Electronic Supplementary Information

Assembled structures of dipyrrins and their oligomers bridged by dioxy-boron moieties

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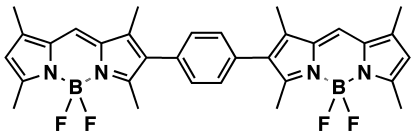
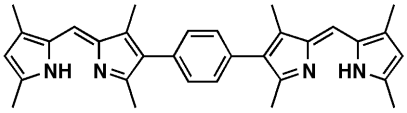
1. Synthetic procedures and spectroscopic data

General Procedures. Starting materials were purchased from Wako Pure Chemical Industries Ltd., Nacalai Tesque Inc., and Sigma-Aldrich Co. and used without further purification unless otherwise stated. UV-visible spectra were recorded on a Hitachi U-3500 spectrometer. Fluorescence spectra were recorded on a Hitachi F-4500 fluorescence spectrometer for ordinary solution and a Hamamatsu Quantum Yields Measurements System for Organic LED Materials C9920-02 for measurement of quantum yields. NMR spectra used in the characterization of products were recorded on a JEOL ECA-600 600 MHz spectrometer. All NMR spectra were referenced to solvent. Matrix-assisted laser desorption ionization time-of-flight mass spectrometries (MALDI-TOF-MS) were recorded on a Shimadzu Axima-CFRplus using negative mode. TLC analyses were carried out on aluminum sheets coated with silica gel 60 (Merck 5554). Column chromatography was performed on Sumitomo alumina KCG-1525, Wakogel C-200, C-300, Merck silica gel 60 and 60H, and Bio-Beads^{TM} S-X1 Beads (for gel permeation chromatography (GPC)). GPC-HPLC was performed on a JAI LC-9225 with JAIGEL-2H and JAIGEL-2.5H columns. In contrast to **3b**$_2$, **2b**$_3$, and **3b**$_3$, it is significantly challenging to prepare and isolate **3a**$_2$, **2a**$_3$, and **3a**$_3$ due to their less solubility, resulting in only the observation of the products by MALDI-TOF-MS.

BODIPY dimer, 2a. A 50 mL round-bottomed flask placed with 2-iodo-1,3,5,7-tetramethyl-BODIPY **1a′**[S1] (383.3 mg, 1.02 mmol), benzene-1,4-diboronic acid bispinacol ester (147.8 mg, 0.45 mmol), $Pd(PPh_3)_4$ (117.9 mg, 0.10 mmol), and Na_2CO_3 (648.7 mg, 6.12 mmol) was flushed with nitrogen and charged with a mixture of degassed toluene (50 mL), ethanol (17 mL), and water (6.5 mL). The mixture was heated at 100 °C for 10 h, cooled, then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **2a** (259.0 mg, 0.44 mmol, 98%) as a red solid. R_f = 0.11 (CH_2Cl_2:hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.31 (s, 4H, Ar-H), 7.14 (s, 2H, *meso*-H), 6.09 (s, 2H, pyrrole-H), 2.59 (s, 6H, CH_3), 2.57 (s, 6H, CH_3), 2.29 (s, 6H, CH_3), 2.28 (s, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 534.5 (1.5). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 564.5 (534). MALDI-TOF-MS: *m/z* (% intensity): 570.4 (70), 571.3 (100). Calcd for $C_{32}H_{32}B_2F_4N_4$ ([M + H]$^+$): 571.28. This compound was further characterized by single-crystal X-ray diffraction analysis.



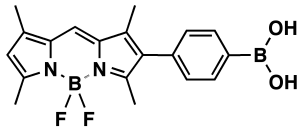
DPR dimer, 2a′. 35% aq. HCl (15 mL) solution was added to an acetone solution (20 mL) of **2a** (56.7 mg, 0.099 mmol) and the mixture was stirred at 80 °C for 5 h. Excess Na_2CO_3 was added to the reaction mixture in ice bath, which was stirred for 1 h. Under reduce pressure, acetone was evaporated, and then the mixture was partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: 5% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **2a′** (42.3 mg, 0.089 mmol, 90%) as a red solid. R_f = 0.21 (10% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.32 (s, 4H, Ar-H), 6.80 (s, 2H, *meso*-H), 5.92 (s, 2H, pyrrole-H), 2.42 (s, 6H, CH_3), 2.37 (s, 6H, CH_3), 2.27 (s, 6H, CH_3), 2.25 (s, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 476.0 (0.41). MALDI-TOF-MS: *m/z* (% intensity): 474.3 (100), 475.3 (65). Calcd for $C_{32}H_{35}N_4$ ([M + H]$^+$): 474.29.



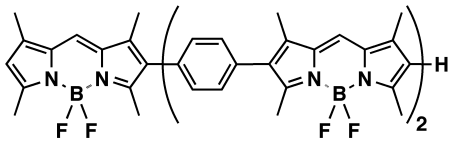
2,6-Diiodo-BODIPY, 1a′′. To a stirred solution of 1,3,5,7-tetramethyl-BODIPY[S2] (248.1 mg, 1.0 mmol) in CH_2Cl_2 (100 mL), *N*-iodosuccinimide (NIS) (495.0 mg, 2.2 mmol) was added at r.t. The reaction mixture was then stirred for 30 min and then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: CH_2Cl_2:hexane = 1:1) to give **1a′′** (489.9 mg, 0.98 mmol, 98%) as a red solid. R_f = 0.52 (CH_2Cl_2:hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.12 (s, 1H, *meso*-H), 2.59 (s, 6H, CH_3), 2.23 (s, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 548.0 (0.93). MALDI-TOF-MS: *m/z* (% intensity): 499.9 (73), 500.9 (100), 501.9 (27). Calcd for $C_{13}H_{14}BF_2N_2$ ([M + H]$^+$): 500.92.

4-BODIPY-phenylboronic acid, 1a′′′. A 200 mL round-bottomed flask placed with **1a′** (347.2 mg, 0.93 mmol), benzene-1,4-diboronic acid (1.231 g, 7.4 mmol), $Pd(PPh_3)_4$ (107.5 mg, 0.09 mmol), and Na_2CO_3 (572.4 mg, 5.6 mmol) was flushed with nitrogen and charged with a mixture of degassed 1,4-dioxane (90 mL) and water (10 mL). The mixture was heated at 100 °C for 15 h, cooled, then partitioned between water and $CHCl_3$. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent:

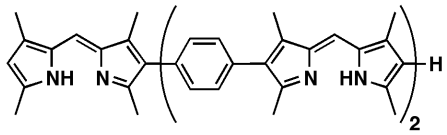
3% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **1a´´´** (195.4 mg, 0.53 mmol, 57%) as a red solid. R_f = 0.40 (3% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.81 (d, J = 7.8 Hz, 2H, Ar-H), 7.31 (d, J = 8.4 Hz, 2H, Ar-H), 7.13 (s, 1H, *meso*-H), 6.09 (s, 1H, pyrrole-H), 2.56 (s, 3H, CH_3), 2.53 (s, 3H, CH_3), 2.28 (s, 3H, CH_3), 2.23 (s, 3H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 522.0 (0.65). MALDI-TOF-MS: *m/z* (% intensity): 367.2 (45), 368.2 (100), 369.2 (20). Calcd for $C_{19}H_{20}B_2F_2N_2O_2$ ([M]$^+$): 368.17.



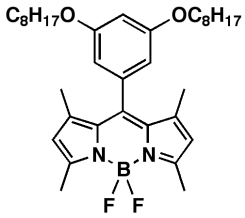
BODIPY trimer, 3a. A 100 mL round-bottomed flask placed with **1a´´** (89.6 mg, 0.18 mmol), **1a´´´** (158.3 mg, 0.43 mmol), $Pd(PPh_3)_4$ (41.4 mg, 0.08 mmol), and Na_2CO_3 (227.8 mg, 2.2 mmol) was flushed with nitrogen and charged with a mixture of degassed DMF (45 mL) and water (5 mL). The mixture was heated at 110 °C for 15 min, cooled, and then partitioned between water and $CHCl_3$. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column ($CHCl_3$:hexane = 3:1) to give **3a** (19.8 mg, 0.022 mmol, 12%) as a red solid. R_f = 0.31 (CH_2Cl_2:hexane = 5:1). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 7.35 (s, 8H, Ar-H), 7.30 (s, 1H, *meso*-H), 7.21 (s, 2H, Ar-H), 6.11 (s, 2H, pyrrole-H), 2.57 (s, 6H, CH_3), 2.54 (s, 6H, CH_3), 2.51 (s, 6H, CH_3), 2.31 (s, 6H, CH_3), 2.28 (s, 12H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 551.5 (1.2). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 585.0 (551). MALDI-TOF-MS: *m/z* (% intensity): 892.4 (73), 893.4 (100). Calcd for $C_{51}H_{49}B_3F_6N_6$ ([M + H]$^+$): 893.42.



DPR trimer, 3a´. A turbid solution of **3a** (12.3 mg, 0.014 mmol) in TFA (30 mL) and water (1.0 mL) was heated at 100 °C for 2 h, cooled, and then partitioned between water and CH_2Cl_2, then the organic layer was washed by 10% Na_2CO_3 aq. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: 8% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **3a´** (6.6 mg, 0.0088 mmol, 63%) as a yellow solid. R_f = 0.30 (8% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.35 (s, 8H, Ar-H), 7.32 (s, 3H, *meso*-H), 6.23 (s, 2H, pyrrole-H), 2.60 (s, 6H, CH_3), 2.57 (s, 6H, CH_3), 2.55 (s, 6H, CH_3), 2.42 (s, 6H, CH_3), 2.40 (s, 6H, CH_3), 2.39 (s, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 508.0 (0.58). MALDI-TOF-MS: *m/z* (% intensity): 749.4 (100), 750.5 (50). Calcd for $C_{51}H_{52}N_6$ ([M + H]$^+$): 749.43.

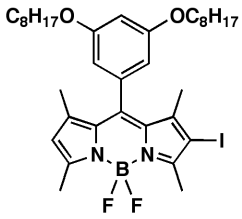


8-(3,5-Dioctyloxyphenyl)-BODIPY, 1b. 2,4-Dimethylpyrrole[S3] (3.600 g, 37.9 mmol) and 3,5-dioctyloxybenzaldehyde[S4] (623.5 mg, 17.2 mmol) were added to a 1 L round-bottomed flask containing N_2-degassed CH_2Cl_2 (500 mL). Two drops of TFA was added and the solution was stirred under nitrogen at r.t. for 1 day. After the addition of a solution of DDQ (3.904 g, 17.2 mmol) in CH_2Cl_2 (200 mL), stirring was continued for 30 min. Et_3N (12 mL) and $BF_3{\cdot}OEt_2$ (3 mL) were successively added, and after 30 min, the reaction mixture was washed with water and dried over anhydrous Na_2SO_4. The solvent was evaporated and the residue was then chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2:hexane = 1:2) to give **1b** (1.072 g, 1.8 mmol, 10%) as a red waxy solid. R_f = 0.55 (CH_2Cl_2:hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 6.52 (s, 1H, Ar-H), 6.41 (s, 2H, Ar-H), 5.98 (s, 2H, pyrrole-H), 3.91 (t, J = 6.6 Hz, 4H, OCH_2), 2.55 (s, 6H, CH_3), 1.79–1.71 (m, 4H, CH_2), 1.56 (s, 6H, CH_3), 1.44–1.40 (m, 4H, CH_2), 1.32–1.25 (m, 16H, $(CH_2)_4$), 0.88 (t, J = 6.6 Hz, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 502.0 (0.90). MALDI-TOF-MS: *m/z* (% intensity): 579.4 (46), 580.4 (100), 581.4 (57). Calcd for $C_{35}H_{51}BF_2N_2O_2$ ([M]$^+$): 580.40.

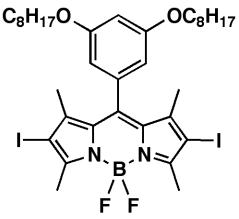


2-Iodo-8-(3,5-dioctyloxyphenyl)-BODIPY, 1b´. To a stirred solution of **1b** (1.074 g, 1.85 mmol) in CH_2Cl_2 (100 mL), NIS (416.2 mg, 1.85 mmol) was added at r.t. The reaction mixture was then stirred for 30 min and then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2:hexane = 1:2) to give **1b´** (654.8 mg, 0.93 mmol, 50%) as a red waxy solid. R_f = 0.38 (CH_2Cl_2:hexane = 1:2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 6.54 (s, 1H, Ar-H), 6.38 (s, 2H, Ar-H), 6.05 (s, 1H, pyrrole-H), 3.91 (t, J = 6.6 Hz, 4H, OCH_2), 2.62 (s, 3H, CH_3), 2.56 (s, 3H, CH_3), 1.79–1.72 (m, 4H, CH_2), 1.57 (s, 6H, CH_3), 1.44–1.40 (m, 4H, CH_2), 1.32–1.25 (m, 16H, $(CH_2)_4$), 0.88 (t, J = 6.6 Hz, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 516.0 (0.77). MALDI-TOF-MS: *m/z* (% intensity): 705.3 (71), 706.3 (100), 707.3 (56). Calcd for

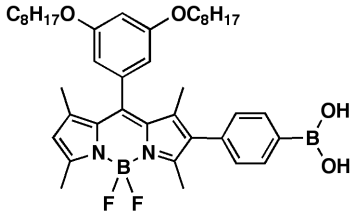
$C_{35}H_{50}BF_2IN_2O_2$ ([M]$^+$): 706.30.



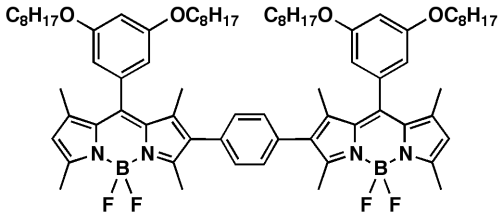
2,6-Diodo-8-(3,5-dioctyloxyphenyl)-BODIPY, 1b´´. To a stirred solution of **1b** (63.9 mg, 0.11 mmol) in CH_2Cl_2 (100 mL), NIS (54.0 mg, 0.24 mmol) was added at r.t. The reaction mixture was then stirred for 30 min and then partitioned between water and CH_2Cl_2. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel column (Wakogel C-300; eluent: CH_2Cl_2:hexane = 1:2) to give **1b´´** (51.7 mg, 0.062 mmol, 56%) as a red solid. R_f = 0.46 (CH_2Cl_2:hexane = 1:2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 6.56 (s, 1H, Ar-H), 6.34 (d, J = 2.4 Hz, 2H, Ar-H), 3.91 (t, J = 6.6 Hz, 4H, OCH_2), 2.64 (s, 6H, CH_3), 1.80–1.73 (m, 4H, CH_2), 1.57 (s, 6H, CH_3), 1.44–1.40 (m, 4H, CH_2), 1.32–1.25 (m, 16H, $(CH_2)_4$), 0.88 (t, J = 6.6 Hz, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 534.5 (0.84). MALDI-TOF-MS: *m/z* (% intensity): 831.2 (56), 832.2 (100), 833.2 (64). Calcd for $C_{35}H_{49}BF_2I_2N_2O_2$ ([M]$^+$): 832.19.



4-(8-(3,5-Dioctyloxyphenyl)-BODIPY)phenylboronic acid, 1b´´´. A 100 mL round-bottomed flask placed with **1b´** (382.5 mg, 0.54 mmol), benzene-1,4-diboronic acid (716.0 mg, 4.3 mmol), $Pd(PPh_3)_4$ (62.4 mg, 0.05 mmol), and Na_2CO_3 (343.4 mg, 3.2 mmol) was flushed with nitrogen and charged with a mixture of degassed 1,4-dioxane (40 mL) and water (4 mL). The mixture was heated at 100 °C for 15 h, cooled, then partitioned between water and $CHCl_3$. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: 1% MeOH/CH_2Cl_2) to give **1b´´´** (328.5 mg, 0.47 mmol, 87%) as a red solid. R_f = 0.30 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 8.26 (d, J = 7.8 Hz, 2H, Ar-H), 7.32 (d, J = 7.8 Hz, 2H, Ar-H), 6.54 (s, 2H, Ar-H), 6.47 (s, 2H, Ar-H), 6.04 (s, 1H, pyrrole-H), 3.94 (t, J = 6.0 Hz, 4H, OCH_2), 2.59 (s, 3H, CH_3), 2.56 (s, 3H, CH_3), 1.79–1.72 (m, 4H, CH_2), 1.57 (s, 6H, CH_3), 1.44–1.40 (m, 4H, CH_2), 1.32–1.25 (m, 16H, $(CH_2)_4$), 0.88 (t, J = 7.2 Hz, 6H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 522.0 (0.65). MALDI-TOF-MS: *m/z* (% intensity): 680.4 (50), 681.4 (100), 682.4 (55). Calcd for $C_{41}H_{56}B_2FN_2O_4$ ([M – F]$^+$): 681.44.

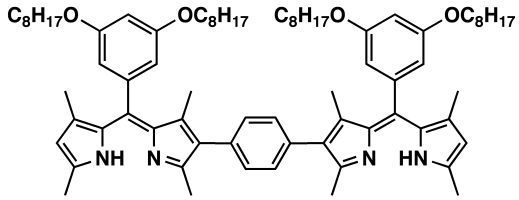


8-(3,5-Dioctyloxyphenyl)-BODIPY dimer, 2b. A 50 mL round-bottomed flask placed with **1b´** (14.8 mg, 0.021 mmol), benzene-1,4-diboronic acid (1.7 mg, 0.010 mmol), $Pd(PPh_3)_4$ (2.3 mg, 0.0020 mmol), and Na_2CO_3 (12.7 mg, 0.12 mmol) was flushed with nitrogen and charged with a mixture of degassed DMF (30 mL) and water (3 mL). The mixture was heated at 100 °C for 20 min, cooled, then partitioned between water and $CHCl_3$. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: CH_2Cl_2:hexane = 4:1) to give **2b** (328.5 mg, 0.0032 mmol, 32%) as a red solid. R_f = 0.35 (CH_2Cl_2:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.17 (s, 4H, Ar-H), 6.52 (t, J = 2.4 Hz, 2H, Ar-H), 6.45 (d, J = 2.4 Hz, 4H, Ar-H), 6.01 (s, 2H, pyrrole-H), 3.92 (t, J = 6.0 Hz, 8H, OCH_2), 2.58 (s, 6H, CH_3), 2.54 (s, 6H, CH_3), 1.78–1.73 (m, 8H, CH_2), 1.58 (s, 6H, CH_3), 1.50 (s, 6H, CH_3), 1.44–1.39 (m, 8H, CH_2), 1.31–1.25 (m, 32H, $(CH_2)_4$), 0.87 (t, J = 7.2 Hz, 12H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 527.5 (1.70). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 555.4 (527.0). MALDI-TOF-MS: *m/z* (% intensity): 1234.8 (38), 1235.8 (100), 1236.8 (72), 1237.8 (30). Calcd for $C_{76}H_{105}B_2F_4N_4O_4$ ([M + H]$^+$): 1235.83.

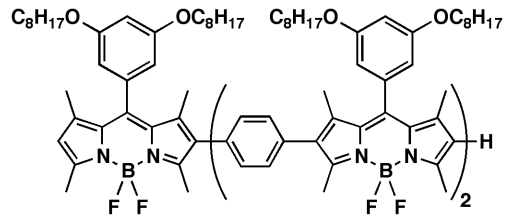


***Meso*-(3,5-dioctyloxyphenyl)-DPR dimer, 2b´.** A turbid solution of **3b** (10.0 mg, 8.1 μmol) in TFA (15 mL) and water (0.5 mL) was heated at 100 °C for 2 h, cooled, then partitioned between water and CH_2Cl_2, then the organic layer was washed by 10% Na_2CO_3 aq. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: 10% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **2b´** (9.0 mg, 7.9 μmol, 97%) as a yellow solid. R_f = 0.60 (10% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 7.17 (s, 4H, Ar-H), 6.50 (s, 6H, Ar-H), 5.85 (s, 2H, pyrrole-H), 3.92 (t, J = 6.0 Hz, 8H, OCH_2), 2.36 (s, 12H, CH_3), 1.77–1.72

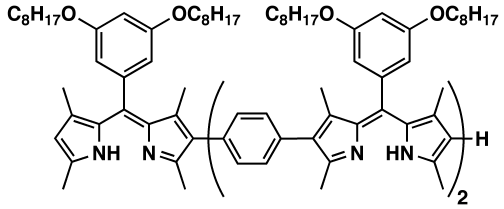
(m, 8H, CH_2), 1.49 (s, 6H, CH_3), 1.47 (s, 6H, CH_3), 1.47 (s, 6H, CH_3), 1.42–1.39 (m, 8H, CH_2), 1.30–1.26 (m, 32H, $(CH_2)_4$), 0.87 (t, J = 6.6 Hz, 12H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 481.0 (0.57). MALDI-TOF-MS: *m/z* (% intensity): 1139.8 (100), 1140.8 (84), 1141.8 (38). Calcd for $C_{76}H_{106}N_4O_4$ ([M + H]$^+$): 1138.82.



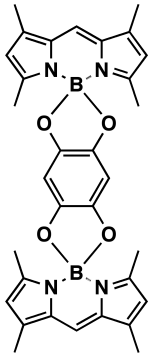
8-(3,5-Dioctyloxyphenyl)-BODIPY trimer, 3b. A 100 mL round-bottomed flask placed with **1b´´** (50.0 mg, 0.06 mmol), **1b´´´** (100.0 mg, 0.14 mmol), $Pd(PPh_3)_4$ (13.9 mg, 0.012 mmol), and Na_2CO_3 (76.3 mg, 0.72 mmol) was flushed with nitrogen and charged with a mixture of degassed DMF (40 mL) and water (4 mL). The mixture was heated at 110 °C for 15 min, cooled, and then partitioned between water and $CHCl_3$. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: CH_2Cl_2:hexane = 3:1) and recrystallized from CH_2Cl_2/MeOH to give **3b** (71.1 mg, 0.038 mmol, 63%) as a red solid. R_f = 0.31 (CH_2Cl_2:hexane = 3:1). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 7.18 (s, 8H, Ar-H), 6.53 (t, J = 2.4 Hz, 2H, Ar-H), 6.49 (d, J = 2.4 Hz, 1H, Ar-H), 6.49 (d, J = 2.4 Hz, 6H, Ar-H), 6.02 (s, 2H, pyrrole-H), 3.92 (t, J = 6.6 Hz, 12H, OCH_2), 2.58 (s, 6H, CH_3), 2.57 (s, 6H, CH_3), 2.55 (s, 6H, CH_3), 1.78–1.73 (m, 12H, CH_2), 1.58 (s, 6H, CH_3), 1.53 (s, 6H, CH_3), 1.51 (s, 6H, CH_3), 1.44–1.38 (m, 12H, CH_2), 1.31–1.25 (m, 48H, $(CH_2)_4$), 0.87 (t, J = 6.6 Hz, 18H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 543.0 (2.4). Fluorescence (CH_2Cl_2, λ_{em}[nm] (λ_{ex}[nm])): 572.6 (543). MALDI-TOF-MS: *m/z* (% intensity): 1889.2 (51), 1890.2 (100), 1891.2 (88), 1892.2 (57), 1893.2 (28). Calcd for $C_{117}H_{158}B_3F_6N_6O_6$ ([M + H]$^+$): 1890.24.



***Meso*-(3,5-dioctyloxyphenyl)-DPR trimer, 3b´.** A turbid solution of **3b** (71.1 mg, 0.038 mmol) in TFA (30 mL) and water (1.0 mL) was heated at 100 °C for 20 min, cooled, and then partitioned between water and CH_2Cl_2, then the organic layer was washed by 10% Na_2CO_3 aq. The combined extracts were dried over anhydrous Na_2SO_4, and evaporated. The residue was then chromatographed over silica gel flash column (eluent: 10% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **3b´** (62.0 mg, 0.036 mmol, 95%) as a yellow solid. R_f = 0.30 (10% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, CD_2Cl_2, 20 °C): δ (ppm) 7.18 (s, 8H, Ar-H), 6.55 (s, 3H, Ar-H), 6.54 (s, 6H, Ar-H), 5.85 (s, 2H, pyrrole-H), 3.92 (t, J = 6.6 Hz, 12H, OCH_2), 2.39 (s, 6H, CH_3), 2.37 (s, 12H, CH_3), 1.77–1.72 (m, 12H, CH_2), 1.49 (s, 6H, CH_3), 1.47 (s, 6H, CH_3), 1.47 (s, 6H, CH_3), 1.44–1.38 (m, 12H, CH_2), 1.32–1.25 (m, 48H, $(CH_2)_4$), 0.86 (t, J = 6.6 Hz, 18H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 493.0 (0.81). MALDI-TOF-MS: *m/z* (% intensity): 1746.2 (100), 1747.3 (50). Calcd for $C_{117}H_{160}N_6O_6$ ([M + H]$^+$): 1746.24.

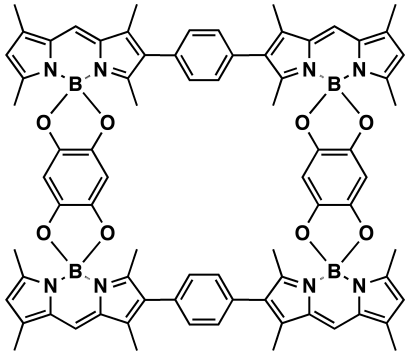


Boron-bridged duplex of 1a, $1a_2$. BODIPY **1a**[S2] (20.0 mg, 0.081 mmol) was dissolved in dry CH_2Cl_2 (5 mL) in the presence of $AlCl_3$ (27.0 mg, 0.20 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., and then a solution of 1,2,4,5-tetrahydroxybenzene[S5] (3.8 mg, 0.027 mmol) in dry CH_3CN (1 mL) was added to the mixture at r.t. The resulting mixture was refluxed for 10 min, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **$1a_2$** (3.0 mg, 0.0054 mmol, 20%) as a brown solid. R_f = 0.45 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.06 (s, 2H, *meso*-H), 6.34 (s, 2H, Ar-H), 6.01 (s, 4H, pyrrole-H), 2.25 (s, 12H, CH_3), 2.14 (s, 12H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 507.5 (1.2). MALDI-TOF-MS: *m/z* (% intensity): 558.3 (50), 559.3 (100). Calcd for $C_{32}H_{32}B_2N_4O_4$ ([M + H]$^+$): 559.26.

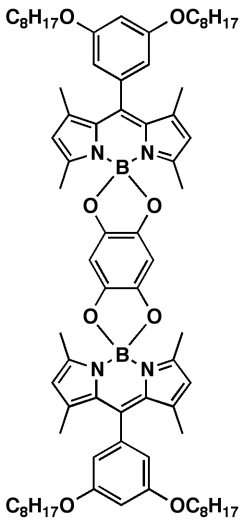


Boron-bridged duplex of 2a, $2a_2$. BODIPY dimer **2a** (6.6 mg, 0.0012 mmol) was dissolved in dry CH_3CN (12 mL) in the presence of $AlCl_3$ (7.8 mg, 0.0060 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., then a solution of 1,2,4,5-tetrahydroxybenzene[S5] (1.3 mg, 0.0096 mmol) in dry CH_3CN (12 mL) was added to the mixture at r.t. The resulting mixture was refluxed for 10 min, and the crude mixture was concentrated

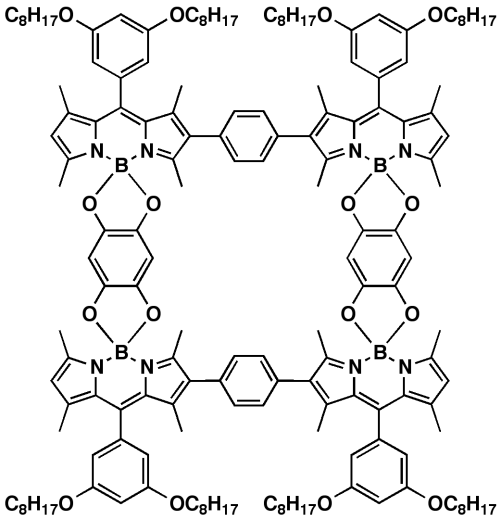
under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: 1% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **2a**$_2$ (0.2 mg, 0.0016 mmol, 26%) as a red solid. R_f = 0.50 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.19 (s, 8H, Ar-H), 7.08 (s, 4H, *meso*-H), 6.42 (s, 4H, Ar-H), 6.05 (s, 4H, pyrrole-H), 2.28 (s, 12H, CH_3), 2.25 (s, 12H, CH_3), 2.19 (s, 12H, CH_3), 2.11 (s, 12H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 507.5 (2.0). MALDI-TOF-MS: *m/z* (% intensity): 1265.6 (100), 1266.6 (90). Calcd for $C_{76}H_{68}B_4N_8O_8$ ($[M + H]^+$): 1265.55.



Boron-bridged duplex of 1b, 1b$_2$. BODIPY **1b** (15.8 mg, 0.027 mmol) was dissolved in dry CH_2Cl_2 (15 mL) in the presence of $AlCl_3$ (9.0 mg, 0.068 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., and then a solution of 1,2,4,5-tetrahydroxybenzene[S5] (1.9 mg, 0.013 mmol) in dry CH_3CN (15 mL) was added to the mixture at r.t. The resulting mixture was refluxed for 10 min, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **1b**$_2$ (12.2 mg, 0.010 mmol, 80%) as a brown solid. R_f = 0.80 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 6.52 (t, J = 2.4 Hz, 4H, Ar-H), 6.43 (d, J = 2.4 Hz, 2H, Ar-H), 6.42 (s, 2H, Ph-H), 5.94 (s, 4H, pyrrole-H), 3.93 (t, J = 6.6 Hz, 8H, OCH_2), 2.16 (s, 3H, CH_3), 1.78–1.75 (m, 8H, CH_2), 1.54 (s, 3H, CH_3), 1.45–1.41 (m, 8H, CH_2), 1.32–1.27 (m, 32H, $(CH_2)_4$), 0.89 (t, J = 6.6 Hz, 12H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 500.5 (1.4). MALDI-TOF-MS: *m/z* (% intensity): 1223.8 (58), 1224.8 (100), 1225.8 (78), 1226.8 (42). Calcd for $C_{76}H_{106}B_2N_4O_8$ ($[M]^+$): 1223.82.

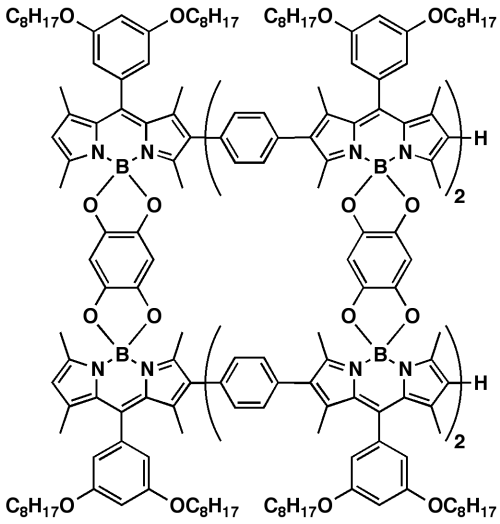


Boron-bridged duplex of 2b, 2b$_2$. BODIPY dimer **2b** (3.9 mg, 0.0032 mmol) was dissolved in dry CH_3CN (10 mL) in the presence of $AlCl_3$ (2.1 mg, 0.016 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., and then a solution of 1,2,4,5-tetrahydroxybenzene[S5] (0.4 mg, 0.0028 mmol) in dry CH_3CN (5 mL) was added the mixture at r.t. The resulting mixture was refluxed for 10 min, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: 1% MeOH/CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **2b**$_2$ (2.0 mg, 0.77 μmol, 55%) as a red solid. R_f = 0.60 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.03 (s, 8H, Ar-H), 6.51 (t, J = 2.4 Hz, 4H, Ar-H), 6.45 (d, J = 2.4 Hz, 8H, Ar-H), 6.42 (s, 4H, Ar-H), 5.97 (s, 4H, pyrrole-H), 3.91 (t, J = 6.0 Hz, 16H, OCH_2), 2.18 (s, 12H, CH_3), 2.10 (s, 12H, CH_3), 1.77–1.73 (m, 16H, CH_2), 1.56 (s, 6H, CH_3), 1.43 (s, 6H, CH_3), 1.44–1.39 (m, 16H, CH_2), 1.30–1.25 (m, 64H, $(CH_2)_4$), 0.87 (t, J = 6.6 Hz, 24H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 525.0 (2.1). MALDI-TOF-MS: *m/z* (% intensity): 2594.6 (94), 2595.6 (100). Calcd for $C_{164}H_{212}B_4N_8O_{16}$ ($[M + H]^+$): 2595.64.

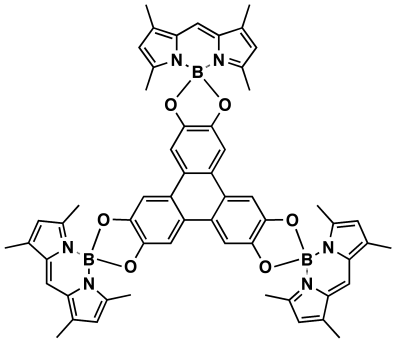


Boron-bridged duplex of 3b, 3b$_2$. BODIPY dimer **3b**

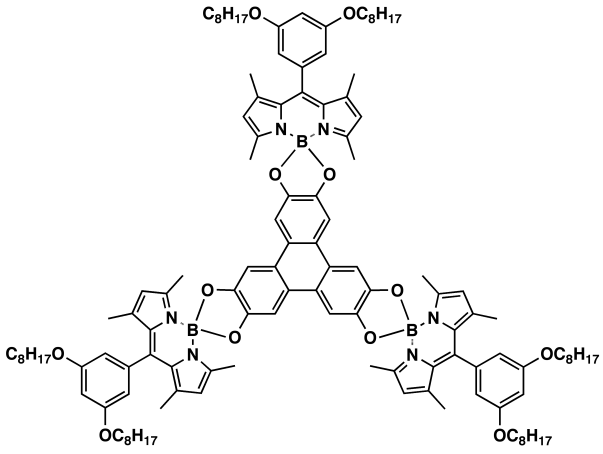
(9.4 mg, 0.0050 mmol) was dissolved in dry CH_2Cl_2 (10 mL) in the presence of $AlCl_3$ (5.0 mg, 0.037 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., and then a solution of 1,2,4,5-tetrahydroxybenzene[S5] (1.0 mg, 0.0075 mmol) in dry CH_3CN (10 mL) was added to the mixture at r.t. The resulting mixture was refluxed for 10 min, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **3b**$_2$ (6.1 mg, 0.0015 mmol, 62%) as a purple solid. R_f = 0.20 (1% MeOH/CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.07 (d, J = 2.4 Hz, 16H, Ar-H), 6.51 (t, J = 2.4 Hz, 4H, Ar-H), 6.49 (t, J = 2.4 Hz, 2H, Ar-H), 6.47 (d, J = 1.8 Hz, 4H, Ar-H), 6.46 (d, J = 1.8 Hz, 8H, Ar-H), 6.42 (s, 4H, Ar-H), 6.41 (s, 2H, Ar-H), 5.97 (s, 4H, pyrrole-H), 3.92 (t, J = 6.0 Hz, 24H, OCH_2), 2.19 (s, 12H, CH_3), 2.13 (s, 12H, CH_3), 2.12 (s, 12H, CH_3), 1.76–1.74 (m, 24H, CH_2), 1.56 (s, 12H, CH_3), 1.43 (s, 24H, CH_3), 1.43–1.39 (m, 24H, CH_2), 1.30–1.25 (m, 96H, $(CH_2)_4$), 0.88–0.84 (m, 36H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 540.5 (3.8). MALDI-TOF-MS: *m/z* (% intensity): 3963.4 (64), 3964.5 (90), 3965.5 (100), 3966.5 (95), 3967.5 (85), 3968.5 (65). Calcd for $C_{252}H_{320}B_6N_{12}O_{24}$ ($[M]^+$): 3965.47.



Boron-bridged triplex of 1a, 1a$_3$. BODIPY **1a** (25.0 mg, 0.095 mmol) was dissolved in dry $CHCl_3$ (10 mL) in the presence of $AlCl_3$ (31.7 mg, 0.248 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., and then a solution of 2,3,6,7,10,11-hexahydroxytriphenylene hydrate (10.2 mg, 0.032 mmol) in dry CH_3CN (2 mL) was added the mixture at r.t. The resulting mixture was stirred for 10 min, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/hexane to give **1a**$_3$ (24.6 mg, 0.0026 mmol, 82%) as a brown solid. R_f = 0.45 (CH_2Cl_2). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.83 (s, 6H, triphenylene-H), 7.12 (s, 3H, *meso*-H), 6.02 (s, 6H, pyrrole-H), 2.27 (s, 18H, CH_3), 2.13 (s, 18H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 509.0 (1.6). MALDI-TOF-MS: *m/z* (% intensity): 946.4 (36), 947.4 (82), 948.4 (100), 949.4 (76), 950.5 (42). Calcd for $C_{57}H_{51}B_3N_6O_6$ ($[M]^+$): 948.42. This compound was further characterized by single-crystal X-ray diffraction analysis.

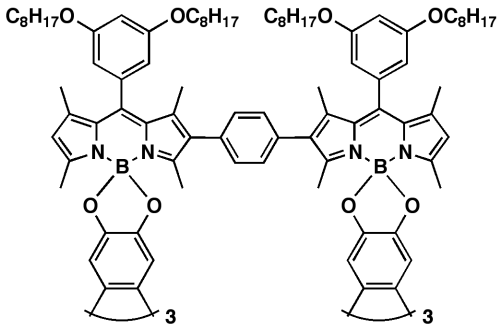


Boron-bridged triplex of 1b, 1b$_3$. BODIPY **1b** (42.3 mg, 0.073 mmol) was dissolved in dry $CHCl_3$ (5 mL) in the presence of $AlCl_3$ (24.3 mg, 0.183 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., and then a solution of 2,3,6,7,10,11-hexahydroxytriphenylene hydrate (7.2 mg, 0.022 mmol) in dry CH_3CN (1 mL) was added to the mixture at r.t. The resulting mixture was stirred for 10 min, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: CH_2Cl_2) and recrystallized from CH_2Cl_2/MeOH to give **1b**$_3$ (17.3 mg, 0.0089 mmol, 40%) as a brown solid. R_f = 0.60 (CH_2Cl_2:hexane = 1:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.87 (s, 6H, triphenylene-H), 6.54 (t, J = 1.8 Hz, 3H, Ar-H), 6.47 (d, J = 1.8 Hz, 6H, Ar-H), 5.96 (s, 6H, pyrrole-H), 3.95 (t, J = 6.6 Hz, 12H, OCH_2), 2.16 (s, 18H, CH_3), 1.80–1.76 (m, 12H, CH_2), 1.58 (s, 18H, CH_3), 1.47–1.42 (m, 12H, CH_2), 1.34–1.29 (m, 48H, $(CH_2)_4$), 0.90–0.88 (t, J = 6.6 Hz, 18H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 503.0 (2.1). MALDI-TOF-MS: *m/z* (% intensity): 1944.3 (46), 1945.2 (100), 1946.3 (92), 1947.2 (76), 1948.2 (35). Calcd for $C_{123}H_{159}B_3N_6O_{12}$ ($[M]^+$): 1945.23.

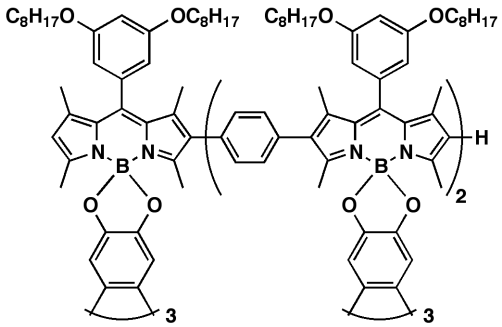


Boron-bridged triplex of 2b, 2b$_3$. BODIPY dimer **2b** (16.0 mg, 0.013 mmol) was dissolved in dry $CHCl_3$ (25 mL) in the presence of $AlCl_3$ (8.7 mg, 0.065 mmol)

under nitrogen. The mixture was stirred for 5 min at r.t., andthen a solution of 2,3,6,7,10,11-hexahydroxytriphenylene hydrate (2.8 mg, 0.0087 mmol) in dry CH_3CN (5 mL) was added to the mixture at r.t. The resulting mixture was refluxed for 10 min, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: CH_2Cl_2) and chromatographed over GPC-HPLC (eluent: $CHCl_3$) to give **2b**$_3$ (11.1 mg, 0.0027 mmol, 62%) as a purple solid. R_f = 0.50 (CH_2Cl_2:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.83 (s, 12H, triphenylene-H), 7.02 (s, 12H, Ar-H), 6.53 (t, J = 2.4 Hz, 6H, Ar-H), 6.49 (d, J = 2.4 Hz, 12H, Ar-H), 5.96 (s, 6H, pyrrole-H), 3.94 (t, J = 6.6 Hz, 24H, OCH_2), 2.14 (s, 18H, CH_3), 2.03 (s, 18H, CH_3), 1.79–1.74 (m, 24H, CH_2), 1.56 (s, 18H, CH_3), 1.48 (s, 18H, CH_3), 1.46–1.41 (m, 24H, CH_2), 1.35–1.25 (m, 96H, $(CH_2)_4$), 0.89–0.86 (t, J = 6.6 Hz, 36H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 527.0 (4.3). MALDI-TOF-MS: *m/z* (% intensity): 4111.5 (55), 4112.5 (85), 4113.5 (93), 4114.5 (100), 4115.5 (95), 4116.6 (82), 4117.6 (57). Calcd for $C_{264}H_{325}B_6N_{12}O_{24}$ ($[M + H]^+$): 4114.51.



Boron-bridged triplex of 3b, 3b$_3$. BODIPY trimer **3b** (19.9. mg, 0.011 mmol) was dissolved in dry $CHCl_3$ (25 mL) in the presence of $AlCl_3$ (10.5 mg, 0.079 mmol) under nitrogen. The mixture was stirred for 5 min at r.t., and then a solution of 2,3,6,7,10,11-hexahydroxytriphenylene hydrate (3.4 mg, 0.0011 mmol) in dry CH_3CN (5 mL) was added to the mixture at r.t. The resulting mixture was refluxed for 3 h, and the crude mixture was concentrated under reduced pressure. The residue was then chromatographed over activated basic alumina column (Sumitomo KCG-1525; eluent: CH_2Cl_2) and chromatographed over GPC-HPLC (eluent: $CHCl_3$) to give **3b**$_3$ (0.6 mg, 0.088 μmol, 3%) as a purple solid. R_f = 0.53 (CH_2Cl_2:hexane = 4:1). ^{1}H NMR (600 MHz, $CDCl_3$, 20 °C): δ (ppm) 7.83 (s, 12H, triphenylene-H), 7.78 (s, 6H, triphenylene-H), 7.02 (s, 24H, Ar-H), 6.53–6.49 (m, 27H, Ar-H), 5.96 (s, 6H, pyrrole-H), 3.93 (t, J = 6.0 Hz, 36H, OCH_2), 2.14 (s, 18H, CH_3), 2.03 (s, 18H, CH_3), 2.02 (s, 18H, CH_3), 1.79–1.72 (m, 36H, CH_2), 1.57 (s, 18H, CH_3), 1.48–1.25 (m, 216H, CH_3 and $(CH_2)_4$), 0.89–0.86 (m, 54H, CH_3). UV/vis (CH_2Cl_2, λ_{max}[nm] (ε, 10^5 $M^{-1}cm^{-1}$)): 542.0 (6.4). MALDI-TOF-MS: *m/z* (% intensity): 6282.8 (100), 6283.9 (96). Calcd for $C_{405}H_{489}B_9N_{18}O_{36}$ ($[M]^+$): 6282.81.



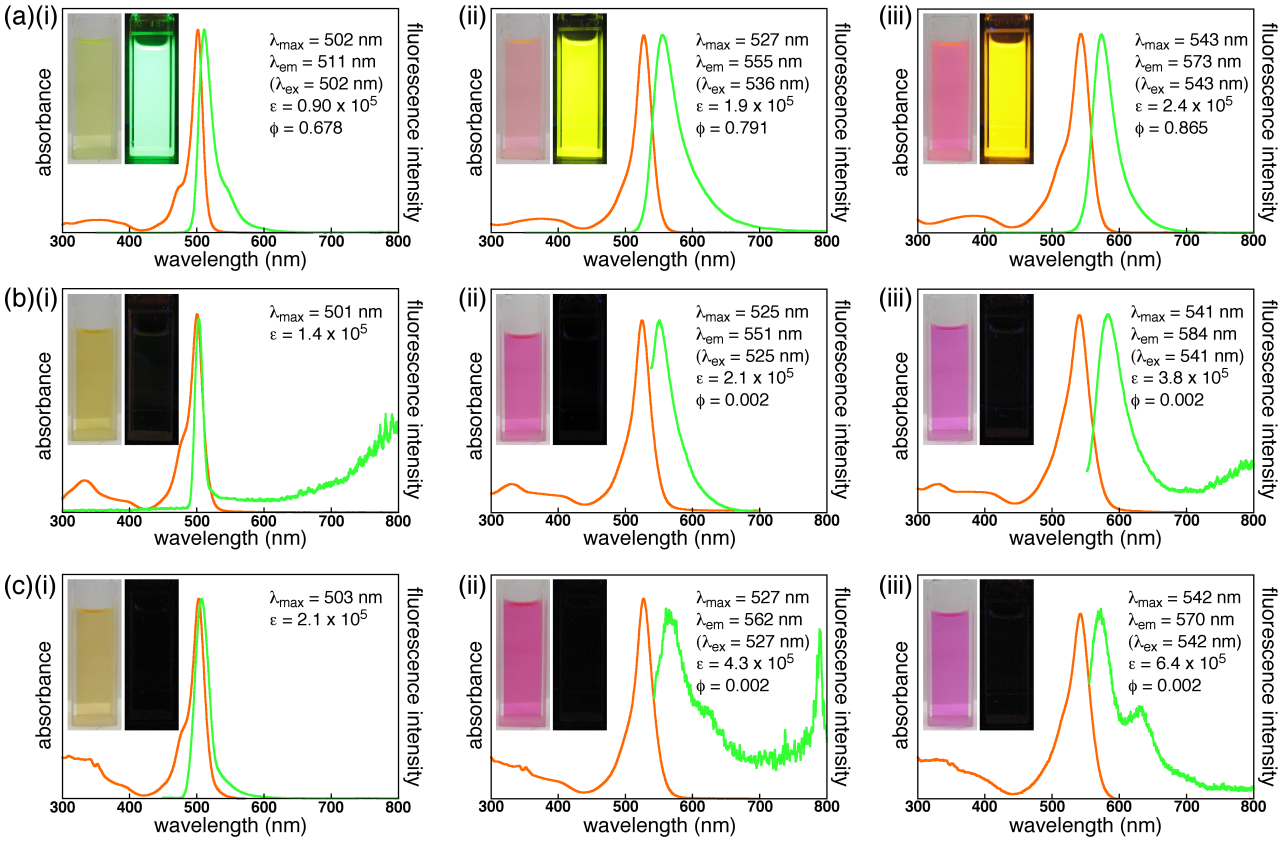
[S1] C.-W. Wan, A. Burghart, J. Chen, F. Bergström, L. B.-Å. Johansson, M. F. Wolford, T. G. Kim, M. R. Topp, R. M. Hochstrasser and K. Burgess, *Chem. Eur. J.,* 2003, **9**, 4430−4441.

[S2] L. Wu and K. Burgess, *Chem. Commun.,* 2008, 4933−4935.

[S3] (a) H. Fischer, *Org. Syn.,* 1935, **15**, 17–19; (b) H. Fischer, *Org. Syn.,* 1935, **15**, 20–21.

[S4] N. Aratani, A. Tskagi, Y. Yanagawa, T. Matsumoto, T. Kawai, Z.-S. Yoon, D. Kim and A. Osuka, *Chem. Eur. J.*, 2005, **11**, 3389−3404.

[S5] R.-W. Paul, S.-H. Louis, H. Asada and V.-D. Stanley, *J. Org. Chem*., 1985, **50**, 4276–4281.



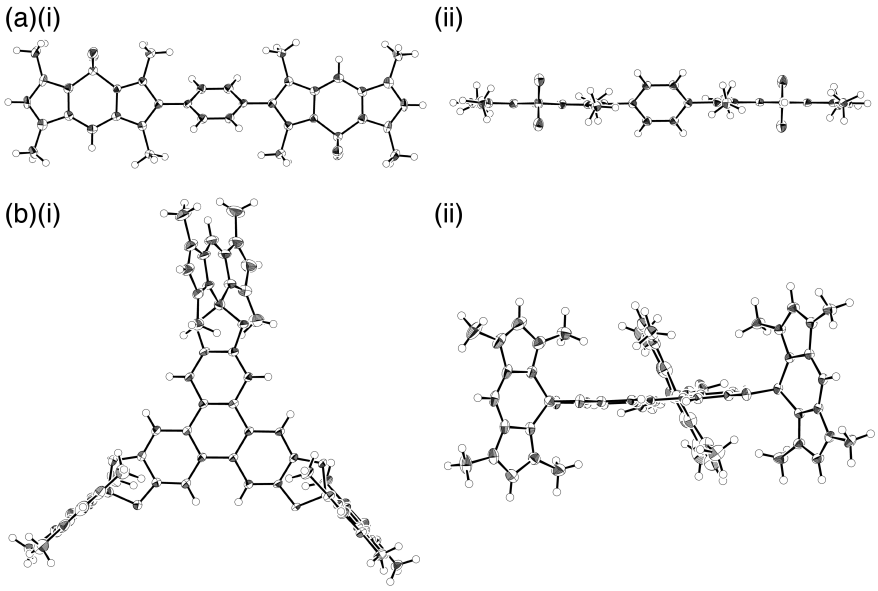
Supporting Figure 1 UV/vis absorption and fluorescence spectra (represented as orange and yellow green lines, respectively) of (a)(i) **1b**, (ii) **2b**, and (iii) **3b**, (b)(i) **1b**$_2$, (ii) **2b**$_2$, and (iii) **3b**$_2$, and (c)(i) **1b**$_3$, (ii) **2b**$_3$, and (iii) **3b**$_3$ in CH_2Cl_2. In the case of **1b**$_2$ and **1b**$_3$, it is difficult to observe fluorescence emissions due to the significantly low quantum yields and the overlap with absorption bands. In addition, as for the UV/vis and fluorescence quantum yield measurements for **3b**$_3$, we used more amounts of the compound obtained from several synthesis. The procedure in the experimental section is a representative one among several trials, even though it showed the significantly low yield of 3%. A small value in the quantum yield (0.002) is comparable to those of the related compounds (**2b**$_2$, **3b**$_2$, and **2b**$_3$).

2. X-ray crystallographic data

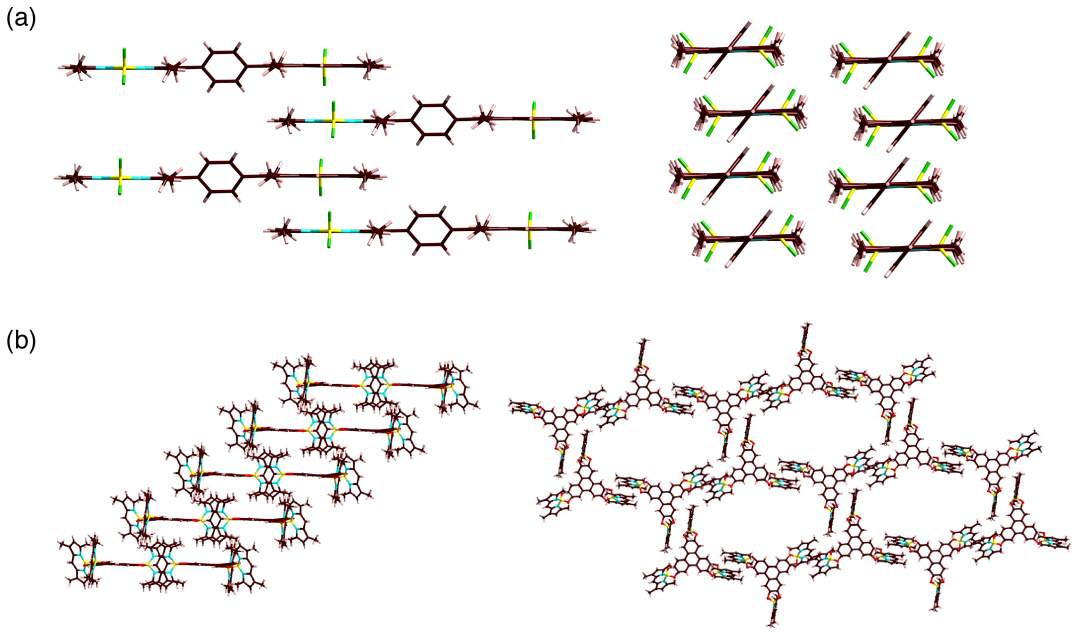
Method for single-crystal X-ray analysis: Crystallographic data for the precursor of metal coordination ligand are summarized in Supporting Table 1. A single crystal of **2a** was obtained by vapor diffusion of hexane into $CHCl_3$. The data crystal was a red prism of approximate dimensions 0.20 mm × 0.10 mm × 0.10 mm. Data were collected at 93 K on a Rigaku RAXIS-RAPID diffractometer with graphite monochromated Cu-Kα radiation (λ = 1.54187 Å) , and structure was solved by direct method. A single crystal of **1a**$_3$ was obtained by vapor diffusion of hexane into $CHCl_3$. The data crystal was a red prism of approximate dimensions 0.20 mm × 0.20 mm × 0.20 mm. Data were collected at 103 K on a Rigaku CCD diffractometer (Saturn 724 with MicroMax-007) with Varimax Mo optics using graphite monochromated Mo-Kα radiation (λ = 0.71075 Å), and structure was solved by direct method. In each compound, the non-hydrogen atoms were refined anisotropically. The calculations were performed using the Crystal Structure crystallographic software package of Molecular Structure Corporation for **2a**[S6] and of CrystalClear for **1a**$_3$. The scattering arising from the presence of disordered solvents in the crystals was removed by use of the utility SQUEEZE in the PLATON software package.[S7,8] CIF files (CCDC-929906 and 929907) can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Supporting Table 1 Crystallographic details for compound **2a** and **1a**$_3$.

	2a	**1a**$_3$
formula	$C_{32}H_{32}B_2F_4N_4 \cdot CHCl_3$	$C_{57}H_{51}B_3N_6O_6$
fw	808.97	948.48
crystal size, mm	0.20 × 0.10 × 0.10	0.20 × 0.20 × 0.20
crystal system	triclinic	triclinic
space group	*P*-1 (no. 2)	*P*-1 (no. 2)
a, Å	6.9862(2)	10.6177(3)
b, Å	11.3882(3)	19.8727(2)
c, Å	12.5660(4)	20.9723(5)
α, °	70.3780(18)	64.525(8)
β, °	73.462(2)	77.294(10)
γ, °	86.088(2)	69.346(9)
V, Å^3	902.32(5)	3725.98(14)
ρ_{calcd}, gcm^{-3}	1.489	0.845
Z	1	2
T, K	93(2)	103(2)
μ(Cu-Kα), mm^{-1}	4.797	0.055
no. of reflns	9206	30415
no. of unique reflns	3206	16325
variables	230	651
$\lambda_{Cu\text{-}K\alpha}$, Å	1.54187	0.055
R_1 ($I > 2\sigma(I)$)	0.0546	0.0695
wR_2 ($I > 2\sigma(I)$)	0.1327	0.2178
GOF	1.099	1.099



Supporting Figure 2 Ortep drawing of single-crystal X-ray structures ((i) top and (ii) side view) of (a) **2a** and (b) **1a**$_3$. Thermal ellipsoids are scaled to the 50% probability level.

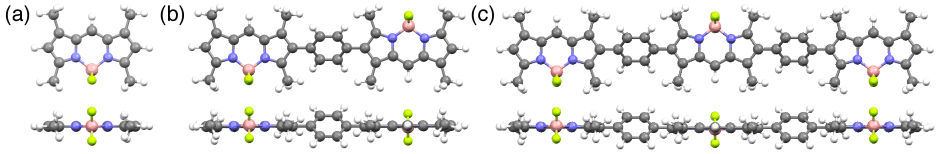


Supporting Figure 3 Packing diagrams of (a) **2a** and (b) **1a**$_3$.

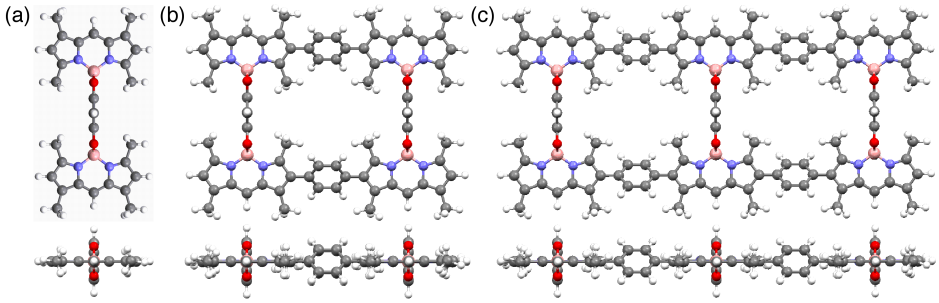
[S6] *CrystalStructure (Ver. 3.8), Single Crystal Structure Analysis Software,* Rigaku/MSC and Rigaku Corporation, 2006.
[S7] A. L. Spek, *PLATON, A Multipurpose Crystallographic Tool*; Utrecht University: Utrecht, 2005.
[S8] P. van der Sluis and A. L. Spek, *Acta Crystallogr. Sect. A*, 1990, **46**, 194–201.

3. Optimization of boron-bridged complexes

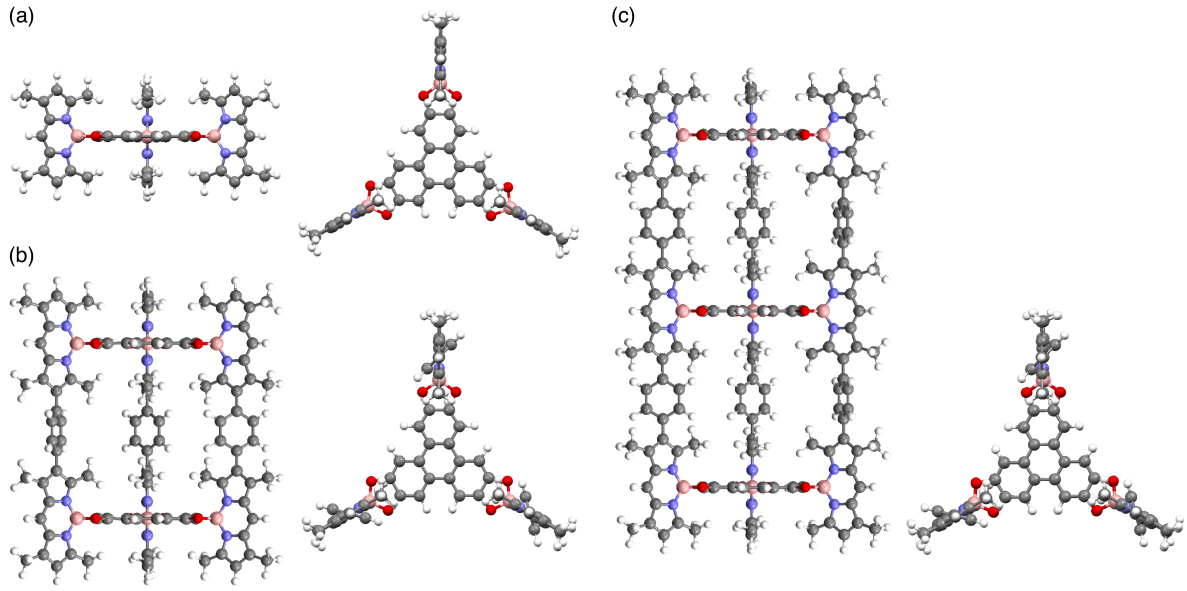
DFT and semi-empirical calculations. Ab initio and semi-empirical calculations of boron-bridged complexes were carried out by using Gaussian 03 program[S7] and a DELL optiplex 960 computer and a Mac mini computer, respectively. The structures were optimized, and the total electronic energies were calculated at the B3LYP level using a 6-31G(d,p) basis set for **1a**, **1a**$_2$, and **1a**$_3$ and at AM1 level for **2a**, **3a**, **2a**$_2$, **3a**$_2$, **2a**$_3$, and **3a**$_3$.



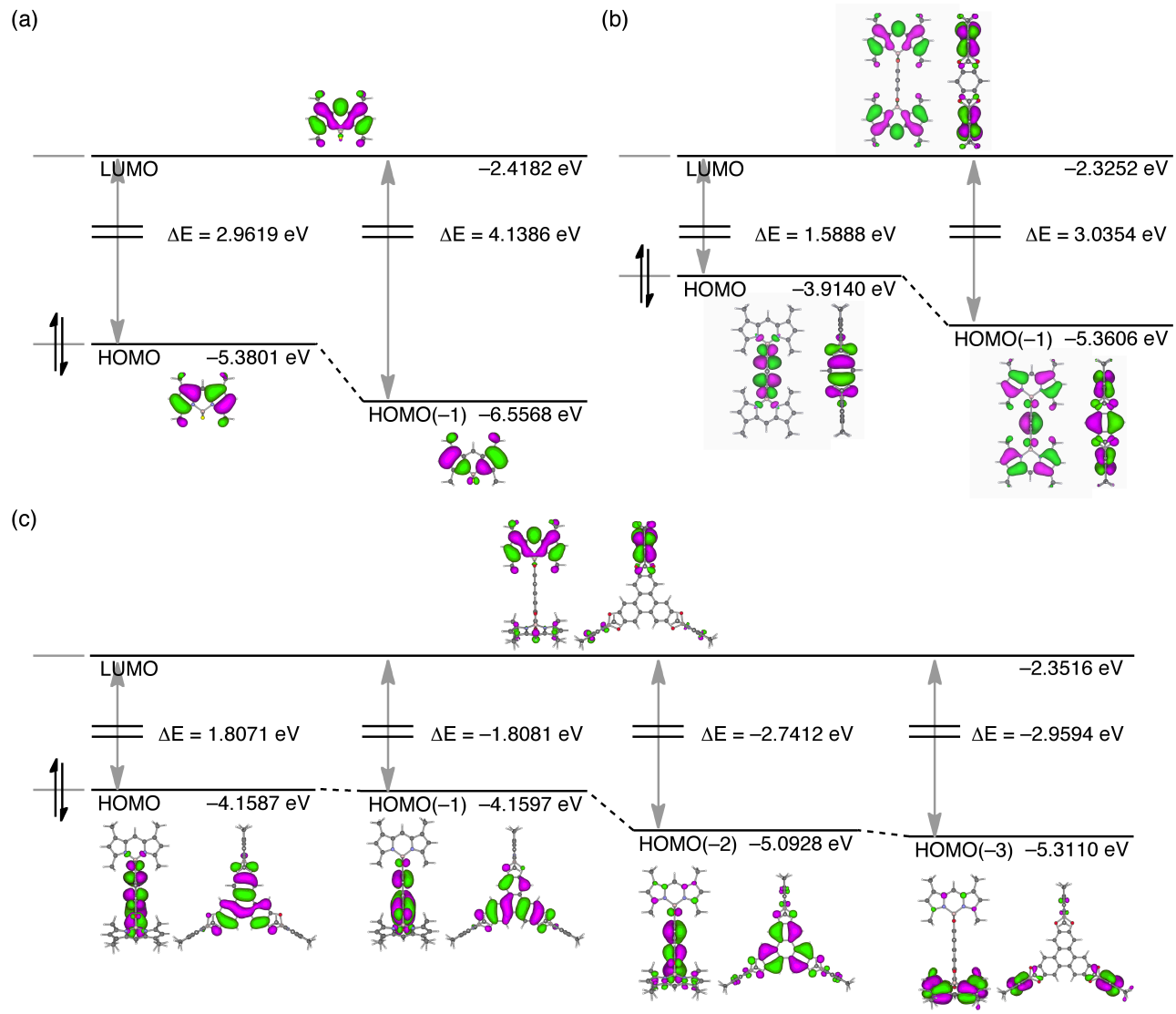
Supporting Figure 4 Optimized structures of (a) **1a** at B3LYP/6-31G(d,p) level and (b) **2a** and (c) **3a** at AM1 level.



Supporting Figure 5 Optimized structures of (a) **1a**$_2$ at B3LYP/6-31G(d,p) level and (b) **2a**$_2$ and (c) **3a**$_2$ at AM1 level.



Supporting Figure 6 Optimized structures of (a) **1a**$_3$ at B3LYP/6-31G(d,p) level and (b) **2a**$_3$ and (c) **3a**$_3$ at AM1 level.



Supporting Figure 7 Diagram of molecular orbitals and their energy levels for (a) **1a**, (b) **1a**$_2$, and (c) **1a**$_3$ as representative forms of the boron-bridged assemblies at B3LYP/6-31+G(d,p)//B3LYP/6-31G(d,p) level. In contrast to **1a**, the molecular orbitals of the duplex **1a**$_2$ and the triplex **1a**$_3$ showed the orbitals localized on the bridging π-conjugated moieties between those on BODIPY units. This theoretical study suggested that the photoexcited intramolecular electron transfer may occur in the multiplexes, resulting the significant quenching of emission.

Cartesian Coordination of 1a (DFT)
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Cartesian Coordination of 3a (AM1)

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H,-2.926239001,2.1946838525,4.1098512132
H,-3.754102234,2.417258583,6.4430861541
H,-1.5684247587,-1.1426624793,7.5597517546
H,-0.7402313953,-1.365085555,5.2265475163

H,-2.5776341406,-0.1659576137,15.2794544739
H,-2.3051718174,1.620845178,15.4093711141
H,-3.4821663431,0.8007012876,16.5348497054
H,-7.8457395153,2.6080339934,12.7709812248
H,-8.2589631983,0.9233386834,13.3000453876
H,-8.106048142,2.2461767615,14.5320567254
H,-0.8572888111,-0.84796694,9.8334368454
H,-0.4729871013,0.7270633027,10.647994986
H,-5.5633228407,0.9238077357,7.0756023275
N,4.5127092541,-1.0530644899,-10.307483677
N,5.3814719955,-1.2499279947,-12.6830901977
N,-0.4318529639,0.035624977,-1.5165960029
N,-1.299547191,0.2448272506,0.8597959964
N,-4.0636545354,1.0276657435,13.1836544836
N,-3.1978740785,0.8056494222,10.8094416041
B,5.8177108148,-1.3356141825,-11.1631665545
B,-2.7617411385,0.7317182733,12.3324605353
C,-4.1735958824,1.0573916606,14.5352114334
C,-2.4140256745,0.6048329562,9.7214093385
C,-3.2058252614,0.7872501791,8.5115390481
C,-7.6864701162,1.8465757543,13.5753850121
C,-0.9768201493,0.2637418986,9.7610781328
C,-5.6781192089,1.3929250059,8.0857621217
C,1.0552590419,-0.3114251842,0.4127578357
C,1.7672023454,-0.479423818,-2.050370172
C,-2.6306092301,1.4535184078,4.8682958771
C,-3.0925895976,1.5793944928,6.1740563212
C,-2.7154735514,0.6545064536,7.1604638196
C,-1.8640075222,-0.401502717,6.8012509971
C,-1.4019173984,-0.5273413327,5.495525908
C,-1.7791400671,0.3975620304,4.5092555956
C,-3.0777879155,0.8135891858,15.4939266572
C,0.012592711,-0.0648424412,1.2998560665
C,-4.5083984067,1.1180438693,10.3681148588
C,-6.2652046437,1.5336125381,13.7225959738
C,2.3159187211,-0.5333566455,-9.7728258981
C,4.4057263709,-1.0390835774,-8.9558183736
C,6.1630363416,-1.4373585416,-13.7755855049
C,5.368212558,-1.2624856958,-14.9763557264
C,4.0668468594,-0.9598424314,-14.5756115749
C,3.0253048645,-0.7017087076,-12.2368220325
C,5.5132308695,-1.3008137205,-8.0132686559
C,4.0658630114,-0.9488363031,-13.1230564308
C,3.0349910712,-0.7169338456,-8.5800412857
C,0.9021680296,-0.1927056252,-9.9353097936
C,3.2436877406,-0.750395201,-10.8622009522
C,1.6704405239,0.4314232022,-6.8702210112
C,1.1816627333,0.5346543324,-5.5722518513
C,1.5448484298,-0.403674377,-4.5941969919
C,2.4129715324,-1.4469521015,-4.9525487754
C,2.9016003769,-1.5502477731,-6.2505681882
C,2.538541731,-0.6118880364,-7.2287556724
C,2.9007238131,-0.7086038083,-15.4221656761
C,7.6030859389,-1.7620642665,-13.7607202348
C,-5.5527821332,1.3661975205,11.2554098299
C,-5.3364654293,1.3184555119,12.6266590958
C,0.8378599728,-0.2638044483,-0.9603188291
C,-3.520331145,0.782691542,1.9101730945
C,1.1848643625,-0.3352680627,3.5820746942
C,-1.4311458784,0.2790961492,-3.8115037001
C,3.1815456404,-0.8166332249,-1.8862849274
C,0.0150104842,-0.0570013865,2.7484032963
C,-1.2886283184,0.2647678627,3.1581467425
C,-2.0824064066,0.4445936936,1.9480511951
C,1.0485637347,-0.2986345024,-3.2427480288
C,-0.3240500476,0.0207066566,-2.8676027201
C,-4.5099179052,1.111659242,8.9208231098
C,-5.5408344043,1.371540391,14.9037116675
F,-1.8271974571,1.6165339763,12.5921143054
F,6.3070524712,-2.5217277791,-10.88640848
F,-2.2367303466,1.4941937495,-0.9481954609
B,-1.7379320478,0.314966283,-0.6622532713

Cartesian Coordination of $1a_2$ (DFT)

-1808.6535902 hartree

H,-7.7516873908,-4.0286471004,-0.1102334411
H,1.9852989788,-2.6520062454,0.8751655907
H,1.9861544837,2.6515723,-0.8807471823
H,2.4858294105,4.1156243903,-0.0027602089
H,1.9830807881,2.6536310939,0.8766037778
H,7.7520407489,-4.0285944888,0.099098017
H,8.2179660236,-2.4656207121,0.7792612375
H,8.1362348319,-2.6770095312,-0.9708963379
H,2.4858126875,-4.1154783294,-0.0032744301
H,1.9839416593,-2.652889076,-0.8821879373
H,-8.2153557381,-2.4651901074,-0.7908344639
H,-8.1393643363,-2.6778144404,0.9594315071
H,-1.981741238,-2.6524656737,-0.8635425099
H,-2.4857888171,-4.1155817336,0.0133963473
H,-1.9874917372,-2.6526254196,0.8938028608
H,-7.7524361264,4.0285970568,0.0899340625
H,-8.2212679823,2.4655529058,0.7679217314
H,-8.1321318801,2.6771390602,-0.9818510967
H,-2.4859010799,4.1155157673,0.0118011969
H,-1.9782445476,2.6516351565,-0.8615501748
H,-1.991159181,2.6533617535,0.8957582667
H,0.0012593146,0.0000450695,2.5325206207
H,-0.001258916,-0.0000704619,-2.5310539659
H,7.4594224,0.0000662821,0.0002502594
H,5.0859930053,4.4541797197,0.0071260125
H,5.0860039,-4.4540448828,-0.0105802866
H,7.7521442921,4.0286502592,-0.0999427266
H,8.2187911132,2.4651666513,-0.7784372455
H,8.1352010419,2.6778693906,0.9714739741
N,4.3035403648,1.2568723025,-0.0001023133
N,4.3035456334,-1.2567429192,-0.002635536
N,-4.303533743,-1.256868197,0.00387282
N,-4.303554788,1.2567451854,0.0015221837
O,-2.4645308837,0.0003892749,1.1770572164
O,2.4645148732,0.0004512585,-1.1755758123
O,2.4656753467,-0.0003626917,1.1746049161
O,-2.4656582317,-0.0004973873,-1.1731224722
C,-2.5201056287,3.0239388437,0.012800786
C,-0.0007053254,-0.0000546018,-1.4470595061
C,1.1781164077,0.0001240815,-0.6995795566
C,1.1788230145,-0.0001165373,0.6998974846
C,5.0934054356,-3.3721222793,-0.0089028237
C,3.9369701739,-2.5579997162,-0.0052773442
C,6.3740091897,0.0000667701,-0.0002633002
C,5.7019081944,1.2137210164,0.003201099

C,6.2080430392,2.5449266355,0.0078121297
C,5.09339592,3.3722562546,0.0060312094
C,5.7019143041,-1.2135876795,-0.0045086584
C,3.9369646227,2.5581322678,0.0016033415
C,2.5200339259,-3.0239017205,-0.0037143758
H,-7.4593932328,-0.0000966693,-0.0112589046
H,-5.0859786678,-4.4541747972,0.0117277714
C,7.6511833539,-2.9475468799,-0.0252559034
C,2.5200356344,3.0240475789,-0.0016042333
C,7.6511551856,2.947695781,0.0251145314
C,6.2080534595,-2.5447914453,-0.0091740049
H,-5.0860417884,4.4540459676,-0.0043414691
C,0.0007061758,0.0000185782,1.4485204877
C,-1.1781037919,0.0001037672,0.7010467709
C,-1.1788342917,-0.0001856408,-0.6984298536
C,-5.0933882526,-3.3722544924,0.0089555117
C,-7.651215608,-2.9476844968,0.0151878086
C,-2.5200229004,-3.0240053134,0.0133227257
C,-7.6510824303,2.9475663259,-0.0341447703
C,-3.9369592395,-2.5581203751,0.0090462993
C,-5.7019005805,1.2135772093,-0.0071726172
C,-3.9369989717,2.5580079714,0.0029926327
C,-5.093423991,3.3721218661,-0.0047551898
C,-6.2080381423,2.5447831118,-0.0120186761
C,-6.2080387351,-2.5449356788,0.0041229156
C,-5.7018984112,-1.2137321827,0.0002949441
C,-6.3739896078,-0.0000854721,-0.0066976008
B,3.3487750983,0.0000575212,-0.0009482005
B,-3.348774278,-0.0000600563,0.0024591408

Cartesian Coordination of $2a_2$ (AM1)

-0.470285 hartree

H,2.1694251854,-5.4338810218,3.3726629983
H,2.1604132443,-5.4713299706,6.9658866817
H,2.5999888131,-5.5173075897,8.7382176471
H,2.6258988357,-3.9410607347,7.8159551117
H,-5.6669471617,-1.7259994338,5.4163380707
H,5.3277148357,-5.3172905354,5.1831296371
H,11.1897324735,-4.8841856691,3.8213847604
H,10.9453998677,-3.6935946042,2.4710287126
H,10.5995080082,-5.4537736435,2.2033029878
H,3.0704710551,-2.4490687611,1.6384680434
H,2.9331408675,-1.3476831538,0.1894317263
H,3.4357244257,-0.6795647658,1.8105837511
H,7.734306266,-0.6790047614,-2.0370440248
H,8.0497763525,-2.465467203,-2.0542742609
H,8.9555031232,-1.4002313319,-0.8975787586
H,3.9433850828,0.7989045585,-0.1378718891
H,3.4039646253,-1.0532245125,5.736868373
H,0.5830154313,-5.7367088118,10.2952005835
H,-1.9929279424,-5.8280834922,11.211490981
H,-3.274079045,-5.2286842681,10.0712976435
H,-2.4164663506,-4.0647142263,11.1664056005
H,-5.0402802325,-1.0356719711,6.9726148692
H,-5.3271808741,-2.8216996253,6.8283860356
H,-3.553446736,-3.4483342214,8.338476963
H,2.8350302971,2.0904241748,-1.9492838531
H,4.6891212172,-0.4622196925,-4.9061696768
H,5.7989958337,-1.7555896229,-3.0922134871
H,-4.688850638,0.4649450484,4.9055572306
H,-5.7994687066,1.7558625089,3.0902858813
H,-3.943582309,-0.8014669748,0.1385849422
H,-2.8346107403,-2.0906451856,1.9513040188
H,9.0016783815,-5.4193976093,5.370593118
H,9.1600362593,-3.0761309908,0.8253791273
H,5.7631289592,-3.7528373583,5.9855782096
H,6.6728808436,-5.2766282601,6.4179055049
N,1.3706305828,2.7271989752,-5.7581714526
N,0.2380181695,4.0249788209,-7.5656601669
N,-1.3691273986,-2.7218029381,5.7610944749
N,5.8318337685,-2.4724946317,1.533065869
N,6.9263756347,-3.7674978956,3.3658200481
N,-6.9280348924,3.7615159876,-3.3690291044
N,-5.8334011085,2.4668945777,-1.5360571117
N,-0.2364026551,-4.019235573,7.5687466068
O,-0.3792876652,4.332478481,-5.2404356154
O,4.616058749,-4.1836188962,2.7598038633
O,0.3785663155,-4.329413801,5.2430210009
O,5.1871761846,-2.1487956752,3.8540199438
O,0.953212814,-2.298692474,6.3429942425
O,-4.6185849206,4.1802239582,-2.7607013507
O,-0.9507856504,2.3018893182,-6.3422903849
O,-5.1865184199,2.1454793014,-3.8567184351
C,-1.6099140043,3.8880972141,-4.8190932891
C,7.9657715785,-1.5646519949,-1.3923645357
C,4.1008713983,0.512562196,-1.1893910691
C,9.1547263854,-4.4240150537,3.3765087047
C,3.1422851884,-1.9894865996,5.2349748154
C,1.9523047156,-2.6741671129,5.4763692794
C,1.6093465488,-3.8866771815,4.8203544046
C,0.0665218742,-5.1663368288,9.5293271115
C,-2.2873536352,-4.9843187807,10.5388853676
C,2.0949496,-4.9208804216,7.9407619327
C,-4.9767619901,-1.9131158082,6.2778434101
C,0.6838274249,-4.6928199218,8.3051081797
C,-2.5613318777,-2.7766789601,6.5350695216
C,-1.6324873746,-2.0463664275,4.6137991764
C,-3.0305648603,-1.6316545028,4.6081127259
C,-3.6013161568,-2.0835492736,5.8083497348
C,-1.2668914303,-4.7563142727,9.515913848
C,-1.470748186,-4.0299629821,8.2772064374
C,-2.6112979107,-3.4209722816,7.768467406
C,3.4806602276,1.2352871064,-2.2030307025
C,3.6776653376,0.8928819201,-3.5496734233
C,4.5247893959,-0.1839438109,-3.8538646402
C,5.1450257462,-0.9067182374,-2.8401674761
C,-3.6772843048,-0.8914684393,3.5504551865
C,-4.5246478931,0.185482195,3.8535471054
C,-5.1452915059,0.9068874771,2.8391222666
C,-4.9365248512,0.5722481528,1.4922225612
C,-4.1010059412,-0.5140065329,1.1898065927
C,-3.4804248104,-1.2353885991,2.204175957
H,3.5551721738,3.4544342285,-8.3351792413
H,-0.5832150385,5.7365490403,-10.2952773975
H,0.5768207975,2.6501133835,-2.8606953233
H,1.0193110156,0.8823112553,-2.9391799076
H,-0.3502926605,1.5361025762,-3.9532385439
H,5.6679703148,1.7291800137,-5.4142486836
H,5.328705026,2.826371862,-6.8252591832
H,5.0412078537,1.0405726821,-6.9712445075

H,-2.6227110624,3.9298685268,-7.8217330058
H,-2.6035197282,5.5061509758,-8.7441342758
H,-2.1693783297,5.4630851477,-6.97040603
H,1.8359387539,5.2958709868,-11.4970960622
H,2.9499682921,4.1290649054,-10.6614972569
H,2.9515452744,5.8809018809,-10.1917399641
H,-2.1728621873,5.4336507065,-3.3707520367
H,-7.734565989,0.6771206047,2.0366281475
H,-8.9563082193,1.3958020515,0.8961299021
H,-8.051364594,2.4633667219,2.0513017397
H,-3.4356631606,0.676375317,-1.8115984495
H,-2.9341225867,1.3454483197,-0.1905283521
H,-3.0716948998,2.4462047255,-1.6400163766
H,-11.0360410751,5.4108901015,-3.5408684502
H,-10.6220086154,4.8038408912,-1.8793043665
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H,-9.0015329969,5.4192487405,-5.3708404219
H,-9.1613880673,3.071225919,-0.8280001683
H,-1.0187417047,-0.881218183,2.939314308
H,-0.5769029499,-2.6492761144,2.8627938747
H,0.3511200431,-1.5342762682,3.9535325394
C,7.0785578815,-2.4805139979,0.8482188262
C,6.9110868223,-1.768113754,-0.3985987226
C,5.5774346674,-1.3325434024,-0.4453073987
C,8.1354051044,-3.7267474562,2.6160100098
C,4.9313547414,-1.7935068758,0.7781034245
C,6.1820618139,-4.7140007736,5.5876810615
C,10.5401640743,-4.6200928187,2.9499941826
H,-6.6697847458,5.2862136154,-6.4129758134
H,-5.7572977356,3.7626557418,-5.9856609319
H,-5.3283306958,5.3241640136,-5.1740609236
H,-3.4006047974,1.0532330036,-5.7389398694
C,-7.1633986297,4.4395596735,-4.5212683805
C,3.5145894997,-1.559402,1.1209105178
C,3.0313755453,1.6345341576,-4.6065594443
C,1.633425132,2.0497138214,-4.6119632987
C,2.6135741562,3.4289761652,-7.7641706375
C,1.4741335965,4.041738264,-8.2708933976
C,1.2710441449,4.770709535,-9.5081750388
C,-0.0651064465,5.1715812503,-9.5264953635
C,2.5629827906,2.7826065829,-6.5318973209
C,-0.6837183192,4.6935660359,-8.3047077655
C,0.6656204129,1.7597446432,-3.5354790512
C,4.9779268958,1.9173707045,-6.2756343332
C,-2.0973976581,4.9129286934,-7.9449776947
C,2.3001868598,5.0281617313,-10.5153412871
C,3.6024857493,2.0877652419,-5.806107258
C,-2.4361721279,4.5010286006,-3.8785357779
C,-3.6261703811,3.8155401349,-3.6395356741
C,-3.9657209994,2.6013065665,-4.2941354591
C,-5.5782814063,1.3297253585,0.4438267821
C,-7.9666982044,1.5616685189,1.3906799828
C,-3.5153846646,1.5564188545,-1.1222919448
C,-10.552501373,4.5774643043,-2.9728703166
C,-4.932431214,1.7896913809,-0.7800863411
C,-8.1386632615,3.71536677,-2.62212431
C,-8.5518211444,4.8577784743,-4.5577219554
C,-9.1586768639,4.4100779655,-3.3840039268
C,-6.912154262,1.7645294735,0.3966412255
C,-7.0801194533,2.475060268,-0.8511853747
C,-8.2113413798,3.0866222464,-1.3852068275
C,-0.6650714316,-1.7580415733,3.5365225176
C,4.936105352,-0.5736102516,-1.4929108159
C,2.434180726,-4.5012012393,3.8795874301
C,3.6247629226,-3.817220501,3.6391787935
C,3.966178536,-2.6029148972,4.2926695454
C,8.5504178055,-4.863166459,4.5547344506
C,7.1631495189,-4.4408603335,4.5204984972
C,8.2092665004,-3.0938915365,1.3812783996
C,-6.1799131639,4.7206937599,-5.5841591412
C,-1.9509891175,2.675638644,-5.4761826188
C,-3.1403865832,1.9894502889,-5.2362031933
B,-0.0638455172,-3.3412892847,6.2238266694
B,5.6337883119,-3.14181452,2.8800773777
B,-5.6350348288,3.1373575041,-2.8824749307
B,0.0650061874,3.3455098554,-6.2215839435

Cartesian Coordination of $3a_2$ (AM1)

-0.6572965 hartree
H,3.8069799469,-1.057304835,-10.7834581042
H,3.8590436008,-1.0548151952,14.8008703096
H,13.1777164473,-1.0894957639,12.5280245803
H,13.0351504997,-0.7627005422,10.7465533882
H,12.8615420412,-2.4547809328,11.3761369726
H,4.3308428568,-2.8866437923,11.6809209887
H,-3.8064305887,1.0617539052,10.7827674015
H,-3.5574470962,1.287764122,12.5707104209
H,-3.8102224751,-0.3753168131,11.8900601945
H,1.8268692004,1.0651744205,9.5244211319
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Cartesian Coordination of $1a_3$ (DFT)

-3057.80575 hartree

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Cartesian Coordination of 2a$_3$ (AM1)

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Cartesian Coordination of $3a_3$ (AM1)

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[S7] *Gaussian 03* (Revision C.01), M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M.

W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004, Gaussian, Inc., Wallingford CT, 2004.