Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Molecular Design to Enhance Binaphthyl-Based Chiroptics Using Organoboron Chemistry in Isomeric Chiral Scaffolds

Kai Zhang,[a] Jingyi Zhao,[a] Niu Zhang,[b] Jin-Fa Chen,[a] Nan Wang,[a] Xiaodong Yin,[a] Xiaoyan Zheng*[a] and Pangkuan Chen*[a]

[a]Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, Key Laboratory of Cluster Science of the Ministry of Education, School of Chemistry and Chemical Engineering, Beijing Institute of Technology of China, Beijing, 102488, China

[b]Analysis & Testing Centre, Beijing Institute of Technology of China, Beijing, 102488, China

* xiaoyanzheng@bit.edu.cn; pangkuan@bit.edu.cn

Table of Contents

1. Experimental Section

Materials and General Methods: 2-Naphthol, 7-bromo-2-naphthol, 4-(diphenylamino)-phenylboronic acid, K_2CO_3, $Pd(PPh_3)_4$, $FeCl_3 \cdot 6H_2O$, CH_2BrCl, and CH_3I were purchased from Energy Chemical. Tetrahydrofuran (THF), dichloromethane, petroleum ether, methanol, and ethyl acetate were purchased from Sinopharm Chemical Reagent Co., Ltd. The chemicals were used without further purification unless otherwise noted. Anhydrous solvents were distilled from commercial materials with sodium/benzopheneone.

All commercial chemicals were used without further purification. 2,2'-Dihydroxy-1,1'-binaphthyl (**1**), 6,6'-dibromo-2,2'-dihydroxy-1,1'-binaphthyl (**2**), 6,6'-dibromo-1,1'-binaphthyl-2,2'-diyloxymethane (**3**), 6,6'-dibromo-2,2'-dimethoxy-1,1'-binaphthalene (**5**) and 7,7'-dibromo-2,2'-dihydroxy-1,1'-binaphthyl (**7**) were prepared using the similar procedures previously described. [1, 2, 3, 4]

400 MHz ^{1}H, 101 MHz ^{13}C, and 225 MHz ^{11}B NMR spectra were recorded on a Bruker spectrometer. ^{11}B NMR spectra were acquired with boron-free quartz NMR tubes and the spectra were referenced externally to $BF_3 \cdot Et_2O$ (δ = 0). High resolution mass spectral data were obtained via ESI on an Agilent (Q-TOF 6520) analyzer.

UV-visible absorption spectra were recorded on a Cary 300 UV-Vis spectrophotometer. Luminescent spectra were recorded on an Edinburgh Instruments FLS980. Fluorescent quantum efficiencies were determined using a Hamamatsu C11347-11 Quantaurus-QY spectrometer.

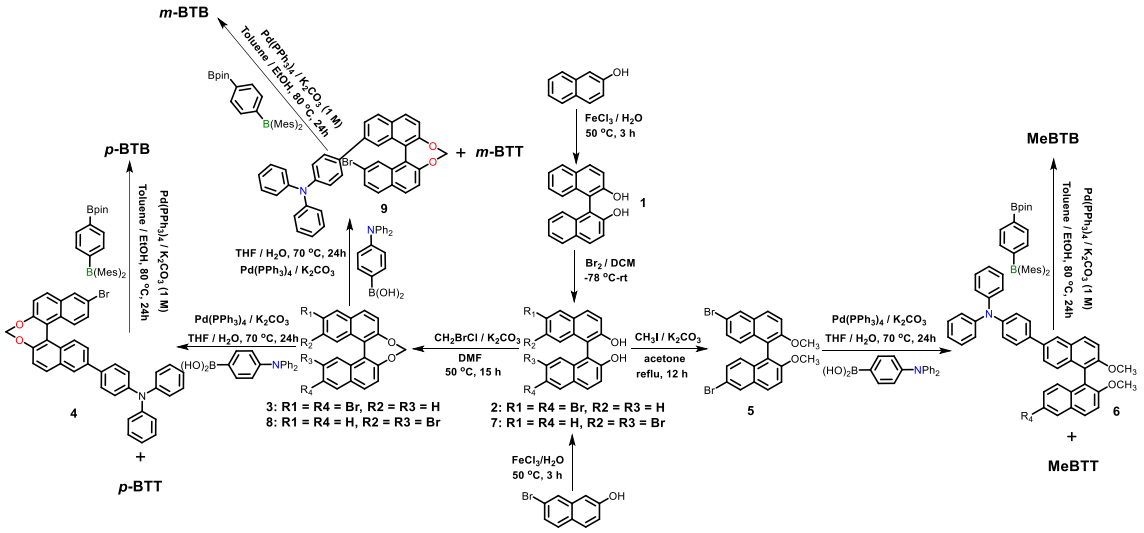
Analytical HPLC was performed on an Agilent 1260 Infinity II instrument equipped with a diode array detector and CHIRALPAK columns (4.6 mm × 250 mm, 3 μm) from Daicel Chiral Technologies. Column temperature was maintained at 30 °C. The CD spectra were measured using a Circular Dichroism spectrometer (J-1500, Jasco). CPL measurements of solutions (c =1.0 × 10^{-5} M) and neat films were performed with circularly polarized luminescence spectrometer (CPL-300, Jasco). Samples were excited with a Xenon ozone-free lamp 150 W LS. The following parameters were used: emission slit width = 3 mm, integration time = 2 second, scan speed = 200 nm/min, accumulations = 2.

The neat films used in this study have been prepared on quartz flakes by spin coating solutions of enantiopure compounds with a concentration of ~ 10 mg/mL. 0.1 mL of the solution was deposited on the quartz flakes fixed within the spin-coater holder, and the film was obtained using a sequence including 60 seconds of rotation, with an acceleration of 1000 rpm/s and a maximum speed of 3000 rpm.

DFT calculations were performed with the Gaussian 09 program. Geometry optimizations and vertical excitations were calculated by means of hybrid density functional CAM-B3LYP with the basis set of 6-31G(d). The input files and orbital representations were generated with Gaussview 5.0 (scaling radii of 75%, isovalue = 0.02). Excitation data were calculated using TD-DFT (CAM-B3LYP functional and 6-31G* basis). The resulting structures were confirmed to be stationary points through vibrational frequency analysis.

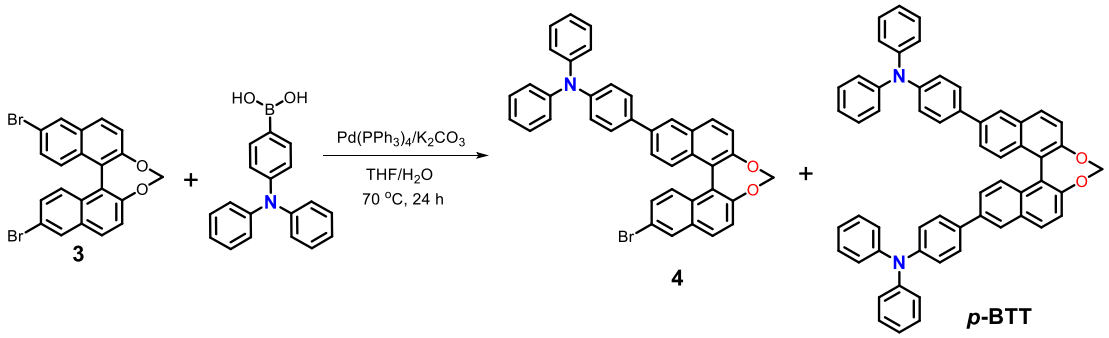
The electronic circular dichroism (ECD) spectra were simulated via TD-DFT calculations of the lowest 30 vertical singlet electronic excitations (CAM-B3LYP functional and 6-31G* basis). Gaussian broadening of the intensities with a parameter σ = 0.20 eV was performed for all ECD spectra. Solvent effects on the spectra were considered by means of the polarizable continuum model [5] (PCM) for dichloromethane (DCM).

2. Synthetic Procedures



Scheme S1. Molecular structures and synthetic route of racemic **MeBTT**, **MeBTB**, ***p*-BTT**, ***p*-BTB**, ***m*-BTT** and ***m*-BTB**.

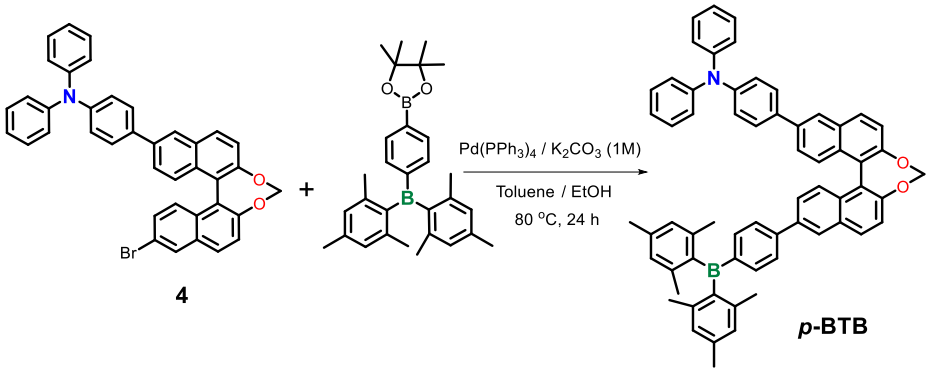
2.1 Synthesis of 4 and *p*-BTT



A mixture of **3** (100 mg, 0.22 mmol), (4-(diphenylamino)phenyl)boronic acid (57 mg, 0.22 mmol), K_2CO_3 (92 mg, 0.66 mmol) and $Pd(PPh_3)_4$ (10 mg, 8.8 μmol) in THF (10 mL) and deionized water (2 mL) was refluxed at 70 °C for 24 h under N_2. After the mixture was cooled down, 10 mL of deionized water was added to the resulting solution and the mixture was extracted with CH_2Cl_2 several times. The organic phase was dried over Na_2SO_4 and was further purified by column chromatography on silica gel using CH_2Cl_2/petroleum ether (1/5, v/v) as eluent to give the product **4** (40 mg, yield: 29%) and ***p*-BTT** (30 mg, yield: 22%) as white solid. Melting point (Mp: >250°C for ***p*-BTT**).

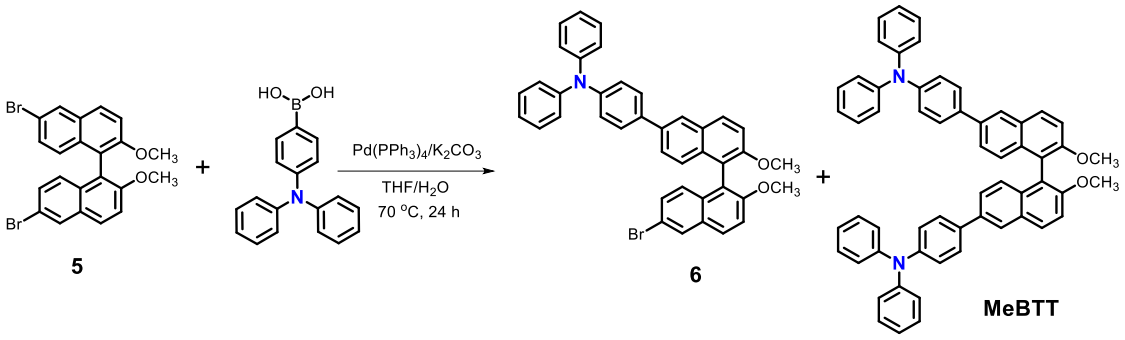
^{1}H NMR (400 MHz, $CDCl_3$) of **4**: δ 8.11 (s, 1H), 8.10 (s, 1H), 8.02 (d, *J* = 9.0 Hz, 1H), 7.89 (d, *J* = 9.0 Hz, 1H), 7.64–7.54 (m, 3H), 7.49 (m, 3H), 7.44 (d, *J* = 9.0 Hz, 1H), 7.40–7.35 (m, 1H), 7.33–7.27 (m, 4H), 7.21–7.10 (m, 6H), 7.07–7.01 (m, 2H), 5.70 (s, 2H); ***p*-BTT**: δ 7.97 (d, *J* = 9.0 Hz, 4H), 7.80 (s, 2H), 7.72–7.64 (m, 2H), 7.45 (d, *J* = 9.0 Hz, 2H), 7.23–7.15 (m, 12H), 7.09–6.95 (m, 12H), 6.92 (d, *J* = 8.4 Hz, 4H), 5.72 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) of **4**: δ 151.5, 151.2, 147.6, 147.4, 137.2, 134.3, 132.9, 132.2, 130.9, 130.7, 130.7, 130.3, 129.4, 129.3, 128.7, 127.9, 127.0, 126.4, 125.7, 125.4, 124.5, 123.9, 123.0, 122.2, 121.3, 119.1, 103.2; ***p*-BTT**: δ 151.7, 147.5, 147.1, 138.3, 134.8, 132.4, 130.8, 130.0, 129.2, 129.0, 127.9, 126.2, 124.6, 124.4, 124.3, 123.7, 122.9, 120.7, 103.2. ESI-HRMS (m/z): calcd. for **4**: $C_{39}H_{26}BrNO_2$ $[M+H]^+$ 620.1225, found 620.1213, calcd. for ***p*-BTT**: $C_{57}H_{40}N_2O_2$ $[M+H]^+$ 785.3168, found 785.3127.

2.2 Synthesis of *p*-BTB



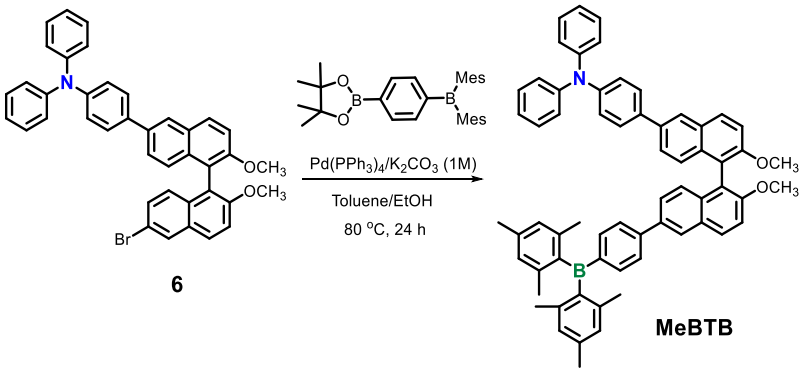
The mixture of **4** (100 mg, 0.16 mmol), 2-(4-(dimesitylboryl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (110 mg, 0.24 mmol), $Pd(PPh_3)_4$ (10 mg, 9 μmol), toluene (6 mL), ethanol (2 mL) and 1 M K_2CO_3 aqueous solution (1 mL) in a round-bottom flask was stirred at 80 ˚C under N_2 atmosphere for 8 h. The mixture was then cooled to r.t. and poured into water (100 mL). After extraction with CH_2Cl_2, the organic phase was dried over Na_2SO_4. Purification by column chromatography on silica using CH_2Cl_2/petroleum ether (1:6, v/v) as eluent yielded a white solid of ***p*-BTB** (56 mg, yield: 40%). Melting point (Mp: 195°C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (s, 1H), 8.11 (s, 1H), 8.08–7.98 (m, 2H), 7.71 (d, *J* = 7.8 Hz, 2H), 7.68–7.55 (m, 8H), 7.54–7.46 (m, 2H), 7.36–7.25 (m, 4H), 7.20–7.10 (m, 6H), 7.08–7.00 (m, 2H), 6.84 (s, 4H), 5.72 (s, 2H), 2.32 (s, 6H), 2.05 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 151.2, 147.7, 147.4, 143.8, 140.8, 138.6, 137.2, 137.1, 134.5, 132.2, 132.1, 131.6, 131.1, 130.7, 130.5, 129.3, 128.2, 127.9, 127.6, 127.4, 126.7, 126.5, 126.1, 125.9, 125.6, 125.5, 125.4, 124.5, 124.0, 123.0, 121.5, 121.3, 103.2, 23.50, 21.2. ^{11}B NMR (225 MHz, $CDCl_3$) δ 74 ppm. ESI-HRMS (m/z): calcd. for $C_{63}H_{52}BNO_2$ $[M+H]^+$ 866.4169, found 866.4134.

2.3 Synthesis of 6 and MeBTT



A mixture of **5** (170 mg, 0.36 mmol), (4-(diphenylamino)phenyl)boronic acid (103 mg, 0.36 mmol), K_2CO_3 (148 mg, 1.08 mmol) and $Pd(PPh_3)_4$ (21 mg, 14.4 μmol) in THF (10 mL) and deionized water (2 mL) was refluxed at 70 °C under N_2 for 24 h. After the mixture was cooled down, 10 mL of deionized water was added to the resulting solution and the mixture was extracted with CH_2Cl_2 several times. The organic phase was dried over Na_2SO_4 and was further purified by column chromatography on silica gel using CH_2Cl_2/petroleum ether (1/5, v/v) as eluent to give the product **6** (60 mg, yield: 26%) and **MeBTT** (65 mg, yield: 29%) as white solid. Melting point (Mp: 164°C). ^{1}H NMR (400 MHz, $CDCl_3$) of **7**: δ 8.10–7.96 (m, 3H), 7.89 (d, *J* = 9.0 Hz, 1H), 7.54 (d, *J* = 9.0 Hz, 2H), 7.51–7.41 (m, 3H), 7.31–7.22 (m, 6H), 7.19–7.07 (m, 6H), 7.06–6.98 (m, 3H), 3.78 (d, *J* = 2.0 Hz, 6H); **MeBTT**: δ 8.14–7.94 (m, 4H), 7.62–7.52 (m, 4H), 7.52–7.41 (m, 4H), 7.31–7.22 (m, 8H), 7.19 (d, *J* = 9.0 Hz, 2H), 7.17–7.10 (m, 12H), 7.06–6.98 (m, 4H), 3.79 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) of **7**: δ 155.2, 154.9, 147.7, 147.0, 135.8, 135.0, 132.8, 132.5, 130.2, 129.8, 129.8, 129.6, 129.5, 129.3, 128.5, 127.8, 127.2, 125.9, 125.5, 125.2, 124.4, 124.0, 122.9, 119.8, 118.7, 117.3, 115.1, 114.4, 56.8; **MeBTT**: δ 155.0, 147.7, 146.9, 135.7, 135.2, 133.0, 129.6, 129.5, 129.4, 127.8, 125.8, 125.8, 125.1, 124.4, 124.0, 122.8, 119.5, 114.6, 57.0 ppm. ESI-HRMS (m/z): calcd. for **7**: $C_{39}H_{26}BrNO_2$ $[M+H]^+$ 636.1538, found 636.1552, calcd. for **MeBTT**: $C_{58}H_{44}N_2O_2$ $[M+H]^+$ 801.3481, found 801.3497.

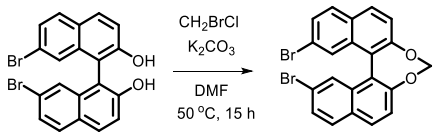
2.4 Synthesis of MeBTB



The mixture of **6** (100 mg, 0.16 mmol), 2-(4-(dimesitylboryl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (0.11 g, 0.24 mmol), $Pd(PPh_3)_4$ (15 mg, 9 μmol), toluene (6 mL), ethanol (2 mL) and 1 M K_2CO_3 aqueous solution (1 mL) in a round-

bottom flask was stirred at 80 ˚C under N_2 atmosphere for 8 h. The mixture was then cooled to r.t. and poured into water (100 mL). After extraction with CH_2Cl_2, the organic phase was dried over Na_2SO_4. Purification by column chromatography on silica using CH_2Cl_2/petroleum ether (1:6, v/v) as eluent yielded a white solid of **MeBTB** (60 mg, yield: 43%). Melting point (Mp: 182°C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 2.0 Hz, 1H), 8.09–7.96 (m, 3H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.57–7.52 (m, 3H), 7.50–7.41 (m, 3H), 7.30–7.22 (m, 5H), 7.20 (d, *J* = 9.0 Hz, 1H), 7.18–7.09 (m, 6H), 7.06–6.98 (m, 2H), 6.83 (s, 4H), 3.79 (d, *J* = 6.0 Hz, 6H), 2.31 (s, 6H), 2.04 (s, 12H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.3, 155.0, 147.7, 146.9, 144.4, 141.8, 140.8, 140.1, 138.5, 137.1, 135.7, 135.6, 135.1, 133.5, 133.0, 129.9, 129.7, 129.5, 129.4, 129.3, 128.1, 127.8, 126.5, 126.2, 125.9, 125.9, 125.7, 125.2, 124.4, 124.0, 122.9, 119.4, 119.3, 114.6, 56.9, 23.5, 21.2. ^{11}B NMR (225 MHz, $CDCl_3$) δ 74 ppm. ESI-HRMS (m/z): calcd. for $C_{63}H_{52}BNO_2$ $[M+H]^+$ 882.4482, found 882.4505.

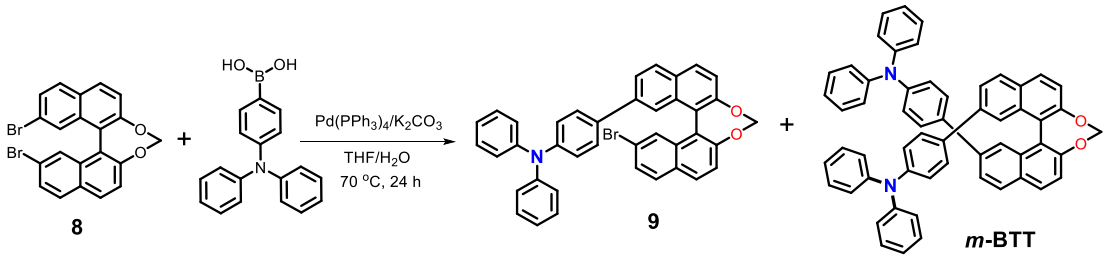
2.5 Synthesis of 8



7 **8**

A mixture of **7** (100 mg, 0.23 mmol), CH_2BrCl (0.44 mL, 6.90 mmol), and K_2CO_3 (311 mg, 2.25 mmol) in dry DMF (3 mL) was stirred at 50 °C for 15 h under N_2 atmosphere. The reaction mixture was poured into water and EtOAc. The aqueous layer was extracted with EtOAc. The organic layers were combined and washed with water three times. After dried over Na_2SO_4, the solvent was evaporated under vacuo to give a residue. The residue was purified by column chromatography to afford **8** (82 mg, yield: 80%) as a white solid powder. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 9.0 Hz, 2H), 7.81 (d, *J* = 9.0 Hz, 2H), 7.64 (d, *J* = 2.0 Hz, 2H), 7.55 (dd, *J* = 9.0, 2.0 Hz, 2H), 7.48 (d, *J* = 9.0 Hz, 2H), 5.68 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.1, 133.0, 130.6, 130.3, 130.1, 128.7, 128.5, 124.8, 121.4, 121.1. GC-MS (m/z): calcd. for $C_{21}H_{12}Br_2O_2$ $[M^+]$ 455.9, found 456.0.

2.6 Synthesis of 9 and *m*-BTT

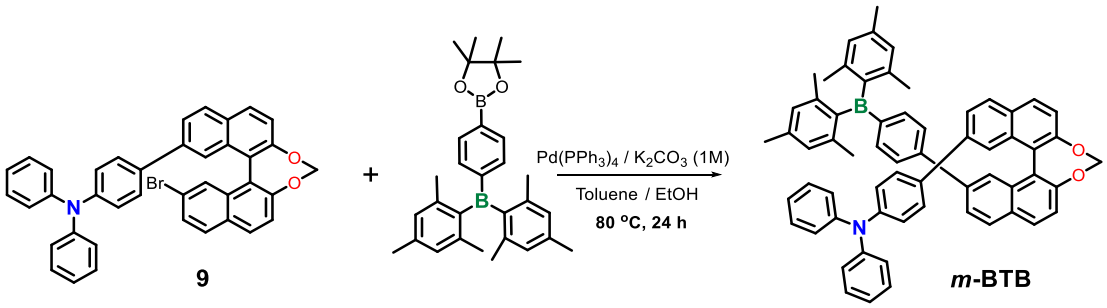


8 **9** ***m*-BTT**

A mixture of **8** (100 mg, 0.22 mmol), (4-(diphenylamino)phenyl)boronic acid (64 mg, 0.33 mmol), K_2CO_3 (91m g, 0.66 mmol) and $Pd(PPh_3)_4$ (10 mg, 8.8 μmol) in THF (10 mL) and deionized water (2 mL) was refluxed at 70 °C under N_2 for 24 h. After the

mixture was cooled down, 10 mL of deionized water was added to the resulting solution and the mixture was extracted with CH_2Cl_2 several times. The organic phase was dried over Na_2SO_4 and was further purified by column chromatography on silica gel using CH_2Cl_2/petroleum ether (1/8, v/v) as eluent to give the product **9** (40 mg, yield: 29%) and ***m*-BTT** (35 mg, yield: 26%) as white solid. Melting point (Mp: 232°C for ***m*-BTT**). ^{1}H NMR (400 MHz, acetone-d_6) of **7**: δ 8.20–8.10 (m, 3H), 8.02 (d, *J* = 9.0 Hz, 1H), 7.86–7.75 (m, 2H), 7.68–7.51 (m, 4H), 7.41–7.33 (m, 2H), 7.33–7.23 (m, 4H), 7.09–7.01 (m, 6H), 7.00–6.91 (m, 2H), 5.76 (s, 2H); ***m*-BTT:** ^{1}H NMR (101 MHz, $CDCl_3$) δ 7.97 (d, *J* = 9.0 Hz, 4H), 7.80 (s, 2H), 7.68 (m, 2H), 7.45 (d, *J* = 9.0 Hz, 2H), 7.24–7.15 (m, 12H), 7.09–6.95 (m, 12H), 6.92 (d, *J* = 8.0 Hz, 4H), 5.72 (s, 2H). ^{13}C NMR (101 MHz, acetone-d_6) of **7**: δ 147.6, 147.5, 138.7, 134.5, 133.1, 132.0, 130.9, 130.9, 130.7, 130.4, 129.4, 129.4, 128.6, 128.2, 128.0, 125.3, 125.2, 124.6, 124.6, 123.3, 123.2, 123.2, 122.0, 120.9, 120.3, 103.3; ***m*-BTT:** ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.7, 147.5, 147.1, 138.3, 134.8, 132.4, 130.8, 130.0, 129.2, 129.0, 127.9, 126.2, 124.6, 124.4, 124.3, 123.7, 122.9, 120.7, 103.2 ppm. ESI-HRMS (m/z): calcd. for **7**: $C_{39}H_{26}BrNO_2$ $[M+H]^+$ 620.1225, found 620.1226, calcd. for ***m*-BTT**: $C_{57}H_{40}N_2O_2$ $[M+H]^+$ 785.3168, found 785.3157.

2.7 Synthesis of *m*-BTB



The mixture of **9** (100 mg, 0.16 mmol), 2-(4-(dimesitylboryl)phenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (110 mg, 0.24 mmol), $Pd(PPh_3)_4$ (10 mg, 9 μmol), toluene (6 mL), ethanol (2 mL) and 1 M K_2CO_3 aqueous solution (1 mL) in a round-bottom flask was stirred at 80 ˚C under N_2 atmosphere for 8 h. The mixture was then cooled to r.t. and poured into water (100 mL). After extraction with CH_2Cl_2, the organic phase was dried over Na_2SO_4. Purification by column chromatography on silica using CH_2Cl_2/petroleum ether (1:4, v/v) as eluent yielded a white solid of ***m*-BTB** (57 mg, yield: 40%). Melting point (Mp: 202°C). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04–7.95 (m, 4H), 7.92 (s, 1H), 7.82–7.73 (m, 2H), 7.72–7.64 (m, 1H), 7.46 (dd, *J* = 13.0, 9.0 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.23–7.11 (m, 6H), 7.06–6.94 (m, 6H), 6.90 (d, *J* = 8.0 Hz, 2H), 6.77 (s, 4H), 5.72 (s, 2H), 2.28 (s, 6H), 1.93 (s, 12H). ^{13}C NMR (101 MHz, CDCl3) δ 151.8, 151.8, 147.6, 147.1, 144.1, 141.6, 140.8, 138.6, 138.4, 138.2, 136.9, 134.8, 132.4, 132.3, 131.3, 130.8, 130.1, 130.0, 129.2, 129.0, 128.1, 128.0, 126.7, 126.5, 126.1, 125.4, 124.8, 124.71, 124.4, 124.2, 123.6, 122.9, 121.3, 120.7, 103.2, 23.4, 21.2. ^{11}B NMR (225 MHz, $CDCl_3$) δ 73 ppm. ESI-HRMS (m/z): calcd. for $C_{63}H_{52}BNO_2$ $[M+H]^+$ 866.4169, found 866.4143.

Reference:

[1] N. Lv, M. Xie, W. Gu, H. Ruan, S. Qiu, C. Zhou and Z. Cui, *Org. Lett.*, 2013, **15**, 2382.

[2] (a) J.-W. Park, M. D. Ediger and M. M. Green, *J. Am. Chem. Soc.*, 2001**, 123***,* 49; (b) K. Takaishi, S. Hinoide, T. Matsumoto and T. Ema, *J. Am. Chem. Soc.*, 2019, **141**, 11852.

[3] J.-K. Ou-Yang, Y.-Y. Zhang, M.-L. He, J.-Tao Li, X. Li, X.-L. Zhao, C.-H. Wang, Y. Yu, D.-X. Wang, L. Xu and H.-B. Yang, *Org. Lett.*, 2014, **16**, 664.

[4] (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785; (b) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 1372; (c) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648.

[5] G. Scalmani and M. J. Frisch, *J. Chem. Phys.* 2010, **132**, 114110.

3. Characterization by NMR Spectroscopy

3.1 NMR Spectra of 4

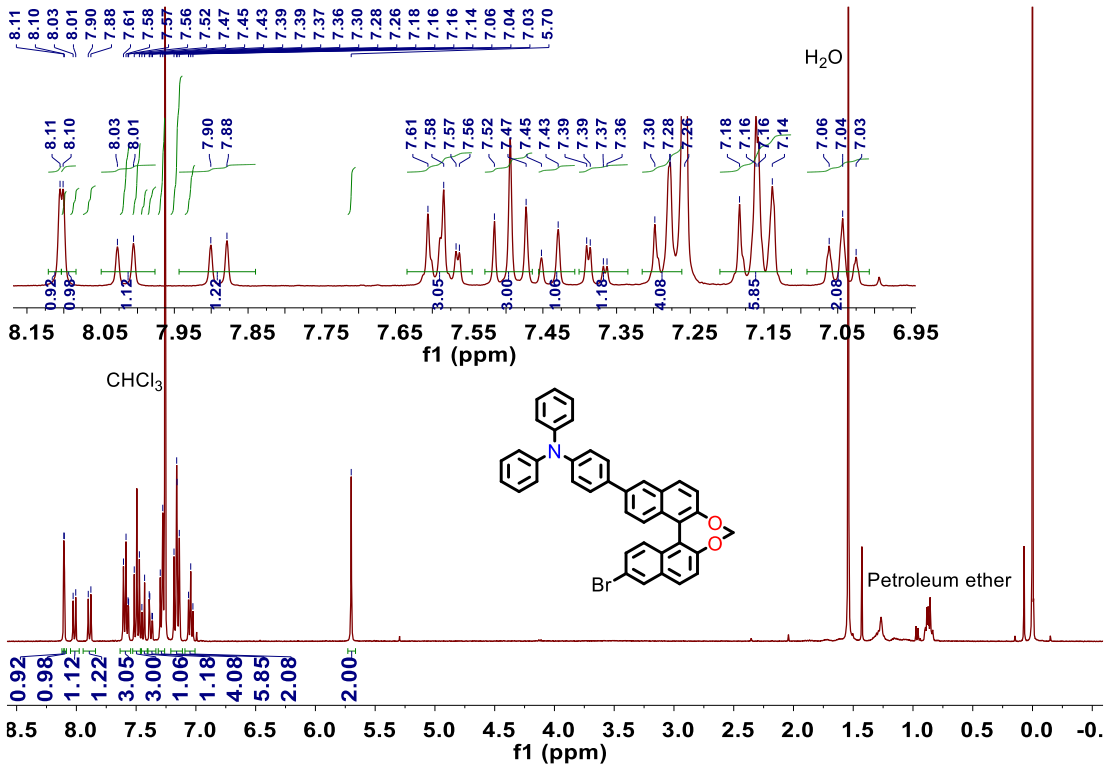


Figure S1. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **4**.

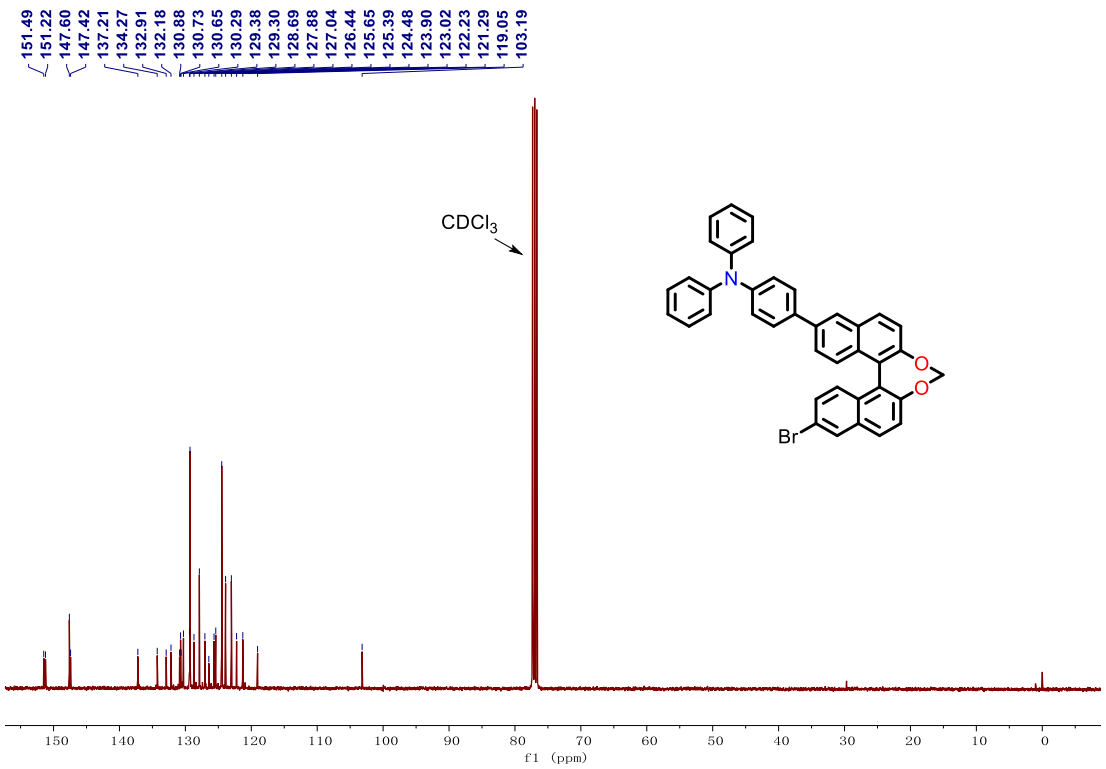


Figure S2. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **4**.

3.2 NMR Spectra of *p*-BTT.

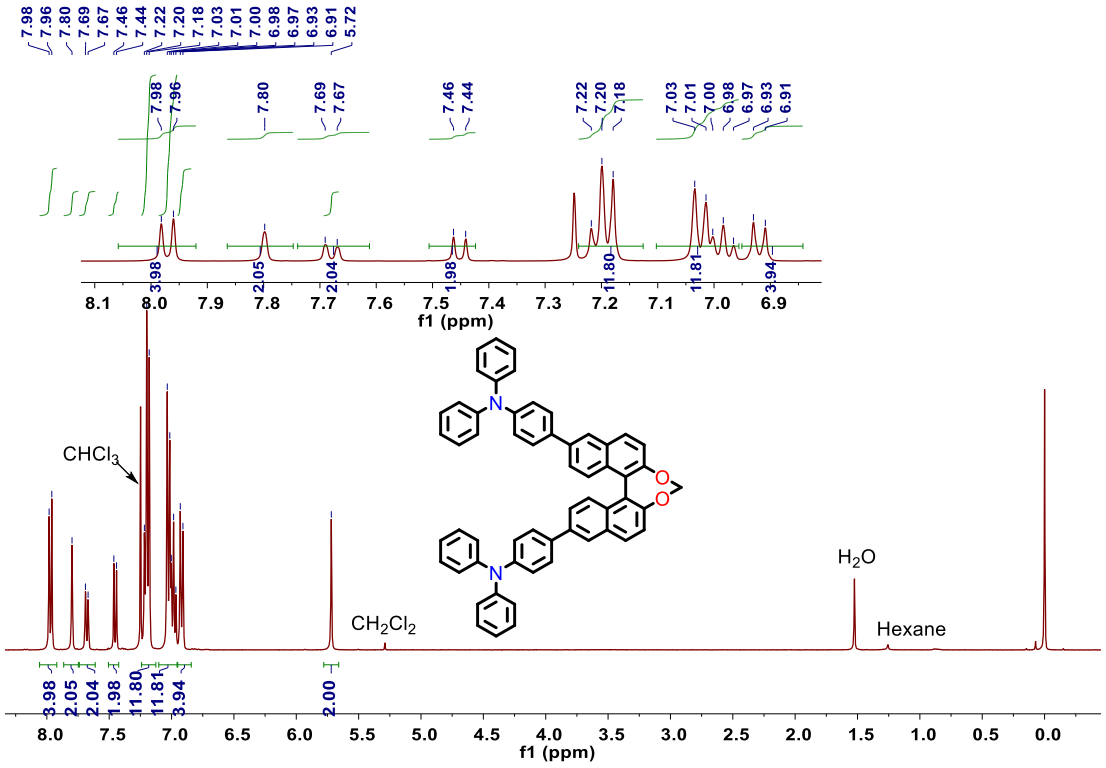


Figure S3. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of ***p*-BTT**.

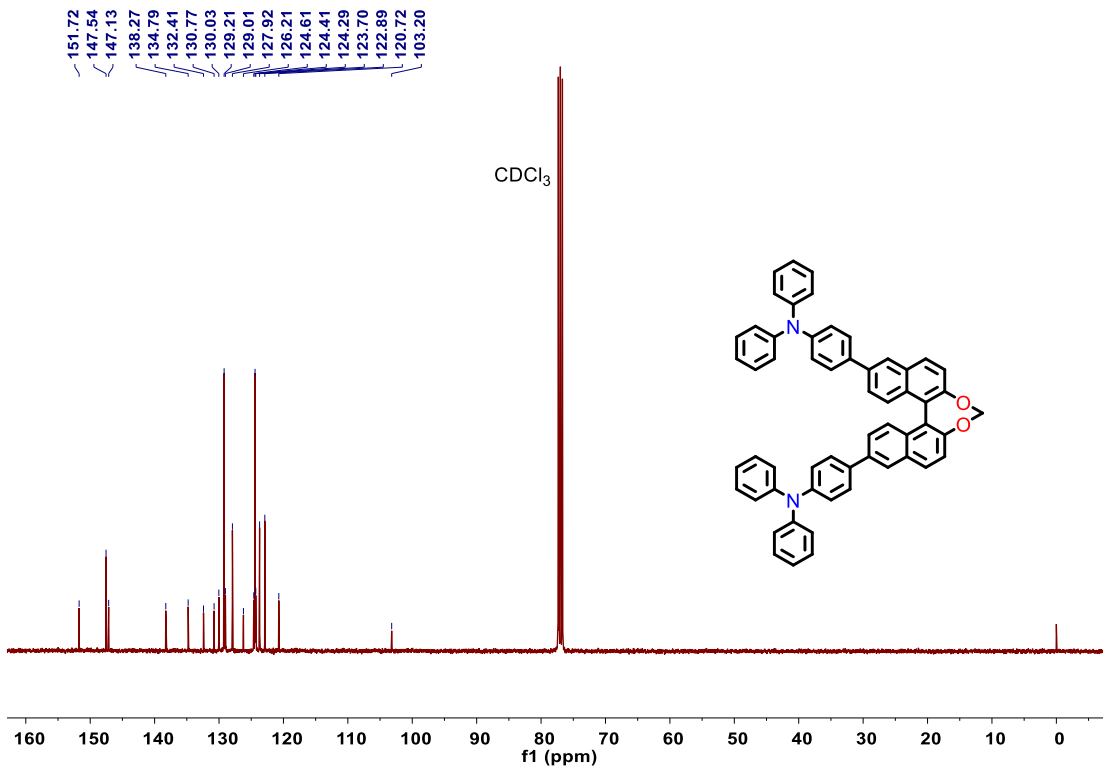


Figure S4. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of ***p*-BTT**.

3.3 NMR Spectra of *p*-BTB.

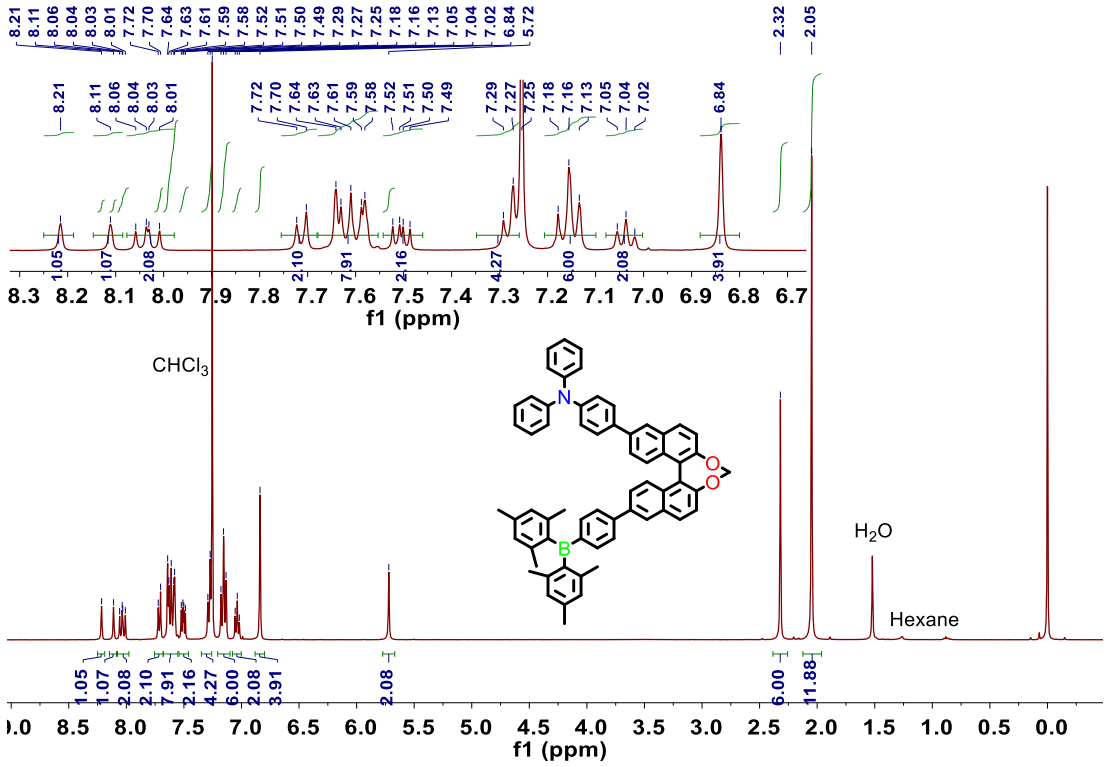


Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of ***p*-BTB**.

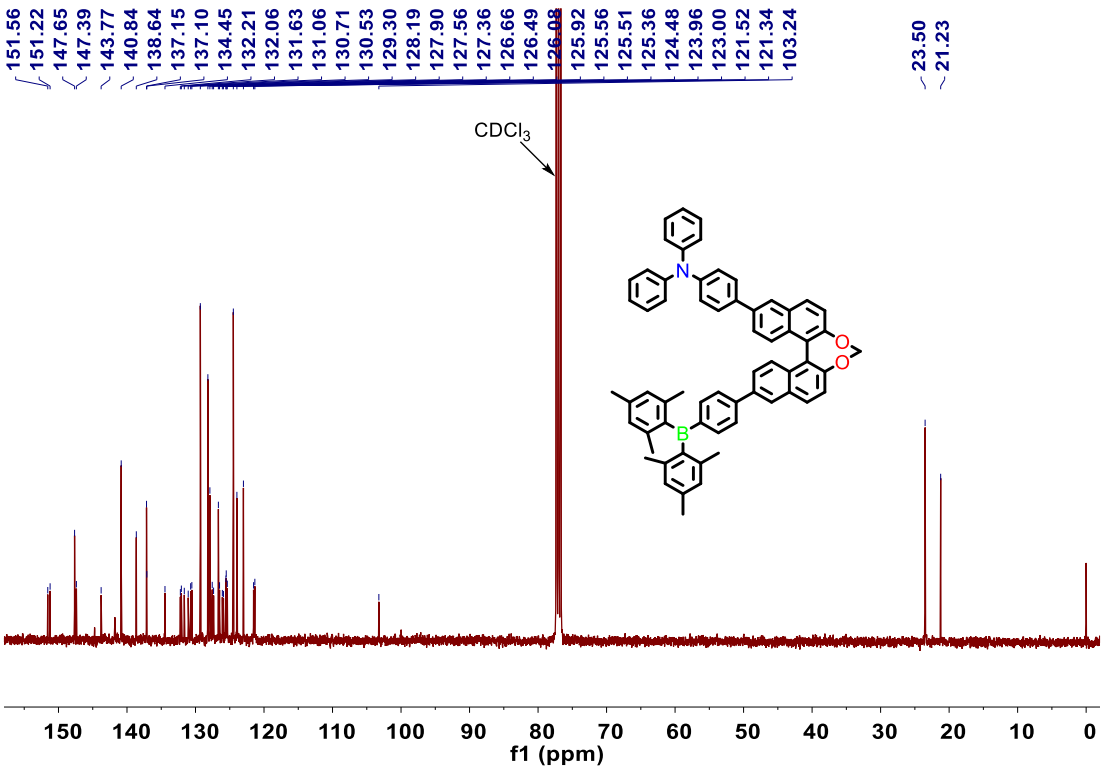


Figure S6. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of ***p*-BTB**.

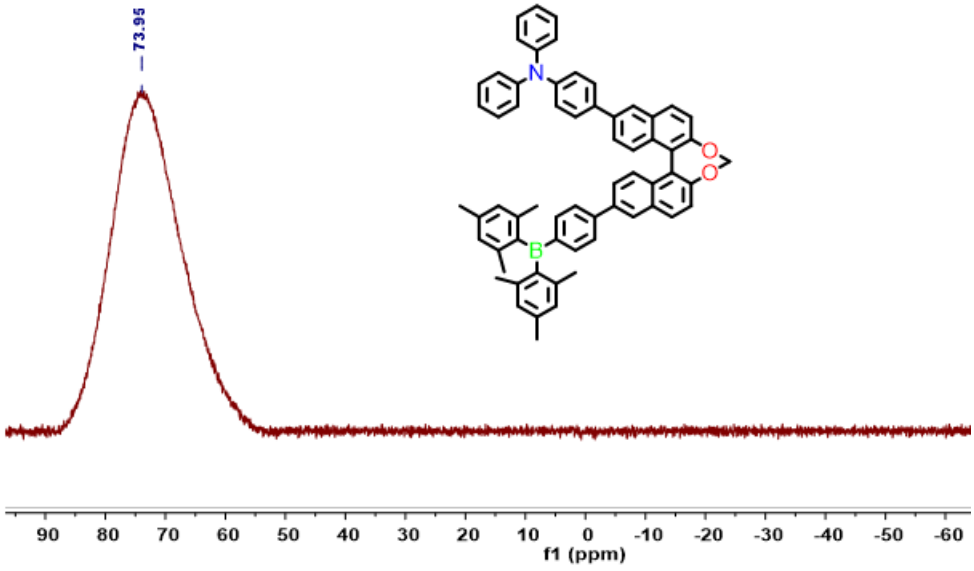


Figure S7.^{11}B NMR (225 MHz, C_6D_6) spectrum of ***p*-BTB**.

3.4 NMR Spectra of 7

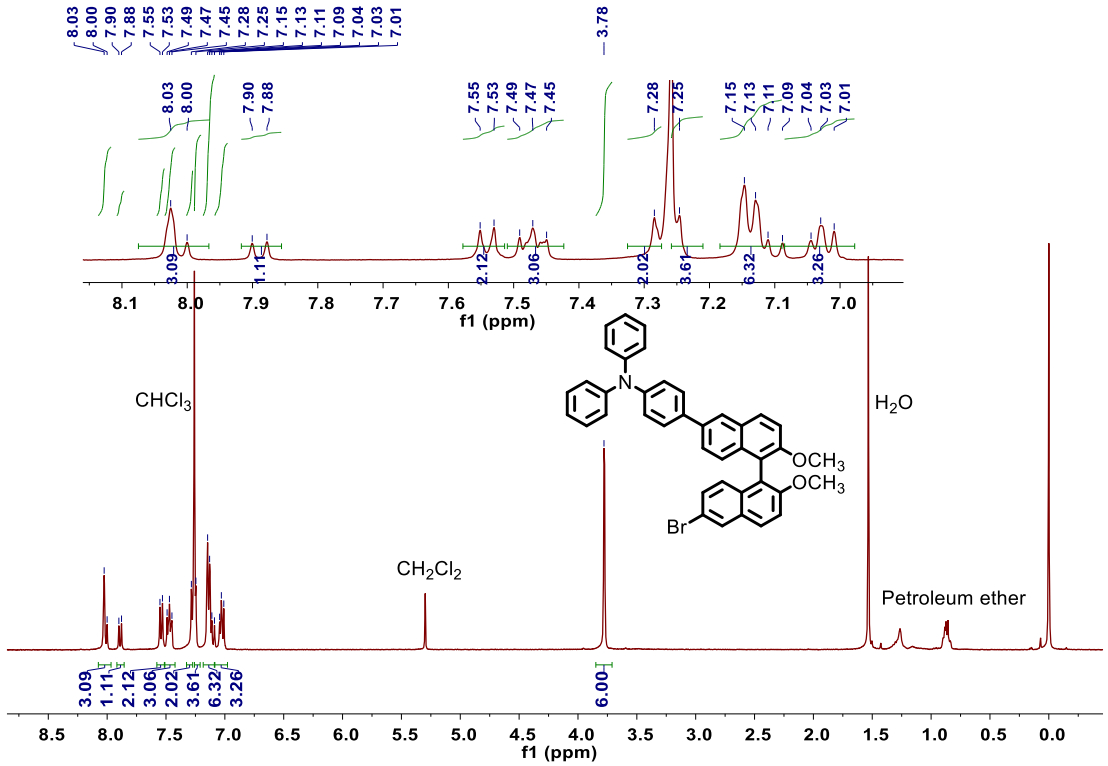


Figure S8. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **7**.

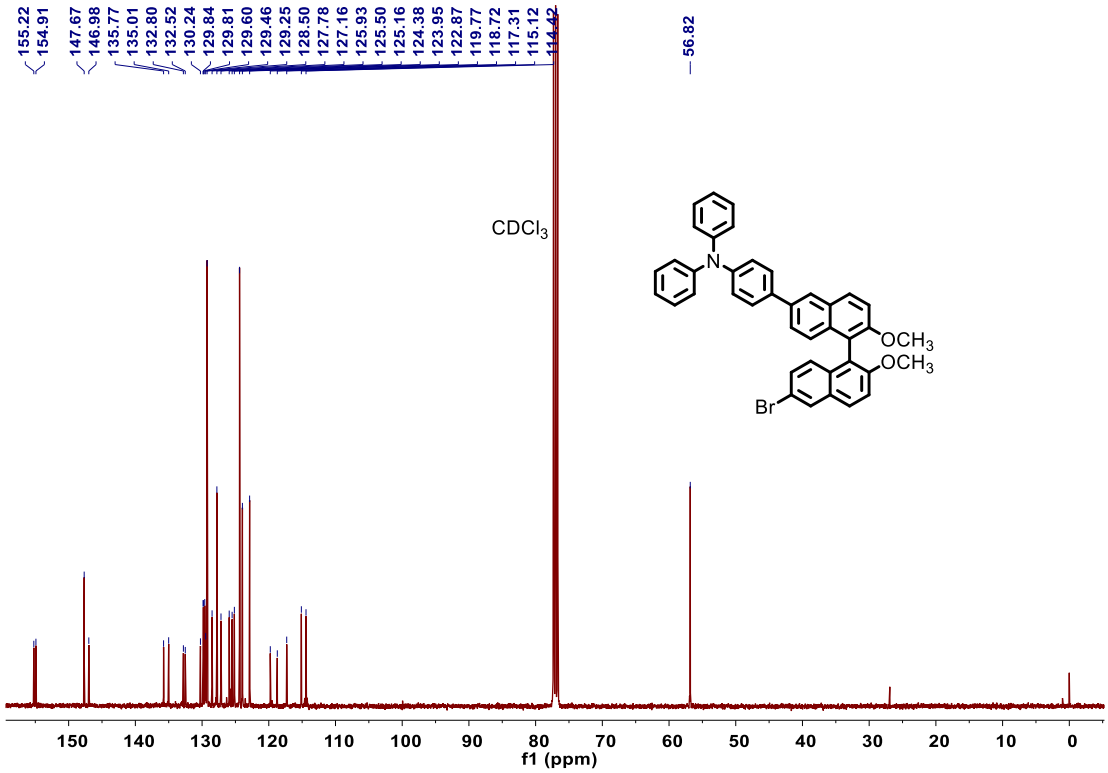


Figure S9. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **7**.

3.5 NMR Spectra of MeBTT

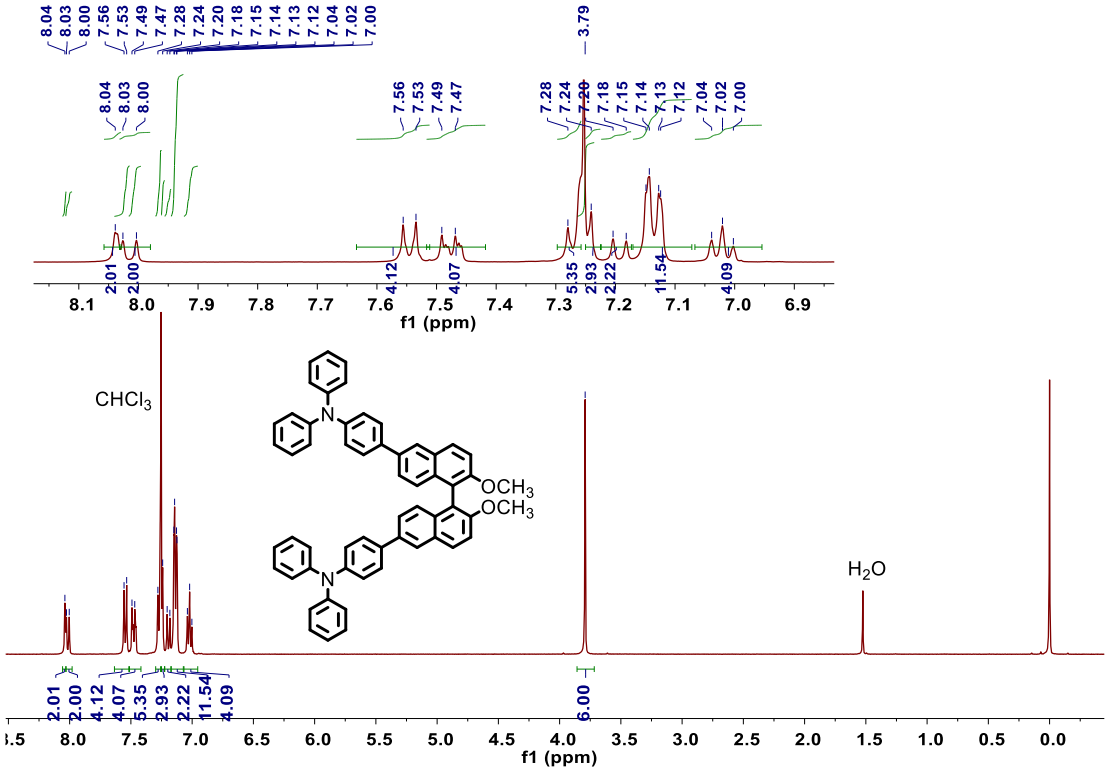


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **MeBTT**.

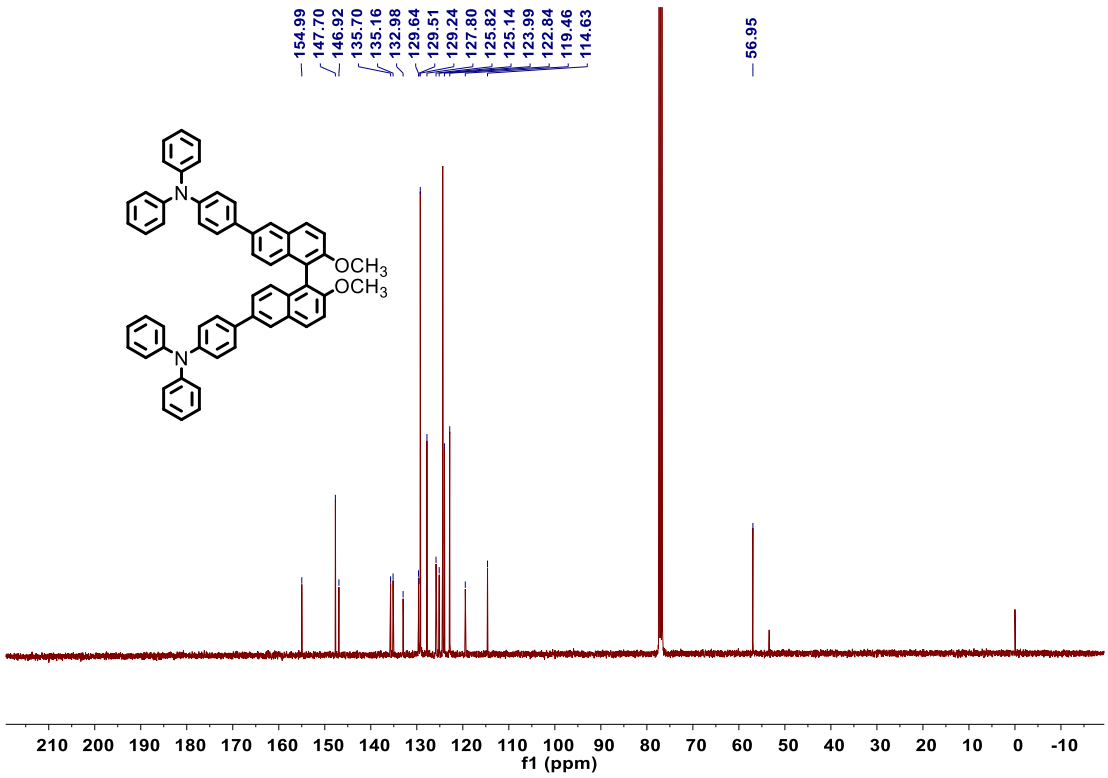


Figure S11. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **MeBTT**.

3.6 NMR Spectra of MeBTB

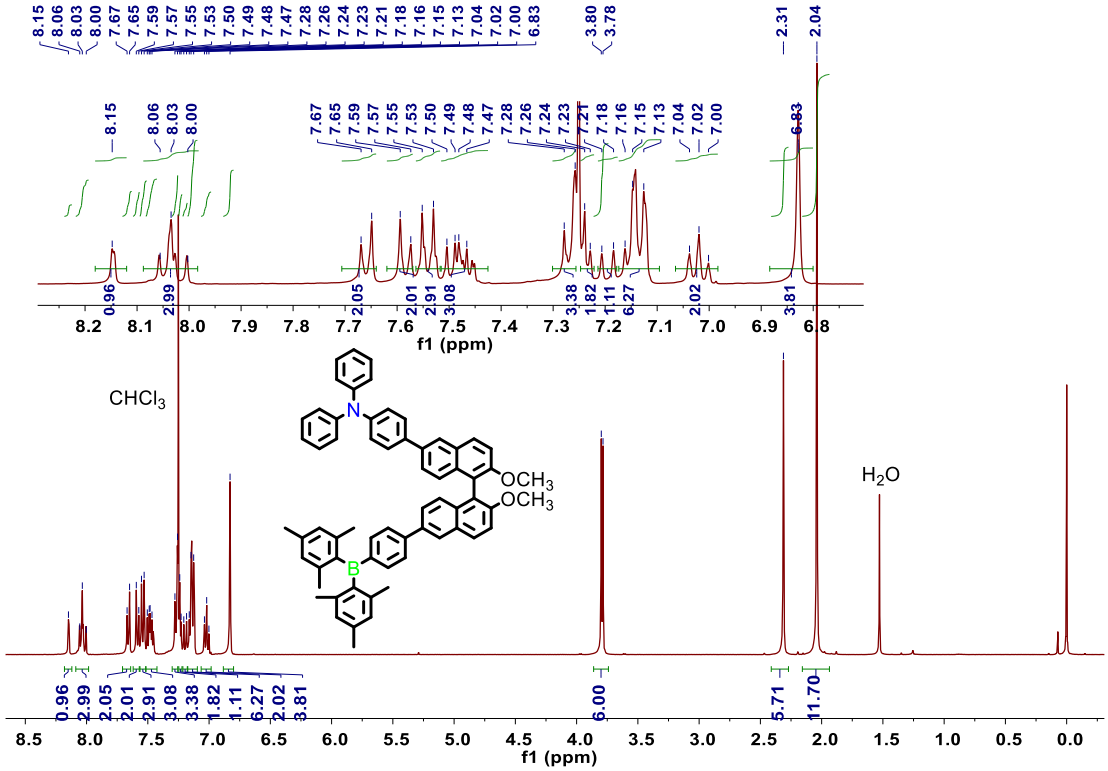


Figure S12. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of **MeBTB**.

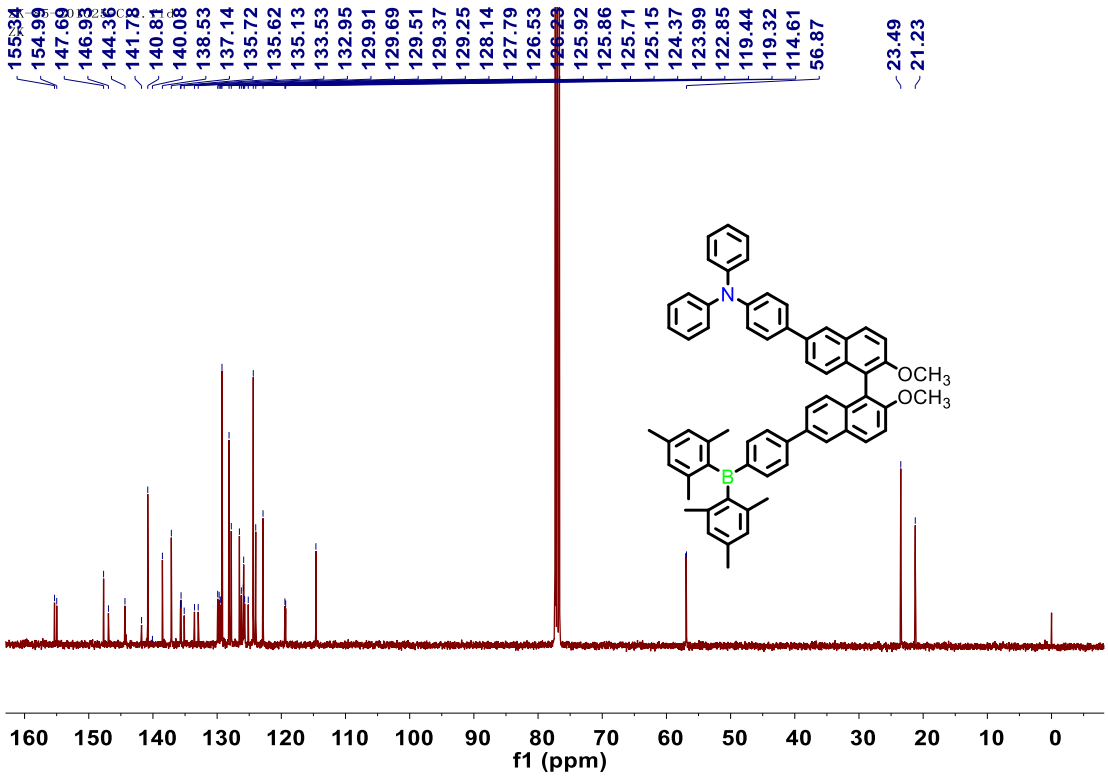


Figure S13. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **MeBTB**.

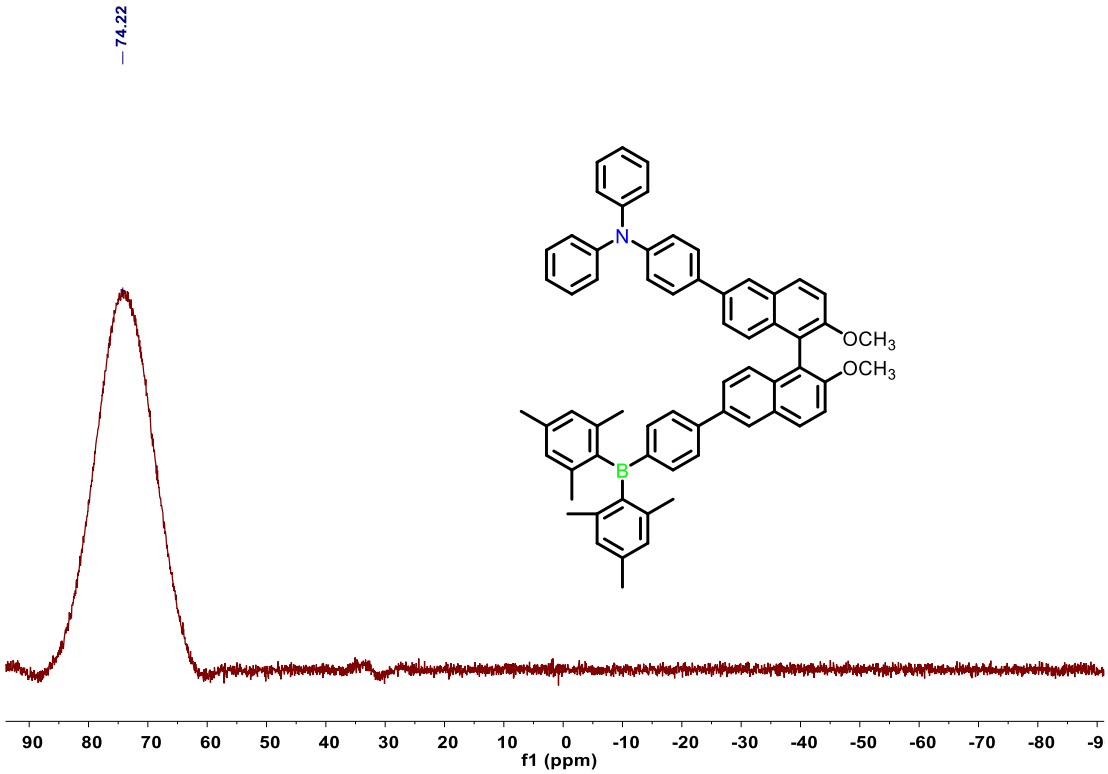


Figure S14.[11]B NMR (225 MHz, C_6D_6) spectrum of **MeBTB**.

3.7 NMR Spectra of 8.

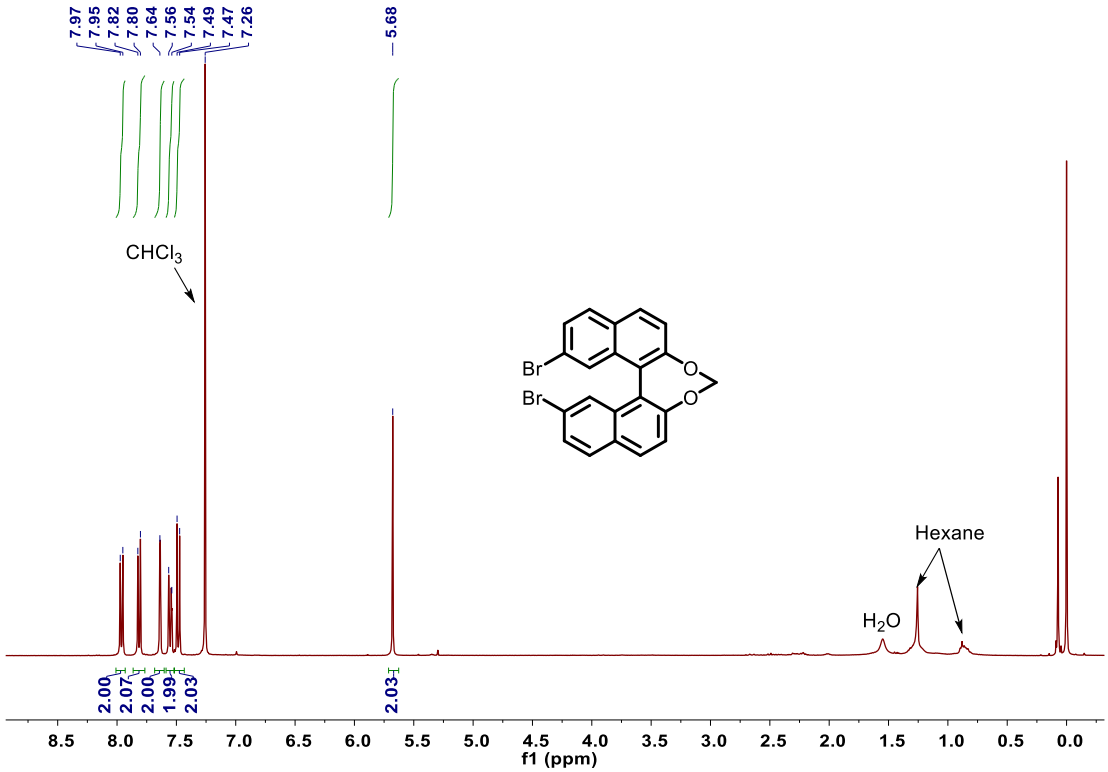


Figure S15. [1]H NMR (400 MHz, $CDCl_3$) spectrum of **8**.

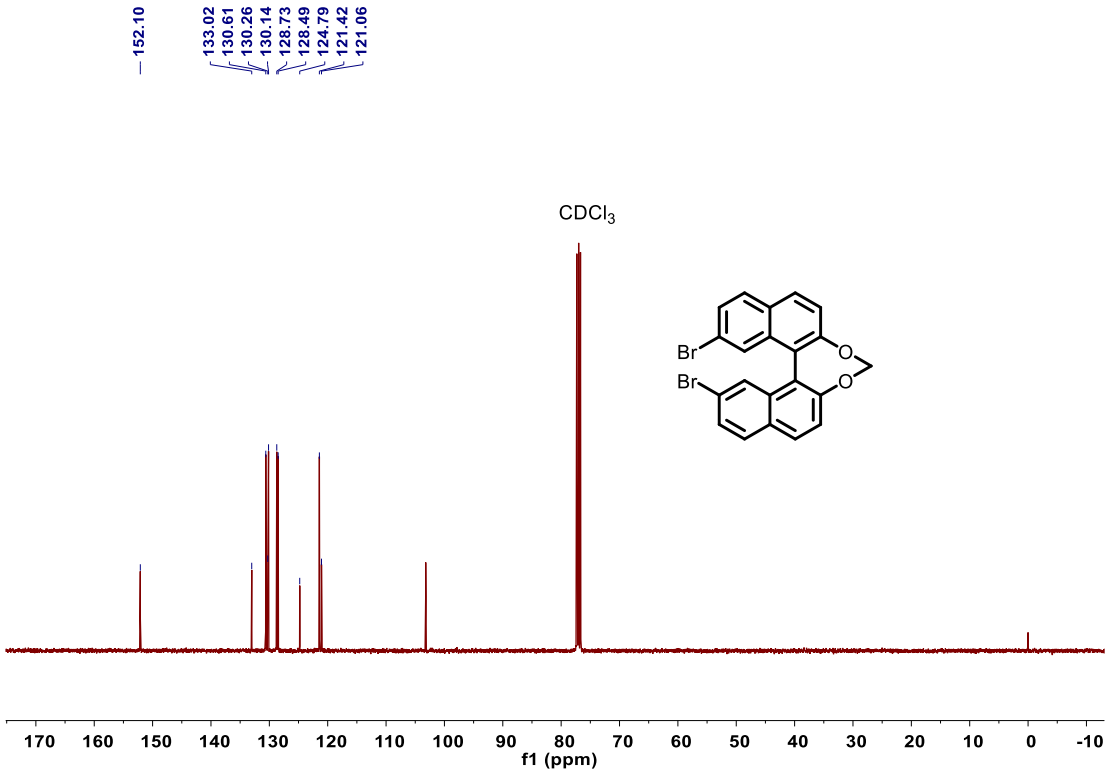


Figure S16. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of **8**.

3.8 NMR Spectra of 9

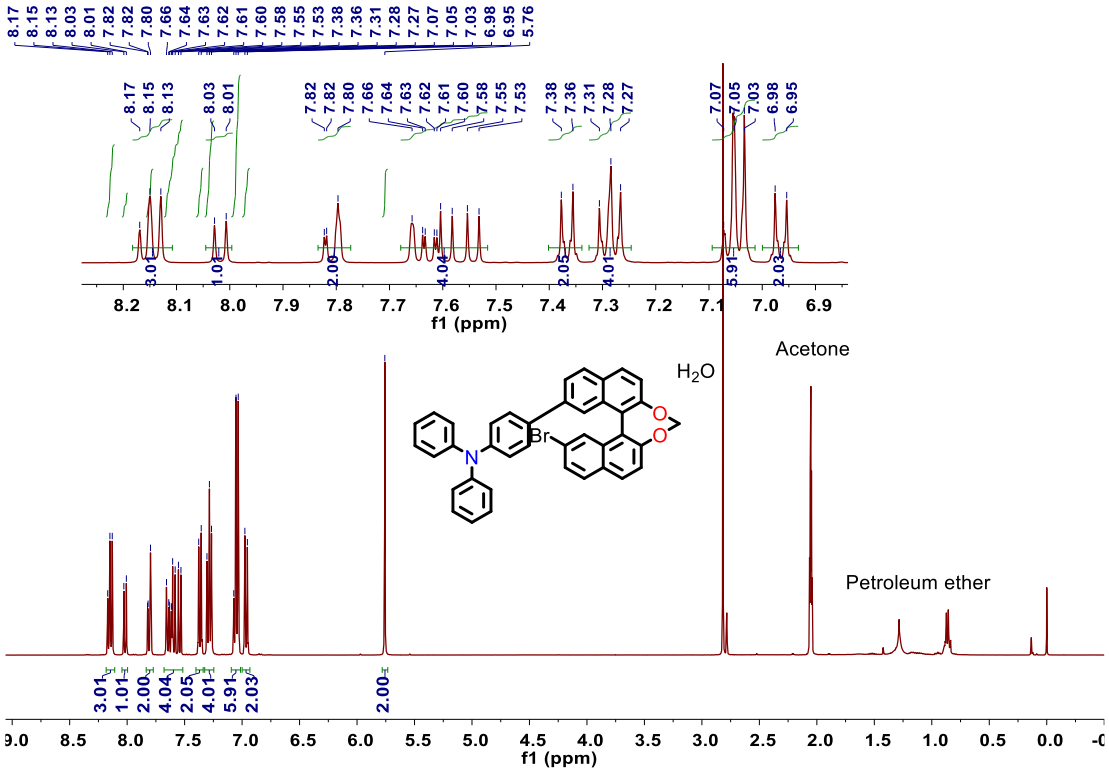


Figure S17. ^{1}H NMR (400 MHz, Acetone-d6) spectrum of **9**.

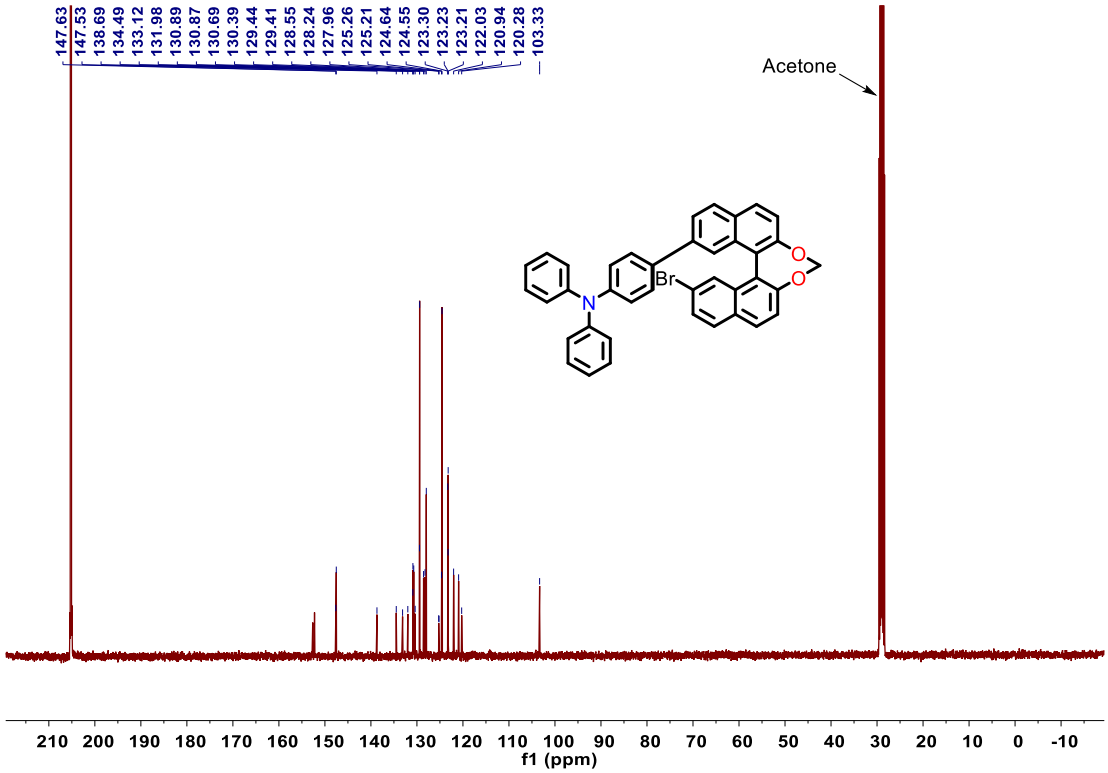


Figure S18. ^{13}C NMR (101 MHz, Acetone-d6) spectrum of **9**.

3.9 NMR Spectra of *m*-BTT.

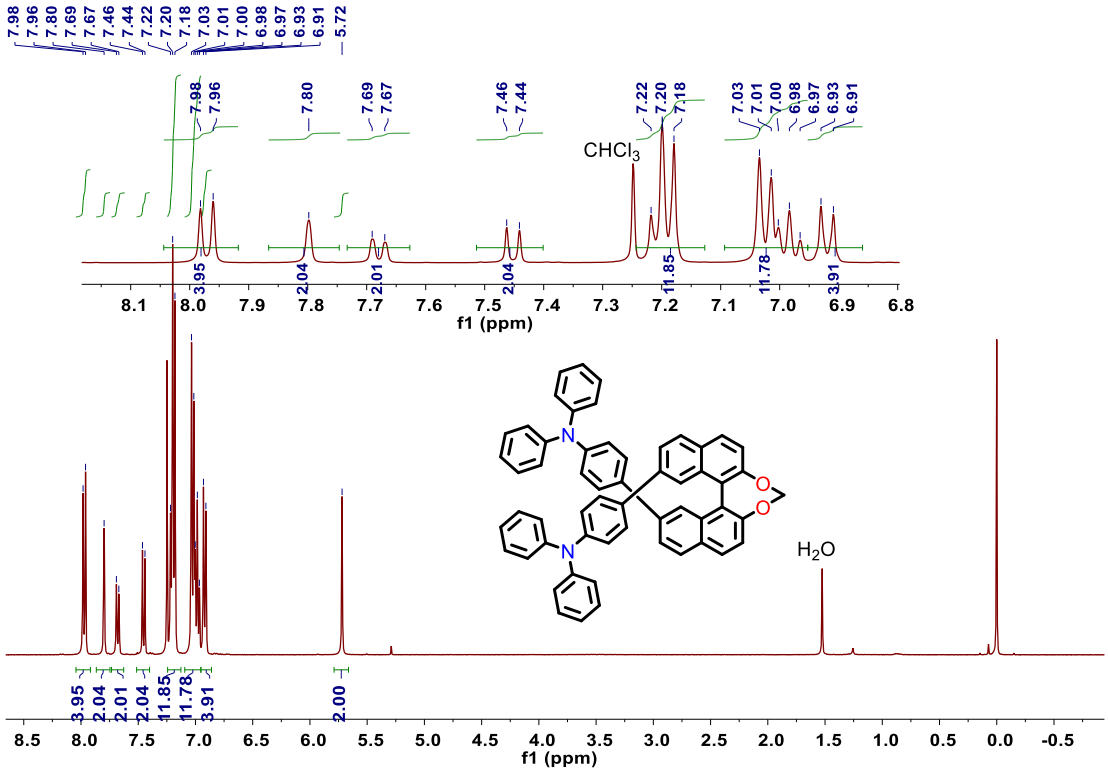


Figure S19. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of ***m*-BTT**.

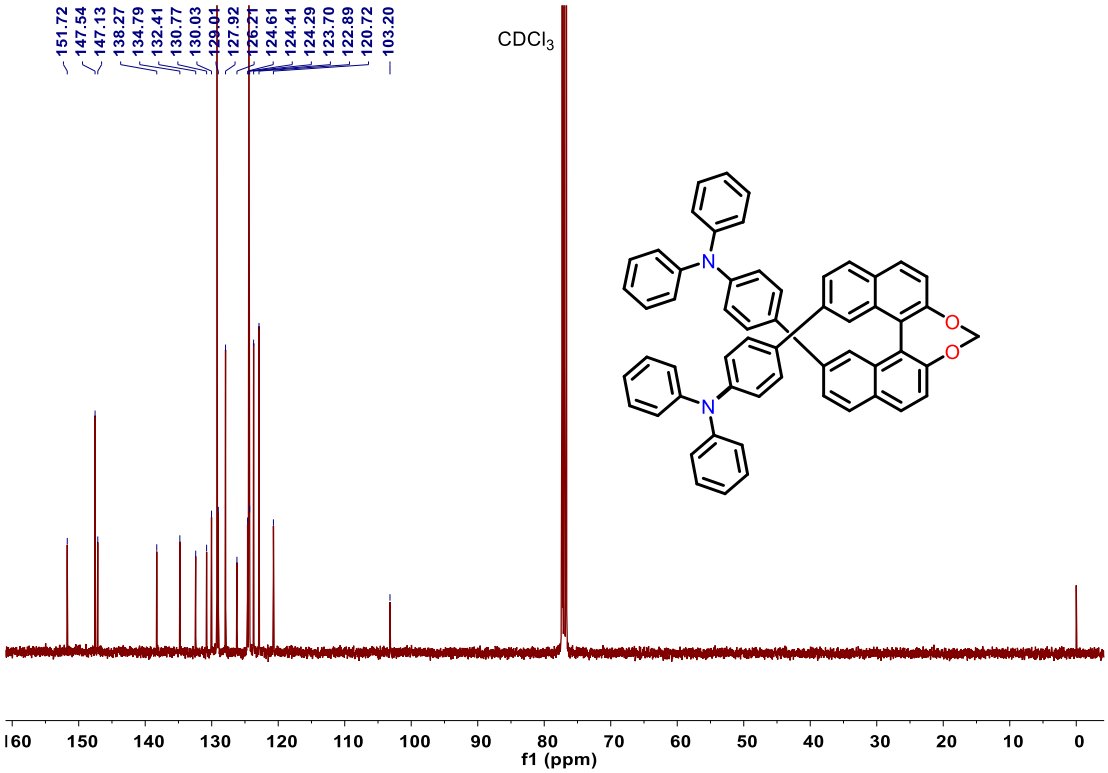


Figure S20. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of ***m*-BTT**.

3.10 NMR Spectra of *m*-BTB

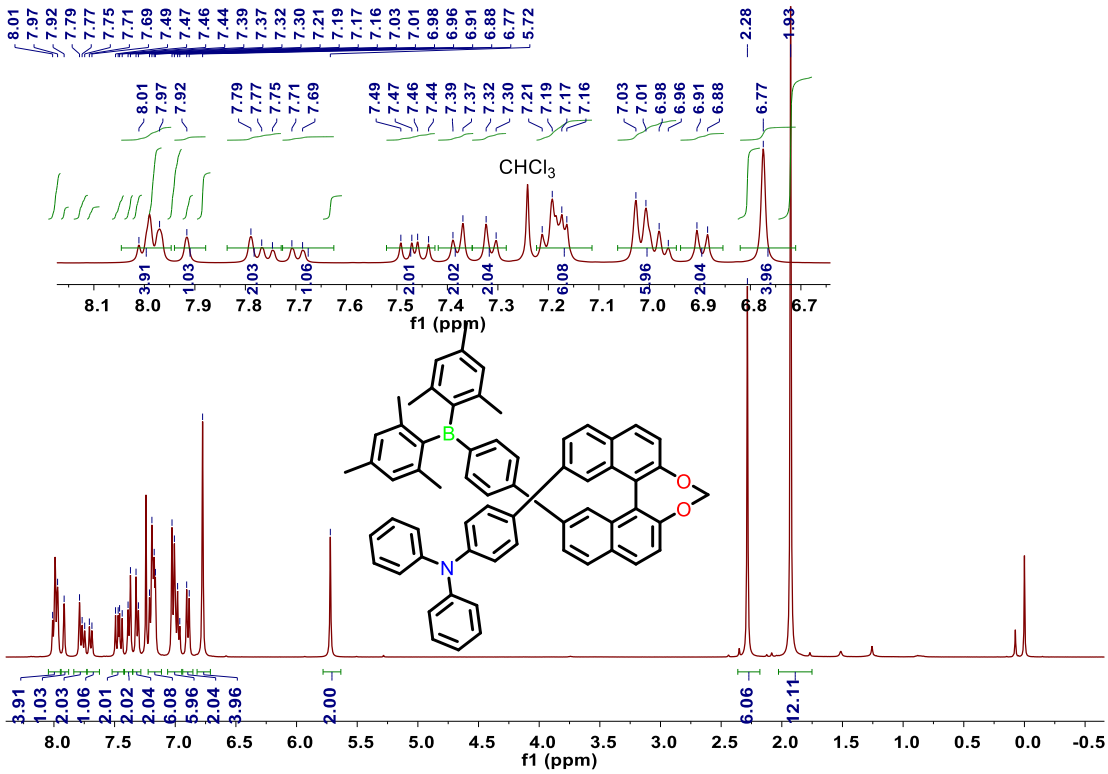


Figure S21. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of ***m*-BTB**.

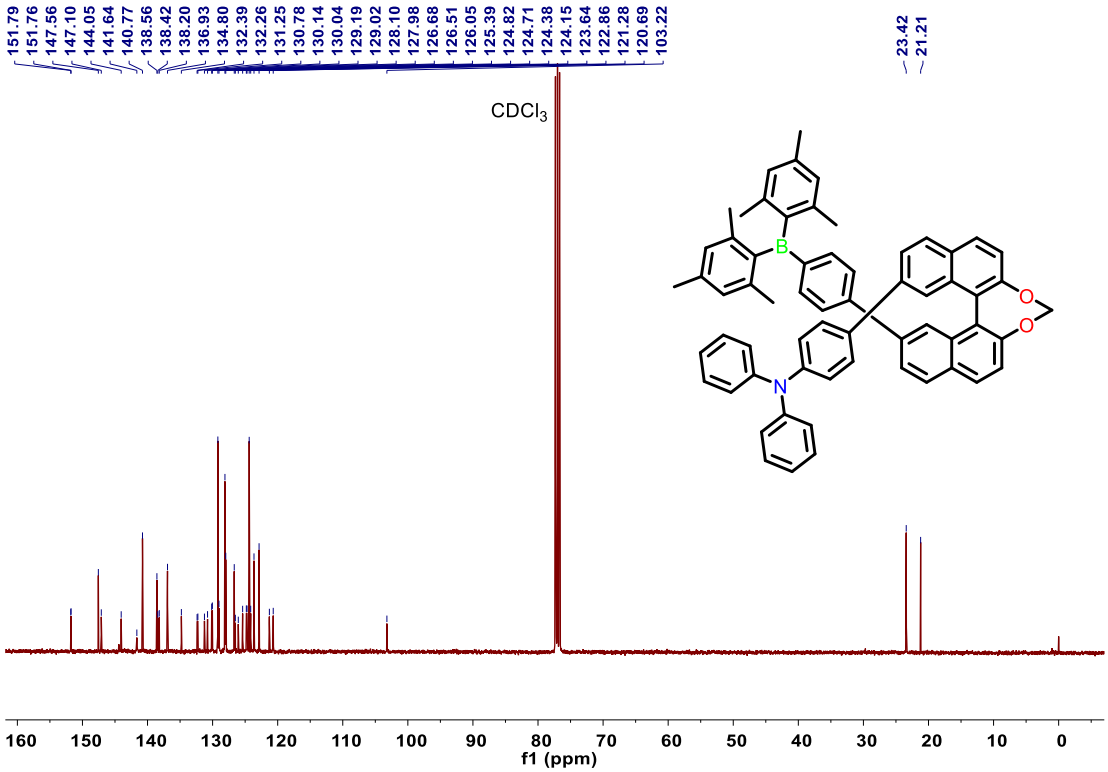


Figure S22. ^{13}C NMR (101 MHz, $CDCl_3$) spectrum of ***m*-BTB**.

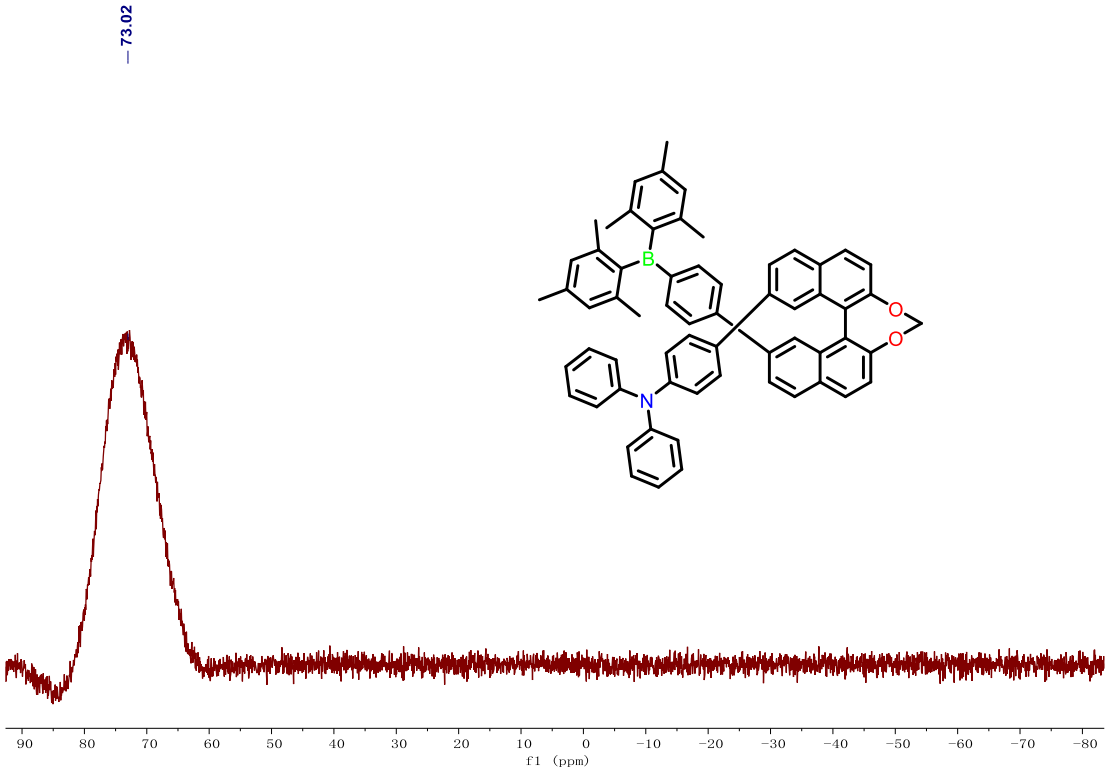


Figure S23.^{11}B NMR (225 MHz, $CDCl_3$) spectrum of ***m*-BTB**.

4. PL Spectra and Transient PL Decay Curves

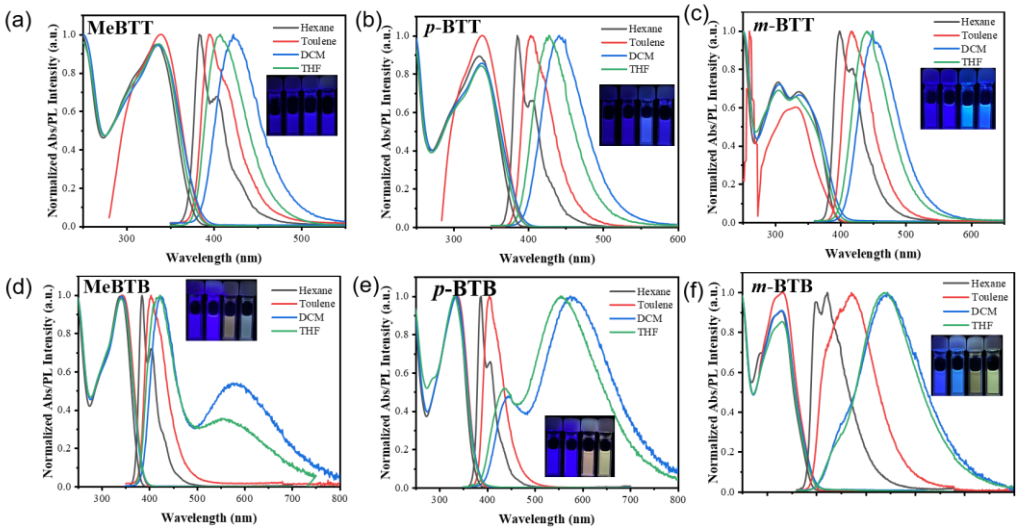


Figure S24. Absorption and emission spectra of (a) **MeBTT**, (b)**MeBTB**, (c) ***p*-BTT**, (d) ***p*-BTB,** (e) ***m*-BTT** and (f) ***m*-BTB** in solvents (c =1.0×10^{-5} M) of different polarities under N_2 at 298 K. Inset: photographs showing the emission colors of **MeBTT**, **MeBTB**, ***p*-BTT**, ***p*-BTB,** ***m*-BTT** and ***m*-BTB** in solutions (c = 0.01 mM) under 365 nm UV irradiation.

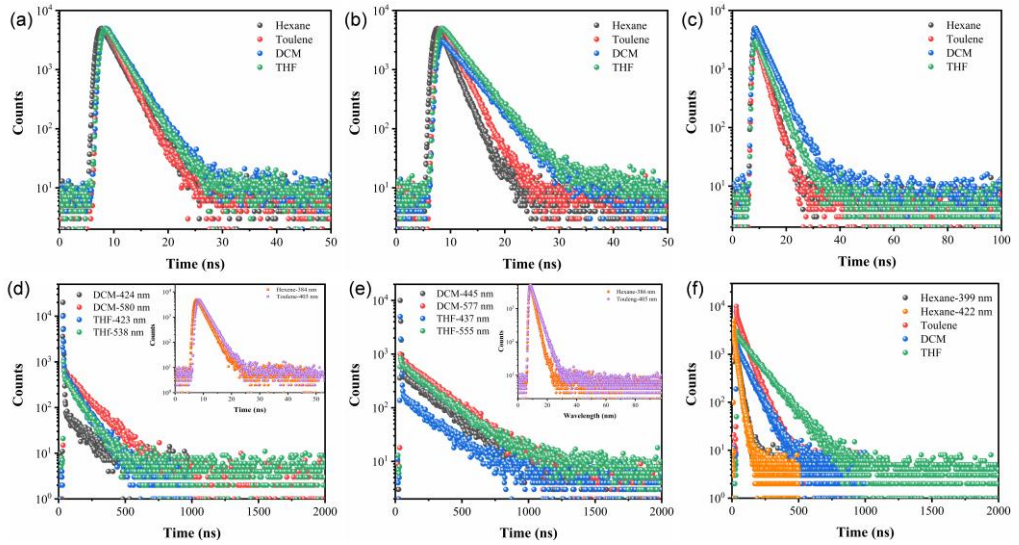


Figure S25. PL decay curves of (a) **MeBTT**, (b)**MeBTB**, (c) ***p*-BTT**, (d) ***p*-BTB,** (e) ***m*-BTT** and (f) ***m*-BTB** in solvents (c = 1.0 × 10^{-5} M) of different polarities under N_2 at 298 K.

Table S1. Absorption and emission properties of **MeBTT** in solvents (c =1.0 × 10^{-5} M) of different polarities under N_2 at 298 K.

	Solvent	λ_{abs} (nm)	λ_{em} (nm)	Φ_{PL} (%)	τ (ns)		Rel %	χ^2
					τ_1	$\tau_{ave.}$		
MeBTT	Hexane	335	384	60.5	2.57	2.57	100	1.293
	Toulene	339	395	77.2	2.30	2.30	100	1.263
	DCM	335	422	81.4	2.98	2.98	100	1.188
	THF	336	408	85.5	2.84	2.84	100	1.251

Table S2. Absorption and emission properties of **MeBTB** in solvents (c =1.0 × 10^{-5} M) of different polarities under N_2 at 298 K.

	Solvent	λ_{abs} (nm)	λ_{em} (nm)	Φ_{PL} (%)	τ (ns)			Rel %	χ^2
					τ_1	τ_2	$\tau_{ave.}$		
MeBTB	Hexane	341	384	61.3	2.02		2.02	100	1.228
	Toulene	343	403	80.5	2.26		2.26	100	1.291
	DCM	342	424	8.6	2.96	133.3	22.08	85.33/14.67	1.243
			580		6.61	136	133.53	1.91/98.09	1.132
	THF	341	423	10.8	2.79	94.71	66.33	30.87/69.13	1.127
			553		3.72	95.83	92.13	4.01/95.99	1.172

Table S3. Absorption and emission properties of ***p*-BTT** in solvents (c =1.0 × 10^{-5} M) of different polarities under N_2 at 298 K.

	Solvent	λ_{abs} (nm)	λ_{em} (nm)	Φ_{PL} (%)	τ (ns)		Rel %	χ^2
					τ_1	$\tau_{ave.}$		
***p*-BTT**	Hexane	336	386	63.2	1.99	1.99	100	1.283
	Toulene	338	403	82.6	2.33	2.33	100	1.233
	DCM	338	441	89.8	3.95	3.95	100	1.279
	THF	337	430	96.0	3.64	3.64	100	1.238

Table S4. Absorption and emission properties of ***p*-BTB** in solvents (c =1.0×10^{-5} M) of different polarities under N_2 at 298 K.

***p*-BTB**	Solvent	λ_{abs} (nm)	λ_{em} (nm)	Φ_{PL} (%)	τ (ns)			Rel %	χ^2
					τ_1	τ_2	$\tau_{ave.}$		

	Hexane	335	386	63.0	2.1		2.1	100	1.192
	Toulene	337	404	81.6	3.15		3.15	100	0.995
	DCM	332	445	15.1	4.17	221.50	158.65	28.92/71.08	1.123
			577		3.26	223.90	223.02	0.40/99.60	1.100
	THF	332	437	15.5	3.92	219.30	148.6	32.83/67.17	1.107
			555		9.76	222.30	219.11	1.50/98.50	1.046

Table S5. Absorption and emission properties of ***m*-BTT** in solvents (c =1.0×10^{-5} M) of different polarities under N_2 at 298 K.

	Solvent	**λ_{abs} (nm)**	**λ_{em} (nm)**	**Φ_{PL} (%)**	**τ (ns)**		**Rel %**	**χ^2**
					τ_1	**$\tau_{ave.}$**		
***m*-BTT**	Hexane	337	399	69.6	2.48	2.48	100	1.260
	Toulene	336	416	88	2.75	2.75	100	1.212
	DCM	336	453	100	4.27	4.27	100	1.232
	THF	332	441	95.8	3.88	3.88	100	1.254

Table S6. Absorption and emission properties of ***m*-BTB** in solvents (c =1.0×10^{-5} M) of different polarities under N_2 at 298 K.

		λ_{abs} (nm)	**λ_{em} (nm)**	**Φ_{PL} (%)**	**τ (ns)**			**Rel %**	**χ^2**
					τ_1	**τ_2**	**$\tau_{ave.}$**		
***m*-BTB**	Hexane	332	399	21.4	1.69	22.24	21.29	4.61/95.39	1.252
			422		10.32	24.98	22.62	16.09/83.91	1.224
	Toulene	332	473	18.7	3.57	57.56	56.15	2.62/97.38	1.283
	DCM	332	545	6.1	5.62	76.01	74.46	2.20/97.80	1.039
	THF	332	538	6.3	124.8		124.8	100	1.235

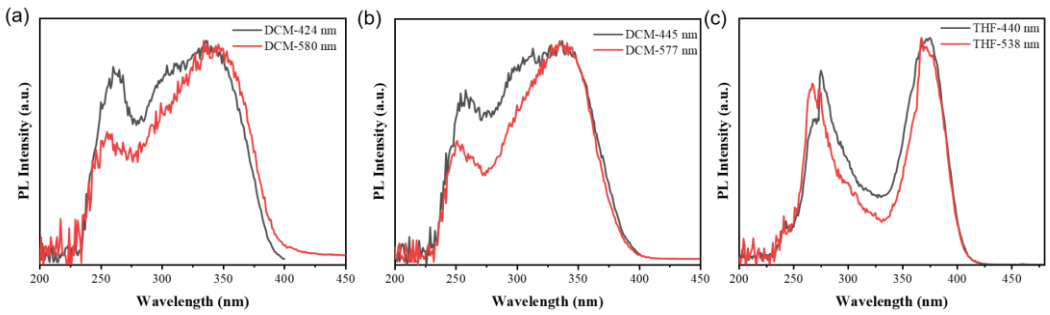


Figure S26. Excitation spectra of (a) **MeBTB** and (b) ***p*-BTB** and (c) ***m*-BTB** in CH_2Cl_2 and THF (c =1.0 × 10^{-5} M) under N_2 at 298 K.

Table S7. Emission properties of **MeBTT**, **MeBTB**, ***p*-BTT**, ***p*-BTB, *m*-BTT** and ***m*-BTB** solid powder at 298 K.

	λ_{em} [nm] in air	φ_{PL} (%)	τ [ns]				Rel %	χ^2
			τ_1	τ_2	τ_3	$\tau_{ave.}$		
MeBTT	425	21	0.92	1.82		1.41	46.60/53.40	1.290
MeBTB	465	23	35.68	119.3		93.77	30.52/69.48	1.109
***p*-BTT**	420	26	1.63	3.66		1.88	87.72/12.28	1.219
***P*-BTB**	457	28	35.77	108.9		81.46	37.52/62.48	1.215
***m*-BTT**	433	59	1.95	4.32		2.05	95.59/4.41	1.242
***m*-BTB**	462	30	7.88	48.41	111.2	69.44	6.74/55.43/37.84	1.288

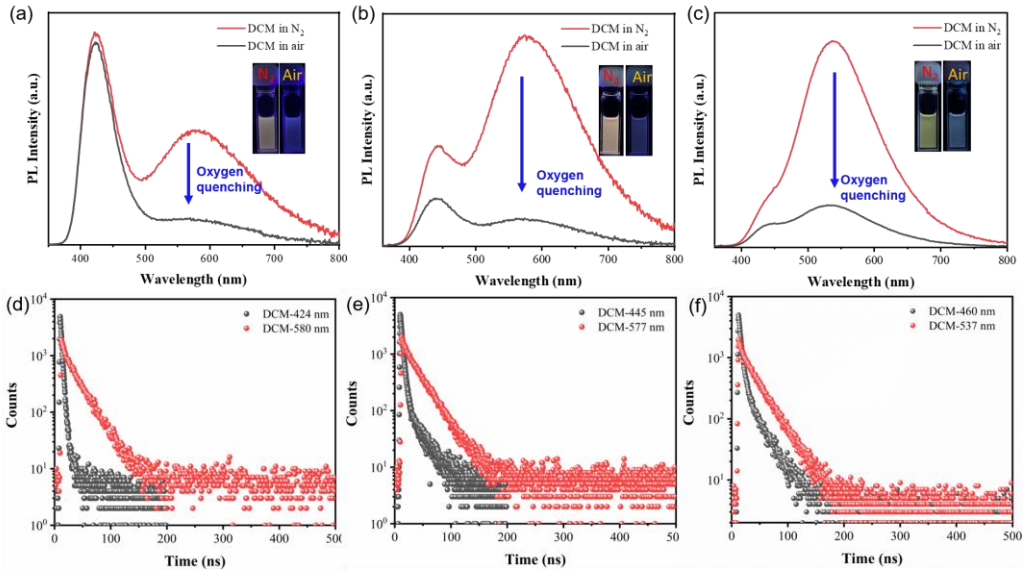


Figure S27. PL spectra and decay curves of (a) **MeBTB**, (b) ***p*-BTB** and (c) ***m*-BTB** in oxygen-free and air-saturated CH_2Cl_2 (c =1.0 × 10^{-5} M) at 298 K and PL decay curves of (d) **MeBTB**, (e) ***p*-BTB** and (f) ***m*-BTB** in air-saturated CH_2Cl_2 at 298 K.

Table S8. Emission properties of **MeBTB**, ***p*-BTB** and ***m*-BTB** in oxygen-free and air-saturated CH_2Cl_2 (c = 1.0 × 10^{-5} M) at 298 K

	Atmosphere	λ_{em} [nm]	φ_{PL} (%)	τ [ns]			Rel %	χ^2
				τ_1	τ_2	$\tau_{ave.}$		
MeBTB	N_2	424	8.6	2.96	133.3	22.08	85.33/14.67	1.243
		580		6.61	136	133.53	1.91/98.09	1.132
	Air	423	3.8	2.67	21.27	3.29	96.65/3.35	1.075
		580		3.78	24.86	22.96	9.02/90.98	1.141
***p*-BTB**	N_2	445	15.1	4.17	221.5	158.65	28.92/71.08	1.123

		577		3.26	223.9	223.02	0.40/99.60	1.100
	Air	445	3.1	3.55	26.03	7.73	81.39/ 18.61	1.225
		577		4.44	27.23	25.99	5.44/94.56	1.163
***m*-BTB**	N_2	460	6.1	4.88	74.01	59.59	20.86/79.14	1.128
		545		5.62	76.01	74.46	2.20/97.80	1.039
	Air	460	3	4.22	25.85	11.44	66.62/33.38	1.040
		537		4.96	28.85	26.93	8.02/91.98	1.146

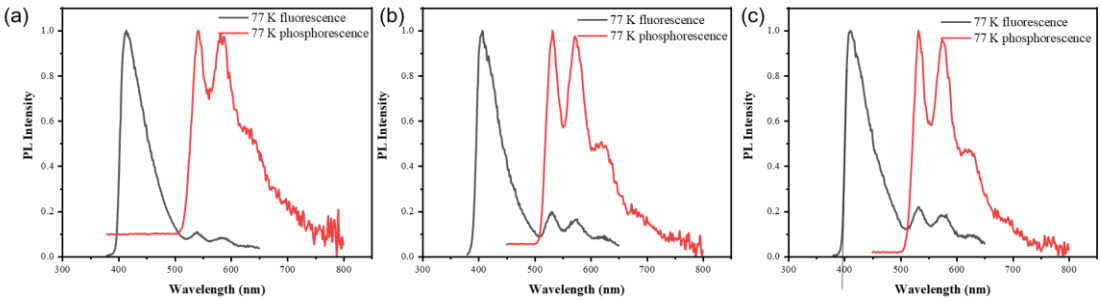


Figure S28. Fluorescence and phosphorescence spectra of **MeBTB**, ***p*-BTB** and ***m*-BTB** in MTHF at 77 K.

5. Chiral HPLC Trace Analysis

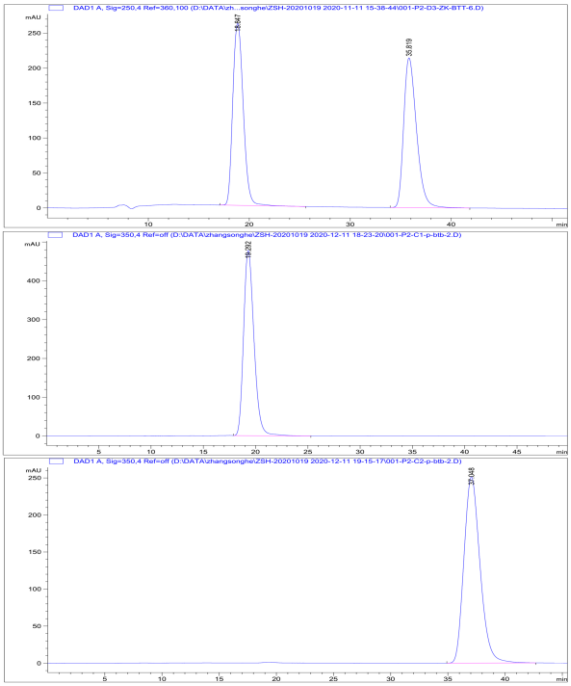


Figure S29. HPLC chromatogram used for chiral resolution of enantiomers of ***p*-BTT** by a preparative HPLC equipped with a Daicel Chiralpak IF column with *n*-hexane/isopropanol = 95:5, flow = 3.0 mL/min.

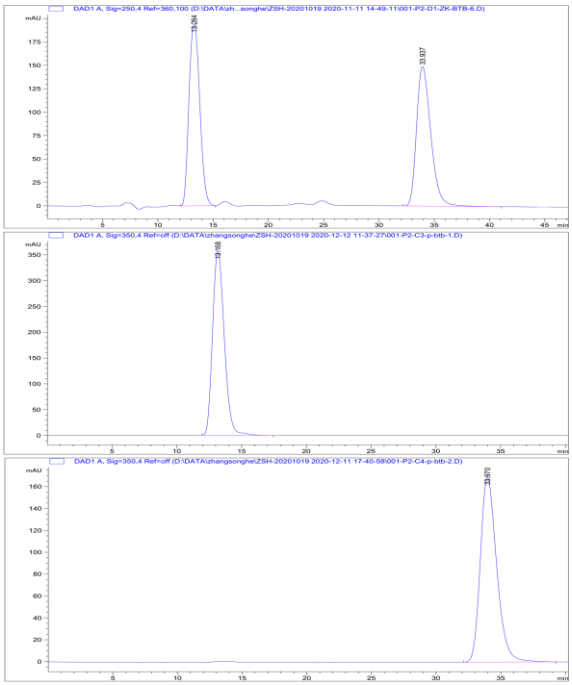


Figure S30. HPLC chromatogram used for chiral resolution of enantiomers of ***p*-BTB** by a preparative HPLC equipped with a Daicel Chiralpak IF column with *n*-hexane/isopropanol = 95:5, flow = 3.0 mL/min.

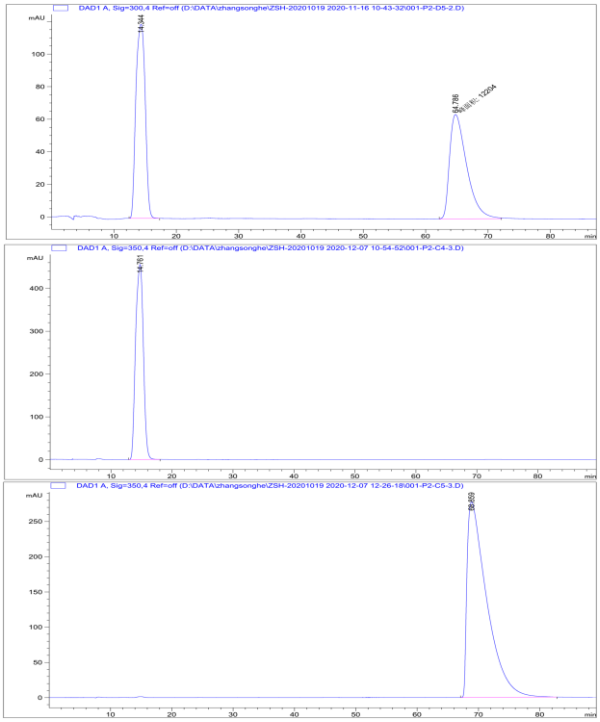


Figure S31. HPLC chromatogram used for chiral resolution of enantiomers of ***m*-BTT** by a preparative HPLC equipped with a Daicel Chiralpak IB column with *n*-hexane/isopropanol = 90:10, flow = 3.0 mL/min.

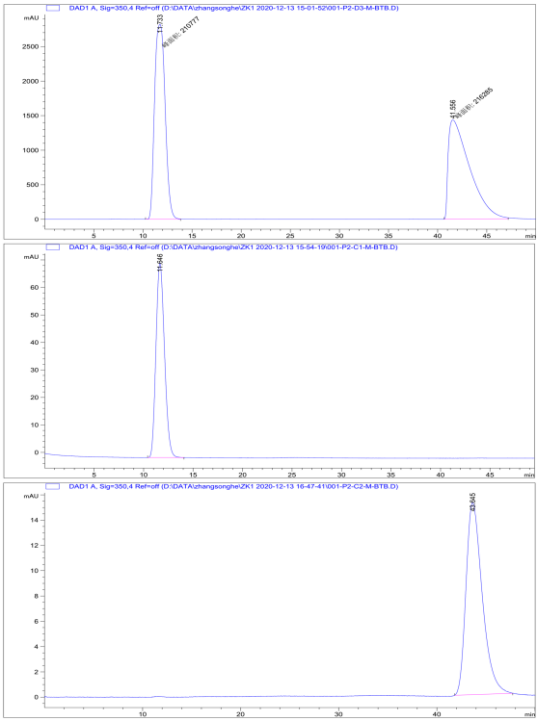


Figure S32. HPLC chromatogram used for chiral resolution of enantiomers of ***m*-BTB** by a preparative HPLC equipped with a Daicel Chiralpak IB column with *n*-hexane/isopropanol = 90:10, flow = 3.0 mL/min.

Table S9. Summary of the HPLC analysis of ***p*-BTT**, ***p*-BTB**, ***m*-BTT** and ***m*-BTB**.

	Fraction	Retention Time / min	Area / %	Enantiomeric excess (ee)	[α] / ° T =25 °C λ = 589 nm
rac-***p*-BTT**	Peak1	18.8	49.94	-	-
	Peak2	35.8	50.06	-	-
enantiopure	**(*S*)-*p*-BTT**	19.3	100	> 99%	+563
***p*-BTT**	**(*R*)-*p*-BTT**	37.0	100	> 99%	–616
rac-***p*-BTB**	Peak1	13.3	49.83	-	-
	Peak2	33.9	50.17	-	-
enantiopure	**(*S*)-*p*-BTB**	13.2	100	> 99%	+488
***p*-BTB**	**(*R*)-*p*-BTB**	34.0	100	> 99%	–521
rac-***m*-BTT**	Peak1	14.3	50.3	-	-
	Peak2	64.8	49.7	-	-
enantiopure	**(*R*)-*m*-BTT**	14.8	100	> 99%	–1262
***m*-BTT**	**(*S*)-*m*-BTT**	68.9	100	> 99%	+1044
rac-***m*-BTB**	Peak1	11.7	49.36	-	-
	Peak2	41.6	50.64	-	-
enantiopure	**(*R*)-*m*-BTB**	11.6	100	> 99%	–1174
***m*-BTB**	**(*S*)-*m*-BTB**	43.6	100	> 99%	+1084

6. CPL Spectra in Different Solutions

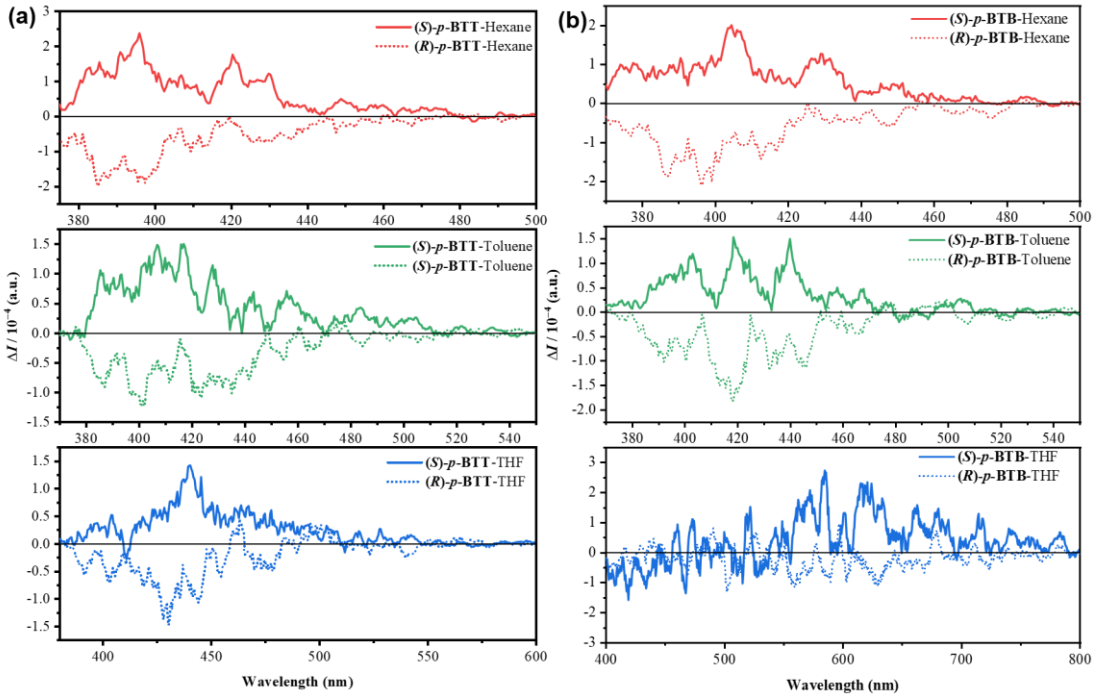


Figure S33. CPL spectra of enantiomers for (a) ***p*-BTT**, (b) ***p*-BTB**, after optical resolution in solvents (c = 0.01 mM) with different polarities under N_2 at 298 K.

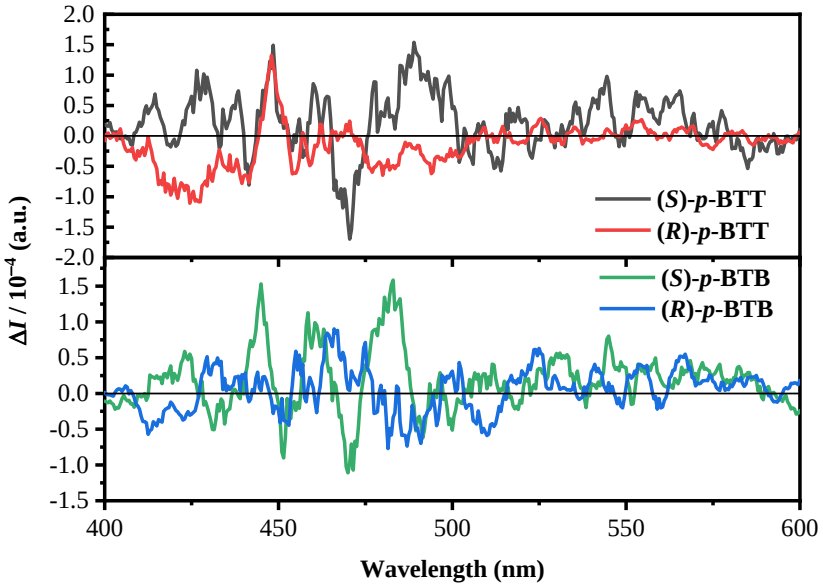
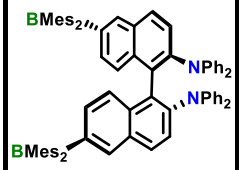


Figure 34. CPL spectra of enantiomers for ***p*-BTT** and ***p*-BTB** neat films after optical resolution at 298 K.

Table S10. Summary of the photophysical and chiroptical data of **BNPh$_2$-BNaph** in various solvents reported by Zhao and Peng (see *ACIE*, 2019, *58*, 4840–4846).

Compound	Solvents	λ_{abs}	λ_{em}	Φ_{PL}	g_{lum} 10^{-3} (λ_{em}/nm)	
					(+)-BNPh$_2$-BNaph	(-)-BNPh$_2$-BNaph
 BNPh2-BNaph	cyclohexane	398	440	0.75	–1.17 (455)	+1.53 (453)
	benzene	398	456	0.68	–0.25(450) +0.42(519)	+0.53 (463) –0.33 (521)
	chloroform	296	472	0.58	--	--
	THF	396	482	0.51	–0.46 (446) +0.74(510)	+0.29 (463) –0.46 (528)
	MOE	396	487	0.52	--	--
	MeCN	390	512	0.26	+1.19 (524)	–0.52 (521)

7. Thermochromic Emissions and Aggregation-induced Emission Properties

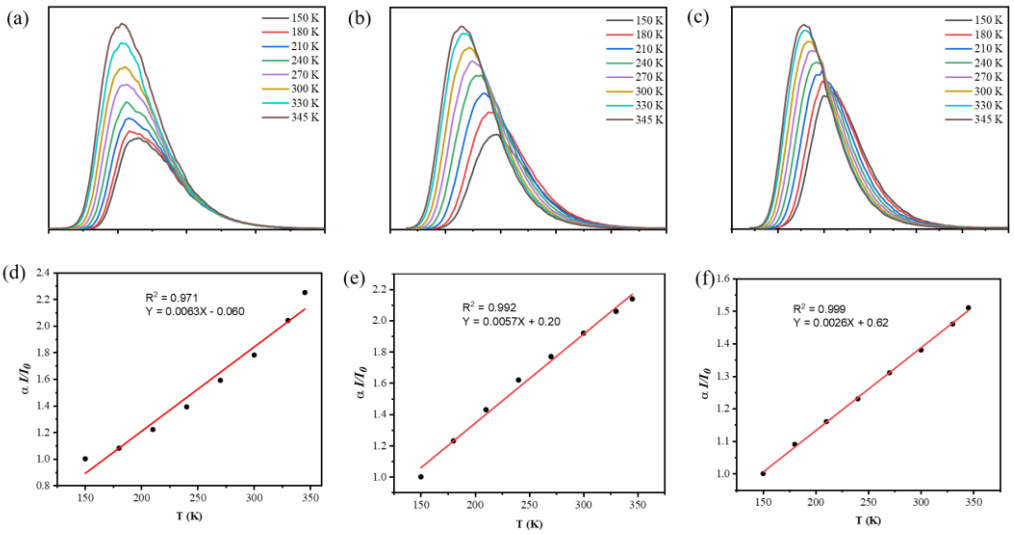


Figure S35. Temperature-dependent spectra and plot of relative PL intensity (α I/I_0) at λ_{max} versus T of (a, d) **MeBTT**, (b, e) ***p*-BTT** and (c, f) ***m*-BTT** in 2-MeTHF (c = 0.03 mM) recorded between 150 and 345 K under N_2 atmosphere, where I_0 = emission intensity at 150 K, I = emission intensity at different temperature.

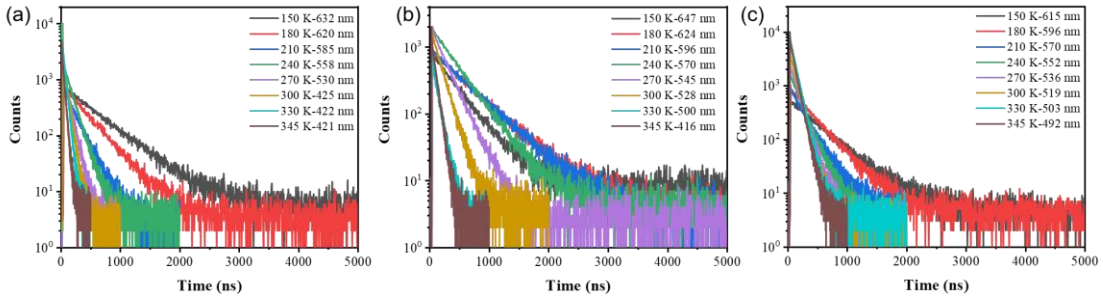


Figure S36. Temperature-dependent transient decay spectra of (a) **MeBTB**, (b) ***p*-BTB** and (c) ***m*-BTB** in MTHF (c = 0.03 mM) recorded between 150 and 345 K under N_2.

Table S11. Temperature-dependent photophysical properties and fitting results of temperature-dependent transient decay spectra of **MeBTB** in MTHF (c = 0.03 mM) under N_2.

T [K]	λ_{max} [nm]	τ [ns]			Rel %	χ^2	CIE [x,y]
		τ_1	τ_2	$\tau_{ave.}$			
150	632	523.10		523.10	100	1.217	[0.34, 0.22]
180	620	356.70		356.70	100	1.166	[0.35, 0.25]
210	585	196.60		196.60	100	1.064	[0.32, 0.28]
240	558	5.91	125.00	122.22	2.33/97.67	1.136	[0.29, 0.29]
270	530	3.86	85.61	82.50	3.81/96.19	1.058	[0.23, 0.23]
300	425	2.77	60.78	54.81	10.30/89.70	1.075	[0.19,0.14]
330	422	2.73	42.45	40.85	4.03/95.97	1.078	[0.17,0.08]
345	421	3.07	32.55	31.69	2.93/97.07	1.206	[0.16,0.06]

Table S12. Temperature-dependent photophysical properties and fitting results of temperature-dependent transient decay spectra of ***p*-BTB** in MTHF (c = 0.03 mM) under N_2.

T [K]	λ_{max} [nm]	τ [ns]			Rel %	χ^2	CIE [x,y]
		τ_1	τ_2	$\tau_{ave.}$			
150	647	368.80		368.80	100	1.121	[0.46, 0.31]
180	624	537.90		537.90	100	1.088	[0.50, 0.39]
210	596	521.00		521.00	100	1.214	[0.47, 0.45]
240	570	345.90		345.90	100	1.217	[0.41, 0.47]
270	545	216.70		216.70	100	1.017	[0.34, 0.45]
300	528	141.90		141.90	100	1.289	[0.26, 0.32]
330	500	87.27		87.27	100	1.104	[0.19, 0.15]
345	416	3.87	68.26	66.12	3.32/96.68	1.035	[0.18,0.10]

Table S13. Temperature-dependent photophysical properties and fitting results of temperature-dependent transient decay spectra of ***m*-BTB** in MTHF (c = 0.03 mM) under N_2.

T [K]	λ_{max} [nm]	τ [ns]			Rel %	χ^2	CIE [x,y]
		τ_1	τ_2	$\tau_{ave.}$			
150	615	468.00		468.00	100	1.170	[0.50, 0.42]
180	596	345.70		345.70	100	1.194	[0.47, 0.45]
210	570	226.10		226.10	100	1.061	[0.42, 0.47]
240	552	161.90		161.90	100	1.113	[0.37, 0.49]
270	536	123.20		123.20	100	1.123	[0.32, 0.48]
300	519	99.38		99.38	100	1.173	[0.27, 0.42]
330	503	6.91	85.93	84.46	1.86/98.14	1.185	[0.22, 0.33]
345	492	4.31	78.58	73.91	2.25/97.75	1.172	[0.20, 0.28]

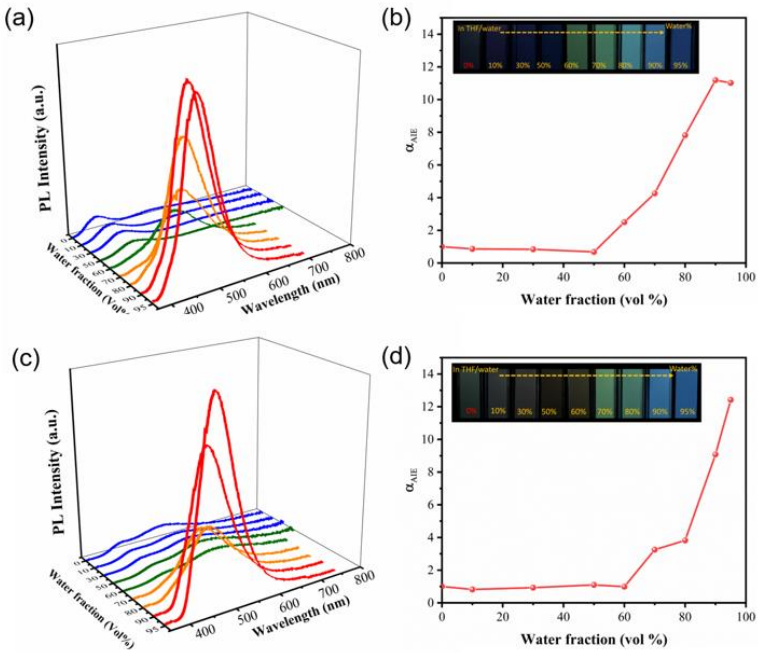


Figure 37. (a, c) Emission spectra of ***p*-BTB** and ***m*-BTB** (c =1.0 × 10^{-5} M) in THF/water mixtures with different water content. (b, d) Plot of relative PL intensity (α_{AIE}) at λ_{max} versus f_w of the THF/water mixtures of ***p*-BTB** and ***m*-BTB**, where α_{AIE} = I/I_0 and I_0 = emission intensity in pure THF solution. Inset: photographs of ***p*-BTB** and ***m*-BTB** in THF and THF/water mixtures with different water content taken under 365 nm UV light.

8. DFT and TD-DFT Computations and Electrochemical Measurements

DFT and TD-DFT calculations were performed using the Gaussian 09 suite of programs.[6] Geometry optimizations and vertical excitations of all compounds were obtained at the CAM-B3LYP/6-31G* and (TD) CAM-B3LYP/6-31G* level of theory, [7, 8] and the resulting structures were confirmed to be stationary points through vibrational frequency analysis.

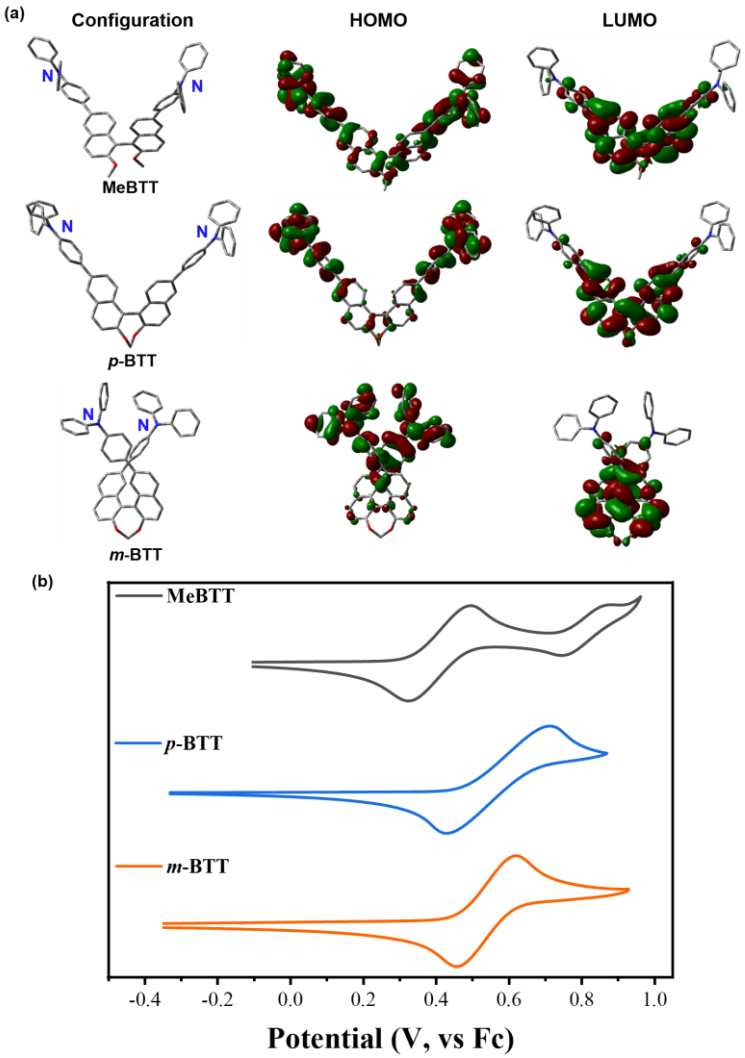


Figure S38. The DFT optimized structures and frontier molecular orbital plots of **MeBTT**, ***p*-BTT** and ***m*-BTT** (iso = 0.02, CAM-B3LYP/6-31G*) in the ground state. Hydrogen atoms are omitted. (b) Cyclic voltammetry of **MeBTT**, ***p*-BTT** and ***m*-BTT** showing the oxidation waves in CH_2Cl_2 (*vs* Fc^+/Fc) with *n*-Bu_4NPF_6 (*c* = 0.1 M) as the electrolyte, υ = 100 mV/s.

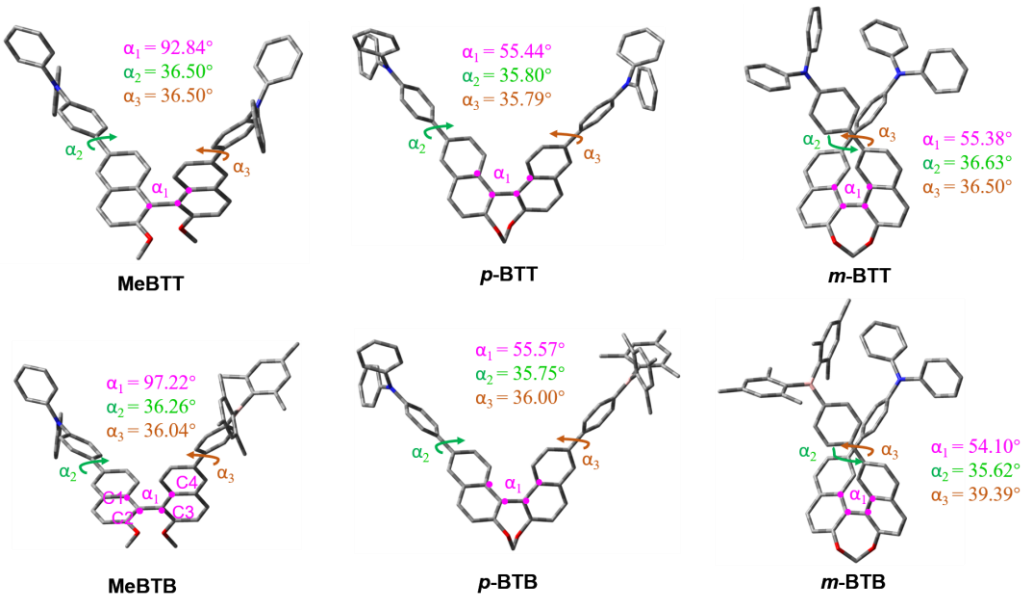


Figure S39. The optimized structures (CAM-B3LYP/6-31G*) in the ground state. Hydrogen atoms are omitted. The angles between the adjacent aryl rings are shown for comparison.

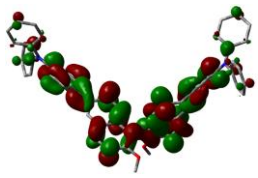
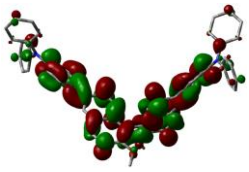
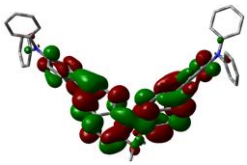
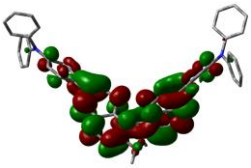
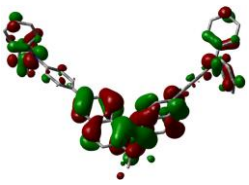
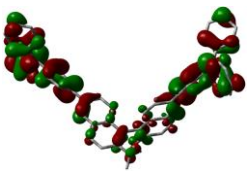
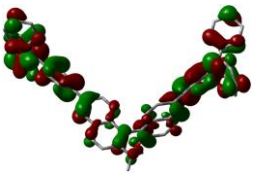
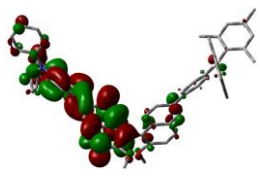
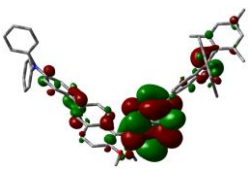
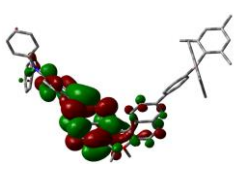
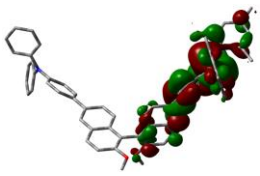
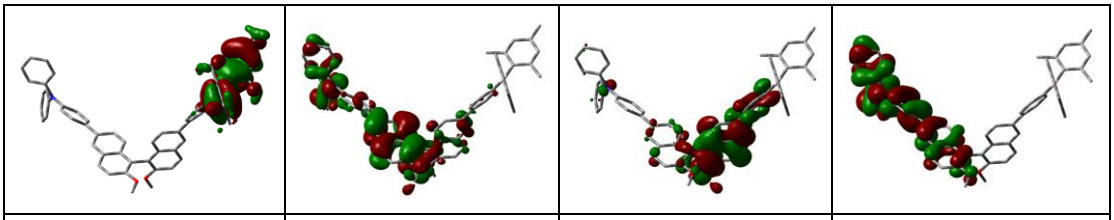
			
LUMO+3	LUMO+2	LUMO+1	LUMO
			
HOMO-3	HOMO-2	HOMO-1	HOMO

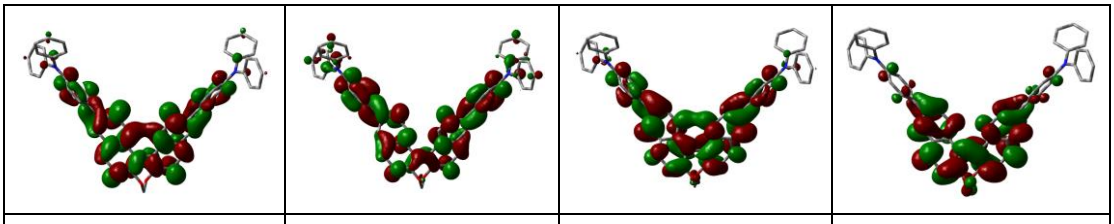
Figure S40. Molecular orbitals contributing to the DFT calculated transitions of **MeBTT** (iso = 0.02, CAM-B3LYP/6-31G*) in the ground state.

			
LUMO+3	LUMO+2	LUMO+1	LUMO

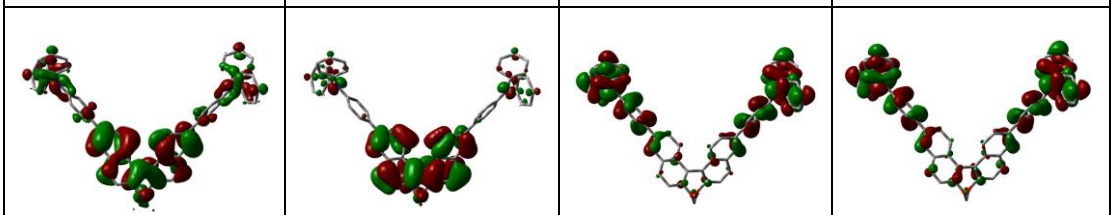


HOMO-3	HOMO-2	HOMO-1	HOMO

Figure S41. Molecular orbitals contributing to the DFT calculated transitions of **MeBTB** (iso = 0.02, CAM-B3LYP/6-31G*) in the ground state.

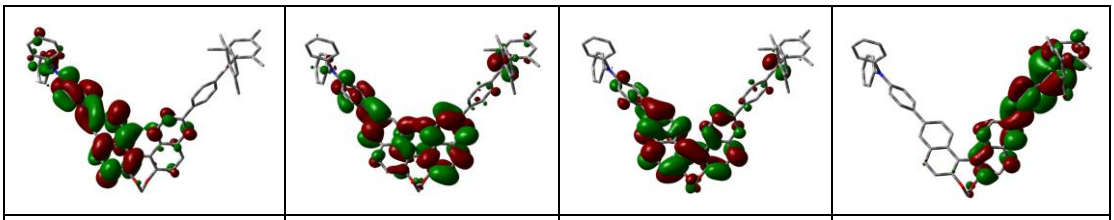


LUMO+3	LUMO+2	LUMO+1	LUMO

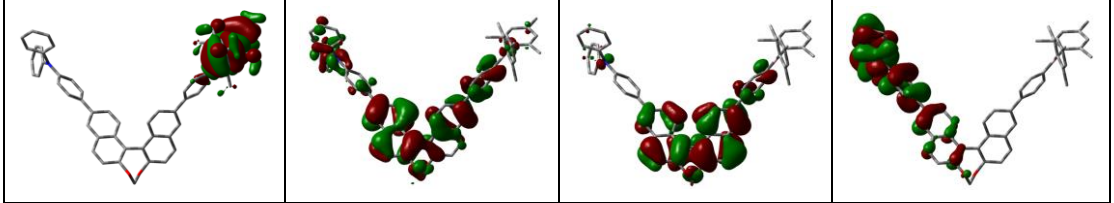


HOMO-3	HOMO-2	HOMO-1	HOMO

Figure S42. Molecular orbitals contributing to the DFT calculated transitions of ***p*-BTT** (iso = 0.02, CAM-B3LYP/6-31G*) in the ground state.



LUMO+3	LUMO+2	LUMO+1	LUMO



HOMO-3	HOMO-2	HOMO-1	HOMO

Figure S43. Molecular orbitals contributing to the DFT calculated transitions of ***p*-BTB** (iso = 0.02, CAM-B3LYP/6-31G*) in the ground state.

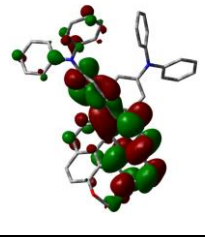
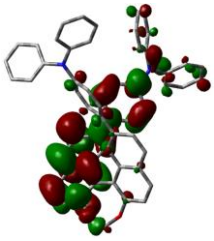
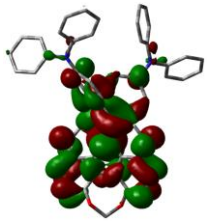
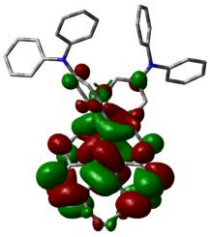
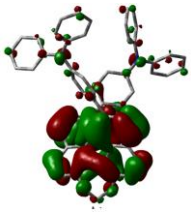
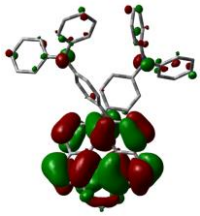
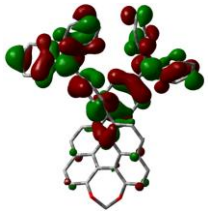
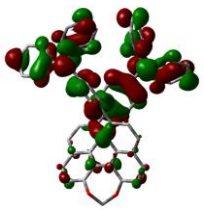
			
LUMO+3	LUMO+2	LUMO+1	LUMO
			
HOMO-3	HOMO-2	HOMO-1	HOMO

Figure S44. Molecular orbitals contributing to the DFT calculated transitions of ***m*-BTT** (iso = 0.02, CAM-B3LYP/6-31G*) in the ground state.

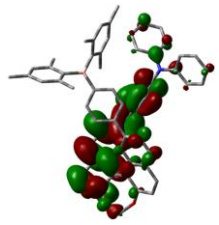
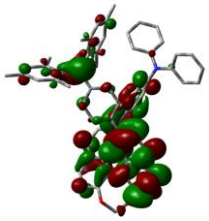
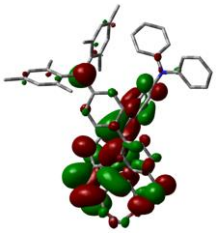
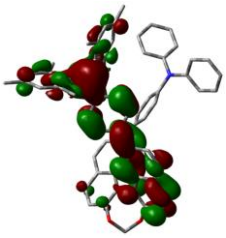
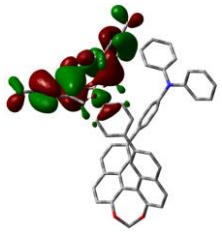
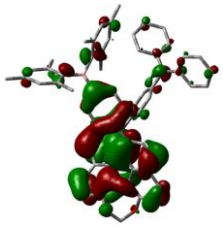
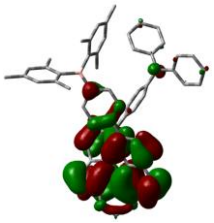
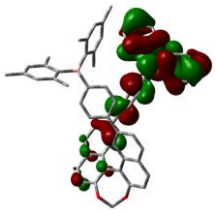
			
LUMO+3	LUMO+2	LUMO+1	LUMO
			
HOMO-3	HOMO-2	HOMO-1	HOMO

Figure S45. Molecular orbitals contributing to the DFT calculated transitions of ***m*-BTB** (iso = 0.02, CAM-B3LYP/6-31G*) in the ground state.

Table S14. Summary of the TD-DFT calculations about selected transitions and oscillator strengths in CH_2Cl_2 (CAM-B3LYP/6-31G*) in the ground state.

Compound	Transition	λ, nm (eV)	Oscillator Strength, *f*	Orbital Contributions
MeBTT	$S_0 \rightarrow S_1$	4.0247 (308.06)	0.7263	HOMO→LUMO+1 (34%) HOMO-1→LUMO (27%)
	$S_0 \rightarrow S_2$	4.0248 (308.05)	0.9033	HOMO→LUMO (31%) HOMO-1→LUMO+1 (30%)

	$S_0 \rightarrow S_3$	4.21 (295)	0.8960	HOMO→LUMO+2 (31%) HOMO-1→LUMO+3 (20%) HOMO-2→LUMO (15%)
	$S_0 \rightarrow S_4$	4.31 (287)	0.1671	HOMO-1→LUMO+2 (28%) HOMO→LUMO+3 (24%)
	$S_0 \rightarrow S_5$	4.45 (279)	0.0446	HOMO→LUMO+2 (55%)
MeBTB	$S_0 \rightarrow S_1$	3.98 (312)	1.0146	HOMO-1→LUMO (58%)
	$S_0 \rightarrow S_2$	4.02 (308)	0.7979	HOMO→LUMO+1 (62%)
	$S_0 \rightarrow S_3$	4.10 (303)	0.1431	HOMO-3→LUMO (85%)
	$S_0 \rightarrow S_4$	4.20 (295)	0.6392	HOMO-1→LUMO+2 (30%) HOMO→LUMO+3 (21%) HOMO-1→LUMO+1 (12%)
	$S_0 \rightarrow S_5$	4.30 (288)	0.1080	HOMO-3→LUMO (96%)
	$S_0 \rightarrow S_6$	4.41(281)	0.0125	HOMO-4→LUMO (54%) HOMO-1→LUMO (12%)
***p*-BTT**	$S_0 \rightarrow S_1$	4.02 (309)	0.7008	HOMO-1→LUMO+1 (33%) HOMO→LUMO (28%) HOMO→LUMO+2 (15%)
	$S_0 \rightarrow S_2$	4.04(307)	1.0888	HOMO→LUMO+1 (32%) HOMO-1→LUMO (30%) HOMO-1→LUMO+2 (13%)
	$S_0 \rightarrow S_3$	4.20(295)	0.8254	HOMO-2→LUMO+1 (53%) HOMO→LUMO+2 (13%)
	$S_0 \rightarrow S_4$	4.33(286)	0.1377	HOMO-1→LUMO+2 (17%) HOMO→LUMO+3 (17%) HOMO-3→LUMO (10%) HOMO-2→LUMO+3 (10%)
	$S_0 \rightarrow S_5$	4.43(280)	0.0404	HOMO-2→LUMO (17%) HOMO-4→LUMO (15%) HOMO-1→LUMO (10%)
	$S_0 \rightarrow S_6$	4.46(278)	0.0302	HOMO→LUMO (41%)
***p*-BTB**	$S_0 \rightarrow S_1$	4.02(308)	0.8039	HOMO→LUMO+1 (38%) HOMO→LUMO+2 (24%) HOMO→LUMO+3 (14%)
	$S_0 \rightarrow S_2$	4.077(304)	0.5850	HOMO-3→LUMO (33%) HOMO-1→LUMO (19%) HOMO-2→LUMO (12%) HOMO-4→LUMO (11%)
	$S_0 \rightarrow S_3$	4.083(304)	0.5000	HOMO-3→LUMO (47%) HOMO-1→LUMO (12%) HOMO-2→LUMO (12%)
	$S_0 \rightarrow S_4$	4.21(294)	0.7265	HOMO-1→LUMO+1 (47%)

				HOMO→LUMO+3 (11%)
	$S_0 \rightarrow S_5$	4.35(285)	0.0210	HOMO-1→LUMO+1 (15%) HOMO→LUMO+3 (14%)
	$S_0 \rightarrow S_6$	4.41(281)	0.0029	HOMO-4→LUMO (22%) HOMO-1→LUMO (14%)
***m*-BTT**	$S_0 \rightarrow S_1$	3.78(328)	0.3943	HOMO→LUMO (42%) HOMO-1→LUMO+1 (20%) HOMO-2→LUMO (20%)
	$S_0 \rightarrow S_2$	3.97(312)	1.2197	HOMO-1→LUMO (36%) HOMO→LUMO+1 (34%)
	$S_0 \rightarrow S_3$	4.21(295)	0.5307	HOMO-2→LUMO (54%) HOMO-1→LUMO+1 (18%)
	$S_0 \rightarrow S_4$	4.30(288)	0.0240	HOMO→LUMO+3 (12%) HOMO-2→LUMO+1 (10%)
	$S_0 \rightarrow S_5$	4.35(285)	0.1006	HOMO-2→LUMO+2 (17%) HOMO-5→LUMO (14%) HOMO-1→LUMO+3 (11%)
	$S_0 \rightarrow S_6$	4.43(279.4)	0.0133	HOMO-1→LUMO (40%)
***m*-BTB**	$S_0 \rightarrow S_1$	3.89(319)	0.2830	HOMO→LUMO+1 (35%) HOMO-1→LUMO (19%) HOMO-1→LUMO+1 (12%)
	$S_0 \rightarrow S_2$	4.09(303)	0.2739	HOMO-3→LUMO (56%)
	$S_0 \rightarrow S_3$	4.10(302)	1.0038	HOMO-3→LUMO (19%) HOMO-1→LUMO (18%) HOMO→LUMO+1 (14%) HOMO-2→LUMO (10%)
	$S_0 \rightarrow S_4$	4.24(293)	0.2850	HOMO→LUMO (27%) HOMO-1→LUMO+1 (15%) HOMO-2→LUMO (13%)
	$S_0 \rightarrow S_5$	4.32(287)	0.0814	HOMO→LUMO (56%) HOMO-1→LUMO+1 (14%)
	$S_0 \rightarrow S_6$	4.37(284)	0.0022	HOMO-4→LUMO (15%) HOMO-6→LUMO+1 (10%)

Table S15. Summary of the DFT calculations (CAM-B3LYP/6-31G*) in the ground state.

	E_{HOMO}[a] (eV)	E_{LUMO}[a] (eV)	E_{gap}[b] (eV)	$E_{TD\text{-}DFT}$[c] (eV)
MeBTT	–6.19	0.01	6.20	4.02
MeBTB	–6.21	–0.67	5.54	3.98
***p*-BTT**	–6.28	–0.33	5.95	4.02
***p*-BTB**	–6.28	–0.74	5.54	4.02
***m*-BTT**	–6.27	–0.37	5.90	3.78
***m*-BTB**	–6.30	–0.73	5.57	2.89

[a] Obtained by DFT calculation (CAM-B3LYP/6-31G*). [b] HOMO-LUMO energy gap: $E_{gap} = E_{LUMO} - E_{HOMO}$. [c] $E_{gap} = E_{LUMO} - E_{HOMO}$ (CAM-B3LYP/6-31G*). [c] Vertical excitation of the lowest transition ($S_0 \rightarrow S_1$) calculated by TD-DFT (CAM-B3LYP/6-31G*).

Table S16. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of **MeBTT** in the ground state.

Atom	X	Y	Z	Atom	X	Y	Z
C	0.513193	3.709554	0.541101	C	-10.0986	-0.51886	0.877855
C	0.355223	4.538031	1.638067	H	3.149614	3.763845	3.411747
O	-0.75789	5.318935	1.652362	H	1.182098	5.208049	3.533263
O	0.757907	5.318882	-1.65242	H	-1.18212	5.208032	-3.53327
C	-0.35522	4.537997	-1.63809	H	-3.14965	3.763819	-3.41173
C	-0.51319	3.709556	-0.54111	H	1.162567	1.959141	-1.43598
C	1.658222	2.868992	0.464839	H	3.130245	0.520873	-1.52013
C	2.621483	2.881731	1.511293	H	4.48888	2.090431	2.23368
C	2.416463	3.747163	2.610481	H	-4.48888	2.090421	-2.23366
C	1.314314	4.555739	2.679442	H	-3.13023	0.520903	1.520171
C	-1.31433	4.55571	-2.67946	H	-1.16258	1.959159	1.436009
C	-2.41648	3.747145	-2.61048	H	5.209965	-0.1227	2.392692
C	-2.62149	2.88172	-1.51128	H	7.206802	-1.54064	2.273966
C	-1.65823	2.868995	-0.46483	H	7.37741	-0.9439	-1.96753
C	1.889085	1.993872	-0.63166	H	5.41887	0.522484	-1.84118
C	2.9963	1.194127	-0.67921	H	-5.41882	0.522382	1.841225
C	3.965885	1.199313	0.362662	H	-7.37735	-0.944	1.967568

C	3.759018	2.040802	1.430297	H	-7.20687	-1.54053	-2.27397
C	-3.75902	2.040801	-1.43027	H	-5.21004	-0.1226	-2.39269
C	-3.96589	1.199315	-0.36263	H	9.947832	-3.85246	-1.48511
C	-2.99631	1.194146	0.679235	H	9.615439	0.249069	-0.28343
C	-1.88909	1.993897	0.631678	H	11.47955	0.842429	-1.78621
C	5.157163	0.320451	0.287212	H	12.61084	-0.9137	-3.13231
C	5.688956	-0.28265	1.431844	H	11.83495	-3.26849	-2.9629
C	6.813224	-1.09145	1.368704	H	-10.6981	-3.06425	-1.42387
C	7.437946	-1.34608	0.144417	H	-10.8238	-5.12601	-2.77346
C	6.907572	-0.75885	-1.00777	H	-8.83246	-6.59448	-3.0046
C	5.794307	0.06431	-0.93147	H	-6.72052	-5.97579	-1.85027
C	-5.79428	0.064253	0.931507	H	-6.60894	-3.93139	-0.47382
C	-6.90754	-0.75891	1.007796	H	-11.4795	0.842424	1.786309
C	-7.43795	-1.34608	-0.1444	H	-12.6109	-0.91373	3.132303
C	-6.81327	-1.09139	-1.36869	H	-11.835	-3.26854	2.962795
C	-5.689	-0.28259	-1.43183	H	-9.94792	-3.85249	1.485011
C	-5.15717	0.320453	-0.28718	H	-9.61538	0.24908	0.283525
N	8.578533	-2.18061	0.073258	C	8.645549	-3.35992	0.857725
N	-8.57854	-2.18062	-0.07326	C	7.529373	-4.19165	0.985306
C	9.655263	-1.8413	-0.78435	C	9.829921	-3.70819	1.513324
C	-8.64554	-3.35992	-0.85773	C	7.597444	-5.34177	1.761194
C	-9.65527	-1.84131	0.78435	H	6.608963	-3.93143	0.473815
C	10.29043	-2.82525	-1.54749	C	9.895466	-4.86992	2.271939
C	10.09863	-0.51886	-0.8778	H	10.69813	-3.06422	1.423867
C	11.14888	-0.18995	-1.72524	C	8.780314	-5.69138	2.405202
C	11.78571	-1.17267	-2.47682	H	6.720587	-5.97584	1.850239
C	11.35242	-2.49122	-2.37817	H	10.8238	-5.12599	2.77343
C	-9.8299	-3.7082	-1.51334	H	8.832536	-6.5945	3.00456
C	-9.89542	-4.86993	-2.27196	C	-0.97818	6.177833	2.756413
C	-8.78025	-5.69137	-2.40523	H	-1.07055	5.615992	3.692337
C	-7.59739	-5.34174	-1.76122	H	-0.17869	6.920142	2.85572
C	-7.52934	-4.19163	-0.98532	H	-1.91847	6.689888	2.552246
C	-11.1489	-0.18996	1.725295	C	0.978147	6.177837	-2.75643
C	-11.7857	-1.1727	2.476816	H	1.918467	6.689851	-2.55229
C	-11.3525	-2.49126	2.378112	H	1.070448	5.616055	-3.6924
C	-10.2905	-2.82528	1.547431	H	0.178658	6.920165	-2.85564

Table S17. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of **MeBTB** in the ground state.

Atom	X	Y	Z	Atom	X	Y	Z
C	1.763917	3.786381	0.321871	1	-0.07261	2.263775	1.313797
C	1.608876	4.66022	1.383823	1	6.311884	-0.10303	2.421381
O	0.520793	5.474801	1.344353	H	8.267873	-1.58056	2.397173
O	2.192508	5.165731	-1.99699	H	8.522426	-1.17259	-1.86258
C	1.01388	4.491265	-1.94359	H	6.606542	0.353448	-1.8319
C	0.762528	3.779471	-0.78331	H	-4.43661	1.261149	1.736628
C	2.882741	2.907715	0.303347	H	-6.55084	0.037251	1.924309
C	3.824387	2.932109	1.36893	H	-6.32859	-0.99425	-2.22993
C	3.623754	3.844799	2.430158	H	-4.22582	0.251116	-2.42849
C	2.545885	4.688028	2.444988	H	10.99415	-4.13252	-1.21392
C	0.078654	4.503519	-3.00686	H	10.76891	0.026462	-0.19954
C	-1.09371	3.806556	-2.89666	H	12.66929	0.497432	-1.70031
C	-1.39439	3.061234	-1.73325	H	13.76481	-1.34932	-2.95135
C	-0.45434	3.052322	-0.6658	H	12.91699	-3.67051	-2.68906
C	3.10736	1.981871	-0.75184	H	-10.5996	-3.44638	-3.38044
C	4.189703	1.14749	-0.74453	H	-6.99426	-5.44058	-2.2586
C	5.139246	1.166033	0.315478	H	-10.7252	1.638131	2.403719
C	4.937068	2.055113	1.344764	H	-10.5599	-2.38016	3.839047
C	-2.60342	2.333491	-1.61133	C	9.679168	-3.49614	1.088581
C	-2.90322	1.609604	-0.48123	C	8.538861	-4.29049	1.238934
C	-1.95694	1.606223	0.58159	C	10.84481	-3.84488	1.77666
C	-0.7807	2.296131	0.493258	C	8.564785	-5.40366	2.069359
C	6.305058	0.250707	0.298308	H	7.632831	-4.03013	0.702442
C	6.800929	-0.31761	1.476383	C	10.86815	-4.97047	2.590268
C	7.901969	-1.16007	1.466891	H	11.73162	-3.22961	1.669455
C	8.538317	-1.48506	0.265382	C	9.728953	-5.75404	2.74621
C	8.043363	-0.93308	-0.91958	H	7.669611	-6.00883	2.175572
C	6.953743	-0.07581	-0.89725	H	11.78241	-5.22745	3.116545
C	-4.84407	0.762173	0.862815	H	9.748185	-6.6286	3.388372
C	-6.0427	0.072313	0.964814	B	-7.96123	-1.37162	-0.01268
C	-6.61787	-0.58121	-0.13678	C	-9.07124	1.433613	0.355928
C	-5.92538	-0.49184	-1.35524	H	-8.14974	1.929521	0.678136
C	-4.73902	0.215778	-1.47252	H	-8.90245	1.089267	-0.66644
C	-4.17303	0.854978	-0.36258	H	-9.85899	2.191711	0.326429

N	9.655112	-2.35369	0.248961	C	-8.90364	-3.40389	2.039056
C	10.75275	-2.08439	-0.60718	H	-9.13095	-3.87245	1.078416
C	-8.27583	-2.51312	-1.06188	H	-7.81973	-3.47236	2.181831
C	-8.95946	-1.00278	1.157962	H	-9.37221	-4.00008	2.826366
C	11.36811	-3.1196	-1.31682	C	-11.6728	0.037947	4.39307
C	11.23663	-0.781	-0.75245	H	-12.3572	-0.78298	4.626437
C	12.30714	-0.52107	-1.59853	H	-11.111	0.26034	5.307916
C	12.92392	-1.55456	-2.29686	H	-12.2687	0.922637	4.152765
C	12.45029	-2.85419	-2.14621	C	-10.4528	-1.35973	-1.75072
C	-9.44851	-2.48444	-1.85173	H	-10.8311	-1.24234	-0.73238
C	-9.69479	-3.4943	-2.77869	H	-10.0158	-0.39905	-2.04435
C	-8.8244	-4.56727	-2.9488	H	-11.3051	-1.54261	-2.41023
C	-7.6812	-4.60291	-2.15907	6	-6.10386	-3.73751	-0.44861
C	-7.38672	-3.59609	-1.23984	H	-5.27642	-3.21203	-0.93667
C	-10.3395	0.623587	2.330559	H	-6.1806	-3.3331	0.562645
C	-10.7452	-0.32386	3.262905	H	-5.82052	-4.79061	-0.36591
C	-10.2525	-1.61868	3.12574	C	-9.10588	-5.64205	-3.96572
C	-9.38584	-1.97272	2.094778	H	-8.74222	-5.35041	-4.95807
C	-9.4513	0.313428	1.300682	H	-8.61252	-6.58132	-3.70092
H	4.340606	3.87005	3.245821	H	-10.179	-5.83305	-4.05832
H	2.416136	5.375984	3.270747	C	0.305003	6.382567	2.409604
H	0.284595	5.065061	-3.90917	H	-0.61464	6.914347	2.165741
H	-1.80908	3.819247	-3.71382	H	0.176414	5.860896	3.364291
H	2.395233	1.935248	-1.56831	H	1.125014	7.103658	2.497219
H	4.318222	0.436463	-1.55465	C	2.511289	5.899759	-3.16556
H	5.651985	2.115225	2.160746	H	2.569302	5.250582	-4.04601
H	-3.31184	2.378159	-2.43374	H	1.785214	6.698902	-3.35016
H	-2.16559	1.021516	1.471877	H	3.490518	6.341449	-2.98133

Table S18. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***p*-BTT** in the ground state.

Atom	X	Y	Z	Atom	X	Y	Z
C	0	7.68611	0	C	10.1571	-2.8144	-3.2259
C	-0.6406	4.74429	-0.3781	C	9.56677	-3.9562	-2.6932
C	-0.9364	5.85542	-1.1398	C	8.6878	-3.8618	-1.6217
O	-0.0444	6.90768	-1.1734	C	9.00212	-1.4732	-1.5837
O	0.04444	6.90767	1.1734	H	-0.8959	8.30517	0.10403

C	0.93639	5.85542	1.13978	H	0.89588	8.30517	-0.104
C	0.64061	4.74429	0.37809	H	-3.8883	4.96291	-2.5471
C	-1.6119	3.69462	-0.3109	H	-2.2509	6.83839	-2.5284
C	-2.7838	3.77505	-1.1152	H	2.25088	6.83839	2.52839
C	-2.9927	4.91345	-1.9351	H	3.88828	4.9629	2.54706
C	-2.0981	5.94618	-1.9311	H	-0.6278	2.5096	1.21219
C	2.09808	5.94617	1.93106	H	-2.3084	0.75645	1.26934
C	2.99272	4.91345	1.93506	H	-4.6325	2.82982	-1.678
C	2.78382	3.77505	1.11519	H	4.63246	2.82981	1.67801
C	1.61188	3.69462	0.31092	H	2.30838	0.75645	-1.2693
C	-1.4912	2.58094	0.56209	H	0.62775	2.5096	-1.2122
C	-2.4438	1.60057	0.60089	H	-5.0441	0.61591	-2.2897
C	-3.596	1.64904	-0.2294	H	-6.7464	-1.1449	-2.2077
C	-3.7436	2.73471	-1.061	H	-6.094	-1.5776	2.00789
C	3.74361	2.7347	1.06096	H	-4.4364	0.22245	1.9373
C	3.59603	1.64903	0.22943	H	4.43639	0.22245	-1.9373
C	2.4438	1.60057	-0.6009	H	6.09398	-1.5776	-2.0079
C	1.49119	2.58094	-0.5621	H	6.74635	-1.1449	2.20768
C	-4.6071	0.56635	-0.1825	H	5.04405	0.61591	2.28966
C	-5.2793	0.15191	-1.3369	H	-8.2196	-4.7532	1.21838
C	-6.2373	-0.8491	-1.2971	H	-8.7893	-0.5054	1.14265
C	-6.5453	-1.4916	-0.0939	H	-10.323	-0.6745	3.06784
C	-5.8708	-1.0926	1.06408	H	-10.838	-2.8905	4.06769
C	-4.9272	-0.0779	1.01689	H	-9.7801	-4.9305	3.12211
C	4.92724	-0.0779	-1.0169	H	9.75262	-3.4144	1.18041
C	5.87075	-1.0926	-1.0641	H	9.91771	-5.0644	3.00806
C	6.54533	-1.4916	0.09385	H	7.86034	-6.0387	4.00436
C	6.23733	-0.8491	1.29705	H	5.63814	-5.3506	3.13078
C	5.2793	0.15191	1.33693	H	5.47857	-3.7267	1.27994
C	4.60711	0.56635	0.18255	H	10.3234	-0.6745	-3.0678
N	-7.5135	-2.5205	-0.0495	H	10.8377	-2.8905	-4.0677
N	7.5135	-2.5206	0.04948	H	9.78007	-4.9305	-3.1221
C	-8.4004	-2.6178	1.05337	H	8.21957	-4.7532	-1.2184
C	7.60488	-3.4601	1.10833	H	8.78926	-0.5054	-1.1426
C	8.4004	-2.6178	-1.0534	C	-7.6049	-3.4601	-1.1083
C	-8.6878	-3.8618	1.62171	C	-6.4501	-4.0157	-1.6662
C	-9.0021	-1.4732	1.58374	C	-8.8528	-3.8459	-1.6054
C	-9.8653	-1.5738	2.66738	C	-6.5452	-4.9297	-2.7079

C	-10.157	-2.8144	3.22593	H	-5.4786	-3.7267	-1.2799
C	-9.5668	-3.9562	2.6932	C	-8.9403	-4.7749	-2.6344
C	8.85279	-3.8459	1.6054	H	-9.7526	-3.4144	-1.1804
C	8.94028	-4.7749	2.63438	C	-7.789	-5.3188	-3.1955
C	7.78902	-5.3188	3.19555	H	-5.6381	-5.3506	-3.1308
C	6.54523	-4.9297	2.70788	H	-9.9177	-5.0645	-3.0081
C	6.45006	-4.0157	1.66624	H	-7.8603	-6.0387	-4.0043
C	9.86529	-1.5738	-2.6674				

Table S19. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***p*-BTB** in the ground state.

Atom	X	Y	Z	Atom	X	Y	Z
C	1.756593	7.925283	-0.08356	H	1.833297	2.698794	-1.24031
C	2.076259	4.935653	0.327897	H	3.319882	0.778357	-1.2728
C	2.484978	6.016873	1.080179	H	5.837938	2.62368	1.665522
O	1.709931	7.158395	1.097459	H	-3.36186	3.576002	-1.73838
O	1.633807	7.14293	-1.24964	H	-1.28996	1.30166	1.248253
C	0.634497	6.193011	-1.21046	H	0.573285	2.860145	1.176521
C	0.806309	5.064658	-0.43601	H	6.017408	0.386277	2.296321
C	2.930776	3.788159	0.276265	H	7.532604	-1.53839	2.233595
C	4.101009	3.752517	1.086074	H	6.847965	-1.93851	-1.97899
C	4.425401	4.870452	1.896423	H	5.381134	0.020589	-1.9279
C	3.645548	5.991843	1.877541	H	-3.46557	1.040452	1.916654
C	-0.50689	6.399686	-2.00938	H	-5.34617	-0.52771	2.010264
C	-1.5075	5.469932	-2.0075	H	-5.85895	-0.17614	-2.22938
C	-1.42545	4.325026	-1.17456	H	-3.99324	1.413357	-2.32504
C	-0.27256	4.126558	-0.36335	H	8.649946	-5.30685	-1.15029
C	2.696516	2.68496	-0.58677	H	9.62806	-1.13431	-1.12263
C	3.540581	1.609658	-0.61171	H	11.14043	-1.47424	-3.04164
C	4.688529	1.545215	0.223235	H	11.43872	-3.74034	-4.01403
C	4.946454	2.616841	1.045789	H	10.18814	-5.65647	-3.04758
C	-2.49149	3.394568	-1.11534	H	-9.98692	-2.82023	-3.45101
C	-2.46419	2.311319	-0.2687	H	-6.03585	-4.42513	-3.65719
C	-1.32886	2.146522	0.569127	H	-9.47495	0.087679	3.656733
C	-0.27519	3.016344	0.522367	H	-8.54311	-4.07894	3.619673
C	5.582231	0.36332	0.188946	C	8.15522	-3.93637	1.156626
C	6.206189	-0.1073	1.348643	C	6.949119	-4.36817	1.715215
C	7.058085	-1.20008	1.319646	C	9.356876	-4.44053	1.661258
C	7.301554	-1.88029	0.122609	C	6.949738	-5.27737	2.764947

C	6.672795	-1.42548	-1.04035	H	6.01296	-3.98661	1.323207
C	5.837068	-0.32029	-1.00417	C	9.347979	-5.36406	2.698403
C	-3.98297	0.771791	1.001438	H	10.29603	-4.10557	1.235335
C	-5.05017	-0.11194	1.051844	C	8.146808	-5.78457	3.260089
C	-5.75943	-0.48321	-0.10132	H	6.004511	-5.6014	3.18849
C	-5.34471	0.094344	-1.31202	H	10.28995	-5.74676	3.077987
C	-4.29408	0.996837	-1.36922	H	8.143519	-6.50043	4.075006
C	-3.59083	1.349698	-0.21149	B	-6.953	-1.49306	-0.03956
N	8.161116	-3.00197	0.089354	C	-8.27774	0.816516	1.418967
C	9.036139	-3.19753	-1.00975	H	-7.38479	1.352465	1.754611
C	-7.35263	-2.28395	-1.34993	H	-8.2649	0.835357	0.32835
C	-7.71732	-1.6861	1.331814	H	-9.14791	1.387132	1.75233
C	9.202384	-4.47007	-1.56285	C	-7.1874	-4.18766	1.343351
C	9.746741	-2.12299	-1.55164	H	-7.50587	-4.34342	0.310946
C	10.59705	-2.31961	-2.63185	H	-6.0948	-4.11726	1.336741
C	10.76797	-3.58882	-3.17518	H	-7.45012	-5.0779	1.918611
C	10.06945	-4.66152	-2.63063	C	-9.78838	-2.18597	5.121605
C	-8.65805	-2.20692	-1.88792	H	-10.2991	-3.15063	5.177716
C	-8.9786	-2.90065	-3.05233	H	-9.07698	-2.14772	5.953707
C	-8.0512	-3.70166	-3.71218	H	-10.5262	-1.3974	5.286291
C	-6.77348	-3.79019	-3.17213	C	-9.73373	-1.35599	-1.25511
C	-6.40765	-3.08963	-2.02323	H	-9.88663	-1.61006	-0.20449
C	-8.99795	-0.76965	3.187701	H	-9.48156	-0.29148	-1.29578
C	-9.08467	-2.0133	3.801908	H	-10.6841	-1.4832	-1.77768
C	-8.48421	-3.09421	3.162468	C	-4.98418	-3.25359	-1.53674
C	-7.81869	-2.95537	1.947114	H	-4.33532	-2.47063	-1.94046
C	-8.31772	-0.58669	1.983982	H	-4.89859	-3.20449	-0.45026
H	2.714844	8.442911	-0.18843	H	-4.57881	-4.21539	-1.85995
H	0.932858	8.639635	0.008172	C	-8.41663	-4.43215	-4.97687
H	5.317716	4.831044	2.513075	H	-8.27633	-3.79172	-5.85446
H	3.888978	6.86862	2.466921	H	-7.79532	-5.31956	-5.11856
H	-0.55958	7.296505	-2.6162	H	-9.4639	-4.7444	-4.9685
H	-2.38944	5.608773	-2.62461				

Table S20. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***m*-BTT** in the ground state.

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.35838	-2.92396	-0.28558	H	-0.04232	-1.30759	0.297542
C	-4.59984	-1.97252	0.546896	C	2.838359	-2.86919	-0.58951

C	-5.42601	-2.95519	1.051792	H	3.160416	-3.84003	-2.48215
O	-6.25053	-3.65129	0.191746	H	2.190085	-1.81876	1.172633
O	-7.01716	-1.62592	-0.71313	N	4.125959	-3.16149	-0.08599
C	-5.88665	-1.5544	-1.50139	N	0.808315	5.137364	0.285017
C	-4.64724	-1.71636	-0.91822	C	5.256636	-3.09967	-0.94043
C	-3.80054	-1.22286	1.471614	C	5.406535	-2.04432	-1.84449
C	-3.79664	-1.59698	2.845343	C	6.238749	-4.09247	-0.88635
C	-4.6137	-2.66595	3.287735	C	6.512094	-1.99265	-2.68384
C	-5.43385	-3.32026	2.411891	H	4.651854	-1.26632	-1.88606
C	-6.0537	-1.26989	-2.87052	C	7.351018	-4.02354	-1.71562
C	-4.95356	-1.17526	-3.67604	H	6.125588	-4.91706	-0.1908
C	-3.65758	-1.4055	-3.15288	C	7.49303	-2.97764	-2.62227
C	-3.49329	-1.69664	-1.76893	H	6.612402	-1.16669	-3.38139
C	-3.03342	-0.09502	1.082421	H	8.10517	-4.80263	-1.66006
C	-2.26392	0.613838	1.978621	H	8.359377	-2.93051	-3.27404
C	-2.24115	0.1986	3.337802	C	4.295044	-3.5168	1.276883
C	-2.98821	-0.86641	3.753186	C	3.407535	-4.40196	1.895222
C	-2.51196	-1.37654	-3.98853	C	5.355255	-2.98886	2.018811
C	-1.26746	-1.64485	-3.49397	C	3.574206	-4.74128	3.231822
C	-1.08785	-1.97497	-2.12346	H	2.58687	-4.82127	1.323248
C	-2.19058	-2.00175	-1.29893	C	5.52621	-3.34796	3.349748
H	-8.10886	-2.77749	0.496766	H	6.044219	-2.297	1.546416
H	-7.75917	-3.52416	-1.10765	C	4.63564	-4.2214	3.966218
H	-4.59675	-2.94116	4.337986	H	2.874906	-5.42928	3.697034
H	-6.08908	-4.12367	2.730114	H	6.355887	-2.92951	3.911314
H	-7.05848	-1.12562	-3.2522	H	4.767526	-4.49436	5.008181
H	-5.06143	-0.94718	-4.73221	C	0.169441	6.372113	0.003133
H	-3.04753	0.208838	0.043234	C	-0.83322	6.861343	0.84506
H	-2.98861	-1.15983	4.799079	C	0.537974	7.118594	-1.11944
H	-2.64305	-1.13369	-5.03917	C	-1.45969	8.068039	0.560612
H	-2.06714	-2.29095	-0.26273	H	-1.119	6.290724	1.722147
H	-1.6511	0.758221	4.05599	C	-0.07995	8.333642	-1.38654
H	-0.40268	-1.59516	-4.14742	H	1.311342	6.741643	-1.77998
C	-1.47379	1.791183	1.543941	C	-1.08494	8.813963	-0.55265
C	-0.21288	2.055976	2.088232	H	-2.23759	8.432956	1.22432
C	-1.95651	2.67468	0.573129	H	0.219213	8.901513	-2.26224
C	0.533429	3.152765	1.685764	H	-1.57104	9.759961	-0.76799
H	0.201326	1.388156	2.837195	C	2.215461	5.026788	0.143794
C	-1.21066	3.764446	0.151796	C	2.782535	3.898092	-0.45464
H	-2.93885	2.512338	0.140989	C	3.053999	6.048237	0.598471

C	0.047198	4.022905	0.705312	C	4.1615	3.792166	-0.58378
H	1.506177	3.334874	2.128887	H	2.13738	3.104751	-0.81647
H	-1.60824	4.428374	-0.60775	C	4.430947	5.943427	0.448148
C	0.262973	-2.28213	-1.59768	H	2.620498	6.924199	1.068866
C	1.201244	-2.97865	-2.3662	C	4.994048	4.814333	-0.13847
C	0.647529	-1.88207	-0.31332	H	4.585577	2.907801	-1.04948
C	2.461543	-3.27812	-1.8725	H	5.067815	6.746743	0.805801
H	0.931837	-3.32677	-3.3586	H	6.070551	4.731879	-0.24766
C	1.911424	-2.16107	0.182146				

Table S21. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***m*-BTB** in the ground state.

Atom	X	Y	Z	Atom	X	Y	Z
C	8.516884	-1.03291	-0.29316	H	-2.82228	2.866906	-1.91097
C	5.685136	-0.33261	0.558856	C	-4.41234	6.382642	-2.05454
C	6.917932	0.119545	0.984158	H	-2.86847	6.973721	-0.68019
O	7.956878	0.204142	0.08055	C	-4.95624	5.351393	-2.81403
O	7.539524	-2.0009	-0.59259	H	-4.78556	3.272925	-3.3463
C	6.513675	-1.55532	-1.40114	H	-4.85161	7.374957	-2.08959
C	5.549163	-0.72169	-0.87246	H	-5.82447	5.529326	-3.44011
C	4.640645	-0.45085	1.534919	C	-1.51947	5.225506	0.924889
C	4.876343	0.002967	2.864034	C	-0.31912	5.75866	1.403092
C	6.148702	0.512461	3.220223	C	-2.65038	5.254416	1.745562
C	7.159991	0.551781	2.302395	C	-0.25267	6.300682	2.680132
C	6.477676	-2.02017	-2.7298	H	0.560395	5.745	0.768322
C	5.462783	-1.62197	-3.55336	C	-2.58038	5.815577	3.014431
C	4.475454	-0.71827	-3.09105	H	-3.58332	4.835641	1.384243
C	4.520082	-0.24165	-1.74976	C	-1.38228	6.337665	3.491903
C	3.373973	-1.01671	1.23932	H	0.687988	6.709541	3.036261
C	2.361217	-1.07086	2.170864	H	-3.46859	5.831018	3.638672
C	2.604107	-0.58144	3.482053	H	-1.32939	6.768932	4.486285
C	3.827926	-0.07631	3.816172	C	-3.18202	-4.43079	0.054039
C	3.440653	-0.2646	-3.94812	C	-2.87143	-5.50425	0.918025
C	2.496493	0.620299	-3.51222	C	-3.68237	-4.73992	-1.23199
C	2.540125	1.130969	-2.18695	C	-3.07071	-6.82029	0.502008
C	3.550617	0.713241	-1.34923	C	-3.84092	-6.06756	-1.6218
H	9.109173	-1.46677	0.517866	C	-3.54282	-7.12671	-0.7691
H	9.142906	-0.81123	-1.16247	H	-2.84928	-7.62966	1.194278
H	6.312436	0.854831	4.237513	H	-4.2178	-6.28139	-2.61944

H	8.149124	0.918279	2.554058	C	-4.13111	-1.86165	0.482707
H	7.258137	-2.69441	-3.06486	C	-3.98653	-0.65614	-0.23544
H	5.410761	-1.97862	-4.57764	C	-5.33949	-2.06958	1.190802
H	3.188468	-1.38633	0.23897	C	-5.017	0.286263	-0.2422
H	4.01978	0.271199	4.827196	C	-6.33438	-1.0975	1.179179
H	3.406004	-0.64627	-4.96453	C	-6.19633	0.090759	0.463456
H	3.615605	1.132883	-0.35335	H	-4.88812	1.202409	-0.81513
H	1.817493	-0.63927	4.227067	H	-7.24841	-1.27314	1.742283
H	1.693915	0.925853	-4.17524	B	-2.96881	-2.93325	0.51131
C	1.022444	-1.58935	1.798868	C	-2.75016	-0.32287	-1.04361
C	-0.13459	-0.9521	2.261964	H	-2.05489	0.301229	-0.47107
C	0.876842	-2.69182	0.949609	H	-2.19335	-1.20597	-1.36044
C	-1.38893	-1.37928	1.853679	H	-3.02465	0.236315	-1.94348
H	-0.04684	-0.08879	2.91471	C	-5.57953	-3.3191	2.006407
C	-0.38355	-3.13191	0.573585	H	-5.48986	-4.22363	1.399796
H	1.759808	-3.21629	0.597431	H	-4.86136	-3.41114	2.828605
C	-1.55248	-2.47999	0.998418	H	-6.57885	-3.3054	2.449172
H	-2.26733	-0.84188	2.1989	C	-7.30025	1.115424	0.447219
H	-0.46805	-3.99879	-0.0756	H	-7.61946	1.372413	1.462511
C	1.494858	2.06977	-1.71487	H	-6.98242	2.03508	-0.05101
C	0.927432	3.022731	-2.5674	H	-8.18352	0.737913	-0.08017
C	1.017504	2.009352	-0.40097	C	-4.0387	-3.66374	-2.23182
C	-0.06853	3.881833	-2.12877	H	-4.83556	-3.01448	-1.86015
H	1.289466	3.117204	-3.58645	H	-3.18331	-3.02036	-2.46264
C	0.011393	2.854096	0.041723	H	-4.3752	-4.10802	-3.17217
H	1.409554	1.258629	0.277823	C	-2.33994	-5.29374	2.319634
C	-0.54804	3.803349	-0.81828	H	-1.2521	-5.17042	2.318672
H	-0.4805	4.623487	-2.80454	H	-2.75733	-4.40771	2.803009
H	-0.35738	2.769099	1.058165	H	-2.57235	-6.15695	2.949547
N	-1.58211	4.661609	-0.37497	C	-3.71081	-8.55496	-1.21661
C	-2.71294	4.892482	-1.19654	H	-4.56266	-8.66368	-1.89421
C	-3.26555	3.855764	-1.95517	H	-2.8223	-8.90602	-1.75452
C	-3.29521	6.161919	-1.25916	H	-3.86234	-9.22471	-0.36561
C	-4.37195	4.089625	-2.76229				

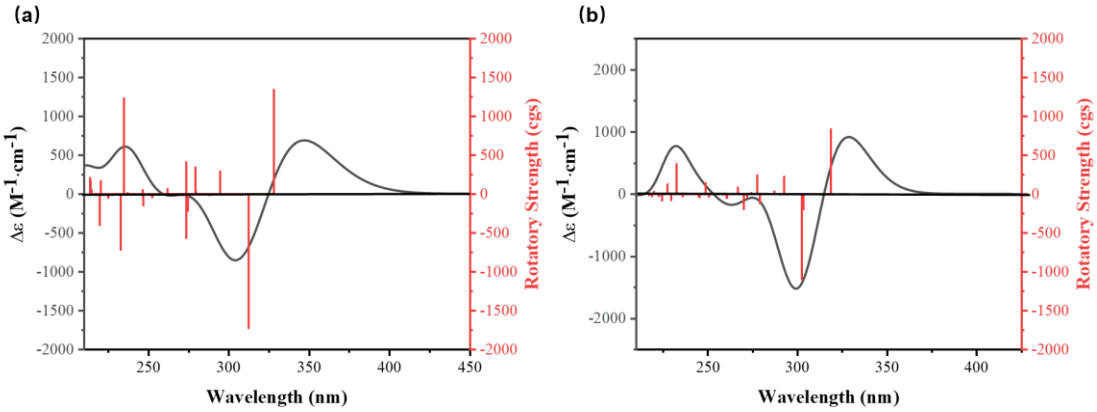


Figure S46. The theoretically calculated ECD spectra of (a) **(*S*)-*m*-BTT** and (b) **(*S*)-*m*-BTB** (CAM-B3LYP/6-31G*).

Table S22. Summary of the theoretical ECD of **(*S*)-m-BTT** and **(*S*)-m-BTB** about selected transitions and oscillator and rotatory strengths in CH_2Cl_2 (CAM-B3LYP/6-31G*).

Compound	Transition	λ, nm (eV)	Oscillator Strength, *f*	*R*, (10^{-40} cgs)	Orbital Contributions
(*S*)-*m*-BTT	$S_0 \rightarrow S_1$	3.78(328)	0.3943	1342.86	HOMO→LUMO (42%) HOMO-1→LUMO+1 (20%) HOMO-2→LUMO (20%)
	$S_0 \rightarrow S_2$	3.97(312)	1.2197	–1720.70	HOMO-1→LUMO (36%) HOMO→LUMO+1 (34%)
	$S_0 \rightarrow S_3$	4.21(295)	0.5307	292.59	HOMO-2→LUMO (54%) HOMO-1→LUMO+1 (18%)
	$S_0 \rightarrow S_4$	4.30(288)	0.0240	–13.24	HOMO-4→LUMO (22%) HOMO→LUMO+3 (12%) HOMO-2→LUMO+1 (10%)
	$S_0 \rightarrow S_5$	4.35(285)	0.1006	–1.22	HOMO-2→LUMO+2 (17%) HOMO-5→LUMO (14%) HOMO-1→LUMO+3 (11%)
	$S_0 \rightarrow S_6$	4.43(279.4)	0.0133	44.93	HOMO-1→LUMO (40%) HOMO-1→LUMO+5 (40%)
	$S_0 \rightarrow S_7$	4.44(279.2)	0.0365	345.02	HOMO→LUMO (40%) HOMO-1→LUMO+5 (40%)
	$S_0 \rightarrow S_8$	4.52(274)	0.1217	–213.03	HOMO-3→LUMO (36%) HOMO-2→LUMO+1 (17%)
	$S_0 \rightarrow S_9$	4.53(273.5)	0.2823	–562.20	HOMO→LUMO+6 (41%) HOMO-1→LUMO+6 (28%) HOMO-1→LUMO+7 (13%)
	$S_0 \rightarrow S_{10}$	4.54(273.3)	0.3734	410.60	HOMO-1→LUMO+7 (37%)

					HOMO→LUMO+7 (33%) HOMO-1→LUMO+6 (11%)
	$S_0 \rightarrow S_{11}$	4.55(272)	0.0036	–3.89	HOMO-2→LUMO+1 (28%) HOMO→LUMO+1 (27%) HOMO-1→LUMO (24%)
	$S_0 \rightarrow S_{12}$	4.74(262)	0.0493	67.19	HOMO-1→LUMO+1 (31%) HOMO→LUMO+10 (28%)
	$S_0 \rightarrow S_{13}$	4.91(252.3)	0.0274	–37.34	HOMO-1→LUMO+10 (31%) HOMO→LUMO+10 (28%)
	$S_0 \rightarrow S_{14}$	4.92(252.1)	0.0335	–32.12	HOMO→LUMO+11 (35%) HOMO-1→LUMO+11 (23%)
	$S_0 \rightarrow S_{15}$	5.00(248)	0.0020	3.82	HOMO-3→LUMO+1 (25%) HOMO→LUMO (13%) HOMO-2→LUMO (11%)
(*S*)-*m*-BTB	$S_0 \rightarrow S_1$	3.89(319)	0.2830	833.59	HOMO→LUMO+1 (35%) HOMO-1→LUMO (19%) HOMO-1→LUMO+1 (12%)
	$S_0 \rightarrow S_2$	4.09(303)	0.2739	–195.61	HOMO-3→LUMO (56%)
	$S_0 \rightarrow S_3$	4.10(302)	1.0038	–1093.62	HOMO-3→LUMO (19%) HOMO-1→LUMO (18%) HOMO→LUMO+1 (14%) HOMO-2→LUMO (10%)
	$S_0 \rightarrow S_4$	4.24(293)	0.2850	225.90	HOMO→LUMO (27%) HOMO-4→LUMO (21%) HOMO-1→LUMO+1 (15%) HOMO-2→LUMO (13%)
	$S_0 \rightarrow S_5$	4.32(287)	0.0814	34.62	HOMO→LUMO (56%) HOMO-1→LUMO+1 (14%)
	$S_0 \rightarrow S_6$	4.37(284)	0.0022	–0.54	HOMO-4→LUMO (15%) HOMO-6→LUMO+1 (10%)
	$S_0 \rightarrow S_7$	4.44(279)	0.0773	–114.06	HOMO→LUMO+5 (16%) HOMO→LUMO+3 (16%)
	$S_0 \rightarrow S_8$	4.47(277)	0.0431	242.32	HOMO→LUMO+5 (66%)
	$S_0 \rightarrow S_9$	4.52(274)	0.0774	14.75	HOMO-5→LUMO (23%) HOMO-1→LUMO+1 (11%)
	$S_0 \rightarrow S_{10}$	4.56(272)	0.3809	–30.30	HOMO→LUMO+6 (88%)
	$S_0 \rightarrow S_{11}$	4.59(270)	0.0446	–188.88	HOMO-5→LUMO (37%) HOMO-1→LUMO+2 (10%)
	$S_0 \rightarrow S_{12}$	4.65(267)	0.0308	87.93	HOMO-7→LUMO (67%)
	$S_0 \rightarrow S_{13}$	4.75(261)	0.3260	–43.74	HOMO-8→LUMO (23%) HOMO-1→LUMO+2 (22%) HOMO-2→LUMO (11%)

					HOMO62→LUMO (10%)
	$S_0 \rightarrow S_{14}$	4.76(260)	0.0696	–46.06	HOMO-2→LUMO+1 (22%) HOMO-1→LUMO+1 (17%) HOMO-2→LUMO (12%)
	$S_0 \rightarrow S_{15}$	4.80(258)	0.0162	–7.06	HOMO-11→LUMO (67%)

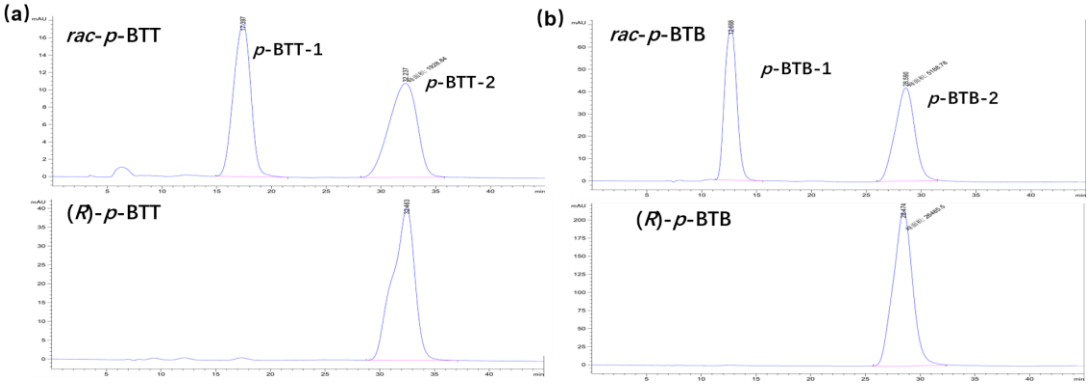


Figure S47. HPLC chromatogram of (a) ***rac*-*p*-BTT** and **(*R*)-*p*-BTT** and **(b) *rac*-*p*-BTB** and **(*R*)-*p*-BTB** by analytical HPLC equipped with a Daicel Chiralpak IF column with *n*-hexane/isopropanol = 90:10, flow = 0.8 mL/min. (The compounds of **(*R*)-*p*-BTT** and **(*R*)-*p*-BTB** were synthesized as described for ***rac*-*p*-BTT** and ***rac*-*p*-BTB,** respectively**,** using (*R*)-1-(2-hydroxynaphthalen-1-yl)naphthalen-2-ol ((*R*)-BINOL) as starting material).

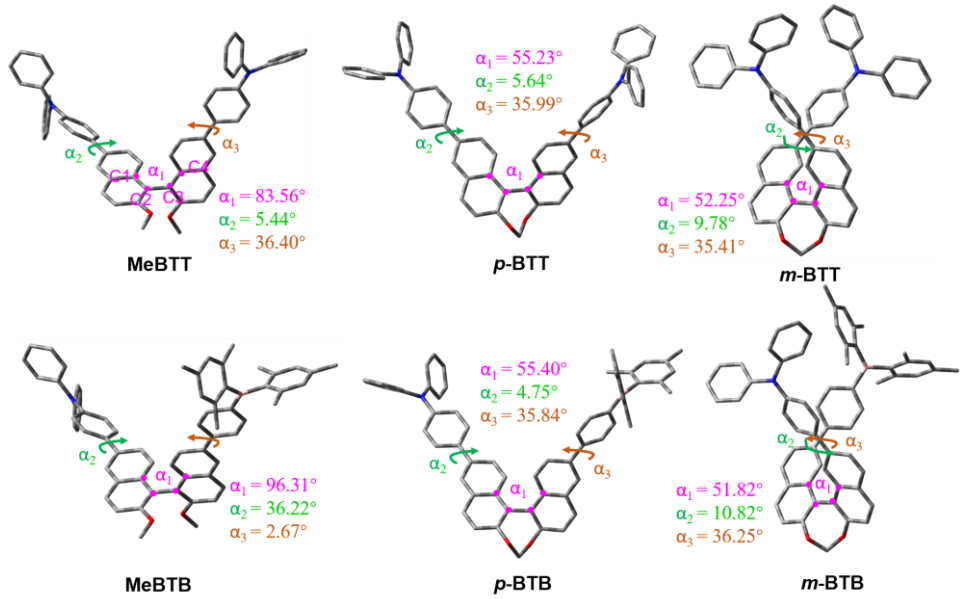


Figure S48. The optimized structures (CAM-B3LYP/6-31G*) in the S_1 excited state. Hydrogen atoms are omitted. The angles between the adjacent aryl rings are shown for comparison.

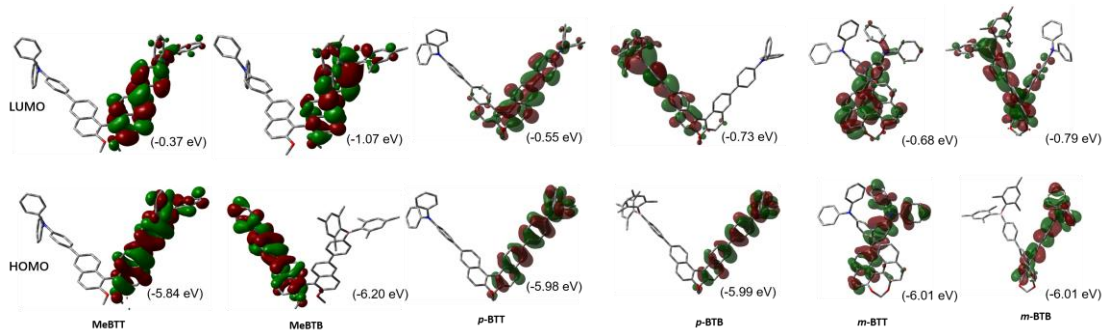


Figure S49. Molecular orbitals contributing to the DFT calculated transitions in the S_1 excited state of ***p*-BTT**, ***m*-BTT**, ***p*-BTB** and ***m*-BTB** in CH_2Cl_2(iso = 0.02, CAM-B3LYP/6-31G*).

Table S23. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of **MeBTT** in the S_1 excited state.

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.57283	3.967221	-0.7608	C	8.809005	-2.01438	-2.23231
C	-0.54437	4.812936	-1.85593	H	-3.38601	3.857539	-3.458
O	0.508412	5.669833	-1.93238	H	-1.53335	5.435045	-3.68816
O	-0.63859	5.818214	1.238774	H	1.397355	5.846293	3.026488
C	0.447326	5.006335	1.270653	H	3.300099	4.310202	2.972262
C	0.518277	4.034889	0.25458	H	-0.98204	2.172934	1.242319
C	-1.65218	3.051441	-0.61961	H	-2.84313	0.609841	1.440488
C	-2.67921	3.004248	-1.60306	H	-4.53209	2.093526	-2.21282
C	-2.60405	3.887092	-2.70462	H	4.467001	2.445899	1.951586
C	-1.5665	4.770531	-2.83418	H	2.852897	0.555987	-1.60749
C	1.455774	5.097865	2.245754	H	0.990422	2.067965	-1.56568
C	2.525028	4.234902	2.214863	H	-5.11747	-0.15991	-2.34139
C	2.645961	3.232614	1.207749	H	-7.0098	-1.70191	-2.10806
C	1.605328	3.155283	0.216877	H	-6.95139	-1.12973	2.139671
C	-1.75734	2.161011	0.484402	H	-5.1007	0.458273	1.901604
C	-2.8053	1.290808	0.595961	H	4.233483	-0.84521	-1.47943
C	-3.8358	1.23384	-0.38409	H	6.102513	-2.36016	-1.49543
C	-3.75149	2.089563	-1.45703	H	7.927173	-0.18416	1.755764
C	3.722369	2.350286	1.170276	H	6.078066	1.360618	1.777054
C	3.855085	1.331131	0.172021	H	-9.3679	-4.18422	1.802745
C	2.804801	1.286802	-0.80863	H	-9.35956	-0.07201	0.591568
C	1.749796	2.14112	-0.79515	H	-11.1646	0.408217	2.202897
C	-4.96101	0.279651	-0.24031	H	-12.1045	-1.41184	3.609942
C	-5.52427	-0.35276	-1.35368	H	-11.1968	-3.71479	3.390393

C	-6.58921	-1.23128	-1.22612	H	10.86007	-2.51554	0.542966
C	-7.11853	-1.52843	0.032939	H	11.95075	-3.15479	2.663979
C	-6.55508	-0.91236	1.153831	H	10.58041	-3.64239	4.677249
C	-5.50285	-0.0201	1.01401	H	8.104131	-3.49915	4.539274
C	5.040718	-0.66695	-0.7797	H	7.012474	-2.8788	2.410982
C	6.094467	-1.53302	-0.79459	H	9.33563	-1.91076	-4.30394
C	7.171174	-1.39534	0.130412	H	9.975402	-4.30642	-4.45107
C	7.108473	-0.32602	1.058629	H	9.805125	-5.74685	-2.43427
C	6.052529	0.542177	1.069435	H	8.988219	-4.80894	-0.30236
C	4.949591	0.42803	0.147986	H	8.541997	-0.96588	-2.16313
N	-8.19801	-2.43359	0.1696	C	-8.23673	-3.6155	-0.61241
N	8.237581	-2.28684	0.125317	C	-7.07781	-4.37045	-0.81514
C	-9.24139	-2.1601	1.089642	C	-9.43505	-4.0436	-1.19106
C	8.865568	-2.65919	1.340748	C	-7.11862	-5.52321	-1.58899
C	8.714312	-2.82571	-1.0953	H	-6.14563	-4.04856	-0.36361
C	-9.76868	-3.17989	1.887153	C	-9.47141	-5.20794	-1.94762
C	-9.75883	-0.86723	1.211781	H	-10.3371	-3.4596	-1.04355
C	-10.7754	-0.60205	2.120406	C	-8.31457	-5.95252	-2.15601
C	-11.3052	-1.62074	2.906349	H	-6.20863	-6.09671	-1.73691
C	-10.7983	-2.91035	2.779687	H	-10.4111	-5.52638	-2.38861
C	10.26091	-2.74082	1.418125	H	-8.34474	-6.85768	-2.75381
C	10.86802	-3.09803	2.613107	C	0.590178	6.558174	-3.03173
C	10.10049	-3.36777	3.7437	H	0.660786	6.018435	-3.98252
C	8.712477	-3.28174	3.667064	H	-0.26677	7.23999	-3.06423
C	8.093458	-2.9319	2.475942	H	1.501803	7.13622	-2.88044
C	9.258864	-2.5505	-3.43045	C	-0.77144	6.817399	2.232673
C	9.622971	-3.89177	-3.5124	H	-1.7027	7.338601	2.011406
C	9.530805	-4.6981	-2.37963	H	-0.83057	6.3791	3.23515
C	9.075517	-4.17611	-1.17846	H	0.060473	7.52951	2.197206

Table S24. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of **MeBTB** in the S_1 excited state.

Atom	X	Y	Z	Atom	X	Y	Z
C	1.818002	3.694632	0.958232	H	-0.01567	2.040582	1.725612
C	1.70859	4.405212	2.140203	H	6.362413	-0.51922	2.302023
O	0.63824	5.234422	2.250507	H	8.296181	-1.99276	1.993114
O	2.210326	5.437079	-1.09235	H	8.421601	-0.95549	-2.16469

C	1.035292	4.793617	-1.1503	H	6.528186	0.564003	-1.84389
C	0.788448	3.874618	-0.10447	H	-3.81276	-0.09134	1.788548
C	2.917281	2.812254	0.769188	H	-5.88116	-1.31098	1.748167
C	3.889834	2.665776	1.795954	H	-6.95004	0.547435	-1.9841
C	3.736615	3.412868	2.987269	H	-4.89516	1.789818	-1.97719
C	2.676479	4.260008	3.163305	H	10.8587	-4.00244	-2.05334
C	0.08744	4.99997	-2.17521	H	10.73985	-0.03738	-0.42866
C	-1.09076	4.304591	-2.16217	H	12.58892	0.631031	-1.91911
C	-1.38827	3.363233	-1.12874	H	13.60545	-1.0216	-3.47175
C	-0.41165	3.165578	-0.09239	H	12.73106	-3.34711	-3.52077
C	3.092337	2.051599	-0.4185	H	-11.8524	-0.74923	-2.80843
C	4.160894	1.212818	-0.57035	H	-8.45085	-2.46159	-4.73802
C	5.142435	1.061935	0.448641	H	-9.32402	-1.26924	4.418599
C	4.985898	1.788923	1.605562	H	-9.36742	-5.04487	2.426293
C	-2.57836	2.654606	-1.11569	C	9.650502	-3.69665	0.376055
C	-2.90417	1.704428	-0.09137	C	8.509328	-4.49985	0.456039
C	-1.90896	1.529351	0.933475	C	10.83828	-4.14452	0.961024
C	-0.73769	2.212138	0.935525	C	8.556519	-5.72031	1.117623
C	6.293105	0.147616	0.256501	H	7.585977	-4.16217	-0.00212
C	6.818125	-0.59437	1.319696	C	10.88214	-5.37485	1.604314
C	7.906903	-1.43527	1.148331	H	11.72612	-3.52374	0.907756
C	8.501188	-1.58228	-0.10861	C	9.742389	-6.16823	1.691456
C	7.975986	-0.85554	-1.18111	H	7.66045	-6.33104	1.171403
C	6.898909	-0.00249	-0.99532	H	11.8134	-5.70794	2.052243
C	-4.48434	0.062353	0.952531	H	9.777938	-7.12563	2.201057
C	-5.66298	-0.62793	0.93226	B	-7.94096	-1.29554	-0.14347
C	-6.62166	-0.50633	-0.12324	C	-8.449	0.248238	2.445177
C	-6.25871	0.405158	-1.15836	H	-7.39702	0.481045	2.643136
C	-5.0902	1.115857	-1.15224	H	-8.71086	0.754958	1.514015
C	-4.12553	0.980047	-0.09338	H	-9.03995	0.691372	3.252352
N	9.605951	-2.44617	-0.29145	C	-8.51502	-4.27494	0.041712
C	10.6741	-2.06411	-1.14261	H	-9.11467	-3.9624	-0.81659
C	-8.76299	-1.4101	-1.49946	H	-7.46877	-4.26577	-0.28195
C	-8.46152	-1.9885	1.18898	H	-8.77553	-5.30992	0.280044
C	11.24481	-2.98935	-2.0211	C	-9.862	-3.90508	4.845902
C	11.17296	-0.75872	-1.11321	H	-10.5929	-4.6922	4.636621
C	12.21432	-0.38745	-1.95412	H	-9.02696	-4.37516	5.379142
C	12.78696	-1.31268	-2.82142	H	-10.3218	-3.18572	5.529336
C	12.2986	-2.61537	-2.84522	C	-10.8347	-0.39804	-0.39042
C	-10.1155	-0.99286	-1.5787	H	-10.8566	-1.08495	0.459011

C	-10.8186	-1.08737	-2.77668	H	-10.3471	0.519618	-0.04432
C	-10.2407	-1.60543	-3.93323	H	-11.8662	-0.14363	-0.6492
C	-8.92083	-2.03295	-3.85506	C	-6.75339	-2.439	-2.72041
C	-8.1798	-1.93744	-2.67623	H	-6.04894	-1.62548	-2.92557
C	-9.14536	-1.87137	3.529974	H	-6.44183	-2.89107	-1.77672
C	-9.39312	-3.23794	3.579481	H	-6.63176	-3.18407	-3.51248
C	-9.1781	-3.97338	2.416467	C	-11.0165	-1.68438	-5.22186
C	-8.73231	-3.37901	1.238868	H	-11.0314	-0.71582	-5.73593
C	-8.68079	-1.24449	2.373001	H	-10.5758	-2.41196	-5.90916
H	4.477708	3.305708	3.774005	H	-12.0581	-1.96965	-5.04501
H	2.584072	4.818776	4.08575	C	0.466682	5.978645	3.444539
H	0.285937	5.706779	-2.97046	H	-0.44691	6.556286	3.305673
H	-1.82139	4.463491	-2.94939	H	0.34949	5.32247	4.313542
H	2.354877	2.131268	-1.20987	H	1.304035	6.663723	3.61494
H	4.25241	0.628837	-1.48067	C	2.548317	6.370527	-2.11071
H	5.725628	1.717261	2.397938	H	2.589061	5.884911	-3.09044
H	-3.27974	2.844421	-1.91827	H	1.833917	7.198882	-2.137
H	-2.08742	0.822115	1.732958	H	3.535541	6.747614	-1.84837

Table S25. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***p*-BTT** in the S_1 excited state.

Atom	X	Y	Z	Atom	X	Y	Z
C	0.033614	7.713095	0.417987	C	10.02149	-2.68391	-3.57533
C	-0.6501	4.790617	-0.08943	C	9.436973	-3.84997	-3.09087
C	-0.95255	5.958327	-0.79735	C	8.578991	-3.80859	-1.99923
O	-0.0454	6.999154	-0.79307	C	8.903303	-1.42612	-1.84397
O	0.099565	6.873648	1.548284	H	-0.85508	8.33144	0.576311
C	0.981003	5.817397	1.435501	H	0.932014	8.331279	0.327294
C	0.652407	4.747306	0.629166	H	-3.94758	5.153467	-2.16081
C	-1.61031	3.75892	-0.04834	H	-2.29445	7.010714	-2.09653
C	-2.82375	3.873306	-0.81425	H	2.34334	6.722346	2.830311
C	-3.03658	5.063838	-1.57639	H	3.965526	4.836717	2.711241
C	-2.12838	6.090074	-1.54646	H	-0.61096	2.494672	1.415347
C	2.166215	5.861384	2.194846	H	-2.2518	0.756951	1.437666
C	3.052553	4.823504	2.123481	H	-4.65045	2.982726	-1.40933
C	2.809229	3.727947	1.256749	H	4.663468	2.739974	1.720155
C	1.613433	3.695909	0.484293	H	2.233841	0.829026	-1.25208
C	-1.47697	2.585019	0.770765	H	0.571886	2.594199	-1.06066
C	-2.41265	1.601328	0.777822	H	-6.04839	1.627975	-1.27223

C	-3.60513	1.657062	-0.02388	H	-7.67094	-0.15285	-1.2831
C	-3.76697	2.84758	-0.79674	H	-5.07464	-2.56316	1.190292
C	3.756144	2.682358	1.125603	H	-3.42927	-0.80699	1.1969
C	3.573105	1.638576	0.248859	H	4.341175	0.312178	-2.00645
C	2.396944	1.639561	-0.54901	H	5.978819	-1.49717	-2.20892
C	1.45609	2.625412	-0.43588	H	6.74531	-1.27769	2.003626
C	-4.56228	0.608637	-0.02678	H	5.062909	0.492192	2.216743
C	-5.80898	0.714106	-0.74451	H	-7.81717	-5.16176	-0.02417
C	-6.73518	-0.28883	-0.75234	H	-7.49429	-1.6802	2.469747
C	-6.51284	-1.49935	-0.04336	H	-7.77893	-3.09308	4.477462
C	-5.28503	-1.63402	0.673136	H	-8.09971	-5.54451	4.243188
C	-4.36073	-0.63263	0.672948	H	-8.12612	-6.56884	1.980708
C	4.85317	-0.0374	-1.11541	H	9.692322	-3.53251	0.795744
C	5.784888	-1.05688	-1.23708	H	9.87261	-5.28215	2.526471
C	6.485415	-1.51777	-0.11836	H	7.823194	-6.28573	3.510184
C	6.215527	-0.93283	1.122526	H	5.593023	-5.52405	2.721931
C	5.26886	0.073384	1.236721	H	5.417385	-3.79924	0.966469
C	4.571193	0.550131	0.122176	H	10.19881	-0.5556	-3.31011
N	-7.44891	-2.52187	-0.05242	H	10.68554	-2.71838	-4.4329
N	7.442281	-2.55192	-0.23855	H	9.638103	-4.8015	-3.57355
C	-7.63708	-3.33049	1.0956	H	8.115175	-4.7184	-1.63371
C	7.543086	-3.54899	0.765135	H	8.702816	-0.48169	-1.34965
C	8.307419	-2.59485	-1.36159	C	-8.23362	-2.76496	-1.2079
C	-7.82027	-4.71271	0.962614	C	-7.64601	-2.71546	-2.47752
C	-7.61978	-2.75245	2.37092	C	-9.60145	-3.03773	-1.08574
C	-7.78482	-3.55076	3.49342	C	-8.42052	-2.9392	-3.60614
C	-7.97061	-4.92436	3.362377	H	-6.58385	-2.51735	-2.56692
C	-7.98948	-5.498	2.092209	C	-10.3637	-3.26386	-2.22181
C	8.795603	-3.97604	1.214876	H	-10.0584	-3.05963	-0.10279
C	8.891674	-4.96119	2.189416	C	-9.78059	-3.21424	-3.48617
C	7.744996	-5.5216	2.743651	H	-7.95507	-2.90849	-4.58604
C	6.496874	-5.09147	2.303892	H	-11.4244	-3.46955	-2.11926
C	6.392637	-4.12054	1.316037	H	-10.3825	-3.38843	-4.37186
C	9.745155	-1.47308	-2.94783				

Table S. 26. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***p*-BTB** in the S_1 excited state.

Atom	X	Y	Z	Atom	X	Y	Z
C	1.753388	7.95251	-0.47861	H	3.277283	0.788101	-1.45157

C	2.101639	4.975461	0.048337	H	5.864829	2.749315	1.424618
C	2.52009	6.105859	0.757433	H	-3.38414	3.519579	-1.82128
O	1.733253	7.240287	0.735451	H	-1.21946	1.366681	1.191055
O	1.607789	7.119983	-1.60722	H	0.634074	2.931464	1.008434
C	0.613865	6.1688	-1.5021	H	7.093302	1.239641	1.336988
C	0.812112	5.072593	-0.68811	H	8.519364	-0.70152	1.364255
C	2.943813	3.844818	0.023162	H	5.74836	-2.80057	-1.20151
C	4.151633	3.829048	0.806091	H	4.296971	-0.88153	-1.22605
C	4.481891	4.991796	1.569469	H	-3.3747	1.114138	1.925443
C	3.691922	6.111019	1.524006	H	-5.24355	-0.4577	2.125243
C	-0.54976	6.340876	-2.27665	H	-5.87518	-0.2546	-2.10925
C	-1.54731	5.40911	-2.21227	H	-4.02198	1.338927	-2.31096
C	-1.43734	4.297937	-1.33835	H	8.169897	-5.68532	0.038637
C	-0.26155	4.135426	-0.55165	H	8.283438	-2.15842	-2.40957
C	2.6953	2.690095	-0.79617	H	8.470686	-3.56851	-4.43069
C	3.520523	1.611943	-0.79107	H	8.524187	-6.04285	-4.22549
C	4.701324	1.540393	0.026545	H	8.381956	-7.09213	-1.97884
C	4.978829	2.707502	0.802358	H	-10.0133	-2.9631	-3.13112
C	-2.4961	3.365091	-1.2154	H	-6.0598	-4.55764	-3.37852
C	-2.44054	2.314035	-0.33022	H	-9.33866	0.199046	3.855441
C	-1.28181	2.185916	0.482184	H	-8.39475	-3.96477	3.936606
C	-0.23446	3.058305	0.373991	C	8.804399	-3.35972	1.269105
C	5.541222	0.39583	0.041453	C	8.191193	-3.2606	2.52368
C	6.773729	0.362347	0.790087	C	10.13782	-3.77707	1.178814
C	7.588789	-0.73269	0.808475	C	8.906161	-3.57835	3.66889
C	7.258672	-1.906	0.079177	H	7.154408	-2.9502	2.588213
C	6.041721	-1.90385	-0.66776	C	10.84007	-4.09608	2.331142
C	5.227471	-0.81114	-0.67683	H	10.61646	-3.83779	0.207918
C	-3.91583	0.812079	1.034197	C	10.2315	-3.99727	3.58052
C	-4.97686	-0.07405	1.144633	H	8.420171	-3.50802	4.636705
C	-5.71606	-0.48829	0.025192	H	11.87483	-4.41391	2.253321
C	-5.33754	0.049284	-1.21563	H	10.78691	-4.24473	4.479073
C	-4.29373	0.954206	-1.33288	B	-6.90174	-1.50044	0.153697
C	-3.56003	1.350204	-0.20817	C	-8.19723	0.855603	1.566765
N	8.081789	-3.02133	0.097323	H	-7.28928	1.399513	1.847446
C	8.214406	-3.83143	-1.05745	H	-8.22991	0.838894	0.475493
C	-7.32981	-2.33971	-1.11731	H	-9.05198	1.441329	1.916683
C	-7.63114	-1.64829	1.549789	C	-7.09576	-4.14836	1.632355
C	8.246927	-5.22683	-0.94078	H	-7.45735	-4.35296	0.621867
C	8.292219	-3.23907	-2.3239	H	-6.00444	-4.06995	1.574547

C	8.401924	-4.03638	-3.45385	H	-7.32474	-5.0158	2.256805
C	8.437921	-5.42344	-3.33894	C	-9.6104	-2.02476	5.40363
C	8.362288	-6.01154	-2.07753	H	-10.1161	-2.98948	5.505457
C	-8.64852	-2.28778	-1.62491	H	-8.88008	-1.95484	6.21834
C	-8.99463	-3.02491	-2.75501	H	-10.3487	-1.23319	5.558453
C	-8.08002	-3.8455	-3.40872	C	-9.71329	-1.41848	-0.99717
C	-6.78871	-3.90865	-2.89792	H	-9.84361	-1.63716	0.065299
C	-6.39763	-3.16483	-1.78499	H	-9.46624	-0.35422	-1.07907
C	-8.8702	-0.67283	3.403976	H	-10.6754	-1.56612	-1.49457
C	-8.93834	-1.89519	4.061978	C	-4.96034	-3.30382	-1.33064
C	-8.34993	-2.99558	3.444876	H	-4.32809	-2.52505	-1.76954
C	-7.71407	-2.89627	2.209792	H	-4.84765	-3.22771	-0.2472
C	-8.21905	-0.52875	2.178965	H	-4.55353	-4.2705	-1.64066
H	2.708957	8.464466	-0.62646	C	-8.47337	-4.62384	-4.63671
H	0.930009	8.669332	-0.40358	H	-8.36127	-4.0149	-5.54154
H	5.388605	4.983601	2.167171	H	-7.84903	-5.51269	-4.76308
H	3.949586	7.010116	2.074441	H	-9.51852	-4.94315	-4.58943
H	-0.62189	7.213122	-2.91722	H	1.832705	2.69159	-1.45162
H	-2.44622	5.52094	-2.81104				

Table S. 27. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***m*-BTT** in the S_1 excited state.

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.92599	-0.74689	0.043748	H	-0.44792	-1.27998	0.31268
C	-4.95927	-0.64293	0.735928	C	1.897395	-3.45702	-0.81984
C	-6.02448	-1.36246	1.278493	H	1.913926	-4.30516	-2.79678
O	-7.04816	-1.7675	0.439451	H	1.584182	-2.43634	1.048045
O	-7.25381	0.412444	-0.39066	N	3.070413	-4.12209	-0.39603
C	-6.17882	0.190681	-1.2265	N	2.22917	4.626247	0.376605
C	-5.00138	-0.32437	-0.70188	C	4.162413	-4.27766	-1.28771
C	-3.91488	-0.19736	1.639917	C	4.569814	-3.21759	-2.10256
C	-3.96137	-0.6482	3.009769	C	4.848711	-5.49299	-1.36077
C	-5.01835	-1.42993	3.458564	C	5.635648	-3.37701	-2.97889
C	-6.06794	-1.77333	2.605461	H	4.046163	-2.26941	-2.04552
C	-6.30874	0.585389	-2.56817	C	5.92551	-5.6386	-2.22611
C	-5.24922	0.445197	-3.42494	H	4.533932	-6.32142	-0.73538
C	-4.04128	-0.13917	-2.97562	C	6.323029	-4.58514	-3.04364
C	-3.91248	-0.54906	-1.61785	H	5.938279	-2.54367	-3.60564
C	-2.90762	0.680623	1.259636	H	6.448218	-6.58923	-2.26964

C	-1.86574	1.113781	2.141998	H	7.159974	-4.70434	-3.72401
C	-1.91492	0.603883	3.481828	C	3.160581	-4.63856	0.921813
C	-2.90414	-0.23067	3.889098	C	2.07754	-5.30866	1.497746
C	-2.95516	-0.35427	-3.863	C	4.336685	-4.48704	1.661659
C	-1.80918	-0.97031	-3.44668	C	2.169391	-5.80629	2.791286
C	-1.68071	-1.43072	-2.10873	H	1.164105	-5.43629	0.926983
C	-2.72636	-1.22073	-1.23472	C	4.427065	-5.00415	2.947685
H	-8.55856	-0.41428	0.872702	H	5.178935	-3.96311	1.222783
H	-8.52962	-1.18179	-0.75903	C	3.344285	-5.66211	3.522758
H	-5.03435	-1.75468	4.494995	H	1.318089	-6.32297	3.223851
H	-6.90789	-2.36795	2.946414	H	5.348581	-4.87864	3.507984
H	-7.25181	1.012987	-2.89127	H	3.415278	-6.05858	4.530407
H	-5.33141	0.758336	-4.4614	C	2.015933	5.471437	-0.74374
H	-2.93899	1.076955	0.254939	C	0.801249	6.149719	-0.8907
H	-2.91639	-0.60091	4.910538	C	3.017953	5.625206	-1.70778
H	-3.05248	-0.017	-4.89117	C	0.595755	6.968492	-1.99171
H	-2.65391	-1.6022	-0.22428	H	0.032243	6.040014	-0.1342
H	-1.13615	0.867031	4.187975	C	2.803232	6.451853	-2.80086
H	-0.98393	-1.10322	-4.13867	H	3.954119	5.089212	-1.59847
C	-0.83427	1.989676	1.702353	C	1.593136	7.124886	-2.95078
C	0.096324	2.601451	2.606948	H	-0.34678	7.496614	-2.09412
C	-0.65684	2.324037	0.315852	H	3.58381	6.562307	-3.54672
C	1.083499	3.443894	2.184661	H	1.428779	7.767452	-3.80942
H	-0.00389	2.433156	3.672082	C	3.478244	4.675728	1.047944
C	0.330625	3.167869	-0.11158	C	4.10285	3.492529	1.457011
H	-1.2841	1.857331	-0.43269	C	4.086426	5.908194	1.310627
C	1.234604	3.760355	0.804799	C	5.318653	3.547547	2.123686
H	1.740376	3.91052	2.909521	H	3.637649	2.538235	1.236582
H	0.44665	3.365159	-1.17122	C	5.305104	5.949821	1.971224
C	-0.44923	-2.12551	-1.66783	H	3.595259	6.824728	1.00345
C	0.256142	-2.97323	-2.52874	C	5.926155	4.772876	2.383559
C	0.053108	-1.95736	-0.37226	H	5.799516	2.62451	2.43126
C	1.401257	-3.63581	-2.1148	H	5.76803	6.910026	2.17498
H	-0.11572	-3.14993	-3.5332	H	6.877773	4.811185	2.903275
C	1.206466	-2.60221	0.045137				

Table S. 28. Coordinates (Å) for the optimized structure (CAM-B3LYP/6-31G*) of ***m*-BTB** in the S_1 excited state.

Atom	X	Y	Z	Atom	X	Y	Z
C	-7.92599	-0.74689	0.043748	H	-0.44792	-1.27998	0.31268
C	-4.95927	-0.64293	0.735928	C	1.897395	-3.45702	-0.81984
C	-6.02448	-1.36246	1.278493	H	1.913926	-4.30516	-2.79678
O	-7.04816	-1.7675	0.439451	H	1.584182	-2.43634	1.048045
O	-7.25381	0.412444	-0.39066	N	3.070413	-4.12209	-0.39603
C	-6.17882	0.190681	-1.2265	N	2.22917	4.626247	0.376605
C	-5.00138	-0.32437	-0.70188	C	4.162413	-4.27766	-1.28771
C	-3.91488	-0.19736	1.639917	C	4.569814	-3.21759	-2.10256
C	-3.96137	-0.6482	3.009769	C	4.848711	-5.49299	-1.36077
C	-5.01835	-1.42993	3.458564	C	5.635648	-3.37701	-2.97889
C	-6.06794	-1.77333	2.605461	H	4.046163	-2.26941	-2.04552
C	-6.30874	0.585389	-2.56817	C	5.92551	-5.6386	-2.22611
C	-5.24922	0.445197	-3.42494	H	4.533932	-6.32142	-0.73538
C	-4.04128	-0.13917	-2.97562	C	6.323029	-4.58514	-3.04364
C	-3.91248	-0.54906	-1.61785	H	5.938279	-2.54367	-3.60564
C	-2.90762	0.680623	1.259636	H	6.448218	-6.58923	-2.26964
C	-1.86574	1.113781	2.141998	H	7.159974	-4.70434	-3.72401
C	-1.91492	0.603883	3.481828	C	3.160581	-4.63856	0.921813
C	-2.90414	-0.23067	3.889098	C	2.07754	-5.30866	1.497746
C	-2.95516	-0.35427	-3.863	C	4.336685	-4.48704	1.661659
C	-1.80918	-0.97031	-3.44668	C	2.169391	-5.80629	2.791286
C	-1.68071	-1.43072	-2.10873	H	1.164105	-5.43629	0.926983
C	-2.72636	-1.22073	-1.23472	C	4.427065	-5.00415	2.947685
H	-8.55856	-0.41428	0.872702	H	5.178935	-3.96311	1.222783
H	-8.52962	-1.18179	-0.75903	C	3.344285	-5.66211	3.522758
H	-5.03435	-1.75468	4.494995	H	1.318089	-6.32297	3.223851
H	-6.90789	-2.36795	2.946414	H	5.348581	-4.87864	3.507984
H	-7.25181	1.012987	-2.89127	H	3.415278	-6.05858	4.530407
H	-5.33141	0.758336	-4.4614	C	2.015933	5.471437	-0.74374
H	-2.93899	1.076955	0.254939	C	0.801249	6.149719	-0.8907
H	-2.91639	-0.60091	4.910538	C	3.017953	5.625206	-1.70778
H	-3.05248	-0.017	-4.89117	C	0.595755	6.968492	-1.99171
H	-2.65391	-1.6022	-0.22428	H	0.032243	6.040014	-0.1342
H	-1.13615	0.867031	4.187975	C	2.803232	6.451853	-2.80086
H	-0.98393	-1.10322	-4.13867	H	3.954119	5.089212	-1.59847
C	-0.83427	1.989676	1.702353	C	1.593136	7.124886	-2.95078
C	0.096324	2.601451	2.606948	H	-0.34678	7.496614	-2.09412

C	-0.65684	2.324037	0.315852	H	3.58381	6.562307	-3.54672
C	1.083499	3.443894	2.184661	H	1.428779	7.767452	-3.80942
H	-0.00389	2.433156	3.672082	C	3.478244	4.675728	1.047944
C	0.330625	3.167869	-0.11158	C	4.10285	3.492529	1.457011
H	-1.2841	1.857331	-0.43269	C	4.086426	5.908194	1.310627
C	1.234604	3.760355	0.804799	C	5.318653	3.547547	2.123686
H	1.740376	3.91052	2.909521	H	3.637649	2.538235	1.236582
H	0.44665	3.365159	-1.17122	C	5.305104	5.949821	1.971224
C	-0.44923	-2.12551	-1.66783	H	3.595259	6.824728	1.00345
C	0.256142	-2.97323	-2.52874	C	5.926155	4.772876	2.383559
C	0.053108	-1.95736	-0.37226	H	5.799516	2.62451	2.43126
C	1.401257	-3.63581	-2.1148	H	5.76803	6.910026	2.17498
H	-0.11572	-3.14993	-3.5332	H	6.877773	4.811185	2.903275
C	1.206466	-2.60221	0.045137				

References:

[6] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. H. Petersson, M. Nakatsuji, X. Caricato, H. P. F. Li, A. Hratchian, J. Izmaylov, G. Bloino, J. L. Zheng, M. Sonnenberg, M. Hada, K. Ehara, R. Toyota, J. Fukuda, M. Hasegawa, T. Ishida, Y. Nakajima, O. Honda, H. Kitao, T. Nakai, J. A. Vreven, J. E. Montgomery Jr., F. Peralta, M. Ogliaro, J. J. Bearpark, E. Heyd, K. N. Brothers, V. N. Kudin, T. Staroverov, R. Keith, J. Kobayashi, K. Normand, A. Raghavachari, J. C. Rendell, S. S. Burant, J. Iyengar, M. Tomasi, N. Cossi, J. M. Rega, M. Millam, J. E. Klene, J. B. Knox, V. Cross, C. Bakken, J. Adamo, R. Jaramillo, R. E. Gomperts, O. Stratmann, A. J. Yazyev, R. Austin, C. Cammi, J. W. Pomelli, R. L. Ochterski, K. Martin, V. G. Morokuma, G. A. Zakrzewski, P. Voth, J. J. Salvador, S. Dannenberg, A. D. Dapprich, O. Daniels, J. B. Farkas, J. V. Foresman, J. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09 Revision C.01, 2010.

[7] (a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B,* 1988, **37**, 785−789; (b) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 1372; (c) A. D. Becke, *J. Chem. Phys.* 1993, **98**, 5648.

[8] (a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.*, 1971, **54**, 724; (b) A. D. McLean, G. S. Chandler, *J. Chem. Phys.*, 1980, **72**, 5639.