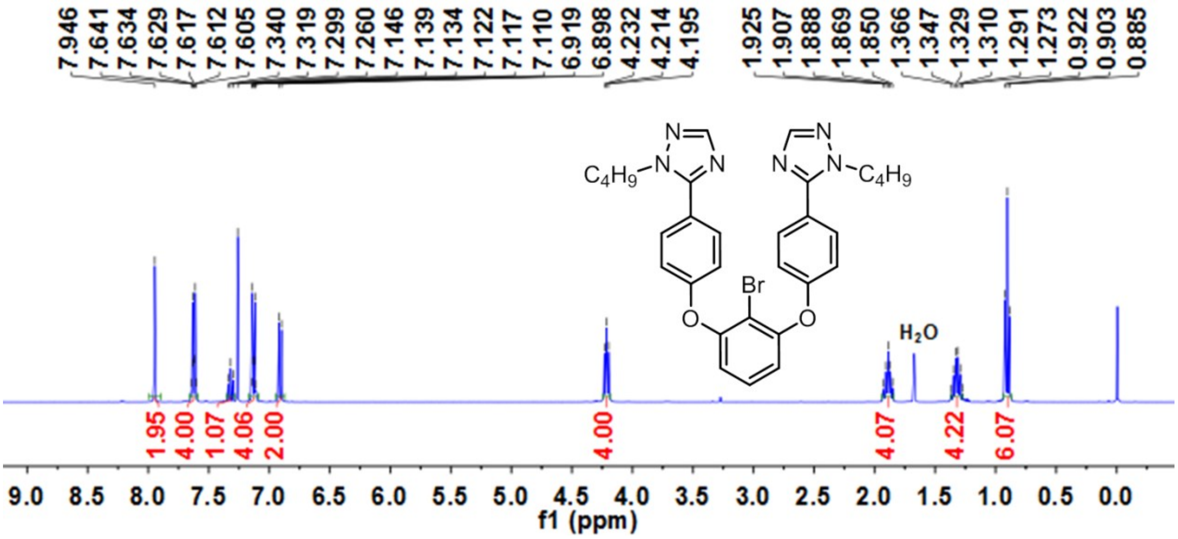


Fig. S33. ^{1}H NMR spectrum of **4a** (400 MHz, $CDCl_3$)

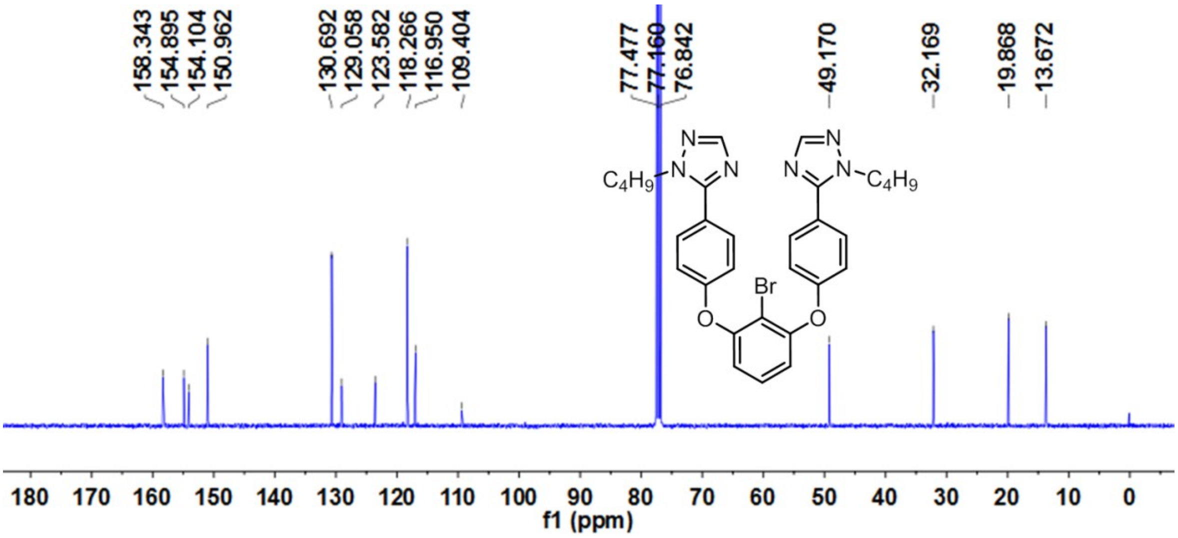


Fig. S34. ^{13}C NMR spectrum of **4a** (101 MHz, $CDCl_3$)

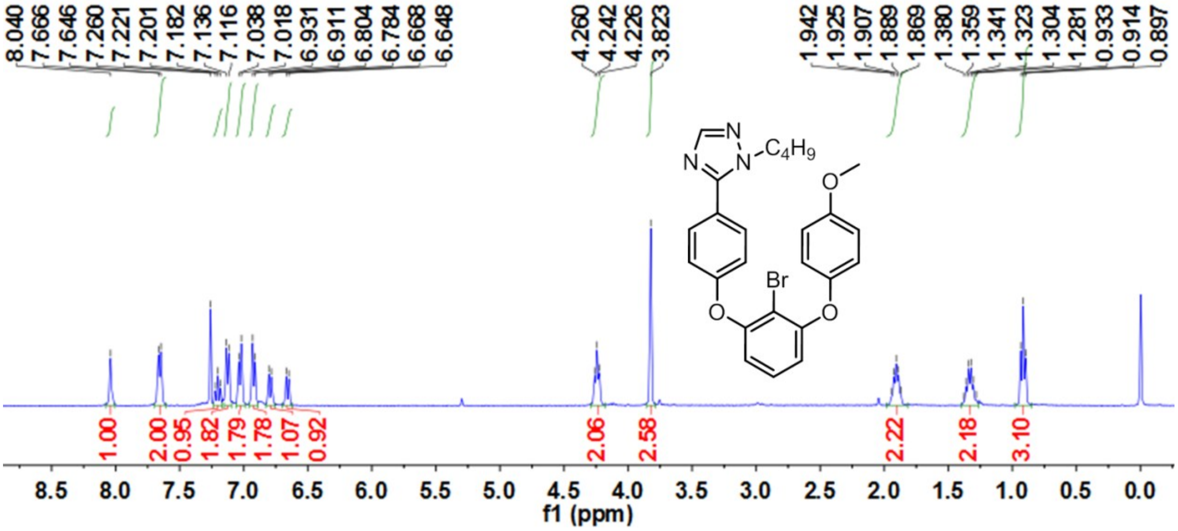


Fig. S35.^{1}H NMR spectrum of **5a** (400 MHz, $CDCl_3$)

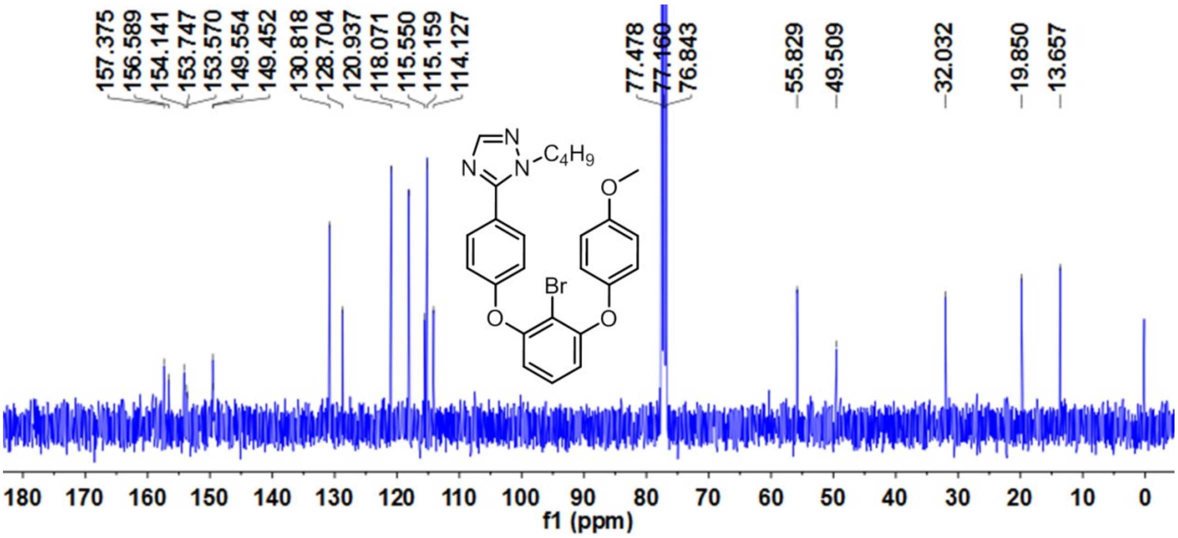


Fig. S36. ^{13}C NMR spectrum of **5a** (101 MHz, $CDCl_3$)

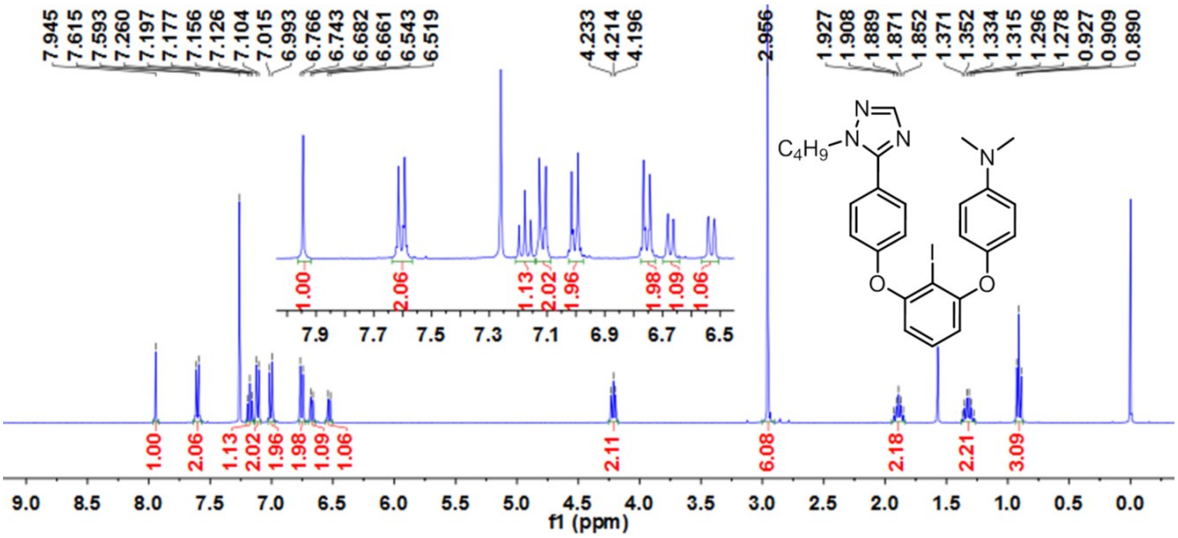


Fig. S37. ^{1}H NMR spectrum of **6a** (400 MHz, $CDCl_3$)

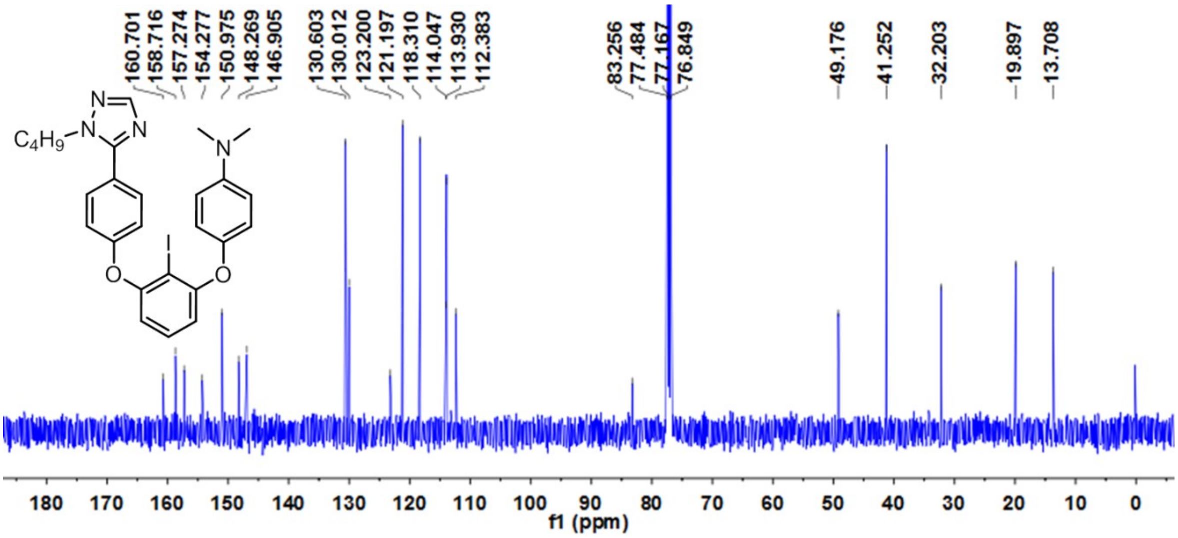


Fig. S38. ^{13}C NMR spectrum of **6a** (400 MHz, $CDCl_3$)

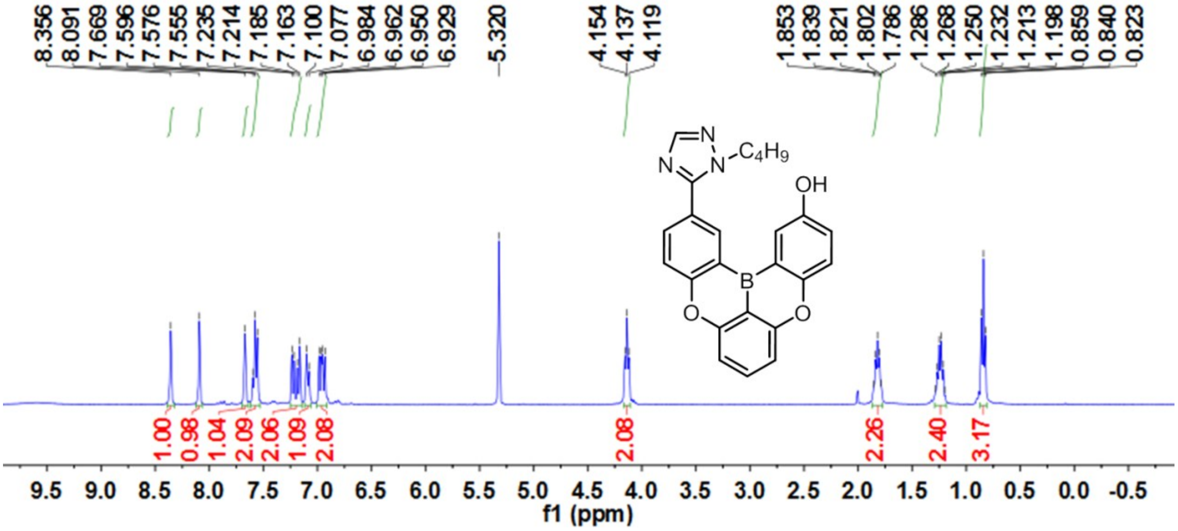


Fig. S39. ^{1}H NMR spectrum of **7a** (400 MHz, CD_2Cl_2)

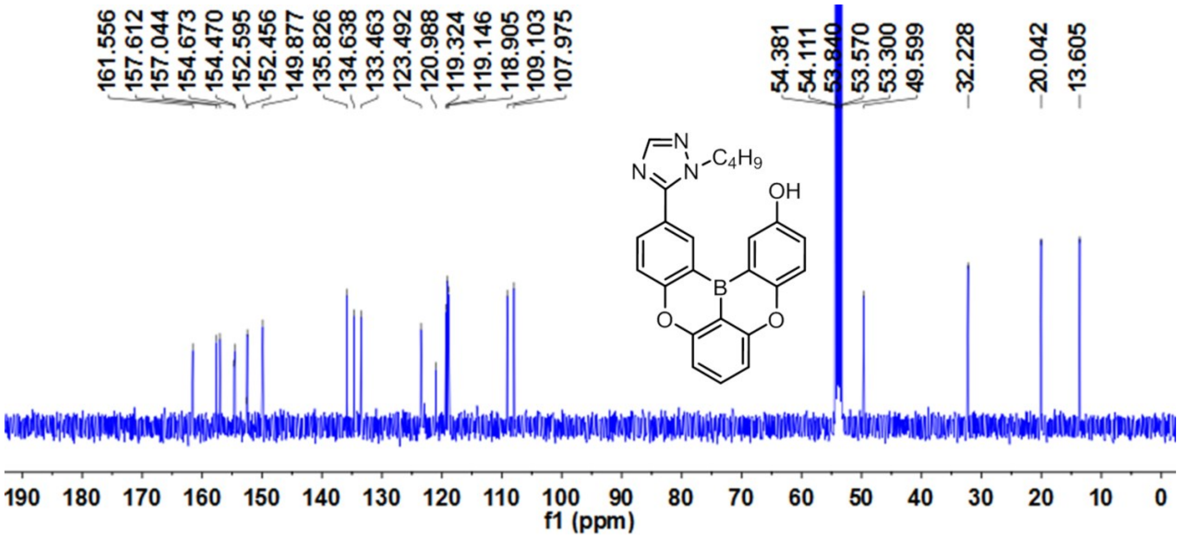


Fig. S40. ^{13}C NMR spectrum of **7a** (101 MHz, CD_2Cl_2)

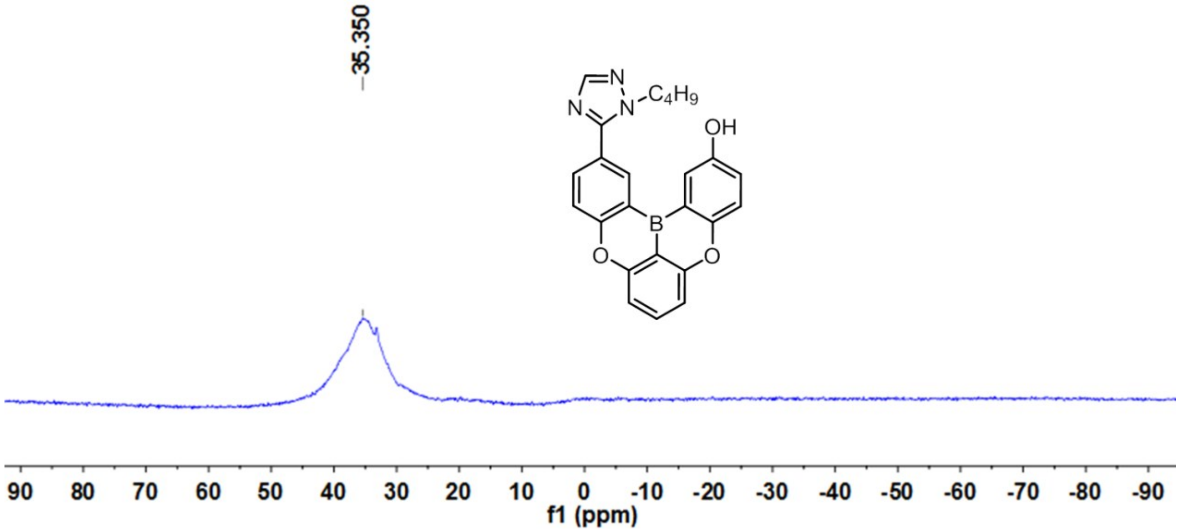


Fig. S41. ^{11}B NMR spectrum of **7a** (225 MHz, CD_2Cl_2)

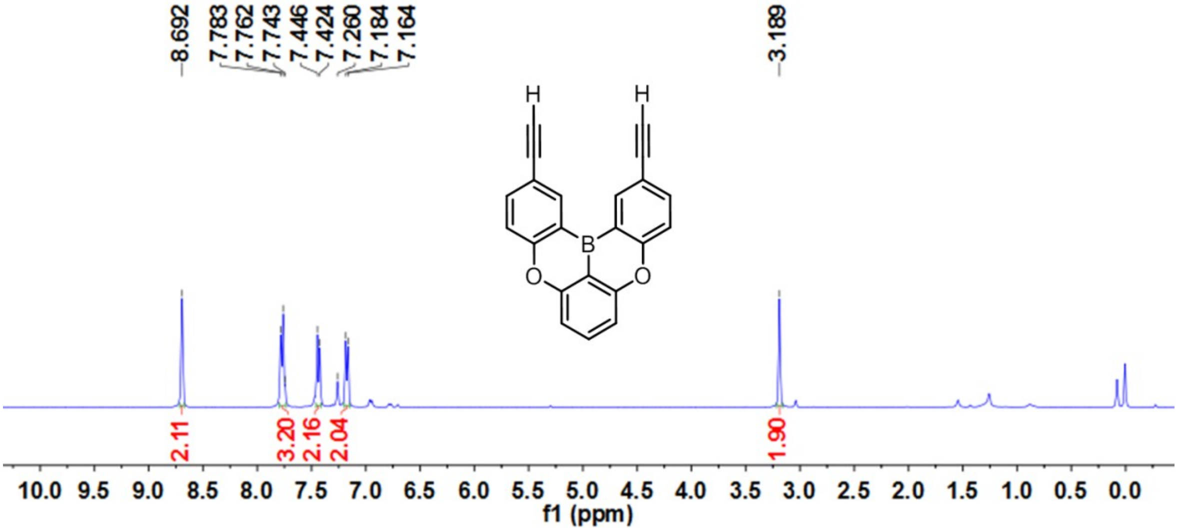


Fig. S42. ^{1}H NMR spectrum of **9a** (400 MHz, $CDCl_3$)

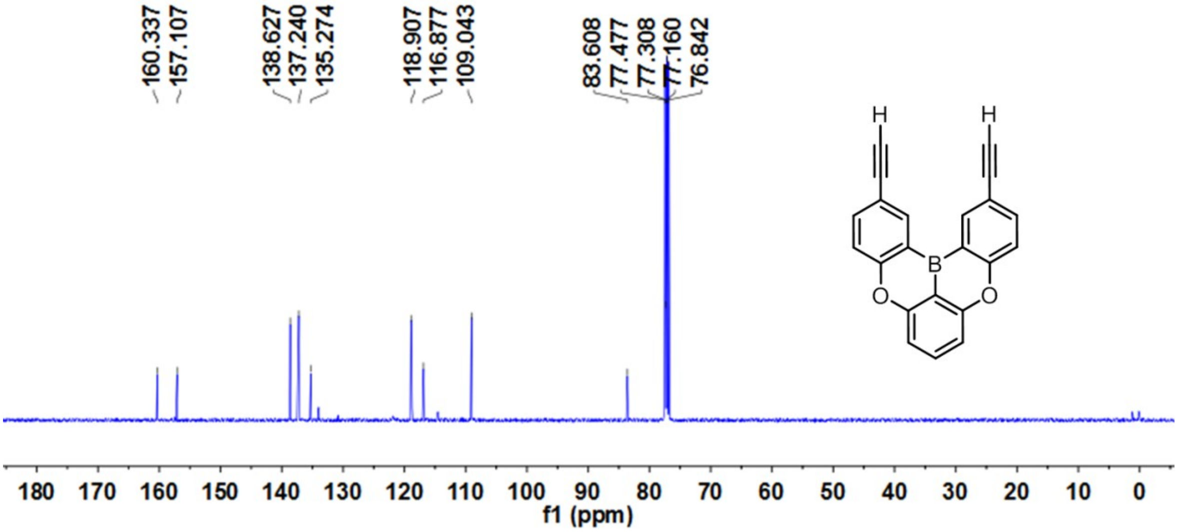


Fig. S43. ^{13}C NMR spectrum of **9a** (101 MHz, $CDCl_3$)

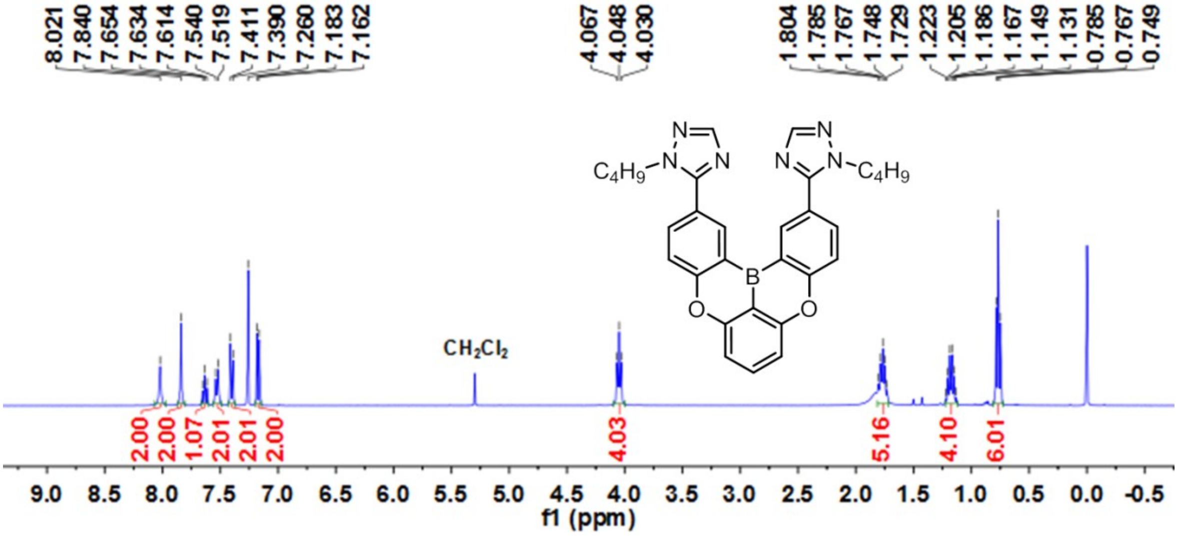


Fig. S44. ^{1}H NMR spectrum of **B1** (400 MHz, $CDCl_3$)

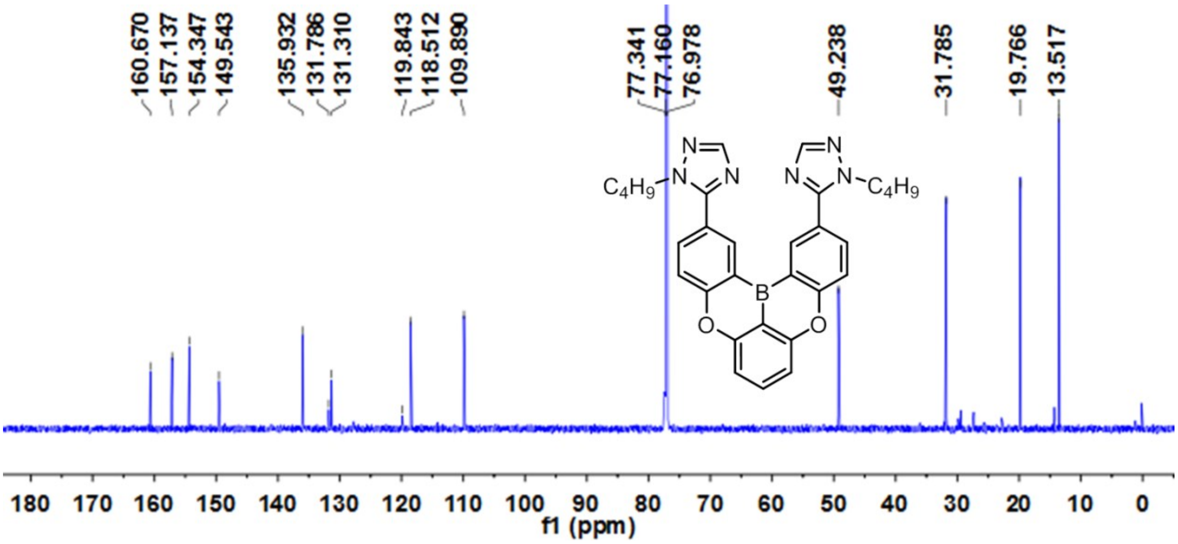


Fig. S45. ^{13}C NMR spectrum of **B1** (176 MHz, $CDCl_3$)

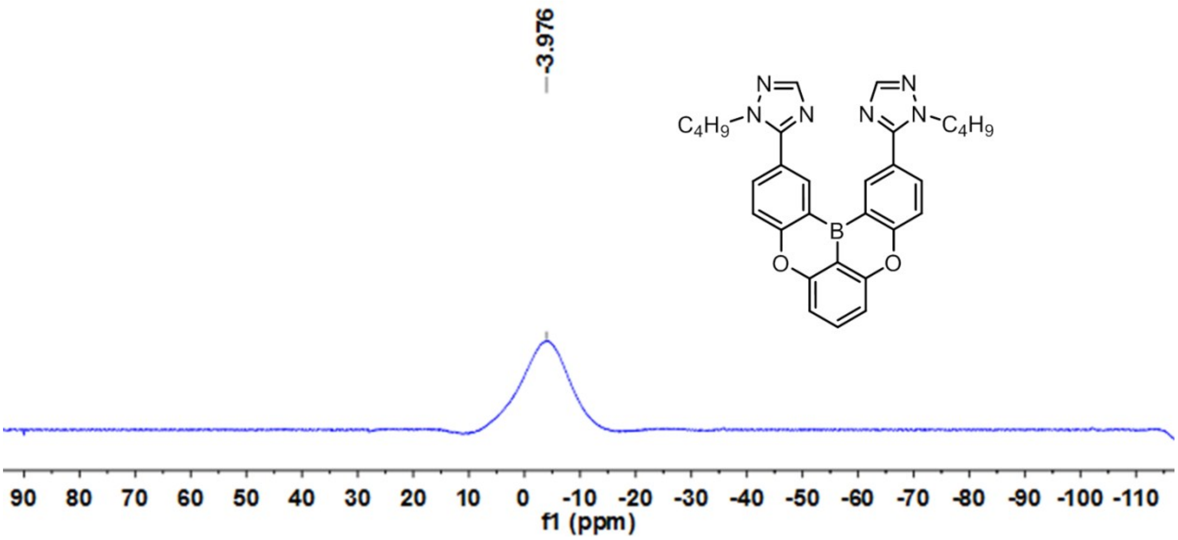


Fig. S46. ^{11}B NMR spectrum of **B1** (225 MHz, $CDCl_3$)

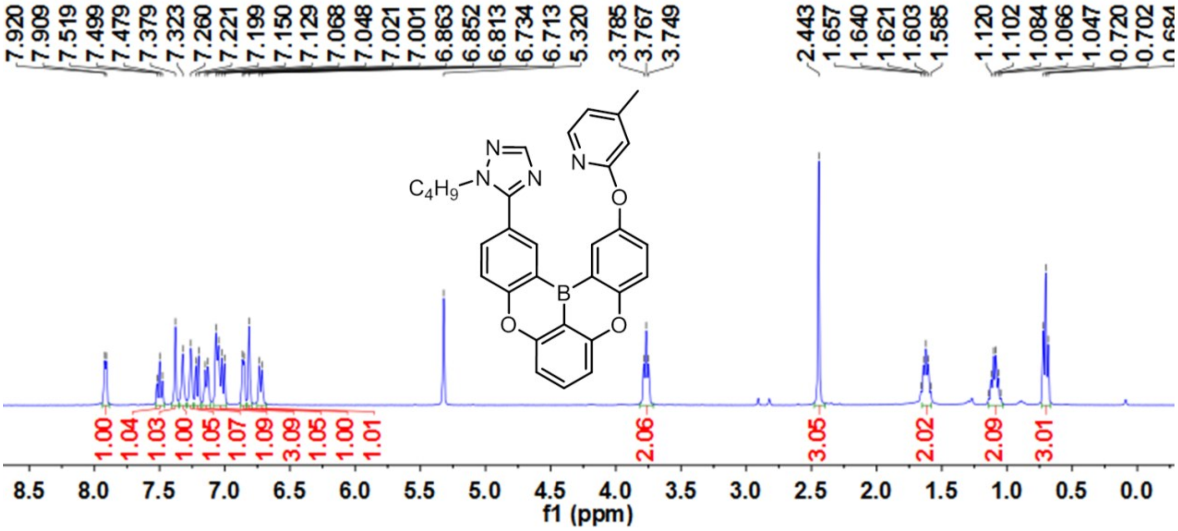


Fig. S47. ^{1}H NMR spectrum of **B2** (400 MHz, CD_2Cl_2)

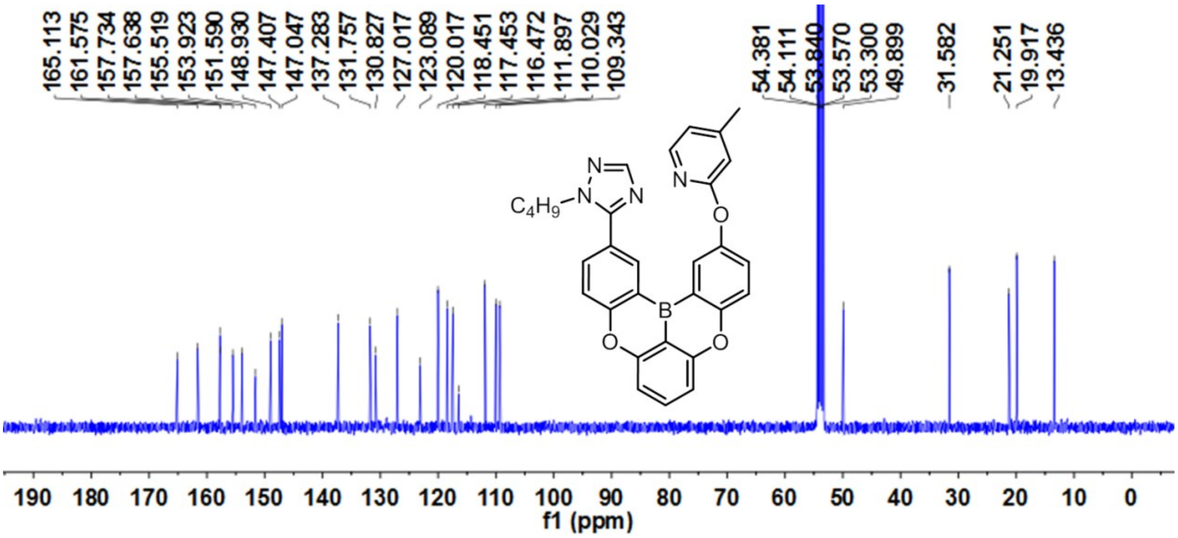


Fig. S48. ^{13}C NMR spectrum of **B2** (101 MHz, CD_2Cl_2)

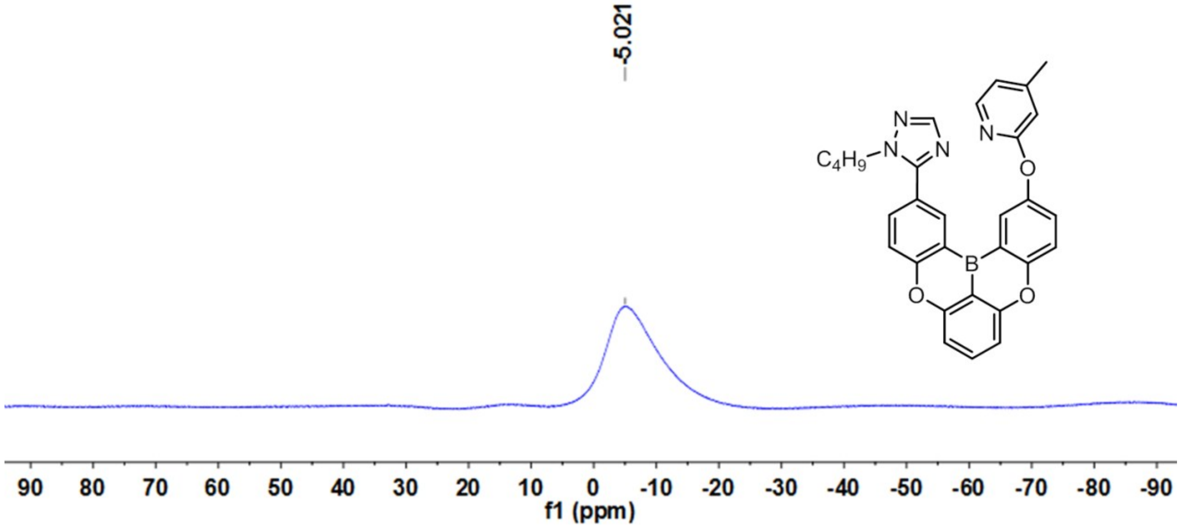


Fig. S49. ^{11}B NMR spectrum of **B2** (225 MHz, CD_2Cl_2)

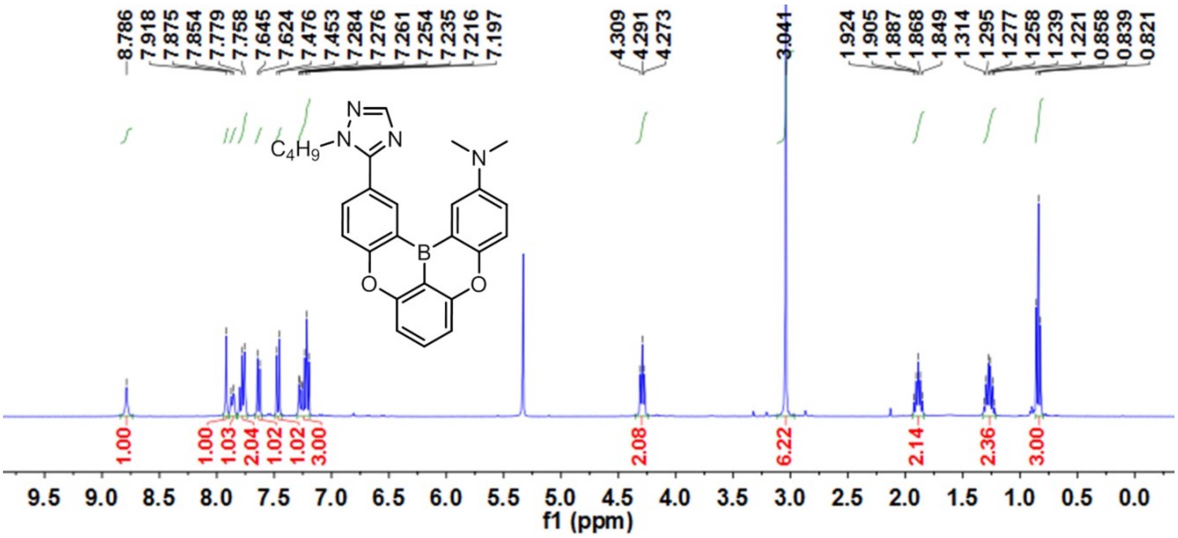


Fig. S50. ^{1}H NMR spectrum of **B3** (400 MHz, CD_2Cl_2)

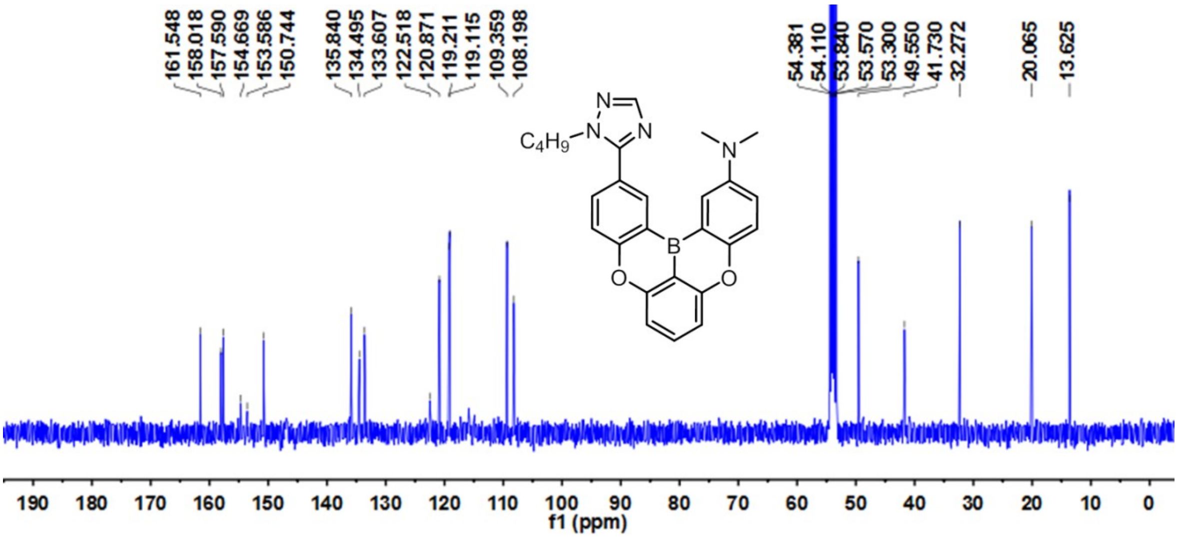


Fig. S51. ^{13}C NMR spectrum of **B3** (101 MHz, CD_2Cl_2)

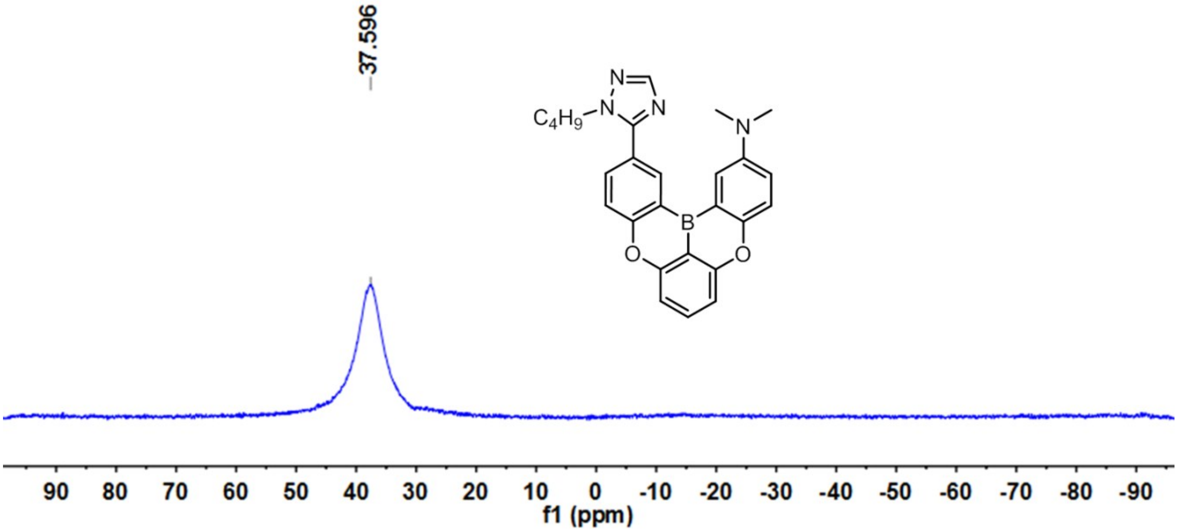


Fig. S52. ^{11}B NMR spectrum of **B3** (128 MHz, CD_2Cl_2)

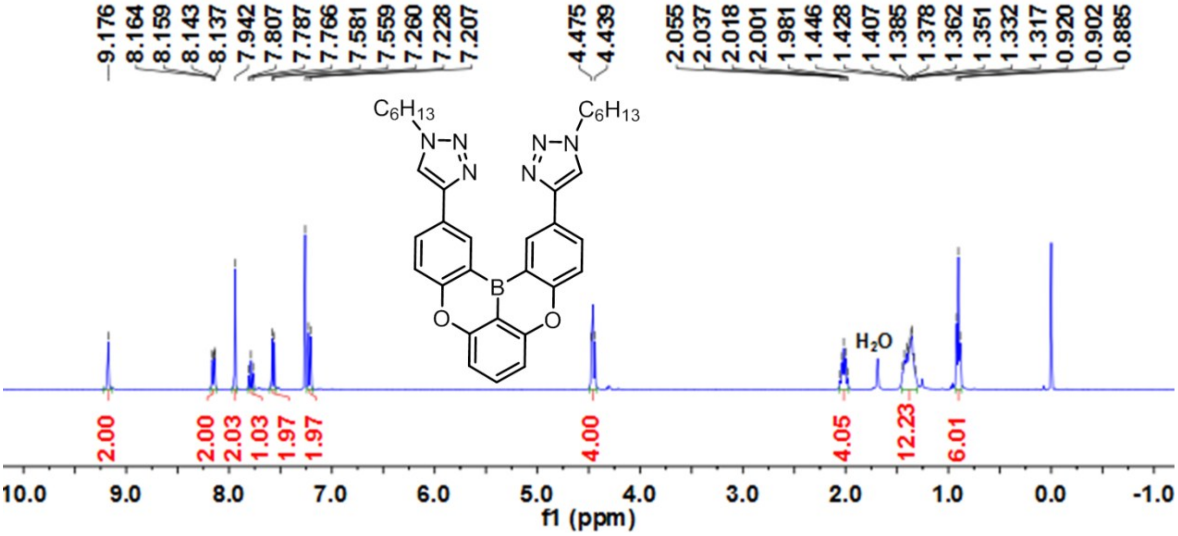


Fig. S53. ^{1}H NMR spectrum of **B4** (400 MHz, $CDCl_3$)

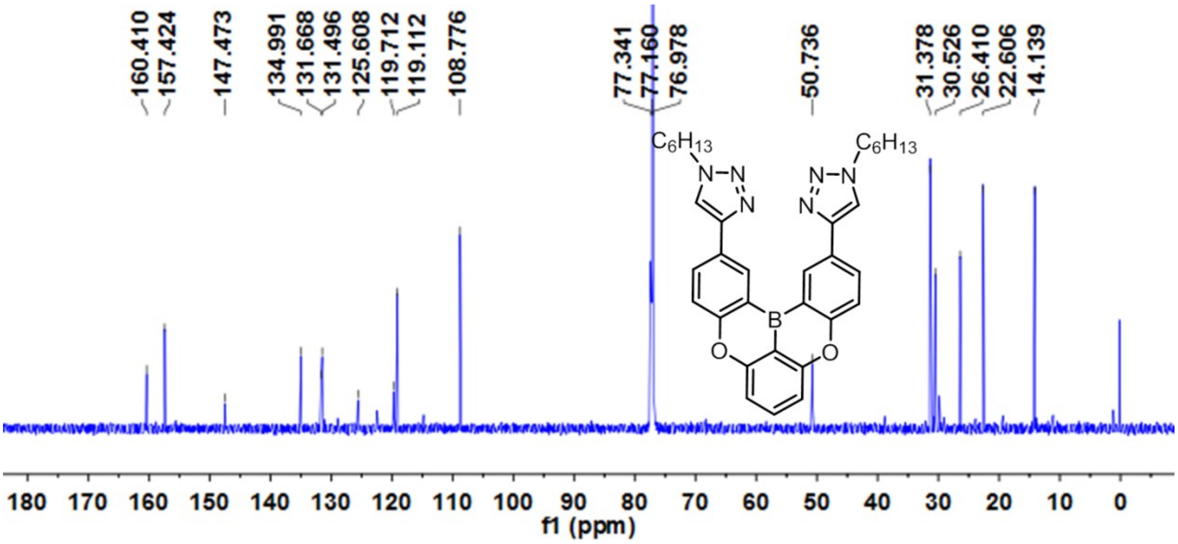


Fig. S54. ^{13}C NMR spectrum of **B4** (176 MHz, $CDCl_3$)

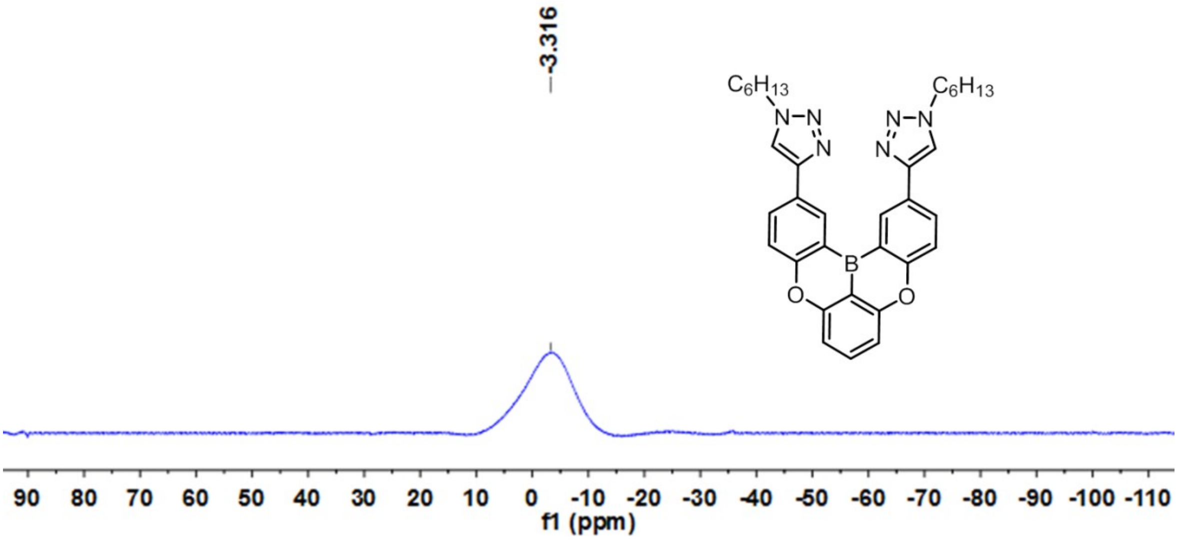


Fig. S55. ^{11}B NMR spectrum of **B4** (225 MHz, $CDCl_3$)

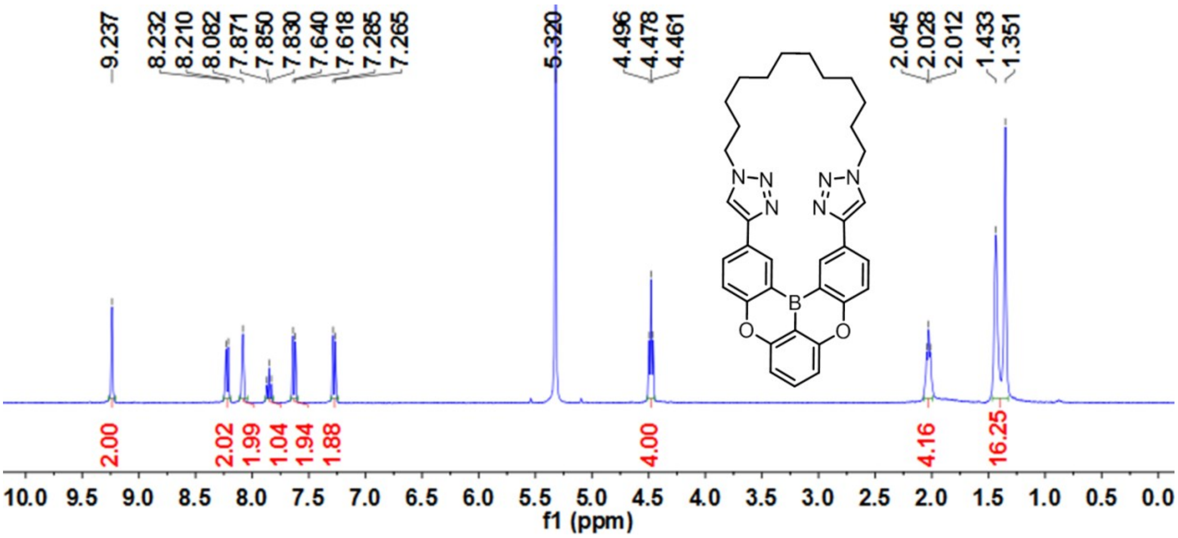


Fig. S56. ^{1}H NMR spectrum of **B5** (400 MHz, CD_2Cl_2)

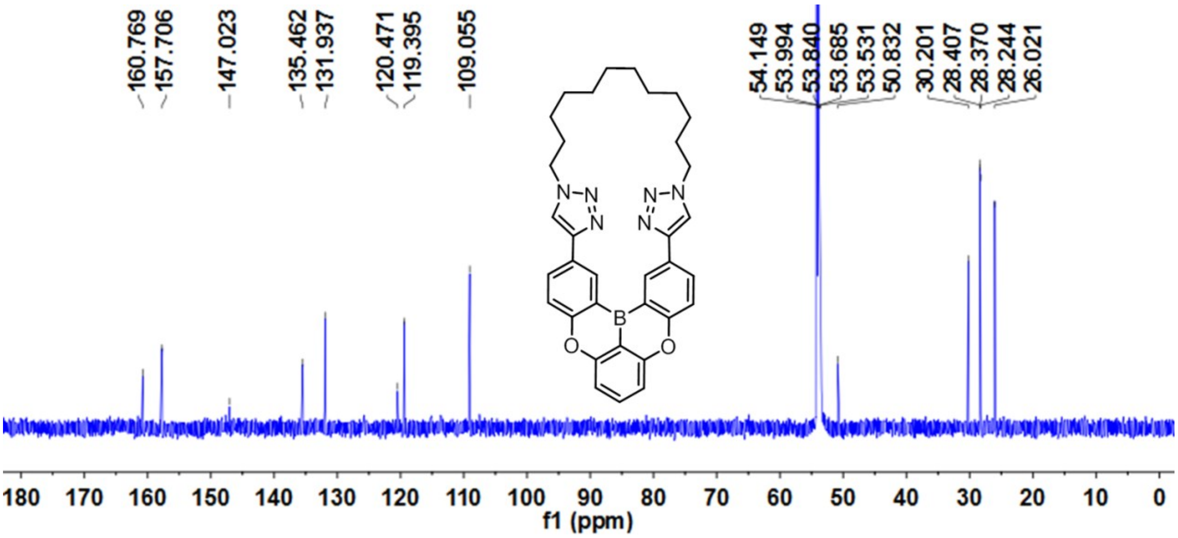


Fig. S57. ^{13}C NMR spectrum of **B5** (176 MHz, CD_2Cl_2)

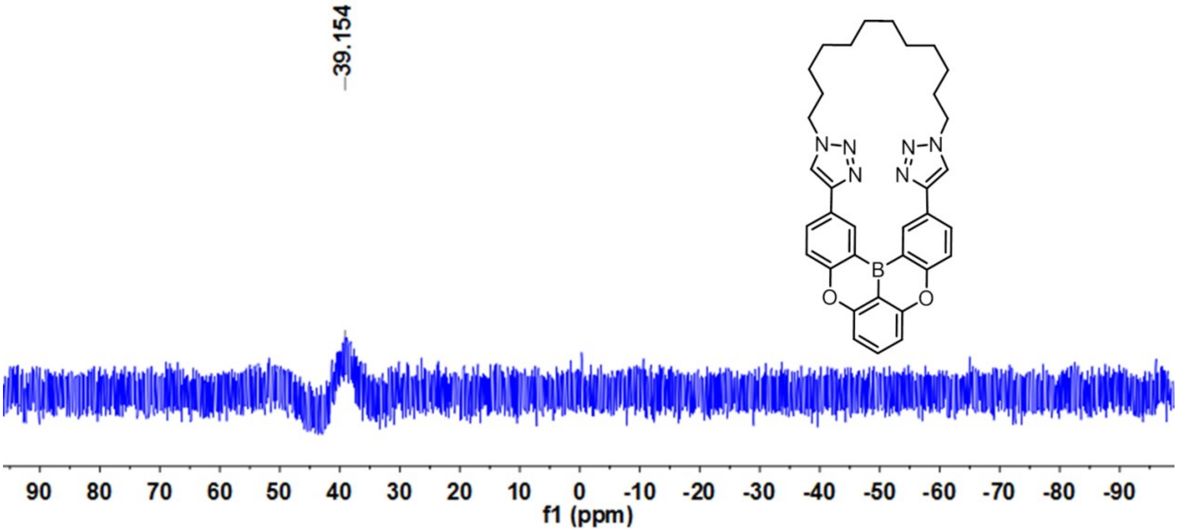


Fig. S58. ^{11}B NMR spectrum of **B5** (225 MHz, CD_2Cl_2)

S7 Crystal structure data

Table S15. X-Ray crystallographic data and structure refinement for **B1**, **B2** and **B3**.

Sample	**B1**	**B2**	**B3**
Empirical formula	$C_{60}H_{58}B_2N_{12}O_4$	$C_{60}H_{50}B_2N_8O_6$	$C_{52}H_{50}B_2N_8O_4$
Formula weight	1032.82	1007.3	872.62
Temperature	180(2) K	180(2) K	180(2) K
Wavelength	0.71073 Å	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/n$	P-1	P2(1)/n
Unit cell dimensions	a = 13.825(7) Å b = 12.616(6) Å c = 15.994(8) Å α = 90° β = 91.612(16)° γ = 90°	a = 11.763(3) Å b = 13.803(4) Å c = 17.801(5) Å α = 87.689(8)° β = 88.933(8)° γ = 86.818(8)°	a = 10.2786(4) Å b = 12.3930(5) Å c = 17.3660(6) Å α = 90° β = 92.5770(10)° γ = 90°
Volume	2788(2) Å^3	2883.0(13) Å^3	2209.89(15) Å^3
Z	56	4	4
Density (calculated)	1.306 Mg/m^3	1.251 Mg/m^3	1.311 Mg/m^3
Absorption coefficient	0.086 mm^{-1}	0.170 mm^{-1}	0.084 mm^{-1}
F(000)	1160	1132	920
Theta range for data collection	2.186 to 27.158°	2.217 to 27.251°	2.259 to 27.572°
Index ranges	-17<=h<=17 -16<=k<=16 -20<=l<=20	-15<=h<=15 -17<=k<=17 -22<=l<=22	-13<=h<=13 -16<=k<=14 -22<=l<=22
Reflections collected	32732	37939	28172
Independent reflections	6158 [R(int) = 0.1053]	12722 [R(int) = 0.1253]	5095 [R(int) = 0.0465]
Completeness to theta =	99.8 %	99.8 %	99.8 %

25.242°			
Absorption correction	Semi-empirical from equivalents		
Max/min transmission	0.759 / 0.650	0.756 / 0.654	0.756 / 0.654
Refinement method	Full-matrix least-squares on F^2		
Data/restraints/parameters	6158 / 0 / 374	12722 / 0 / 726	5095 / 20 / 298
Goodness-of-fit on F^2	1.032	0.999	1.165
Final R indices [I>2sigma(I)]	R1 = 0.0568 wR2 = 0.1287	R1 = 0.0886 wR2 = 0.2147	R1 = 0.0582 wR2 = 0.1798
R indices (all data)	R1 = 0.0901 wR2 = 0.1443	R1 = 0.2055 wR2 = 0.2557	R1 = 0.0853 wR2 = 0.2008
Extinction coefficient	n/a	n/a	n/a
Largest diff. peak and hole (e.Å^{-3})	0.505 and -0.294	0.359 and -0.387	0.887 and -0.429

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for dimer **B1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
B(1)	6441(2)	6771(2)	4700(1)	23(1)
C(1)	5928(1)	5812(2)	4183(1)	22(1)
N(1)	5635(1)	2110(1)	4071(1)	27(1)
O(1)	5560(1)	7059(1)	3038(1)	35(1)
C(2)	5498(1)	6062(2)	3402(1)	27(1)
N(2)	5328(1)	1206(1)	4446(1)	30(1)
O(2)	8190(1)	8139(1)	4882(1)	34(1)
O(3)	7559(2)	3264(2)	5189(1)	63(1)
C(3)	4958(2)	5343(2)	2923(1)	33(1)
N(3)	4440(1)	2592(1)	4824(1)	22(1)
C(4)	4831(2)	4332(2)	3213(1)	31(1)
N(4)	8298(1)	4789(1)	7985(1)	31(1)
C(5)	5256(1)	4031(2)	3978(1)	23(1)
N(5)	8189(1)	3804(1)	8320(1)	37(1)
C(6)	5806(1)	4763(2)	4439(1)	23(1)
N(6)	7826(1)	3784(1)	6937(1)	31(1)
C(7)	7309(1)	6581(2)	5380(1)	23(1)
C(8)	7348(1)	5776(2)	5983(1)	23(1)
C(9)	8100(1)	5666(2)	6579(1)	25(1)
C(10)	8856(1)	6400(2)	6582(1)	31(1)
C(11)	8854(2)	7201(2)	6000(1)	32(1)
C(12)	8091(1)	7285(2)	5417(1)	26(1)
C(13)	6826(1)	7576(2)	4020(1)	24(1)

C(14)	7635(1)	8208(2)	4153(1)	27(1)
C(15)	7940(2)	8947(2)	3573(1)	34(1)
C(16)	7428(2)	9036(2)	2820(1)	35(1)
C(17)	6634(2)	8401(2)	2643(1)	33(1)
C(18)	6354(1)	7685(2)	3244(1)	27(1)
C(19)	5112(1)	2942(2)	4293(1)	23(1)
C(20)	4608(1)	1533(2)	4888(1)	26(1)
C(21)	6478(2)	2089(2)	3533(1)	37(1)
C(22)	6301(2)	1467(2)	2748(2)	52(1)
C(23)	5508(2)	1816(3)	2172(2)	62(1)
C(24)	5442(3)	1186(3)	1358(2)	77(1)
C(25)	8077(1)	4766(2)	7157(1)	26(1)
C(26)	7910(2)	3246(2)	7666(1)	35(1)
C(27)	8475(2)	5681(2)	8556(1)	36(1)
C(28)	7710(2)	5734(2)	9216(1)	39(1)
C(29)	6692(2)	5888(2)	8858(2)	50(1)
C(30)	5930(2)	5888(3)	9512(2)	74(1)
C(31)	8252(2)	3835(3)	4737(2)	69(1)

Table 2. Bond lengths [Å] and angles [°] for dimer **B1**.

B(1)-C(13)	1.590(3)	N(2)-C(20)	1.305(3)	C(5)-C(6)	1.391(3)	C(13)-C(14)	1.385(3)
B(1)-C(7)	1.614(3)	O(2)-C(14)	1.380(2)	C(5)-C(19)	1.479(3)	C(13)-C(18)	1.393(3)
B(1)-C(1)	1.619(3)	O(2)-C(12)	1.385(2)	N(5)-C(26)	1.310(3)	C(14)-C(15)	1.390(3)
B(1)-N(3)	1.662(3)	O(3)-C(31)	1.413(4)	N(6)-C(25)	1.331(3)	C(15)-C(16)	1.385(3)
C(1)-C(6)	1.397(3)	C(3)-C(4)	1.370(3)	N(6)-C(26)	1.351(3)	C(16)-C(17)	1.382(3)
C(1)-C(2)	1.404(3)	N(3)-C(19)	1.350(2)	C(7)-C(12)	1.399(3)	C(17)-C(18)	1.382(3)
N(1)-C(19)	1.328(2)	N(3)-C(20)	1.359(3)	C(7)-C(8)	1.401(3)	C(21)-C(22)	1.495(3)
N(1)-N(2)	1.361(2)	N(3)-B(1)	1.602(3)	C(8)-C(9)	1.396(3)	C(22)-C(23)	1.479(4)
N(1)-C(21)	1.469(3)	C(4)-C(5)	1.394(3)	C(9)-C(10)	1.396(3)	C(23)-C(24)	1.526(4)
O(1)-C(18)	1.384(2)	N(4)-C(25)	1.330(2)	C(9)-C(25)	1.466(3)	C(27)-C(28)	1.516(3)
O(1)-C(2)	1.389(2)	N(4)-N(5)	1.363(2)	C(10)-C(11)	1.373(3)	C(28)-C(29)	1.516(3)
C(2)-C(3)	1.392(3)	N(4)-C(27)	1.467(3)	C(11)-C(12)	1.392(3)	C(29)-C(30)	1.505(4)

C(13)-B(1)-C(7)	107.42(16)	C(6)-C(1)-C(2)	115.00(17)
C(13)-B(1)-C(1)	106.14(15)	C(6)-C(1)-B(1)	127.81(16)
C(7)-B(1)-C(1)	122.74(16)	C(2)-C(1)-B(1)	117.08(16)
C(13)-B(1)-N(3)#1	105.54(15)	C(19)-N(1)-N(2)	111.48(16)
C(7)-B(1)-N(3)#1	107.67(14)	C(19)-N(1)-C(21)	128.16(18)
C(1)-B(1)-N(3)#1	106.17(15)	N(2)-N(1)-C(21)	120.30(16)

C(18)-O(1)-C(2)	118.37(15)	O(2)-C(12)-C(11)	112.74(17)
O(1)-C(2)-C(3)	113.48(16)	O(2)-C(12)-C(7)	123.92(17)
O(1)-C(2)-C(1)	123.13(17)	C(11)-C(12)-C(7)	123.35(18)
C(3)-C(2)-C(1)	123.38(18)	C(14)-C(13)-C(18)	115.86(17)
C(20)-N(2)-N(1)	102.99(16)	C(14)-C(13)-B(1)	123.13(17)
C(14)-O(2)-C(12)	120.51(15)	C(18)-C(13)-B(1)	121.01(17)
C(4)-C(3)-C(2)	119.47(18)	O(2)-C(14)-C(13)	121.40(17)
C(19)-N(3)-C(20)	104.43(16)	O(2)-C(14)-C(15)	115.73(18)
C(19)-N(3)-B(1)#1	131.02(16)	C(13)-C(14)-C(15)	122.87(18)
C(20)-N(3)-B(1)#1	124.52(15)	C(16)-C(15)-C(14)	118.5(2)
C(3)-C(4)-C(5)	119.72(18)	C(17)-C(16)-C(15)	121.03(19)
C(25)-N(4)-N(5)	110.01(16)	C(16)-C(17)-C(18)	118.22(19)
C(25)-N(4)-C(27)	131.06(17)	C(17)-C(18)-O(1)	116.30(17)
N(5)-N(4)-C(27)	118.17(16)	C(17)-C(18)-C(13)	123.43(19)
C(6)-C(5)-C(4)	119.62(18)	O(1)-C(18)-C(13)	120.26(17)
C(6)-C(5)-C(19)	120.77(16)	N(1)-C(19)-N(3)	107.40(17)
C(4)-C(5)-C(19)	119.61(17)	N(1)-C(19)-C(5)	124.33(17)
C(26)-N(5)-N(4)	102.08(16)	N(3)-C(19)-C(5)	128.25(17)
C(5)-C(6)-C(1)	122.73(17)	N(2)-C(20)-N(3)	113.70(18)
C(25)-N(6)-C(26)	102.96(17)	N(1)-C(21)-C(22)	112.84(19)
C(12)-C(7)-C(8)	114.57(17)	C(23)-C(22)-C(21)	117.8(2)
C(12)-C(7)-B(1)	119.53(16)	C(22)-C(23)-C(24)	113.7(3)
C(8)-C(7)-B(1)	125.86(17)	N(6)-C(25)-N(4)	109.18(17)
C(9)-C(8)-C(7)	123.75(18)	N(6)-C(25)-C(9)	124.38(17)
C(10)-C(9)-C(8)	118.66(18)	N(4)-C(25)-C(9)	126.44(18)
C(10)-C(9)-C(25)	122.73(17)	N(5)-C(26)-N(6)	115.8(2)
C(8)-C(9)-C(25)	118.58(17)	N(4)-C(27)-C(28)	111.09(19)
C(11)-C(10)-C(9)	119.84(18)	C(29)-C(28)-C(27)	113.65(18)
C(10)-C(11)-C(12)	119.82(19)	C(30)-C(29)-C(28)	113.4(2)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1

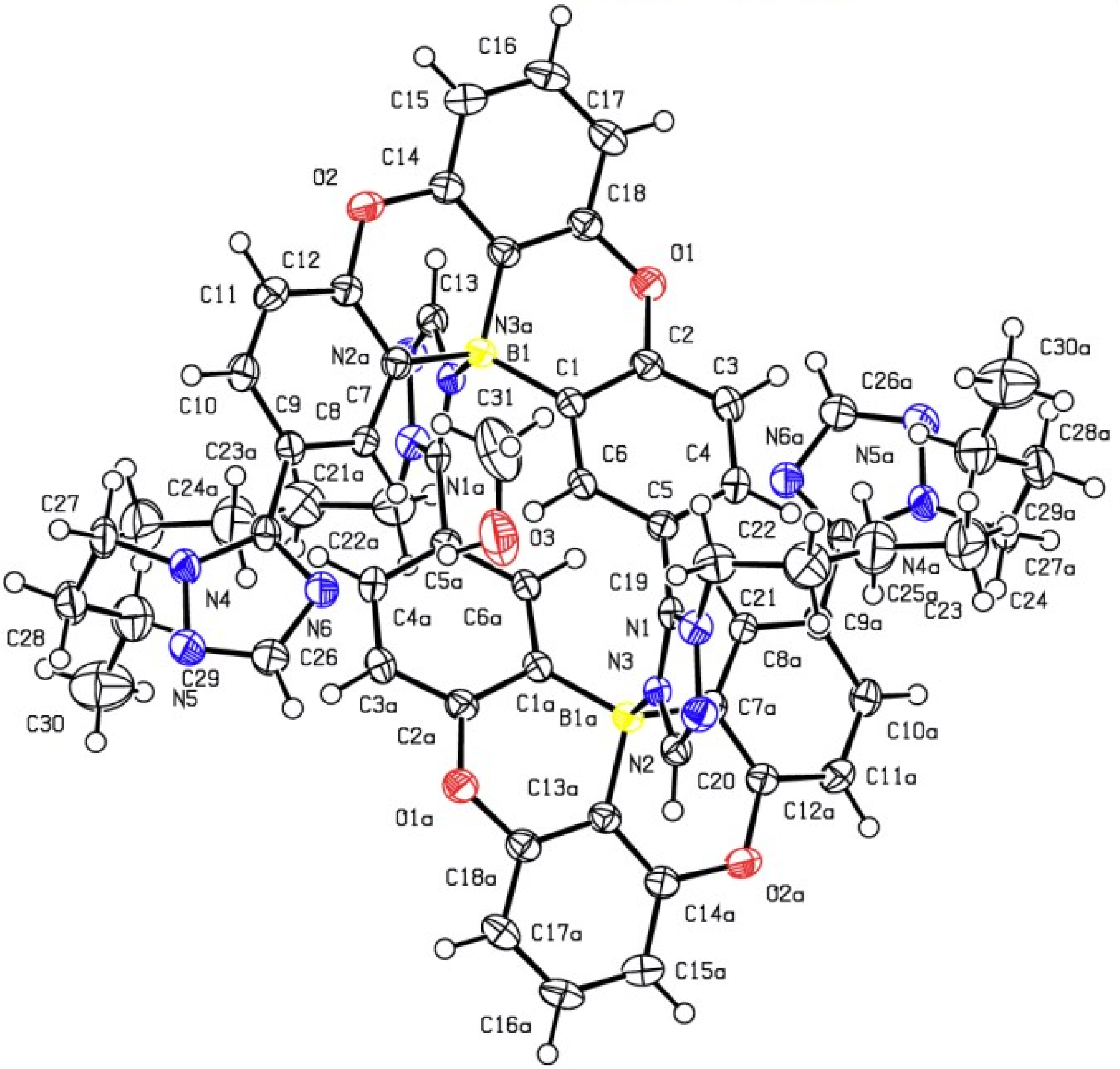
Table 3. Anisotropic displacement parameters (Å^2 x 10^3) for dimer **B1**; the anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2} U^{11}$ + ... + $2hka^* b^* U^{12}$]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	24(1)	23(1)	21(1)	2(1)	0(1)	-1(1)
C(1)	22(1)	26(1)	19(1)	1(1)	0(1)	1(1)
N(1)	25(1)	27(1)	29(1)	-1(1)	1(1)	1(1)

O(1)	39(1)	32(1)	32(1)	11(1)	-11(1)	-6(1)
C(2)	28(1)	26(1)	25(1)	5(1)	-1(1)	-1(1)
N(2)	31(1)	25(1)	33(1)	1(1)	-2(1)	2(1)
O(2)	34(1)	31(1)	35(1)	8(1)	-4(1)	-10(1)
O(3)	103(2)	48(1)	39(1)	-6(1)	-17(1)	9(1)
C(3)	37(1)	38(1)	24(1)	6(1)	-10(1)	-4(1)
N(3)	23(1)	23(1)	19(1)	1(1)	-3(1)	-2(1)
C(4)	33(1)	33(1)	25(1)	-2(1)	-6(1)	-6(1)
N(4)	38(1)	29(1)	25(1)	3(1)	-9(1)	-2(1)
C(5)	23(1)	25(1)	23(1)	-1(1)	2(1)	-1(1)
N(5)	47(1)	32(1)	31(1)	7(1)	-7(1)	-4(1)
C(6)	24(1)	27(1)	17(1)	0(1)	-1(1)	0(1)
N(6)	38(1)	27(1)	27(1)	0(1)	-3(1)	-1(1)
C(7)	24(1)	23(1)	23(1)	-2(1)	1(1)	1(1)
C(8)	24(1)	22(1)	22(1)	-2(1)	-2(1)	-2(1)
C(9)	28(1)	25(1)	22(1)	-1(1)	-3(1)	1(1)
C(10)	25(1)	37(1)	30(1)	1(1)	-7(1)	-2(1)
C(11)	26(1)	35(1)	35(1)	1(1)	-2(1)	-8(1)
C(12)	28(1)	25(1)	26(1)	2(1)	0(1)	-1(1)
C(13)	28(1)	22(1)	24(1)	2(1)	2(1)	2(1)
C(14)	27(1)	26(1)	28(1)	2(1)	2(1)	1(1)
C(15)	31(1)	29(1)	41(1)	6(1)	6(1)	-2(1)
C(16)	42(1)	29(1)	35(1)	12(1)	10(1)	3(1)
C(17)	38(1)	34(1)	27(1)	8(1)	2(1)	5(1)
C(18)	30(1)	25(1)	27(1)	3(1)	1(1)	3(1)
C(19)	22(1)	26(1)	19(1)	-2(1)	-5(1)	-2(1)
C(20)	28(1)	25(1)	24(1)	2(1)	-4(1)	0(1)
C(21)	29(1)	41(1)	42(1)	-1(1)	8(1)	4(1)
C(22)	47(2)	60(2)	50(1)	-11(1)	18(1)	-2(1)
C(23)	50(2)	84(2)	52(2)	-16(2)	6(1)	-12(2)
C(24)	88(2)	93(2)	50(2)	-17(2)	8(2)	-31(2)
C(25)	24(1)	29(1)	24(1)	0(1)	-5(1)	2(1)
C(26)	40(1)	30(1)	33(1)	3(1)	-2(1)	-2(1)
C(27)	45(1)	36(1)	27(1)	-5(1)	-12(1)	-4(1)
C(28)	48(1)	41(1)	29(1)	-2(1)	-10(1)	0(1)
C(29)	46(2)	55(2)	48(1)	2(1)	-8(1)	-2(1)
C(30)	52(2)	75(2)	94(2)	17(2)	11(2)	3(2)
C(31)	76(2)	88(2)	42(2)	-12(2)	1(1)	25(2)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for dimer **B1**.

	x	y	z	U(eq)
H(3A)	7652	3370	5704	95
H(3)	4679	5551	2398	40
H(4)	4455	3838	2895	37
H(6)	6112	4538	4948	27
H(8)	6835	5276	5987	27
H(10)	9371	6346	6986	37
H(11)	9371	7696	5996	39
H(15)	8488	9383	3690	40
H(16)	7625	9541	2418	42
H(17)	6289	8455	2122	40
H(20)	4235	1075	5222	31
H(21A)	7034	1776	3849	45
H(21B)	6652	2825	3384	45
H(22A)	6908	1467	2433	62
H(22B)	6171	723	2908	62
H(23A)	5603	2574	2038	74
H(23B)	4887	1750	2461	74
H(24A)	6070	1197	1090	115
H(24B)	4951	1506	982	115
H(24C)	5261	452	1479	115
H(26)	7774	2509	7703	42
H(27A)	8473	6351	8234	43
H(27B)	9121	5600	8833	43
H(28A)	7731	5070	9546	47
H(28B)	7866	6327	9602	47
H(29A)	6662	6569	8551	60
H(29B)	6547	5314	8451	60
H(30A)	5933	5202	9800	111
H(30B)	5294	6008	9243	111
H(30C)	6068	6454	9917	111
H(31A)	8538	4389	5094	103
H(31B)	7937	4160	4244	103
H(31C)	8761	3350	4558	103



The ORTEP diagram showing the structure of dimer **B1** with labeling schemes

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for dimer **B2**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3333(3)	7863(3)	10492(2)	39(1)
Cl(1)	6288(1)	8463(1)	3217(1)	96(1)
O(1)	2112(2)	6816(2)	9864(2)	51(1)
N(1)	8619(3)	6362(3)	11755(2)	55(1)
B(1)	4316(4)	7010(3)	10558(2)	35(1)
C(2)	2312(4)	7731(3)	10158(2)	45(1)
Cl(2)	6169(2)	6384(1)	3224(1)	152(1)
O(2)	4468(3)	9024(2)	11060(2)	56(1)
N(2)	6168(3)	4852(2)	7873(2)	45(1)

B(2)	3940(4)	917(3)	3599(2)	37(1)
N(3)	6932(3)	4140(3)	7648(2)	51(1)
C(3)	1440(4)	8437(3)	10061(2)	60(1)
O(3)	8633(3)	7110(2)	10571(2)	56(1)
O(4)	6143(3)	818(2)	2810(1)	51(1)
C(4)	1619(5)	9338(4)	10317(3)	68(1)
N(4)	6020(3)	3694(2)	8702(2)	37(1)
N(5)	326(3)	830(3)	5661(2)	51(1)
C(5)	2665(4)	9542(3)	10648(3)	58(1)
O(5)	2206(3)	1918(2)	2612(2)	62(1)
O(6)	1251(3)	2254(2)	5645(2)	57(1)
C(6)	3471(4)	8786(3)	10734(2)	44(1)
N(6)	6740(3)	1745(2)	6286(2)	43(1)
N(7)	6764(3)	1584(3)	7043(2)	51(1)
C(7)	5477(3)	7505(3)	10702(2)	36(1)
N(8)	6370(3)	242(2)	6472(2)	35(1)
C(8)	5450(4)	8469(3)	10940(2)	48(1)
C(9)	6457(5)	8942(3)	11072(3)	69(1)
C(10)	7490(4)	8499(4)	10969(3)	66(1)
C(12)	6592(4)	7075(3)	10603(2)	40(1)
C(11)	7549(4)	7547(3)	10726(2)	47(1)
C(13)	4153(3)	6359(3)	9826(2)	35(1)
C(15)	2761(4)	5686(3)	8998(2)	47(1)
C(14)	3027(4)	6291(3)	9562(2)	41(1)
C(17)	4716(3)	5200(3)	8862(2)	36(1)
C(16)	3610(4)	5135(3)	8648(2)	42(1)
C(18)	4983(3)	5811(3)	9431(2)	35(1)
C(19)	9087(4)	6424(3)	11080(2)	48(1)
C(20)	9995(4)	5861(3)	10822(3)	56(1)
C(21)	10480(4)	5159(4)	11291(3)	56(1)
C(23)	9107(5)	5672(4)	12213(3)	71(2)
C(22)	10027(5)	5061(4)	12013(3)	72(2)
C(24)	11482(5)	4494(4)	11054(3)	89(2)
C(25)	5626(3)	4597(3)	8497(2)	35(1)
C(26)	6794(4)	3448(3)	8159(2)	47(1)
C(27)	6100(5)	5786(4)	7439(2)	67(1)
C(28)	5476(7)	5673(6)	6708(4)	136(3)
C(29)	5686(9)	6332(7)	6131(4)	169(4)
C(30)	5389(11)	6249(6)	5399(4)	202(6)

C(31)	4129(4)	1302(3)	2758(2)	42(1)
C(32)	5214(4)	1198(3)	2409(2)	45(1)
C(33)	5410(4)	1447(3)	1657(2)	52(1)
C(34)	4489(5)	1804(3)	1241(2)	55(1)
C(35)	3426(5)	1949(3)	1558(2)	58(1)
C(36)	3274(4)	1721(3)	2317(2)	45(1)
C(37)	2795(3)	1496(3)	3914(2)	38(1)
C(38)	2063(4)	1955(3)	3399(2)	48(1)
C(39)	1042(4)	2477(4)	3609(3)	68(1)
C(40)	776(4)	2548(4)	4347(3)	63(1)
C(41)	1500(4)	2129(3)	4879(2)	50(1)
C(42)	2481(3)	1615(3)	4674(2)	43(1)
C(43)	5133(3)	932(2)	4019(2)	31(1)
C(44)	6122(4)	825(3)	3591(2)	40(1)
C(45)	7214(4)	733(3)	3892(2)	47(1)
C(46)	7335(4)	743(3)	4651(2)	44(1)
C(47)	6382(3)	892(2)	5113(2)	31(1)
C(48)	5320(3)	989(2)	4796(2)	33(1)
C(49)	693(4)	1548(3)	6035(3)	52(1)
C(50)	504(4)	1686(4)	6795(3)	62(1)
C(51)	-73(4)	1029(5)	7196(3)	76(2)
C(52)	-483(4)	238(4)	6829(3)	71(1)
C(53)	-247(4)	169(4)	6066(3)	58(1)
C(54)	-372(6)	1152(6)	8025(3)	117(3)
C(55)	6507(3)	937(3)	5936(2)	36(1)
C(56)	6544(4)	676(3)	7137(2)	45(1)
C(57)	6907(4)	2718(3)	5951(2)	49(1)
C(58)	8097(4)	3013(3)	5985(3)	63(1)
C(59)	8279(6)	4020(4)	5686(4)	83(2)
C(60)	9279(8)	4442(6)	5862(5)	97(3)
C(61)	6362(7)	7405(4)	2733(4)	118(3)
C(60A)	8020(20)	4370(20)	5054(16)	135(10)

Table 2. Bond lengths [Å] and angles [°] for dimer **B2**.

C(1)-C(2)	1.375(6)
C(1)-C(36)	1.380(5)
C(1)-B(1)	1.606(6)
Cl(1)-C(61)	1.722(6)

O(1)-C(14)	1.377(5)	O(4)-C(44)	1.391(4)	C(10)-C(11)	1.397(6)	C(37)-C(38)	1.379(5)
O(1)-C(2)	1.418(5)	C(4)-C(5)	1.421(7)	C(12)-C(11)	1.357(6)	C(37)-C(42)	1.411(5)
N(1)-C(19)	1.314(5)	N(4)-C(25)	1.344(5)	C(13)-C(18)	1.398(5)	C(38)-C(39)	1.418(6)
N(1)-C(23)	1.340(6)	N(4)-C(26)	1.355(5)	C(13)-C(14)	1.420(6)	C(39)-C(40)	1.351(6)
B(1)-C(7)	1.591(6)	N(4)-B(1)#1	1.659(5)	C(15)-C(16)	1.376(6)	C(40)-C(41)	1.374(6)
B(1)-C(13)	1.632(5)	N(5)-C(49)	1.312(5)	C(15)-C(14)	1.383(5)	C(41)-C(42)	1.373(6)
B(1)-N(4)#1	1.659(5)	N(5)-C(53)	1.343(6)	C(17)-C(16)	1.372(5)	C(43)-C(44)	1.383(5)
C(2)-C(3)	1.383(6)	C(5)-C(6)	1.376(6)	C(17)-C(18)	1.395(5)	C(43)-C(48)	1.412(5)
Cl(2)-C(61)	1.651(6)	O(5)-C(36)	1.375(5)	C(17)-C(12)	1.476(5)	C(44)-C(45)	1.398(6)
O(2)-C(8)	1.369(5)	O(5)-C(38)	1.410(5)	C(19)-C(20)	1.370(6)	C(45)-C(46)	1.364(5)
O(2)-C(6)	1.379(5)	O(6)-C(49)	1.364(5)	C(20)-C(21)	1.364(6)	C(46)-C(47)	1.389(5)
N(2)-C(25)	1.346(5)	O(6)-C(41)	1.404(5)	C(21)-C(22)	1.384(7)	C(47)-C(48)	1.378(5)
N(2)-N(3)	1.363(4)	N(6)-C(55)	1.343(5)	C(21)-C(24)	1.517(6)	C(47)-C(56)	1.479(5)
N(2)-C(27)	1.474(5)	N(6)-N(7)	1.357(4)	C(23)-C(22)	1.385(7)	C(49)-C(50)	1.386(6)
B(2)-C(31)	1.583(6)	N(6)-C(57)	1.470(5)	C(27)-C(28)	1.523(8)	C(50)-C(51)	1.339(7)
B(2)-C(43)	1.603(6)	N(7)-C(56)	1.298(5)	C(28)-C(29)	1.372(10)	C(51)-C(52)	1.408(7)
B(2)-C(37)	1.630(6)	C(7)-C(8)	1.410(5)	C(29)-C(30)	1.367(10)	C(51)-C(54)	1.524(7)
B(2)-N(8)#2	1.670(5)	C(7)-C(12)	1.420(5)	C(31)-C(36)	1.375(6)	C(52)-C(53)	1.387(6)
N(3)-C(26)	1.307(5)	N(8)-C(55)	1.340(5)	C(31)-C(32)	1.411(6)	C(57)-C(58)	1.483(6)
C(3)-C(4)	1.370(7)	N(8)-C(56)	1.372(5)	C(32)-C(33)	1.387(5)	C(58)-C(59)	1.493(7)
O(3)-C(19)	1.327(5)	N(8)-B(2)#2	1.670(5)	C(33)-C(34)	1.381(6)	C(59)-C(60A)	1.24(3)
O(3)-C(11)	1.408(5)	C(8)-C(9)	1.412(6)	C(34)-C(35)	1.370(7)	C(59)-C(60)	1.387(10
O(4)-C(32)	1.384(5)	C(9)-C(10)	1.344(6)	C(35)-C(36)	1.384(6)		

C(2)-C(1)-C(6)	115.5(4)	C(8)-O(2)-C(6)	119.8(3)
C(2)-C(1)-B(1)	121.9(4)	C(25)-N(2)-N(3)	111.9(3)
C(6)-C(1)-B(1)	1 22.6(4)	C(25)-N(2)-C(27)	129.4(4)
C(14)-O(1)-C(2)	117.8(3)	N(3)-N(2)-C(27)	118.6(3)
C(19)-N(1)-C(23)	114.3(4)	C(31)-B(2)-C(43)	107.8(3)
C(7)-B(1)-C(1)	107.3(3)	C(31)-B(2)-C(37)	106.6(3)
C(7)-B(1)-C(13)	121.7(3)	C(43)-B(2)-C(37)	121.7(3)
C(1)-B(1)-C(13)	104.7(3)	C(31)-B(2)-N(8)#2	104.6(3)
C(7)-B(1)-N(4)#1	109.9(3)	C(43)-B(2)-N(8)#2	107.9(3)
C(1)-B(1)-N(4)#1	106.7(3)	C(37)-B(2)-N(8)#2	107.0(3)
C(13)-B(1)-N(4)#1	105.6(3)	C(26)-N(3)-N(2)	102.4(3)
C(1)-C(2)-C(3)	125.1(4)	C(4)-C(3)-C(2)	116.9(5)
C(1)-C(2)-O(1)	119.5(3)	C(19)-O(3)-C(11)	118.5(3)
C(3)-C(2)-O(1)	115.4(4)	C(32)-O(4)-C(44)	119.9(3)

C(3)-C(4)-C(5)	121.4(4)	C(18)-C(17)-C(25)	119.9(4)
C(25)-N(4)-C(26)	104.7(3)	C(17)-C(16)-C(15)	119.2(4)
C(25)-N(4)-B(1)#1	130.1(3)	C(17)-C(18)-C(13)	122.6(4)
C(26)-N(4)-B(1)#1	125.2(3)	N(1)-C(19)-C(20)	126.2(4)
C(49)-N(5)-C(53)	116.0(4)	N(1)-C(19)-O(3)	118.3(4)
C(6)-C(5)-C(4)	117.3(4)	C(20)-C(19)-O(3)	115.5(4)
C(36)-O(5)-C(38)	119.0(3)	C(21)-C(20)-C(19)	118.9(4)
C(49)-O(6)-C(41)	118.4(3)	C(20)-C(21)-C(22)	117.6(4)
C(5)-C(6)-O(2)	114.8(4)	C(20)-C(21)-C(24)	122.7(5)
C(5)-C(6)-C(1)	123.7(4)	C(22)-C(21)-C(24)	119.7(5)
O(2)-C(6)-C(1)	121.4(4)	N(1)-C(23)-C(22)	124.5(5)
C(55)-N(6)-N(7)	111.2(3)	C(23)-C(22)-C(21)	118.5(5)
C(55)-N(6)-C(57)	128.1(3)	N(2)-C(25)-N(4)	107.4(3)
N(7)-N(6)-C(57)	120.6(3)	N(2)-C(25)-C(17)	124.5(3)
C(56)-N(7)-N(6)	103.9(3)	N(4)-C(25)-C(17)	128.1(3)
C(8)-C(7)-C(12)	114.1(4)	N(3)-C(26)-N(4)	113.5(4)
C(8)-C(7)-B(1)	119.6(4)	N(2)-C(27)-C(28)	109.9(5)
C(12)-C(7)-B(1)	126.3(3)	C(29)-C(28)-C(27)	116.7(7)
C(55)-N(8)-C(56)	105.2(3)	C(30)-C(29)-C(28)	125.4(9)
C(55)-N(8)-B(2)#2	130.1(3)	C(36)-C(31)-C(32)	115.8(4)
C(56)-N(8)-B(2)#2	124.6(3)	C(36)-C(31)-B(2)	123.8(4)
O(2)-C(8)-C(7)	123.9(4)	C(32)-C(31)-B(2)	120.3(4)
O(2)-C(8)-C(9)	114.3(4)	O(4)-C(32)-C(33)	116.4(4)
C(7)-C(8)-C(9)	121.8(4)	O(4)-C(32)-C(31)	120.7(3)
C(10)-C(9)-C(8)	121.5(4)	C(33)-C(32)-C(31)	122.9(4)
C(9)-C(10)-C(11)	118.2(4)	C(34)-C(33)-C(32)	117.4(4)
C(11)-C(12)-C(7)	123.1(4)	C(35)-C(34)-C(33)	121.9(4)
C(12)-C(11)-C(10)	121.3(4)	C(34)-C(35)-C(36)	118.8(4)
C(12)-C(11)-O(3)	120.7(4)	O(5)-C(36)-C(31)	120.7(3)
C(10)-C(11)-O(3)	117.9(4)	O(5)-C(36)-C(35)	116.4(4)
C(18)-C(13)-C(14)	114.2(3)	C(31)-C(36)-C(35)	122.8(4)
C(18)-C(13)-B(1)	128.2(4)	C(38)-C(37)-C(42)	115.1(4)
C(14)-C(13)-B(1)	117.5(3)	C(38)-C(37)-B(2)	118.3(3)
C(16)-C(15)-C(14)	120.0(4)	C(42)-C(37)-B(2)	126.5(3)
O(1)-C(14)-C(15)	114.9(4)	C(37)-C(38)-O(5)	124.4(4)
O(1)-C(14)-C(13)	122.0(3)	C(37)-C(38)-C(39)	123.2(4)
C(15)-C(14)-C(13)	123.1(4)	O(5)-C(38)-C(39)	112.4(4)
C(16)-C(17)-C(18)	120.7(4)	C(40)-C(39)-C(38)	118.9(4)
C(16)-C(17)-C(25)	119.3(3)	C(39)-C(40)-C(41)	119.9(4)

C(42)-C(41)-C(40)	121.1(4)	N(5)-C(49)-C(50)	125.3(5)
C(42)-C(41)-O(6)	119.3(4)	O(6)-C(49)-C(50)	116.3(4)
C(40)-C(41)-O(6)	119.5(4)	C(51)-C(50)-C(49)	118.5(5)
C(41)-C(42)-C(37)	121.8(4)	C(50)-C(51)-C(52)	118.9(5)
C(44)-C(43)-C(48)	113.9(3)	C(50)-C(51)-C(54)	121.9(5)
C(44)-C(43)-B(2)	118.0(3)	C(52)-C(51)-C(54)	119.1(5)
C(48)-C(43)-B(2)	128.0(3)	C(53)-C(52)-C(51)	118.0(5)
C(43)-C(44)-O(4)	123.7(4)	N(5)-C(53)-C(52)	123.3(4)
C(43)-C(44)-C(45)	124.0(3)	N(8)-C(55)-N(6)	106.9(3)
O(4)-C(44)-C(45)	112.3(3)	N(8)-C(55)-C(47)	129.1(3)
C(46)-C(45)-C(44)	119.3(4)	N(6)-C(55)-C(47)	124.0(3)
C(45)-C(46)-C(47)	119.8(4)	N(7)-C(56)-N(8)	112.8(3)
C(48)-C(47)-C(46)	119.3(3)	N(6)-C(57)-C(58)	113.6(4)
C(48)-C(47)-C(55)	120.5(3)	C(57)-C(58)-C(59)	114.8(4)
C(46)-C(47)-C(55)	120.3(3)	C(60A)-C(59)-C(58)	126.7(16)
C(47)-C(48)-C(43)	123.6(3)	C(60)-C(59)-C(58)	118.4(7)
N(5)-C(49)-O(6)	118.2(4)	Cl(2)-C(61)-Cl(1)	117.2(4)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+2
#2 -x+1, -y, -z+1

Table 3. Anisotropic displacement parameters ($Å^2$ x 10^3) for dimer **B2**; the anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2}U^{11} + ... + 2hka^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	42(3)	36(2)	37(2)	0(2)	4(2)	9(2)
Cl(1)	91(1)	90(1)	108(1)	-33(1)	-10(1)	16(1)
O(1)	37(2)	52(2)	66(2)	-13(2)	1(1)	0(1)
N(1)	53(2)	67(3)	47(2)	-5(2)	-6(2)	2(2)
B(1)	40(3)	31(2)	35(2)	-1(2)	3(2)	-3(2)
C(2)	46(3)	47(3)	42(2)	-7(2)	3(2)	6(2)
Cl(2)	206(3)	100(1)	148(2)	-6(1)	82(2)	-17(1)
O(2)	59(2)	42(2)	67(2)	-18(2)	-9(2)	11(2)
N(2)	59(2)	46(2)	29(2)	-1(2)	4(2)	-1(2)
B(2)	48(3)	35(3)	29(2)	0(2)	-3(2)	-8(2)
N(3)	61(3)	49(2)	42(2)	-7(2)	15(2)	-7(2)
C(3)	61(3)	59(3)	60(3)	-8(2)	-5(2)	19(3)
O(3)	48(2)	60(2)	60(2)	6(2)	6(2)	-4(2)
O(4)	59(2)	65(2)	28(1)	2(1)	1(1)	10(2)
C(4)	67(4)	55(3)	78(3)	-2(3)	5(3)	27(3)

N(4)	44(2)	39(2)	29(2)	-4(1)	3(2)	3(2)
N(5)	43(2)	54(2)	57(2)	-9(2)	-9(2)	4(2)
C(5)	55(3)	46(3)	72(3)	-7(2)	-2(2)	6(2)
O(5)	57(2)	84(2)	43(2)	9(2)	-19(2)	4(2)
O(6)	46(2)	59(2)	66(2)	-24(2)	3(2)	1(2)
C(6)	47(3)	37(2)	48(2)	-6(2)	2(2)	4(2)
N(6)	56(2)	39(2)	36(2)	-2(2)	-5(2)	-6(2)
N(7)	72(3)	47(2)	35(2)	-3(2)	-10(2)	-4(2)
C(7)	41(3)	36(2)	31(2)	4(2)	-1(2)	0(2)
N(8)	40(2)	34(2)	31(2)	1(1)	-5(1)	-3(1)
C(8)	55(3)	41(3)	48(2)	-4(2)	-2(2)	-1(2)
C(9)	68(4)	40(3)	99(4)	-19(3)	-7(3)	-5(3)
C(10)	43(3)	59(3)	98(4)	-7(3)	-3(3)	-16(3)
C(12)	48(3)	37(2)	34(2)	1(2)	2(2)	-9(2)
C(11)	44(3)	48(3)	48(2)	-3(2)	2(2)	2(2)
C(13)	43(3)	32(2)	29(2)	2(2)	1(2)	1(2)
C(15)	44(3)	45(2)	52(2)	-4(2)	-8(2)	-4(2)
C(14)	41(3)	42(2)	39(2)	3(2)	6(2)	1(2)
C(17)	49(3)	32(2)	25(2)	1(2)	-3(2)	-1(2)
C(16)	48(3)	41(2)	35(2)	-4(2)	-9(2)	2(2)
C(18)	42(2)	36(2)	28(2)	6(2)	-4(2)	-1(2)
C(19)	38(3)	53(3)	54(3)	-3(2)	-3(2)	-4(2)
C(20)	45(3)	62(3)	61(3)	-10(2)	3(2)	-7(2)
C(21)	44(3)	63(3)	61(3)	-13(3)	-7(2)	1(2)
C(23)	72(4)	92(4)	49(3)	-3(3)	-7(3)	7(3)
C(22)	65(4)	73(4)	78(4)	3(3)	-20(3)	8(3)
C(24)	61(4)	107(5)	100(4)	-40(4)	-13(3)	25(3)
C(25)	45(3)	38(2)	23(2)	-3(2)	-4(2)	-6(2)
C(26)	57(3)	43(3)	42(2)	-7(2)	8(2)	-1(2)
C(27)	84(4)	63(3)	52(3)	19(2)	16(3)	-3(3)
C(28)	168(8)	136(6)	105(5)	72(5)	-56(5)	-43(6)
C(29)	237(12)	182(9)	92(6)	39(6)	-51(6)	-54(8)
C(30)	385(18)	121(7)	101(6)	17(5)	-77(8)	-2(9)
C(31)	54(3)	40(2)	33(2)	-3(2)	-8(2)	-5(2)
C(32)	64(3)	41(2)	31(2)	-1(2)	-5(2)	-4(2)
C(33)	70(3)	46(3)	39(2)	0(2)	3(2)	-6(2)
C(34)	91(4)	44(3)	29(2)	10(2)	-10(2)	-10(3)
C(35)	87(4)	46(3)	40(3)	10(2)	-28(3)	-5(3)
C(36)	57(3)	40(2)	39(2)	6(2)	-12(2)	-7(2)

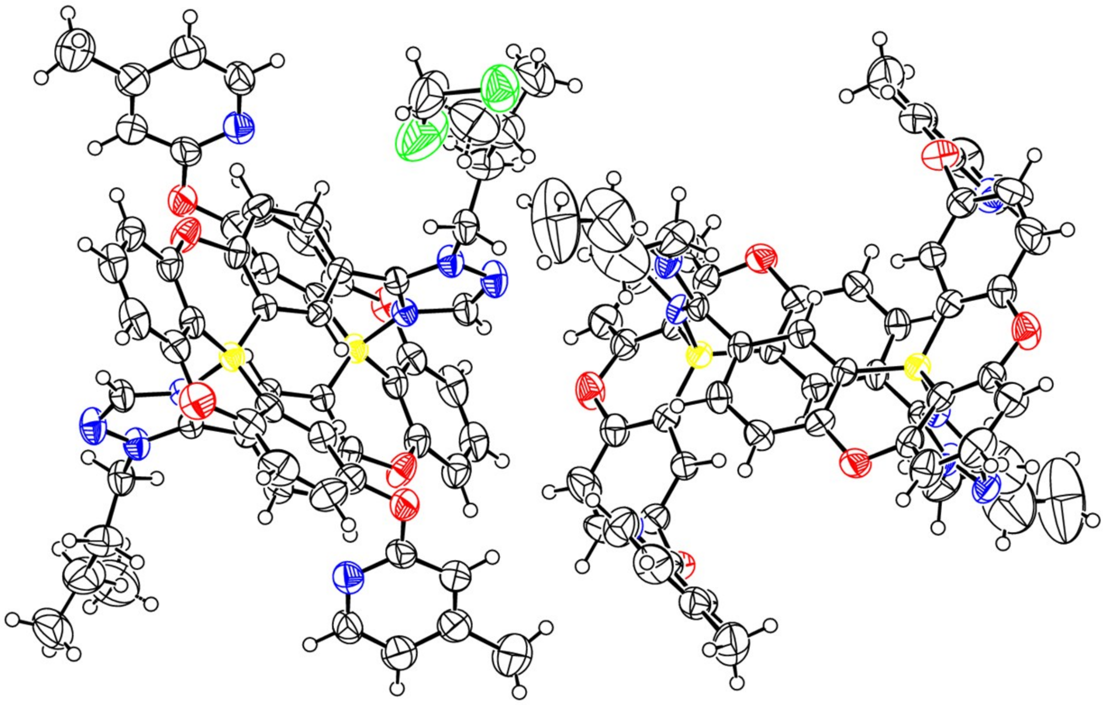
C(37)	38(2)	34(2)	44(2)	0(2)	-11(2)	-3(2)
C(38)	45(3)	46(3)	55(3)	1(2)	-8(2)	-7(2)
C(39)	48(3)	70(3)	85(4)	5(3)	-17(3)	12(3)
C(40)	49(3)	67(3)	70(3)	-1(3)	7(3)	11(2)
C(41)	42(3)	48(3)	59(3)	-9(2)	0(2)	3(2)
C(42)	44(3)	39(2)	45(2)	-4(2)	-8(2)	3(2)
C(43)	37(2)	26(2)	31(2)	2(2)	-3(2)	-1(2)
C(44)	56(3)	40(2)	25(2)	1(2)	-2(2)	2(2)
C(45)	34(3)	65(3)	40(2)	-2(2)	8(2)	4(2)
C(46)	40(3)	51(3)	39(2)	0(2)	-10(2)	6(2)
C(47)	37(2)	25(2)	30(2)	3(2)	1(2)	-1(2)
C(48)	36(2)	29(2)	34(2)	-1(2)	2(2)	0(2)
C(49)	31(3)	60(3)	68(3)	-19(3)	-5(2)	1(2)
C(50)	47(3)	79(4)	62(3)	-21(3)	2(2)	-8(3)
C(51)	49(3)	123(5)	57(3)	-21(3)	-6(3)	-13(3)
C(52)	60(3)	97(4)	55(3)	-6(3)	-4(2)	-12(3)
C(53)	48(3)	65(3)	61(3)	-17(3)	-10(2)	-2(2)
C(54)	114(6)	188(8)	53(3)	-20(4)	5(3)	-43(5)
C(55)	34(2)	35(2)	38(2)	-6(2)	-6(2)	4(2)
C(56)	60(3)	42(3)	34(2)	-5(2)	-4(2)	-10(2)
C(57)	69(3)	37(2)	42(2)	-5(2)	-2(2)	-3(2)
C(58)	53(3)	55(3)	80(3)	6(3)	5(3)	-3(2)
C(59)	88(5)	61(4)	100(5)	2(3)	20(4)	-13(3)
C(60)	117(8)	81(6)	98(6)	-7(5)	2(5)	-49(6)
C(61)	166(7)	74(4)	116(5)	-32(4)	61(5)	-21(4)
C(60A)	81(18)	190(30)	140(20)	-20(20)	-32(16)	-11(18)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for dimer **B2**.

	x	y	z	U(eq)
H(3)	749	8303	9828	73
H(4)	1032	9837	10272	81
H(5)	2803	10175	10804	69
H(9)	6402	9589	11238	82
H(10)	8163	8823	11060	79
H(12)	6672	6426	10444	47
H(15)	1992	5652	8851	56
H(16)	3431	4715	8262	50
H(18)	5760	5856	9555	42

H(20)	10282	5958	10324	67
H(23)	8801	5597	12708	85
H(22)	10341	4586	12363	87
H(24A)	11203	3951	10785	134
H(24B)	11894	4244	11501	134
H(24C)	11994	4858	10723	134
H(26)	7197	2833	8151	57
H(27A)	6877	5998	7326	80
H(27B)	5690	6287	7739	80
H(28A)	5675	5014	6529	164
H(28B)	4648	5712	6821	164
H(29A)	5333	6961	6289	203
H(29B)	6519	6403	6124	203
H(30A)	5890	5750	5167	304
H(30B)	5467	6873	5125	304
H(30C)	4598	6065	5380	304
H(33)	6150	1374	1436	62
H(34)	4595	1953	720	66
H(35)	2805	2202	1263	69
H(39)	553	2773	3237	82
H(40)	89	2886	4498	75
H(42)	2962	1330	5056	51
H(45)	7865	665	3570	56
H(46)	8070	648	4865	53
H(48)	4677	1101	5119	40
H(50)	779	2234	7026	74
H(52)	-909	-234	7095	85
H(53)	-503	-373	5817	69
H(54A)	77	1659	8222	175
H(54B)	-200	538	8307	175
H(54C)	-1185	1337	8080	175
H(56)	6507	347	7616	54
H(57A)	6402	3197	6215	59
H(57B)	6676	2734	5418	59
H(58A)	8593	2553	5698	75
H(58B)	8339	2959	6516	75
H(59A)	8237	4017	5131	100
H(59B)	7634	4447	5864	100
H(60A)	9931	3994	5753	145

H(60B)	9266	4584	6397	145
H(60C)	9345	5047	5560	145
H(61A)	5786	7469	2334	142
H(61B)	7119	7344	2482	142
H(60D)	8222	5046	5011	203
H(60E)	7199	4331	4985	203
H(60F)	8435	3996	4668	203



The ORTEP diagram showing the structure of dimer **B2** with labeling schemes

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for dimer **B3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	1608(1)	3157(1)	4943(1)	39(1)
N(3)	5108(1)	7489(1)	4634(1)	24(1)
N(4)	3710(1)	8019(1)	5442(1)	26(1)
N(2)	4404(1)	8919(1)	5279(1)	29(1)
O(2)	3622(2)	1575(1)	7219(1)	56(1)
C(21)	4114(2)	7166(1)	5059(1)	23(1)
C(22)	5230(2)	8564(1)	4790(1)	26(1)
C(3)	3471(2)	6102(1)	5069(1)	23(1)

C(8)	2730(2)	2391(1)	6056(1)	32(1)
C(7)	1686(2)	2393(2)	5518(1)	36(1)
C(13)	4723(2)	3234(2)	6798(1)	32(1)
C(2)	3953(2)	5264(1)	5533(1)	23(1)
C(1)	3405(2)	4230(1)	5523(1)	24(1)
C(6)	2287(2)	4117(1)	5036(1)	28(1)
C(18)	5618(2)	4026(2)	7029(1)	35(1)
C(23)	2771(2)	8074(2)	6059(1)	35(1)
C(14)	4489(2)	2429(2)	7343(1)	42(1)
C(4)	2361(2)	5941(2)	4600(1)	32(1)
C(5)	1761(2)	4954(2)	4591(1)	36(1)
N(1)	7101(2)	4897(2)	7956(1)	64(1)
C(16)	6001(2)	3223(2)	8271(1)	56(1)
C(9)	2678(2)	1628(2)	6640(1)	43(1)
C(12)	688(2)	1640(2)	5510(1)	48(1)
C(15)	5133(2)	2425(2)	8059(1)	56(1)
C(17)	6255(2)	4066(2)	7756(1)	44(1)
C(11)	715(3)	877(2)	6091(2)	58(1)
C(10)	1670(3)	866(2)	6663(2)	56(1)
B(1)	3948(2)	3165(2)	5972(1)	28(1)
C(24)	3422(2)	8495(2)	6799(1)	51(1)
C(25)	4643(2)	7892(2)	7089(1)	64(1)
C(20)	7228(3)	5791(3)	7467(2)	74(1)
C(26)	5221(3)	8410(3)	7818(1)	93(1)
C(19)	7793(3)	4918(3)	8695(2)	97(1)

Table 2. Bond lengths [Å] and angles [°] for dimer **B3**.

O(1)-C(7)	1.377(2)	N(2)-C(22)	1.305(2)
O(1)-C(6)	1.385(2)	O(2)-C(9)	1.366(3)
N(3)-C(21)	1.349(2)	O(2)-C(14)	1.395(3)
N(3)-C(22)	1.364(2)	C(21)-C(3)	1.476(2)
N(3)-B(1)#1	1.672(2)	C(22)-H(22A)	0.9500
N(4)-C(21)	1.325(2)	C(3)-C(4)	1.386(2)
N(4)-N(2)	1.3606(19)	C(3)-C(2)	1.391(2)
N(4)-C(23)	1.475(2)	C(8)-C(7)	1.390(3)

C(8)-C(9)	1.391(3)	C(16)-C(17)	1.408(4)
C(8)-B(1)	1.588(3)	C(16)-H(16A)	0.9500
C(7)-C(12)	1.386(3)	C(9)-C(10)	1.403(3)
C(13)-C(18)	1.392(3)	C(12)-C(11)	1.383(3)
C(13)-C(14)	1.404(3)	C(12)-H(12A)	0.9500
C(13)-B(1)	1.611(3)	C(15)-H(15A)	0.9500
C(2)-C(1)	1.400(2)	C(11)-C(10)	1.365(4)
C(2)-H(2B)	0.9500	C(11)-H(11A)	0.9500
C(1)-C(6)	1.402(2)	C(10)-H(10A)	0.9500
C(1)-B(1)	1.620(3)	C(24)-C(25)	1.5267(10)
C(6)-C(5)	1.390(3)	C(24)-H(24A)	0.9900
C(18)-C(17)	1.397(3)	C(24)-H(24B)	0.9900
C(18)-H(18A)	0.9500	C(25)-C(26)	1.518(3)
C(23)-C(24)	1.514(3)	C(25)-H(25A)	0.9900
C(23)-H(23A)	0.9900	C(25)-H(25B)	0.9900
C(23)-H(23B)	0.9900	C(20)-H(20A)	0.9800
C(14)-C(15)	1.381(3)	C(20)-H(20B)	0.9800
C(4)-C(5)	1.369(3)	C(20)-H(20C)	0.9800
C(4)-H(4A)	0.9500	C(26)-H(26A)	0.9800
C(5)-H(5A)	0.9500	C(26)-H(26B)	0.9800
N(1)-C(17)	1.383(3)	C(26)-H(26C)	0.9800
N(1)-C(20)	1.406(4)	C(19)-H(19A)	0.9800
N(1)-C(19)	1.439(3)	C(19)-H(19B)	0.9800
C(16)-C(15)	1.371(4)	C(19)-H(19C)	0.9800

C(7)-O(1)-C(6)	119.52(14)	N(3)-C(22)-H(22A)	123.1
C(21)-N(3)-C(22)	104.20(14)	C(4)-C(3)-C(2)	119.68(15)
C(21)-N(3)-B(1)#1	132.56(13)	C(4)-C(3)-C(21)	118.65(15)
C(22)-N(3)-B(1)#1	123.23(13)	C(2)-C(3)-C(21)	121.68(14)
C(21)-N(4)-N(2)	111.74(13)	C(7)-C(8)-C(9)	115.91(17)
C(21)-N(4)-C(23)	129.17(14)	C(7)-C(8)-B(1)	121.74(16)
N(2)-N(4)-C(23)	118.62(13)	C(9)-C(8)-B(1)	122.24(18)
C(22)-N(2)-N(4)	102.78(13)	O(1)-C(7)-C(12)	115.83(19)
C(9)-O(2)-C(14)	120.34(15)	O(1)-C(7)-C(8)	120.41(15)
N(4)-C(21)-N(3)	107.51(14)	C(12)-C(7)-C(8)	123.75(19)
N(4)-C(21)-C(3)	123.82(14)	C(18)-C(13)-C(14)	115.93(18)
N(3)-C(21)-C(3)	128.46(14)	C(18)-C(13)-B(1)	126.01(16)
N(2)-C(22)-N(3)	113.76(15)	C(14)-C(13)-B(1)	118.06(18)
N(2)-C(22)-H(22A)	123.1	C(3)-C(2)-C(1)	122.91(15)

C(3)-C(2)-H(2B)	118.5
C(1)-C(2)-H(2B)	118.5
C(2)-C(1)-C(6)	114.65(15)
C(2)-C(1)-B(1)	127.63(14)
C(6)-C(1)-B(1)	117.66(15)
O(1)-C(6)-C(5)	113.24(15)
O(1)-C(6)-C(1)	123.46(16)
C(5)-C(6)-C(1)	123.29(16)
C(13)-C(18)-C(17)	124.23(19)
C(13)-C(18)-H(18A)	117.9
C(17)-C(18)-H(18A)	117.9
N(4)-C(23)-C(24)	110.68(15)
N(4)-C(23)-H(23A)	109.5
C(24)-C(23)-H(23A)	109.5
N(4)-C(23)-H(23B)	109.5
C(24)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	108.1
C(15)-C(14)-O(2)	114.46(19)
C(15)-C(14)-C(13)	121.3(2)
O(2)-C(14)-C(13)	124.20(19)
C(5)-C(4)-C(3)	119.60(17)
C(5)-C(4)-H(4A)	120.2
C(3)-C(4)-H(4A)	120.2
C(4)-C(5)-C(6)	119.77(16)
C(4)-C(5)-H(5A)	120.1
C(6)-C(5)-H(5A)	120.1
C(17)-N(1)-C(20)	120.60(18)
C(17)-N(1)-C(19)	121.2(3)
C(20)-N(1)-C(19)	118.0(2)
C(15)-C(16)-C(17)	120.1(2)
C(15)-C(16)-H(16A)	120.0
C(17)-C(16)-H(16A)	120.0
O(2)-C(9)-C(8)	121.35(18)
O(2)-C(9)-C(10)	116.60(19)
C(8)-C(9)-C(10)	122.1(2)
C(11)-C(12)-C(7)	117.5(2)
C(11)-C(12)-H(12A)	121.3
C(7)-C(12)-H(12A)	121.3
C(16)-C(15)-C(14)	121.3(2)
C(16)-C(15)-H(15A)	119.4
C(14)-C(15)-H(15A)	119.4
N(1)-C(17)-C(18)	121.2(2)
N(1)-C(17)-C(16)	121.7(2)
C(18)-C(17)-C(16)	117.1(2)
C(10)-C(11)-C(12)	121.8(2)
C(10)-C(11)-H(11A)	119.1
C(12)-C(11)-H(11A)	119.1
C(11)-C(10)-C(9)	118.8(2)
C(11)-C(10)-H(10A)	120.6
C(9)-C(10)-H(10A)	120.6
C(8)-B(1)-C(13)	108.13(15)
C(8)-B(1)-C(1)	106.25(15)
C(13)-B(1)-C(1)	122.11(15)
C(8)-B(1)-N(3)#1	104.28(13)
C(13)-B(1)-N(3)#1	107.94(14)
C(1)-B(1)-N(3)#1	106.80(13)
C(23)-C(24)-C(25)	115.87(18)
C(23)-C(24)-H(24A)	108.3
C(25)-C(24)-H(24A)	108.3
C(23)-C(24)-H(24B)	108.3
C(25)-C(24)-H(24B)	108.3
H(24A)-C(24)-H(24B)	107.4
C(26)-C(25)-C(24)	110.7(2)
C(26)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25A)	109.5
C(26)-C(25)-H(25B)	109.5
C(24)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	108.1
N(1)-C(20)-H(20A)	109.5
N(1)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
N(1)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5

H(26A)-C(26)-H(26C)	109.5	H(19A)-C(19)-H(19B)	109.5
H(26B)-C(26)-H(26C)	109.5	N(1)-C(19)-H(19C)	109.5
N(1)-C(19)-H(19A)	109.5	H(19A)-C(19)-H(19C)	109.5
N(1)-C(19)-H(19B)	109.5	H(19B)-C(19)-H(19C)	109.5

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+2
#2 -x+1, -y, -z+1

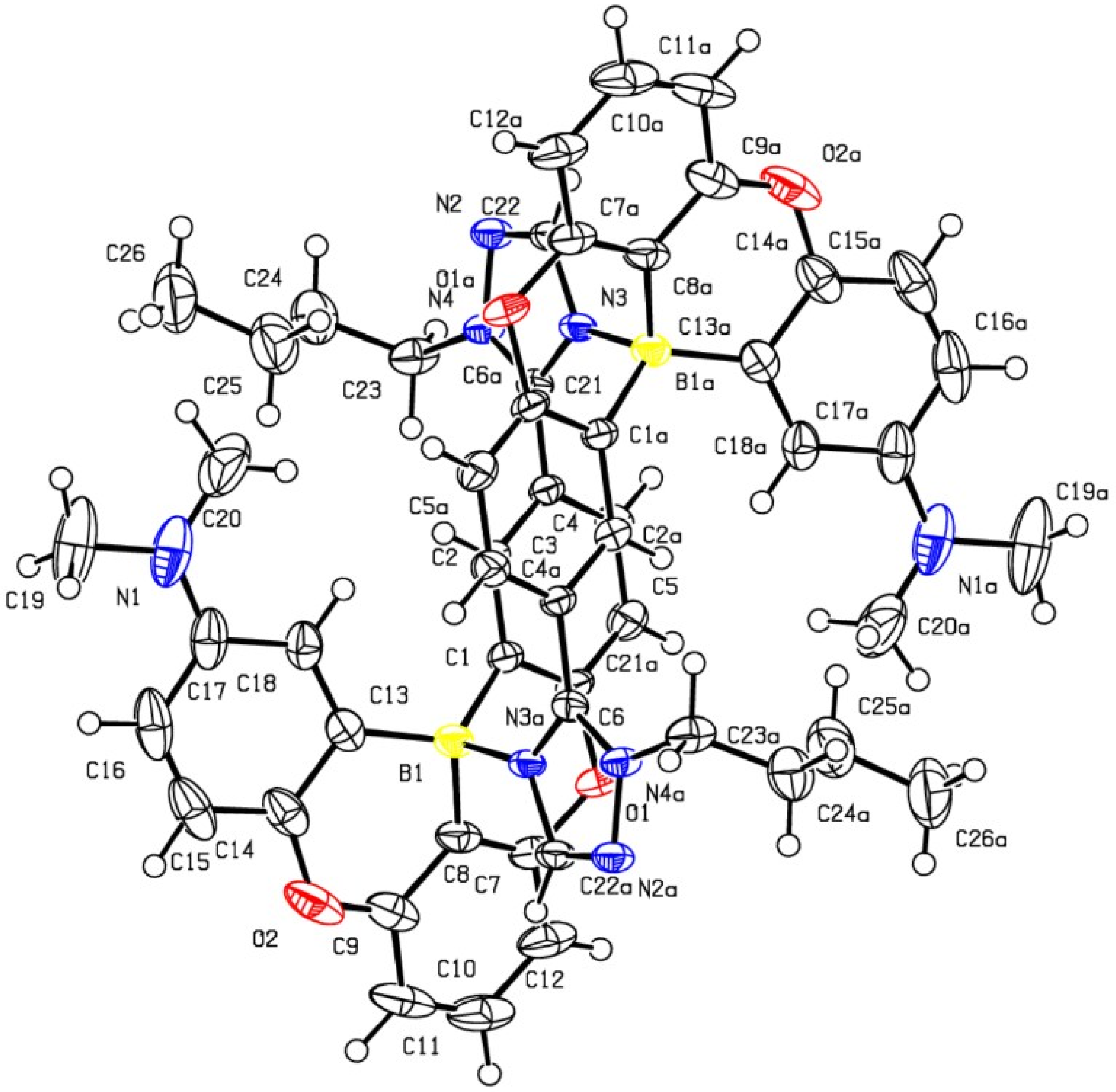
Table 3. Anisotropic displacement parameters ($Å^2$ x 10^3) for dimer **B3**; the anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$h^2 a^{*2}U^{11}$ + ... + 2hka* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	46(1)	28(1)	44(1)	-5(1)	-2(1)	-18(1)
N(3)	31(1)	15(1)	27(1)	1(1)	4(1)	-2(1)
N(4)	28(1)	16(1)	33(1)	-1(1)	5(1)	-2(1)
N(2)	34(1)	17(1)	35(1)	1(1)	6(1)	-2(1)
O(2)	72(1)	36(1)	63(1)	25(1)	19(1)	7(1)
C(21)	24(1)	18(1)	26(1)	2(1)	1(1)	1(1)
C(22)	32(1)	16(1)	31(1)	2(1)	4(1)	-2(1)
C(3)	25(1)	18(1)	25(1)	-3(1)	3(1)	-2(1)
C(8)	40(1)	19(1)	40(1)	-1(1)	18(1)	-2(1)
C(7)	40(1)	23(1)	45(1)	-7(1)	18(1)	-8(1)
C(13)	39(1)	29(1)	28(1)	2(1)	8(1)	12(1)
C(2)	23(1)	20(1)	27(1)	-2(1)	1(1)	-1(1)
C(1)	26(1)	20(1)	26(1)	-3(1)	5(1)	-4(1)
C(6)	33(1)	23(1)	30(1)	-6(1)	4(1)	-10(1)
C(18)	39(1)	40(1)	27(1)	-2(1)	0(1)	12(1)
C(23)	33(1)	26(1)	48(1)	-6(1)	17(1)	-1(1)
C(14)	52(1)	38(1)	37(1)	11(1)	14(1)	20(1)
C(4)	37(1)	28(1)	31(1)	5(1)	-6(1)	-4(1)
C(5)	33(1)	37(1)	36(1)	-1(1)	-10(1)	-10(1)
N(1)	54(1)	98(2)	40(1)	-18(1)	-18(1)	1(1)
C(16)	59(1)	83(2)	27(1)	2(1)	-1(1)	40(1)
C(9)	52(1)	28(1)	50(1)	8(1)	24(1)	5(1)
C(12)	45(1)	32(1)	69(2)	-13(1)	21(1)	-16(1)
C(15)	71(2)	61(2)	37(1)	20(1)	15(1)	38(1)
C(17)	43(1)	61(2)	28(1)	-9(1)	-2(1)	24(1)
C(11)	54(1)	33(1)	88(2)	-7(1)	37(1)	-16(1)
C(10)	72(2)	21(1)	79(2)	9(1)	46(1)	1(1)
B(1)	36(1)	19(1)	30(1)	0(1)	9(1)	0(1)

C(24)	57(1)	60(2)	39(1)	-3(1)	22(1)	0(1)
C(25)	66(2)	84(2)	44(1)	5(1)	8(1)	-11(1)
C(20)	66(2)	98(2)	59(2)	-23(2)	-8(1)	-35(2)
C(26)	106(2)	138(3)	36(1)	1(2)	3(1)	-58(2)
C(19)	66(2)	174(4)	48(2)	-35(2)	-28(1)	26(2)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for dimer **B3**.

	x	y	z	U(eq)
H(22A)	5859	9012	4564	32
H(2B)	4686	5401	5871	28
H(18A)	5807	4575	6669	42
H(23A)	2411	7346	6150	42
H(23B)	2041	8556	5897	42
H(4A)	2018	6512	4287	39
H(5A)	987	4843	4281	43
H(16A)	6431	3207	8767	67
H(12A)	11	1649	5119	58
H(15A)	4972	1858	8410	67
H(11A)	49	345	6092	69
H(10A)	1654	352	7068	68
H(24A)	2780	8473	7207	62
H(24B)	3656	9261	6720	62
H(25A)	4420	7130	7194	77
H(25B)	5294	7899	6686	77
H(20A)	7865	6296	7699	112
H(20B)	7524	5547	6967	112
H(20C)	6383	6152	7393	112
H(26A)	6002	8012	7995	140
H(26B)	5454	9160	7711	140
H(26C)	4580	8392	8219	140
H(19A)	8342	5564	8732	145
H(19B)	7168	4931	9105	145
H(19C)	8341	4273	8752	145



The ORTEP diagram showing the structure of dimer **B3** with labeling schemes

S8 References

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